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#  
#   CIF generated by the Xtal System   #  
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# (Publishing Staff Use Only)
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# 1. SUBMISSION DETAILS  
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_publ_contact_author_name  
  'Skelton, B. W.'  
_publ_contact_author_address  
;  
  Department of Chemistry  
  University of Western Australia  
  35 Stirling Highway  
  Crawley  
  Western Australia 6009
```

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    Australia
;
_publ_contact_author_email      bws@crystal.uwa.edu.au
_publ_contact_author_fax       (+61)_08_9380_1118
_publ_contact_author_phone     (+61)_08-9380_3481

_publ_contact_letter
;   ?                           #<< contact letter
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;   ?                           #<< paper title text
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;   ?                           #<< paper footnote text
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loop_
_publ_author_name
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'Skelton, Brian W.' .
; Department of Chemistry,
University of Western Australia,
35 Stirling Highway,
Crawley,
WA 6009,
Australia.
;

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;   ?                           #<< synopsis if FI,CI,CM,CO papers
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;   ?                           #<< abstract text
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;   ?                           #<< scientific commentary text
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;   ?                           #<< material & crystal preparation text
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_publ_section_exptl_refinement
;   ?                           #<< crystallographic methods used
;

_publ_section_acknowledgements
;   ?                           #<< acknowledgements text
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_publ_section_references

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;
Sheldrick, G M. (1996). SADABS. Program for Empirical Absorption Correction
of Area Detector Data. University of Gottingen, Germany.

Siemens (1995). SMART and SAINT. Area-Detector Control and Integration
Software. Siemens Analytical X-ray Systems Inc., Madison, Wisconsin, USA.

Hall, S.R., King, G.S.D., and Stewart., J.M. (1995).
The Xtal 3.5 User's Manual. University of Western Australia, Lamb: Perth.

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_publ_section_figure_captions
; ? #<< figure captions
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Data block for single structure (one for each study in the paper)
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data_br687

2. EXPERIMENTAL DATA
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_chemical_melting_point ?

_symmetry_cell_setting orthorhombic
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loop_
_symmetry_equiv_pos_as_xyz
+x,+y,+z 1/2-x,-y,1/2+z 1/2+x,1/2-y,-z -x,1/2+y,1/2-z

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_cell_length_b 16.661(3)
_cell_length_c 33.177(7)
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_cell_angle_beta 90.00000
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Bruker SMART CCD diffractometer
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SADABS; Sheldrick, 1996
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_refine_ls_extinction_coef      1582(319)
_refine_ls_abs_structure_details 'Flack xabs refined'

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_refine_ls_abs_structure_Flack -.007(5)

3. Information for the "methods" section

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_computing_data_collection 'Siemens SMART (Siemens, 1995)'
_computing_cell_refinement 'Siemens SAINT (Siemens, 1995)'
_computing_data_reduction 'xtal ADDRREF SORTRF'
_computing_structure_solution xtal
_computing_structure_refinement 'xtal CRYLSQ'
_computing_molecular_graphics xtal
_computing_publication_material 'xtal BONDLA CIFIO'

4. Supplementary data for validation and tables

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_atom_type_scatter_dispersion_real
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Cu ? 0 16 .263 1.266 'Int Tables Vol IV Tables 2.2B and 2.3.1'
C ? 0 448 .002 .002 'Int Tables Vol IV Tables 2.2B and 2.3.1'
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Ir1 .356680(10) 1.003920(10) .857600(10) .01608(11) Uani ? ? 1.00000
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C1022 .6233(5) .9292(4) .8056(2) .027(4) Uani ? ? 1.00000 ? ?

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| C1023 | .6574(5) | .8926(5) | .7717(3) | .037(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C1024 | .6056(5) | .8666(5) | .7402(2) | .031(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1025 | .5200(5) | .8767(5) | .7433(2) | .030(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1026 | .4852(5) | .9138(4) | .7774(2) | .025(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1031 | .5505(4) | .9411(4) | .8942(2) | .023(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1032 | .6265(5) | .9661(5) | .9098(2) | .028(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1033 | .6670(5) | .9189(5) | .9388(2) | .033(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1034 | .6316(5) | .8478(5) | .9515(2) | .037(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C1035 | .5561(5) | .8224(5) | .9363(3) | .035(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1036 | .5153(5) | .8682(4) | .9074(2) | .026(4) | Uani | ? | ? | 1.00000 | ? | ? |
| P2 | -.04720(10) | 1.01862(10) | .84779(5) | .0189(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C2011 | -.0954(4) | .9207(4) | .8391(2) | .022(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C2012 | -.0728(5) | .8793(5) | .8039(2) | .032(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2013 | -.1097(5) | .8066(5) | .7942(3) | .038(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2014 | -.1705(5) | .7753(5) | .8193(3) | .041(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2015 | -.1954(5) | .8169(5) | .8531(3) | .038(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2016 | -.1579(4) | .8881(4) | .8625(2) | .029(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2021 | -.0880(5) | 1.0747(4) | .8047(2) | .022(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C2022 | -.1718(5) | 1.0643(5) | .7938(2) | .029(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2023 | -.2067(5) | 1.1098(5) | .7631(2) | .032(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2024 | -.1586(5) | 1.1669(5) | .7428(3) | .039(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2025 | -.0759(6) | 1.1766(5) | .7526(3) | .043(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2026 | -.0398(5) | 1.1309(5) | .7836(3) | .036(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2031 | -.1037(4) | 1.0604(4) | .8903(2) | .024(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2032 | -.0912(4) | 1.0251(4) | .9287(2) | .028(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2033 | -.1349(5) | 1.0520(5) | .9619(2) | .038(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2034 | -.1897(6) | 1.1171(6) | .9581(3) | .047(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2035 | -.2011(6) | 1.1532(5) | .9210(3) | .046(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2036 | -.1581(5) | 1.1241(5) | .8875(2) | .033(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C111 | .3385(4) | .8867(4) | .84227(19) | .021(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C112 | .3228(4) | .8147(4) | .8377(2) | .023(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C1121 | .3366(4) | .7307(4) | .8302(2) | .021(3) | Uani | ? | ? | 1.00000 | ? | ? |
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| C211 | .0943(4) | .8941(4) | .8701(2) | .023(3) | Uani | ? | ? | 1.00000 | ? | ? |
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| C2123 | .0611(6) | .6053(5) | .8727(3) | .051(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C2124 | .1003(7) | .5766(5) | .9074(4) | .059(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C2125 | .1336(7) | .6298(6) | .9344(3) | .053(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C2126 | .1335(5) | .7121(5) | .9265(2) | .035(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C121 | .3503(4) | 1.0415(4) | .7995(2) | .023(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C122 | .3396(4) | 1.0614(4) | .7647(2) | .021(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C1221 | .3494(4) | 1.0891(4) | .7234(2) | .023(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1222 | .3622(5) | 1.1720(4) | .7159(2) | .030(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1223 | .3770(5) | 1.1988(5) | .6774(3) | .039(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C1224 | .3777(5) | 1.1464(6) | .6448(3) | .042(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C1225 | .3624(6) | 1.0659(6) | .6517(3) | .048(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C1226 | .3480(5) | 1.0361(5) | .6904(2) | .041(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C221 | .1093(4) | .9898(4) | .79586(18) | .021(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C222 | .1319(4) | .9786(4) | .76105(19) | .022(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C2221 | .1433(4) | .9673(5) | .7183(2) | .029(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2222 | .1331(5) | 1.0328(6) | .6924(3) | .048(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2223 | .1386(6) | 1.0275(9) | .6513(3) | .071(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C2224 | .1547(7) | .9528(10) | .6362(3) | .076(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C2225 | .1650(6) | .8848(8) | .6588(4) | .067(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C2226 | .1606(5) | .8923(6) | .7017(3) | .048(6) | Uani | ? | ? | 1.00000 | ? | ? |

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|-------|-----------|------------|------------|----------|------|---|---|---------|---|---|
| C131 | .3522(4) | 1.1215(4) | .8750(2) | .021(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C132 | .3353(4) | 1.1900(4) | .8852(2) | .025(4) | Uani | ? | ? | 1.00000 | ? | ? |
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| C1322 | .2592(6) | 1.2983(5) | .9215(2) | .039(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C1323 | .2513(6) | 1.3775(6) | .9330(3) | .050(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1324 | .3113(7) | 1.4325(5) | .9224(3) | .052(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1325 | .3793(6) | 1.4088(5) | .9001(4) | .057(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1326 | .3887(5) | 1.3296(5) | .8878(3) | .041(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C231 | .1105(4) | 1.1322(4) | .84511(19) | .020(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C232 | .1336(4) | 1.2015(4) | .8394(2) | .023(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C2321 | .1329(4) | 1.2849(4) | .8282(2) | .022(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2322 | .0582(5) | 1.3256(5) | .8258(3) | .035(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2323 | .0560(5) | 1.4066(5) | .8141(3) | .043(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2324 | .1291(5) | 1.4468(4) | .8052(3) | .035(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2325 | .2040(5) | 1.4062(4) | .8082(2) | .031(4) | Uani | ? | ? | 1.00000 | ? | ? |
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| C1422 | .2399(6) | .8951(5) | 1.0065(3) | .035(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C1423 | .2361(7) | .8617(5) | 1.0451(3) | .047(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C1424 | .3057(7) | .8475(5) | 1.0663(3) | .052(6) | Uani | ? | ? | 1.00000 | ? | ? |
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| C1426 | .3888(5) | .8988(5) | 1.0119(2) | .034(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C241 | .1051(4) | 1.0412(4) | .91519(19) | .019(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C242 | .1304(4) | 1.0568(4) | .9494(2) | .023(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2421 | .1482(5) | 1.0826(4) | .9900(2) | .022(3) | Uani | ? | ? | 1.00000 | ? | ? |
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| C2426 | .2275(5) | 1.1116(5) | .9996(2) | .031(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C11 | .4630(7) | 1.1159(7) | .9987(4) | .062(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12 | .4588(8) | 1.1941(10) | .9894(4) | .088(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C13 | .4834(10) | 1.2518(7) | 1.0194(7) | .112(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C14 | .5118(8) | 1.2237(9) | 1.0560(5) | .088(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C15 | .5112(8) | 1.1468(9) | 1.0639(4) | .078(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C16 | .4889(8) | 1.0918(7) | 1.0355(3) | .065(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21 | .3681(6) | .6842(6) | .9456(3) | .048(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C22 | .3664(6) | .6973(5) | .9869(3) | .046(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C23 | .4267(6) | .6670(6) | 1.0119(3) | .049(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C24 | .4904(6) | .6198(6) | .9947(3) | .051(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C25 | .4909(6) | .6052(5) | .9533(3) | .040(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C26 | .4307(6) | .6382(6) | .9299(3) | .050(6) | Uani | ? | ? | 1.00000 | ? | ? |
| H1012 | .53178 | 1.11740 | .90961 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1013 | .58848 | 1.24569 | .90675 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1014 | .63311 | 1.30115 | .84505 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1015 | .62798 | 1.22146 | .78703 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1016 | .56950 | 1.09247 | .78868 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1022 | .65920 | .94640 | .82688 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1023 | .71535 | .88431 | .77111 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1024 | .63168 | .84372 | .71659 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1025 | .48466 | .85757 | .72142 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1026 | .42435 | .92079 | .77987 | .03000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1032 | .65038 | 1.01636 | .90117 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1033 | .71757 | .93646 | .95086 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1034 | .66210 | .81414 | .97004 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1035 | .53004 | .77326 | .94721 | .04700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1036 | .46208 | .85113 | .89579 | .03200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2012 | -.03269 | .90384 | .78446 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2013 | -.09377 | .77533 | .77085 | .04700 | Uiso | ? | ? | 1.00000 | ? | ? |

| | | | | | | | | | | |
|-------|---------|---------|---------|--------|------|---|---|---------|---|---|
| H2014 | -.19804 | .72500 | .81267 | .05700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2015 | -.23544 | .79554 | .87103 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2016 | -.17801 | .91606 | .88551 | .03400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2022 | -.20687 | 1.02673 | .80806 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2023 | -.26301 | 1.10110 | .75557 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2024 | -.18505 | 1.20032 | .72245 | .04700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2025 | -.04116 | 1.21361 | .73800 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2026 | .01930 | 1.13600 | .79135 | .04700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2032 | -.05057 | .98258 | .93221 | .03300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2033 | -.12962 | 1.02592 | .98752 | .04700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2034 | -.21578 | 1.13744 | .98203 | .05500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2035 | -.24118 | 1.19770 | .91838 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2036 | -.16625 | 1.15055 | .86141 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1122 | .23539 | .68787 | .86010 | .03300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1123 | .26663 | .54909 | .85134 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1124 | .38494 | .51173 | .81400 | .04000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1125 | .47255 | .61117 | .78631 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1126 | .44290 | .74797 | .79574 | .03300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1222 | .36215 | 1.21091 | .73729 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1223 | .38389 | 1.25502 | .67260 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1224 | .38847 | 1.16535 | .61747 | .04900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1225 | .35918 | 1.02958 | .62906 | .05300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1226 | .34009 | .97858 | .69431 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1322 | .21624 | 1.26027 | .92852 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1323 | .20478 | 1.39516 | .94853 | .06900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1324 | .30591 | 1.48760 | .93100 | .06200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1325 | .42113 | 1.44908 | .89120 | .07100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1326 | .43794 | 1.31225 | .87251 | .05700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1422 | .19111 | .90582 | .99125 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1423 | .18128 | .84953 | 1.05686 | .05600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1424 | .30213 | .82135 | 1.09176 | .06600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1425 | .43228 | .85923 | 1.06705 | .06000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1426 | .44252 | .91117 | 1.00020 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2122 | .02931 | .70489 | .84019 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2123 | .03770 | .56650 | .85315 | .06600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2124 | .09869 | .52158 | .91310 | .08300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2125 | .16012 | .61033 | .95944 | .06100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2126 | .16055 | .74968 | .94523 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2222 | .12140 | 1.08256 | .70494 | .06200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2223 | .13236 | 1.07604 | .63347 | .08700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2224 | .16091 | .95051 | .60719 | .08200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2225 | .17367 | .83218 | .64678 | .09600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2226 | .17102 | .84695 | .71914 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2322 | .00676 | 1.29864 | .83487 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2323 | .00147 | 1.43249 | .81071 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2324 | .12830 | 1.50165 | .79663 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2325 | .25493 | 1.43426 | .80193 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2326 | .26044 | 1.29899 | .82197 | .03100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2422 | .03488 | 1.05411 | 1.01539 | .03400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2423 | .06573 | 1.09539 | 1.08024 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2424 | .20002 | 1.13381 | 1.09715 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2425 | .30046 | 1.15322 | 1.04457 | .04500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2426 | .26880 | 1.11688 | .97882 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11 | .44944 | 1.07416 | .97780 | .07800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12 | .43606 | 1.21477 | .96549 | .13300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H13 | .48540 | 1.30911 | 1.01327 | .13100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H14 | .53288 | 1.26211 | 1.07746 | .10800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H15 | .52306 | 1.12417 | 1.09002 | .10100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H16 | .49890 | 1.03588 | 1.04100 | .08100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21 | .32698 | .70567 | .92906 | .06800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22 | .32336 | .73077 | .99864 | .05700 | Uiso | ? | ? | 1.00000 | ? | ? |

| | | | | | | | | | | |
|-----|--------|--------|---------|--------|------|---|---|---------|---|---|
| H23 | .42845 | .67969 | 1.04073 | .06700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H24 | .52777 | .59395 | 1.01139 | .06400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H25 | .53344 | .57313 | .94133 | .04900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H26 | .43198 | .62551 | .90153 | .07000 | Uiso | ? | ? | 1.00000 | ? | ? |

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

| | | | | | | |
|-------|------------|------------|------------|------------|------------|-------------|
| Ir1 | .01431(11) | .01840(11) | .01552(11) | -.00033(9) | .00071(9) | -.00042(11) |
| Ir2 | .01417(11) | .02104(12) | .01454(11) | -.00149(9) | .00064(10) | .00060(11) |
| Cu1 | .0180(4) | .0216(4) | .0203(4) | -.0001(3) | .0018(4) | -.0004(4) |
| Cu2 | .0151(4) | .0259(4) | .0205(4) | -.0027(4) | .0001(3) | -.0020(3) |
| Cu3 | .0171(4) | .0210(4) | .0194(4) | -.0005(3) | -.0006(4) | -.0012(3) |
| Cu4 | .0161(3) | .0229(4) | .0185(4) | .0012(4) | .0006(3) | -.0004(3) |
| P1 | .0161(7) | .0163(7) | .0240(8) | .0013(6) | .0022(6) | .0016(8) |
| C1011 | .013(3) | .023(3) | .045(5) | -.000(3) | .000(3) | .003(3) |
| C1012 | .025(4) | .030(4) | .030(4) | -.001(3) | -.003(3) | -.004(3) |
| C1013 | .030(4) | .026(4) | .042(5) | -.002(3) | -.005(4) | -.009(3) |
| C1014 | .037(5) | .026(4) | .049(5) | -.006(3) | -.005(4) | .002(3) |
| C1015 | .045(5) | .029(4) | .035(4) | -.003(4) | .002(4) | .008(3) |
| C1016 | .034(5) | .028(4) | .029(4) | -.002(3) | .002(3) | .004(3) |
| C1021 | .026(4) | .014(3) | .024(4) | .002(3) | .008(3) | .008(3) |
| C1022 | .029(4) | .021(3) | .032(4) | .006(3) | -.001(3) | -.001(3) |
| C1023 | .025(4) | .050(5) | .036(5) | .010(4) | .009(3) | .002(4) |
| C1024 | .036(5) | .033(4) | .023(4) | .004(3) | .014(3) | .002(3) |
| C1025 | .030(4) | .030(4) | .031(4) | -.004(3) | .003(3) | -.003(3) |
| C1026 | .029(4) | .020(3) | .025(4) | -.001(3) | .004(3) | -.004(3) |
| C1031 | .014(3) | .028(4) | .026(4) | .001(3) | -.002(3) | .003(3) |
| C1032 | .024(4) | .031(4) | .029(4) | .004(3) | -.003(3) | .007(3) |
| C1033 | .030(4) | .037(4) | .034(4) | -.003(3) | -.013(3) | .002(3) |
| C1034 | .035(5) | .046(5) | .029(4) | .008(4) | -.010(4) | .011(4) |
| C1035 | .035(4) | .028(4) | .041(5) | .008(3) | -.002(4) | .011(3) |
| C1036 | .028(4) | .025(4) | .023(4) | .002(3) | -.000(3) | .003(3) |
| P2 | .0175(8) | .0200(8) | .0192(8) | -.0025(7) | .0024(6) | -.0001(6) |
| C2011 | .016(3) | .021(3) | .030(4) | -.002(3) | -.008(3) | .000(3) |
| C2012 | .025(4) | .034(4) | .038(5) | -.005(3) | -.001(3) | -.008(3) |
| C2013 | .025(4) | .031(4) | .059(6) | .003(3) | -.000(4) | -.022(4) |
| C2014 | .031(4) | .024(4) | .067(6) | .000(3) | -.011(4) | -.001(4) |
| C2015 | .028(4) | .037(4) | .050(5) | -.010(3) | -.004(4) | .014(4) |
| C2016 | .023(4) | .028(3) | .035(4) | -.003(3) | -.002(3) | .002(3) |
| C2021 | .020(3) | .029(3) | .018(3) | .003(3) | -.000(3) | -.000(3) |
| C2022 | .026(4) | .031(4) | .029(4) | -.002(3) | -.000(3) | -.002(3) |
| C2023 | .025(4) | .042(5) | .030(4) | .005(3) | -.011(3) | -.007(3) |
| C2024 | .043(5) | .039(5) | .034(5) | -.001(4) | -.015(4) | .005(4) |
| C2025 | .048(6) | .052(5) | .030(5) | -.011(4) | -.010(4) | .016(4) |
| C2026 | .032(4) | .042(5) | .034(5) | -.008(4) | -.008(4) | .010(4) |
| C2031 | .022(4) | .033(4) | .017(3) | -.009(3) | .003(3) | -.002(3) |
| C2032 | .021(3) | .037(4) | .027(4) | -.001(3) | -.002(3) | -.001(3) |
| C2033 | .029(4) | .060(6) | .026(4) | -.009(4) | .003(3) | -.001(4) |
| C2034 | .037(5) | .068(7) | .036(5) | -.000(5) | .012(4) | -.024(4) |
| C2035 | .041(5) | .049(5) | .048(6) | .012(4) | .004(4) | -.016(4) |
| C2036 | .041(5) | .033(4) | .024(4) | .005(4) | .005(3) | -.005(3) |
| C111 | .023(4) | .023(3) | .016(3) | -.004(3) | .004(3) | -.005(2) |
| C112 | .016(3) | .030(4) | .021(3) | .001(3) | .001(3) | .003(3) |
| C1121 | .021(4) | .021(3) | .022(4) | -.001(3) | -.005(3) | -.001(3) |
| C1122 | .022(4) | .025(3) | .027(4) | .000(3) | .000(3) | -.008(3) |

| | | | | | | |
|-------|---------|----------|---------|----------|----------|----------|
| C1123 | .031(4) | .026(4) | .032(4) | -.005(3) | -.003(3) | .001(3) |
| C1124 | .034(4) | .026(4) | .037(4) | .000(3) | -.009(4) | -.008(3) |
| C1125 | .026(4) | .030(4) | .032(4) | .000(3) | .001(3) | -.008(3) |
| C1126 | .023(4) | .026(3) | .031(4) | -.004(3) | .000(3) | .001(3) |
| C211 | .019(3) | .029(4) | .021(3) | -.004(3) | -.001(3) | -.005(3) |
| C212 | .022(4) | .026(4) | .026(4) | -.003(3) | .001(3) | .001(3) |
| C2121 | .024(4) | .023(3) | .033(4) | -.002(3) | .007(3) | .003(3) |
| C2122 | .024(4) | .039(4) | .038(5) | -.006(3) | .003(3) | -.006(3) |
| C2123 | .040(5) | .031(4) | .081(7) | -.009(4) | .021(5) | -.011(5) |
| C2124 | .061(7) | .027(4) | .089(8) | .002(5) | .040(6) | .012(5) |
| C2125 | .069(7) | .046(5) | .044(6) | .012(5) | .014(5) | .017(4) |
| C2126 | .046(5) | .038(4) | .022(4) | .003(4) | .000(4) | .003(3) |
| C121 | .023(4) | .020(3) | .024(4) | -.007(3) | -.003(3) | -.001(3) |
| C122 | .022(4) | .026(3) | .016(3) | -.002(3) | .001(3) | -.003(3) |
| C1221 | .018(3) | .035(4) | .017(3) | -.003(3) | .000(3) | .001(3) |
| C1222 | .031(4) | .033(4) | .027(4) | .005(3) | .004(3) | .005(3) |
| C1223 | .038(5) | .043(5) | .035(5) | .009(4) | .000(4) | .018(4) |
| C1224 | .029(4) | .072(6) | .026(4) | -.006(4) | -.001(4) | .011(5) |
| C1225 | .051(5) | .070(6) | .024(4) | -.020(5) | .005(4) | -.012(4) |
| C1226 | .042(5) | .051(5) | .030(4) | -.017(4) | .006(4) | -.009(4) |
| C221 | .020(3) | .029(3) | .014(3) | .002(3) | .000(2) | .002(3) |
| C222 | .021(3) | .023(3) | .022(3) | -.005(3) | -.002(3) | .006(3) |
| C2221 | .019(3) | .044(4) | .025(4) | -.012(3) | .003(3) | -.004(3) |
| C2222 | .029(4) | .084(7) | .031(4) | -.013(5) | .001(4) | .020(5) |
| C2223 | .042(6) | .129(11) | .043(6) | -.007(6) | .002(5) | .015(7) |
| C2224 | .041(6) | .143(13) | .043(7) | .000(7) | .007(5) | -.013(7) |
| C2225 | .039(6) | .087(9) | .077(8) | .005(6) | .014(5) | -.040(7) |
| C2226 | .028(5) | .065(6) | .050(6) | -.004(4) | .005(4) | -.027(5) |
| C131 | .019(3) | .020(3) | .024(4) | -.005(3) | -.002(3) | .003(3) |
| C132 | .024(4) | .028(4) | .024(4) | -.005(3) | -.003(3) | -.002(3) |
| C1321 | .031(4) | .023(4) | .033(4) | .003(3) | -.011(3) | -.002(3) |
| C1322 | .052(6) | .035(4) | .029(4) | .005(4) | -.005(4) | -.002(3) |
| C1323 | .070(7) | .046(5) | .035(5) | .020(5) | -.012(5) | -.013(4) |
| C1324 | .074(7) | .028(4) | .053(6) | .010(5) | -.034(6) | -.005(4) |
| C1325 | .053(6) | .023(4) | .096(8) | -.006(4) | -.035(6) | -.001(5) |
| C1326 | .032(5) | .024(4) | .067(6) | -.002(3) | -.013(4) | .004(4) |
| C231 | .015(3) | .024(3) | .020(3) | -.000(3) | .003(3) | -.001(2) |
| C232 | .015(3) | .032(4) | .021(3) | .002(3) | -.002(3) | -.000(3) |
| C2321 | .022(4) | .027(3) | .018(3) | .000(3) | -.002(3) | .003(3) |
| C2322 | .023(4) | .028(4) | .053(5) | -.001(3) | .002(4) | .011(4) |
| C2323 | .025(4) | .037(5) | .067(6) | .005(4) | -.001(4) | .012(4) |
| C2324 | .039(5) | .024(4) | .042(5) | .001(3) | .003(4) | .006(3) |
| C2325 | .031(4) | .027(4) | .034(4) | -.008(3) | .003(3) | -.002(3) |
| C2326 | .023(4) | .026(4) | .024(4) | .000(3) | .001(3) | -.002(3) |
| C141 | .021(3) | .012(3) | .033(4) | .006(3) | -.007(3) | -.009(3) |
| C142 | .019(3) | .026(4) | .025(4) | .002(3) | .002(3) | -.001(3) |
| C1421 | .037(4) | .015(3) | .021(3) | .000(3) | .001(3) | .001(3) |
| C1422 | .042(5) | .028(4) | .036(5) | .001(3) | .013(4) | .002(3) |
| C1423 | .067(7) | .041(5) | .033(5) | -.006(5) | .020(5) | .006(4) |
| C1424 | .092(8) | .042(5) | .022(4) | -.014(5) | .004(5) | .004(4) |
| C1425 | .072(7) | .047(5) | .026(4) | -.014(5) | -.019(4) | .009(4) |
| C1426 | .042(5) | .035(4) | .026(4) | -.005(4) | -.009(4) | .003(3) |
| C241 | .015(3) | .025(3) | .017(3) | .000(3) | .002(3) | .001(3) |
| C242 | .023(4) | .027(3) | .019(3) | .001(3) | .003(3) | .006(3) |
| C2421 | .031(4) | .019(3) | .017(3) | .003(3) | -.001(3) | -.002(2) |
| C2422 | .027(4) | .026(3) | .025(4) | -.002(3) | .003(3) | -.002(3) |
| C2423 | .044(5) | .032(4) | .023(4) | .006(4) | .006(3) | -.007(3) |
| C2424 | .046(5) | .052(5) | .023(4) | .010(4) | -.007(4) | -.015(4) |
| C2425 | .034(5) | .046(5) | .031(4) | .004(4) | -.004(4) | -.014(4) |
| C2426 | .024(4) | .043(4) | .027(4) | .006(4) | .000(3) | -.004(3) |
| C11 | .051(7) | .072(8) | .064(7) | -.009(6) | -.006(6) | .001(6) |

| | | | | | | |
|-----|----------|----------|----------|----------|----------|----------|
| C12 | .050(7) | .125(13) | .090(10) | .027(8) | .023(7) | .066(9) |
| C13 | .077(10) | .036(6) | .22(2) | .004(6) | .071(13) | .038(10) |
| C14 | .070(9) | .063(9) | .132(14) | -.014(7) | .008(9) | -.038(9) |
| C15 | .071(8) | .096(10) | .066(8) | .002(7) | -.009(7) | -.019(7) |
| C16 | .081(9) | .057(7) | .055(7) | .004(6) | -.021(6) | .008(5) |
| C21 | .040(5) | .059(6) | .045(6) | .003(5) | -.012(4) | -.008(4) |
| C22 | .043(5) | .038(5) | .056(6) | .005(4) | .005(5) | -.007(4) |
| C23 | .052(6) | .044(5) | .050(6) | .002(5) | .004(5) | .006(4) |
| C24 | .048(6) | .044(5) | .060(6) | .011(4) | .002(5) | .016(5) |
| C25 | .045(5) | .034(4) | .042(5) | .000(4) | .014(4) | .005(4) |
| C26 | .043(6) | .043(5) | .064(7) | -.005(4) | -.002(5) | -.015(5) |

5. Molecular Geometry

#-----

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_distance

_geom_bond_publ_flag

#<< enter YES for value to be published

| | | | | | |
|-------|-------|---|---|------------|---|
| Ir1 | P1 | . | . | 2.2676(17) | ? |
| Ir1 | C111 | . | . | 2.039(7) | ? |
| Ir1 | C121 | . | . | 2.028(7) | ? |
| Ir1 | C131 | . | . | 2.043(7) | ? |
| Ir1 | C141 | . | . | 2.021(7) | ? |
| Ir2 | P2 | . | . | 2.2658(17) | ? |
| Ir2 | C211 | . | . | 2.043(7) | ? |
| Ir2 | C221 | . | . | 2.039(6) | ? |
| Ir2 | C231 | . | . | 2.032(7) | ? |
| Ir2 | C241 | . | . | 2.039(6) | ? |
| Cu1 | C111 | . | . | 2.002(7) | ? |
| Cu1 | C112 | . | . | 2.149(7) | ? |
| Cu1 | C211 | . | . | 2.031(7) | ? |
| Cu1 | C212 | . | . | 2.222(7) | ? |
| Cu2 | C121 | . | . | 1.977(7) | ? |
| Cu2 | C122 | . | . | 2.265(7) | ? |
| Cu2 | C221 | . | . | 1.994(6) | ? |
| Cu2 | C222 | . | . | 2.143(7) | ? |
| Cu3 | C131 | . | . | 2.008(7) | ? |
| Cu3 | C132 | . | . | 2.170(7) | ? |
| Cu3 | C231 | . | . | 2.000(6) | ? |
| Cu3 | C232 | . | . | 2.135(7) | ? |
| Cu4 | C141 | . | . | 2.010(7) | ? |
| Cu4 | C142 | . | . | 2.225(7) | ? |
| Cu4 | C241 | . | . | 2.026(6) | ? |
| Cu4 | C242 | . | . | 2.168(7) | ? |
| P1 | C1011 | . | . | 1.818(7) | ? |
| P1 | C1021 | . | . | 1.835(7) | ? |
| P1 | C1031 | . | . | 1.835(7) | ? |
| C1011 | C1012 | . | . | 1.378(11) | ? |
| C1011 | C1016 | . | . | 1.410(11) | ? |
| C1012 | C1013 | . | . | 1.386(10) | ? |
| C1012 | H1012 | . | . | .958 | ? |
| C1013 | C1014 | . | . | 1.381(12) | ? |
| C1013 | H1013 | . | . | .953 | ? |
| C1014 | C1015 | . | . | 1.385(11) | ? |
| C1014 | H1014 | . | . | .980 | ? |
| C1015 | C1016 | . | . | 1.379(11) | ? |

| | | | | | |
|-------|-------|---|---|-----------|---|
| C1015 | H1015 | . | . | .961 | ? |
| C1016 | H1016 | . | . | .967 | ? |
| C1021 | C1022 | . | . | 1.399(10) | ? |
| C1021 | C1026 | . | . | 1.393(10) | ? |
| C1022 | C1023 | . | . | 1.392(11) | ? |
| C1022 | H1022 | . | . | .956 | ? |
| C1023 | C1024 | . | . | 1.402(11) | ? |
| C1023 | H1023 | . | . | .941 | ? |
| C1024 | C1025 | . | . | 1.389(11) | ? |
| C1024 | H1024 | . | . | .966 | ? |
| C1025 | C1026 | . | . | 1.405(10) | ? |
| C1025 | H1025 | . | . | .975 | ? |
| C1026 | H1026 | . | . | .986 | ? |
| C1031 | C1032 | . | . | 1.387(10) | ? |
| C1031 | C1036 | . | . | 1.409(10) | ? |
| C1032 | C1033 | . | . | 1.404(11) | ? |
| C1032 | H1032 | . | . | .964 | ? |
| C1033 | C1034 | . | . | 1.378(12) | ? |
| C1033 | H1033 | . | . | .952 | ? |
| C1034 | C1035 | . | . | 1.379(12) | ? |
| C1034 | H1034 | . | . | .966 | ? |
| C1035 | C1036 | . | . | 1.389(11) | ? |
| C1035 | H1035 | . | . | .987 | ? |
| C1036 | H1036 | . | . | .979 | ? |
| P2 | C2011 | . | . | 1.828(7) | ? |
| P2 | C2021 | . | . | 1.828(7) | ? |
| P2 | C2031 | . | . | 1.815(7) | ? |
| C2011 | C2012 | . | . | 1.406(10) | ? |
| C2011 | C2016 | . | . | 1.380(10) | ? |
| C2012 | C2013 | . | . | 1.386(11) | ? |
| C2012 | H2012 | . | . | .998 | ? |
| C2013 | C2014 | . | . | 1.385(12) | ? |
| C2013 | H2013 | . | . | .967 | ? |
| C2014 | C2015 | . | . | 1.376(13) | ? |
| C2014 | H2014 | . | . | .972(8) | ? |
| C2015 | C2016 | . | . | 1.366(10) | ? |
| C2015 | H2015 | . | . | .946 | ? |
| C2016 | H2016 | . | . | .952 | ? |
| C2021 | C2022 | . | . | 1.404(10) | ? |
| C2021 | C2026 | . | . | 1.402(11) | ? |
| C2022 | C2023 | . | . | 1.388(11) | ? |
| C2022 | H2022 | . | . | .965 | ? |
| C2023 | C2024 | . | . | 1.398(12) | ? |
| C2023 | H2023 | . | . | .949 | ? |
| C2024 | C2025 | . | . | 1.377(13) | ? |
| C2024 | H2024 | . | . | .972 | ? |
| C2025 | C2026 | . | . | 1.403(12) | ? |
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| C2026 | H2026 | . | . | .987 | ? |
| C2031 | C2032 | . | . | 1.415(10) | ? |
| C2031 | C2036 | . | . | 1.378(11) | ? |
| C2032 | C2033 | . | . | 1.381(11) | ? |
| C2032 | H2032 | . | . | .970 | ? |
| C2033 | C2034 | . | . | 1.401(13) | ? |
| C2033 | H2033 | . | . | .959 | ? |
| C2034 | C2035 | . | . | 1.381(13) | ? |
| C2034 | H2034 | . | . | .960 | ? |
| C2035 | C2036 | . | . | 1.396(12) | ? |
| C2035 | H2035 | . | . | .985 | ? |
| C2036 | H2036 | . | . | .980 | ? |
| C111 | C112 | . | . | 1.235(10) | ? |

| | | | | | |
|-------|-------|---|---|-----------|---|
| C112 | C1121 | . | . | 1.440(10) | ? |
| C1121 | C1122 | . | . | 1.383(10) | ? |
| C1121 | C1126 | . | . | 1.402(10) | ? |
| C1122 | C1123 | . | . | 1.395(10) | ? |
| C1122 | H1122 | . | . | .972 | ? |
| C1123 | C1124 | . | . | 1.367(11) | ? |
| C1123 | H1123 | . | . | .982 | ? |
| C1124 | C1125 | . | . | 1.387(11) | ? |
| C1124 | H1124 | . | . | .966 | ? |
| C1125 | C1126 | . | . | 1.401(10) | ? |
| C1125 | H1125 | . | . | .965 | ? |
| C1126 | H1126 | . | . | .982 | ? |
| C211 | C212 | . | . | 1.208(10) | ? |
| C212 | C2121 | . | . | 1.450(10) | ? |
| C2121 | C2122 | . | . | 1.413(11) | ? |
| C2121 | C2126 | . | . | 1.396(11) | ? |
| C2122 | C2123 | . | . | 1.365(12) | ? |
| C2122 | H2122 | . | . | .994 | ? |
| C2123 | C2124 | . | . | 1.396(15) | ? |
| C2123 | H2123 | . | . | .989 | ? |
| C2124 | C2125 | . | . | 1.368(14) | ? |
| C2124 | H2124 | . | . | .937 | ? |
| C2125 | C2126 | . | . | 1.396(12) | ? |
| C2125 | H2125 | . | . | .988 | ? |
| C2126 | H2126 | . | . | .982 | ? |
| C121 | C122 | . | . | 1.214(10) | ? |
| C122 | C1221 | . | . | 1.455(9) | ? |
| C1221 | C1222 | . | . | 1.420(10) | ? |
| C1221 | C1226 | . | . | 1.406(11) | ? |
| C1222 | C1223 | . | . | 1.373(11) | ? |
| C1222 | H1222 | . | . | .961 | ? |
| C1223 | C1224 | . | . | 1.391(12) | ? |
| C1223 | H1223 | . | . | .956 | ? |
| C1224 | C1225 | . | . | 1.383(14) | ? |
| C1224 | H1224 | . | . | .975 | ? |
| C1225 | C1226 | . | . | 1.397(12) | ? |
| C1225 | H1225 | . | . | .964 | ? |
| C1226 | H1226 | . | . | .976 | ? |
| C221 | C222 | . | . | 1.225(9) | ? |
| C222 | C2221 | . | . | 1.443(10) | ? |
| C2221 | C2222 | . | . | 1.397(12) | ? |
| C2221 | C2226 | . | . | 1.393(12) | ? |
| C2222 | C2223 | . | . | 1.370(13) | ? |
| C2222 | H2222 | . | . | .946 | ? |
| C2223 | C2224 | . | . | 1.37(2) | ? |
| C2223 | H2223 | . | . | 1.007 | ? |
| C2224 | C2225 | . | . | 1.37(2) | ? |
| C2224 | H2224 | . | . | .969 | ? |
| C2225 | C2226 | . | . | 1.430(16) | ? |
| C2225 | H2225 | . | . | .973 | ? |
| C2226 | H2226 | . | . | .968 | ? |
| C131 | C132 | . | . | 1.221(10) | ? |
| C132 | C1321 | . | . | 1.467(10) | ? |
| C1321 | C1322 | . | . | 1.401(12) | ? |
| C1321 | C1326 | . | . | 1.397(11) | ? |
| C1322 | C1323 | . | . | 1.380(12) | ? |
| C1322 | H1322 | . | . | .965 | ? |
| C1323 | C1324 | . | . | 1.375(14) | ? |
| C1323 | H1323 | . | . | .953 | ? |
| C1324 | C1325 | . | . | 1.376(15) | ? |
| C1324 | H1324 | . | . | .966 | ? |

| | | | | | |
|-------|-------|---|---|-----------|---|
| C1325 | C1326 | . | . | 1.390(12) | ? |
| C1325 | H1325 | . | . | .994 | ? |
| C1326 | H1326 | . | . | .982 | ? |
| C231 | C232 | . | . | 1.228(9) | ? |
| C232 | C2321 | . | . | 1.439(10) | ? |
| C2321 | C2322 | . | . | 1.379(10) | ? |
| C2321 | C2326 | . | . | 1.398(10) | ? |
| C2322 | C2323 | . | . | 1.404(12) | ? |
| C2322 | H2322 | . | . | .987 | ? |
| C2323 | C2324 | . | . | 1.383(12) | ? |
| C2323 | H2323 | . | . | .982 | ? |
| C2324 | C2325 | . | . | 1.384(11) | ? |
| C2324 | H2324 | . | . | .957 | ? |
| C2325 | C2326 | . | . | 1.376(10) | ? |
| C2325 | H2325 | . | . | .964 | ? |
| C2326 | H2326 | . | . | .988 | ? |
| C141 | C142 | . | . | 1.238(10) | ? |
| C142 | C1421 | . | . | 1.434(10) | ? |
| C1421 | C1422 | . | . | 1.392(11) | ? |
| C1421 | C1426 | . | . | 1.398(11) | ? |
| C1422 | C1423 | . | . | 1.396(12) | ? |
| C1422 | H1422 | . | . | .950 | ? |
| C1423 | C1424 | . | . | 1.341(15) | ? |
| C1423 | H1423 | . | . | .984 | ? |
| C1424 | C1425 | . | . | 1.379(15) | ? |
| C1424 | H1424 | . | . | .952 | ? |
| C1425 | C1426 | . | . | 1.402(11) | ? |
| C1425 | H1425 | . | . | .966 | ? |
| C1426 | H1426 | . | . | .967 | ? |
| C241 | C242 | . | . | 1.232(9) | ? |
| C242 | C2421 | . | . | 1.443(9) | ? |
| C2421 | C2422 | . | . | 1.411(10) | ? |
| C2421 | C2426 | . | . | 1.398(11) | ? |
| C2422 | C2423 | . | . | 1.372(10) | ? |
| C2422 | H2422 | . | . | .953 | ? |
| C2423 | C2424 | . | . | 1.375(12) | ? |
| C2423 | H2423 | . | . | .972 | ? |
| C2424 | C2425 | . | . | 1.394(12) | ? |
| C2424 | H2424 | . | . | .963 | ? |
| C2425 | C2426 | . | . | 1.373(11) | ? |
| C2425 | H2425 | . | . | .953 | ? |
| C2426 | H2426 | . | . | .961 | ? |
| C11 | C12 | . | . | 1.34(2) | ? |
| C11 | C16 | . | . | 1.350(16) | ? |
| C11 | H11 | . | . | 1.007 | ? |
| C12 | C13 | . | . | 1.44(2) | ? |
| C12 | H12 | . | . | .938 | ? |
| C13 | C14 | . | . | 1.38(3) | ? |
| C13 | H13 | . | . | .976 | ? |
| C14 | C15 | . | . | 1.31(2) | ? |
| C14 | H14 | . | . | 1.017 | ? |
| C15 | C16 | . | . | 1.361(17) | ? |
| C15 | H15 | . | . | .965 | ? |
| C16 | H16 | . | . | .963 | ? |
| C21 | C22 | . | . | 1.386(14) | ? |
| C21 | C26 | . | . | 1.368(14) | ? |
| C21 | H21 | . | . | .930 | ? |
| C22 | C23 | . | . | 1.370(14) | ? |
| C22 | H22 | . | . | .970 | ? |
| C23 | C24 | . | . | 1.409(14) | ? |
| C23 | H23 | . | . | .982 | ? |

C24 C25 . . 1.396(14) ?
C24 H24 . . .923 ?
C25 C26 . . 1.355(13) ?
C25 H25 . . .953 ?
C26 H26 . . .963 ?

loop_

_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
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_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle

_geom_angle_publ_flag #<< enter YES for value to be published

P1 Ir1 C111 . . . 92.85(19) ?
P1 Ir1 C121 . . . 90.5(2) ?
P1 Ir1 C131 . . . 97.5(2) ?
P1 Ir1 C141 . . . 98.0(2) ?
C111 Ir1 C121 . . . 93.0(3) ?
C111 Ir1 C131 . . . 169.6(3) ?
C111 Ir1 C141 . . . 87.1(3) ?
C121 Ir1 C131 . . . 88.3(3) ?
C121 Ir1 C141 . . . 171.5(3) ?
C131 Ir1 C141 . . . 90.2(3) ?
P2 Ir2 C211 . . . 94.3(2) ?
P2 Ir2 C221 . . . 91.33(18) ?
P2 Ir2 C231 . . . 94.58(18) ?
P2 Ir2 C241 . . . 101.40(19) ?
C211 Ir2 C221 . . . 92.3(3) ?
C211 Ir2 C231 . . . 170.7(3) ?
C211 Ir2 C241 . . . 89.6(3) ?
C221 Ir2 C231 . . . 90.1(3) ?
C221 Ir2 C241 . . . 166.9(3) ?
C231 Ir2 C241 . . . 86.0(3) ?
C111 Cu1 C112 . . . 34.4(3) ?
C111 Cu1 C211 . . . 174.8(3) ?
C111 Cu1 C212 . . . 152.3(3) ?
C112 Cu1 C211 . . . 150.7(3) ?
C112 Cu1 C212 . . . 120.1(3) ?
C211 Cu1 C212 . . . 32.6(3) ?
C121 Cu2 C122 . . . 32.4(3) ?
C121 Cu2 C221 . . . 173.6(3) ?
C121 Cu2 C222 . . . 140.2(3) ?
C122 Cu2 C221 . . . 141.2(2) ?
C122 Cu2 C222 . . . 109.9(2) ?
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C131 Cu3 C132 . . . 33.7(3) ?
C131 Cu3 C231 . . . 177.4(3) ?
C131 Cu3 C232 . . . 143.4(3) ?
C132 Cu3 C231 . . . 143.7(3) ?
C132 Cu3 C232 . . . 112.5(3) ?
C231 Cu3 C232 . . . 34.3(3) ?
C141 Cu4 C142 . . . 33.5(3) ?
C141 Cu4 C241 . . . 171.8(3) ?
C141 Cu4 C242 . . . 137.8(3) ?
C142 Cu4 C241 . . . 139.9(3) ?
C142 Cu4 C242 . . . 109.5(3) ?
C241 Cu4 C242 . . . 34.0(3) ?
Ir1 P1 C1011 . . . 111.8(2) ?
Ir1 P1 C1021 . . . 116.1(2) ?

| | | | | | | | |
|-------|-------|-------|---|---|---|----------|---|
| Ir1 | P1 | C1031 | . | . | . | 116.7(2) | ? |
| C1011 | P1 | C1021 | . | . | . | 103.9(3) | ? |
| C1011 | P1 | C1031 | . | . | . | 104.7(3) | ? |
| C1021 | P1 | C1031 | . | . | . | 102.2(3) | ? |
| P1 | C1011 | C1012 | . | . | . | 119.7(6) | ? |
| P1 | C1011 | C1016 | . | . | . | 121.0(6) | ? |
| C1012 | C1011 | C1016 | . | . | . | 118.8(6) | ? |
| C1011 | C1012 | C1013 | . | . | . | 120.6(7) | ? |
| C1011 | C1012 | H1012 | . | . | . | 119.4 | ? |
| C1013 | C1012 | H1012 | . | . | . | 119.9 | ? |
| C1012 | C1013 | C1014 | . | . | . | 120.4(7) | ? |
| C1012 | C1013 | H1013 | . | . | . | 118.8 | ? |
| C1014 | C1013 | H1013 | . | . | . | 120.7 | ? |
| C1013 | C1014 | C1015 | . | . | . | 119.5(7) | ? |
| C1013 | C1014 | H1014 | . | . | . | 119.9 | ? |
| C1015 | C1014 | H1014 | . | . | . | 120.5 | ? |
| C1014 | C1015 | C1016 | . | . | . | 120.5(7) | ? |
| C1014 | C1015 | H1015 | . | . | . | 118.4 | ? |
| C1016 | C1015 | H1015 | . | . | . | 121.0 | ? |
| C1011 | C1016 | C1015 | . | . | . | 120.0(7) | ? |
| C1011 | C1016 | H1016 | . | . | . | 120.8 | ? |
| C1015 | C1016 | H1016 | . | . | . | 119.1 | ? |
| P1 | C1021 | C1022 | . | . | . | 117.5(5) | ? |
| P1 | C1021 | C1026 | . | . | . | 122.5(5) | ? |
| C1022 | C1021 | C1026 | . | . | . | 120.0(6) | ? |
| C1021 | C1022 | C1023 | . | . | . | 120.0(7) | ? |
| C1021 | C1022 | H1022 | . | . | . | 120.5 | ? |
| C1023 | C1022 | H1022 | . | . | . | 119.5 | ? |
| C1022 | C1023 | C1024 | . | . | . | 120.3(7) | ? |
| C1022 | C1023 | H1023 | . | . | . | 117.9 | ? |
| C1024 | C1023 | H1023 | . | . | . | 121.7 | ? |
| C1023 | C1024 | C1025 | . | . | . | 119.5(7) | ? |
| C1023 | C1024 | H1024 | . | . | . | 118.0 | ? |
| C1025 | C1024 | H1024 | . | . | . | 122.5 | ? |
| C1024 | C1025 | C1026 | . | . | . | 120.5(7) | ? |
| C1024 | C1025 | H1025 | . | . | . | 118.6 | ? |
| C1026 | C1025 | H1025 | . | . | . | 120.9 | ? |
| C1021 | C1026 | C1025 | . | . | . | 119.7(7) | ? |
| C1021 | C1026 | H1026 | . | . | . | 119.6 | ? |
| C1025 | C1026 | H1026 | . | . | . | 120.7 | ? |
| P1 | C1031 | C1032 | . | . | . | 123.0(6) | ? |
| P1 | C1031 | C1036 | . | . | . | 117.0(5) | ? |
| C1032 | C1031 | C1036 | . | . | . | 119.7(7) | ? |
| C1031 | C1032 | C1033 | . | . | . | 119.5(7) | ? |
| C1031 | C1032 | H1032 | . | . | . | 120.1 | ? |
| C1033 | C1032 | H1032 | . | . | . | 120.4 | ? |
| C1032 | C1033 | C1034 | . | . | . | 120.0(7) | ? |
| C1032 | C1033 | H1033 | . | . | . | 120.7 | ? |
| C1034 | C1033 | H1033 | . | . | . | 119.2 | ? |
| C1033 | C1034 | C1035 | . | . | . | 121.0(8) | ? |
| C1033 | C1034 | H1034 | . | . | . | 119.0 | ? |
| C1035 | C1034 | H1034 | . | . | . | 120.0 | ? |
| C1034 | C1035 | C1036 | . | . | . | 119.8(7) | ? |
| C1034 | C1035 | H1035 | . | . | . | 119.5 | ? |
| C1036 | C1035 | H1035 | . | . | . | 120.6 | ? |
| C1031 | C1036 | C1035 | . | . | . | 119.9(7) | ? |
| C1031 | C1036 | H1036 | . | . | . | 118.5 | ? |
| C1035 | C1036 | H1036 | . | . | . | 121.6 | ? |
| Ir2 | P2 | C2011 | . | . | . | 113.8(2) | ? |
| Ir2 | P2 | C2021 | . | . | . | 117.7(2) | ? |
| Ir2 | P2 | C2031 | . | . | . | 114.9(2) | ? |

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|-------|-------|-------|---|---|---|----------|---|
| C2011 | P2 | C2021 | . | . | . | 100.4(3) | ? |
| C2011 | P2 | C2031 | . | . | . | 104.7(3) | ? |
| C2021 | P2 | C2031 | . | . | . | 103.5(3) | ? |
| P2 | C2011 | C2012 | . | . | . | 117.4(5) | ? |
| P2 | C2011 | C2016 | . | . | . | 124.8(5) | ? |
| C2012 | C2011 | C2016 | . | . | . | 117.5(6) | ? |
| C2011 | C2012 | C2013 | . | . | . | 120.7(7) | ? |
| C2011 | C2012 | H2012 | . | . | . | 120.1 | ? |
| C2013 | C2012 | H2012 | . | . | . | 119.0 | ? |
| C2012 | C2013 | C2014 | . | . | . | 119.4(8) | ? |
| C2012 | C2013 | H2013 | . | . | . | 122.8 | ? |
| C2014 | C2013 | H2013 | . | . | . | 117.8 | ? |
| C2013 | C2014 | C2015 | . | . | . | 120.3(7) | ? |
| C2013 | C2014 | H2014 | . | . | . | 120.5 | ? |
| C2015 | C2014 | H2014 | . | . | . | 119.1 | ? |
| C2014 | C2015 | C2016 | . | . | . | 119.7(8) | ? |
| C2014 | C2015 | H2015 | . | . | . | 121.4 | ? |
| C2016 | C2015 | H2015 | . | . | . | 118.8 | ? |
| C2011 | C2016 | C2015 | . | . | . | 122.3(7) | ? |
| C2011 | C2016 | H2016 | . | . | . | 120.3 | ? |
| C2015 | C2016 | H2016 | . | . | . | 117.4 | ? |
| P2 | C2021 | C2022 | . | . | . | 118.8(5) | ? |
| P2 | C2021 | C2026 | . | . | . | 122.4(6) | ? |
| C2022 | C2021 | C2026 | . | . | . | 118.8(7) | ? |
| C2021 | C2022 | C2023 | . | . | . | 120.5(7) | ? |
| C2021 | C2022 | H2022 | . | . | . | 120.8 | ? |
| C2023 | C2022 | H2022 | . | . | . | 118.6 | ? |
| C2022 | C2023 | C2024 | . | . | . | 120.2(7) | ? |
| C2022 | C2023 | H2023 | . | . | . | 119.6 | ? |
| C2024 | C2023 | H2023 | . | . | . | 120.2 | ? |
| C2023 | C2024 | C2025 | . | . | . | 119.8(8) | ? |
| C2023 | C2024 | H2024 | . | . | . | 118.9 | ? |
| C2025 | C2024 | H2024 | . | . | . | 121.2 | ? |
| C2024 | C2025 | C2026 | . | . | . | 120.5(8) | ? |
| C2024 | C2025 | H2025 | . | . | . | 120.9 | ? |
| C2026 | C2025 | H2025 | . | . | . | 118.6 | ? |
| C2021 | C2026 | C2025 | . | . | . | 120.1(7) | ? |
| C2021 | C2026 | H2026 | . | . | . | 117.2 | ? |
| C2025 | C2026 | H2026 | . | . | . | 122.7 | ? |
| P2 | C2031 | C2032 | . | . | . | 118.0(5) | ? |
| P2 | C2031 | C2036 | . | . | . | 124.0(5) | ? |
| C2032 | C2031 | C2036 | . | . | . | 118.1(6) | ? |
| C2031 | C2032 | C2033 | . | . | . | 120.7(7) | ? |
| C2031 | C2032 | H2032 | . | . | . | 120.5 | ? |
| C2033 | C2032 | H2032 | . | . | . | 118.8 | ? |
| C2032 | C2033 | C2034 | . | . | . | 119.8(7) | ? |
| C2032 | C2033 | H2033 | . | . | . | 121.1 | ? |
| C2034 | C2033 | H2033 | . | . | . | 119.1 | ? |
| C2033 | C2034 | C2035 | . | . | . | 120.0(8) | ? |
| C2033 | C2034 | H2034 | . | . | . | 118.2 | ? |
| C2035 | C2034 | H2034 | . | . | . | 121.7 | ? |
| C2034 | C2035 | C2036 | . | . | . | 119.5(8) | ? |
| C2034 | C2035 | H2035 | . | . | . | 119.6 | ? |
| C2036 | C2035 | H2035 | . | . | . | 120.9 | ? |
| C2031 | C2036 | C2035 | . | . | . | 121.8(7) | ? |
| C2031 | C2036 | H2036 | . | . | . | 119.4 | ? |
| C2035 | C2036 | H2036 | . | . | . | 118.8 | ? |
| Ir1 | C111 | Cu1 | . | . | . | 95.5(3) | ? |
| Ir1 | C111 | C112 | . | . | . | 171.9(6) | ? |
| Cu1 | C111 | C112 | . | . | . | 79.4(5) | ? |
| Cu1 | C112 | C111 | . | . | . | 66.2(4) | ? |

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|-------|-------|-------|---|---|---|----------|---|
| Cu1 | C112 | C1121 | . | . | . | 134.4(5) | ? |
| C111 | C112 | C1121 | . | . | . | 159.2(7) | ? |
| C112 | C1121 | C1122 | . | . | . | 122.5(6) | ? |
| C112 | C1121 | C1126 | . | . | . | 119.2(6) | ? |
| C1122 | C1121 | C1126 | . | . | . | 118.3(6) | ? |
| C1121 | C1122 | C1123 | . | . | . | 121.0(6) | ? |
| C1121 | C1122 | H1122 | . | . | . | 118.3 | ? |
| C1123 | C1122 | H1122 | . | . | . | 120.7 | ? |
| C1122 | C1123 | C1124 | . | . | . | 120.5(7) | ? |
| C1122 | C1123 | H1123 | . | . | . | 120.1 | ? |
| C1124 | C1123 | H1123 | . | . | . | 119.4 | ? |
| C1123 | C1124 | C1125 | . | . | . | 119.9(7) | ? |
| C1123 | C1124 | H1124 | . | . | . | 121.2 | ? |
| C1125 | C1124 | H1124 | . | . | . | 118.8 | ? |
| C1124 | C1125 | C1126 | . | . | . | 119.9(7) | ? |
| C1124 | C1125 | H1125 | . | . | . | 121.6 | ? |
| C1126 | C1125 | H1125 | . | . | . | 118.5 | ? |
| C1121 | C1126 | C1125 | . | . | . | 120.4(7) | ? |
| C1121 | C1126 | H1126 | . | . | . | 119.8 | ? |
| C1125 | C1126 | H1126 | . | . | . | 119.8 | ? |
| Ir2 | C211 | Cu1 | . | . | . | 91.7(3) | ? |
| Ir2 | C211 | C212 | . | . | . | 173.2(6) | ? |
| Cu1 | C211 | C212 | . | . | . | 82.4(5) | ? |
| Cu1 | C212 | C211 | . | . | . | 65.0(4) | ? |
| Cu1 | C212 | C2121 | . | . | . | 125.1(5) | ? |
| C211 | C212 | C2121 | . | . | . | 169.4(7) | ? |
| C212 | C2121 | C2122 | . | . | . | 119.7(7) | ? |
| C212 | C2121 | C2126 | . | . | . | 121.5(7) | ? |
| C2122 | C2121 | C2126 | . | . | . | 118.7(7) | ? |
| C2121 | C2122 | C2123 | . | . | . | 120.4(8) | ? |
| C2121 | C2122 | H2122 | . | . | . | 120.4 | ? |
| C2123 | C2122 | H2122 | . | . | . | 119.2 | ? |
| C2122 | C2123 | C2124 | . | . | . | 120.5(9) | ? |
| C2122 | C2123 | H2123 | . | . | . | 120.2 | ? |
| C2124 | C2123 | H2123 | . | . | . | 119.2 | ? |
| C2123 | C2124 | C2125 | . | . | . | 119.7(8) | ? |
| C2123 | C2124 | H2124 | . | . | . | 119.3 | ? |
| C2125 | C2124 | H2124 | . | . | . | 120.8 | ? |
| C2124 | C2125 | C2126 | . | . | . | 120.9(9) | ? |
| C2124 | C2125 | H2125 | . | . | . | 120.4 | ? |
| C2126 | C2125 | H2125 | . | . | . | 118.7 | ? |
| C2121 | C2126 | C2125 | . | . | . | 119.6(8) | ? |
| C2121 | C2126 | H2126 | . | . | . | 119.8 | ? |
| C2125 | C2126 | H2126 | . | . | . | 120.5 | ? |
| Ir1 | C121 | Cu2 | . | . | . | 87.4(3) | ? |
| Ir1 | C121 | C122 | . | . | . | 174.4(6) | ? |
| Cu2 | C121 | C122 | . | . | . | 87.0(5) | ? |
| Cu2 | C122 | C121 | . | . | . | 60.6(4) | ? |
| Cu2 | C122 | C1221 | . | . | . | 133.9(5) | ? |
| C121 | C122 | C1221 | . | . | . | 165.4(7) | ? |
| C122 | C1221 | C1222 | . | . | . | 119.3(6) | ? |
| C122 | C1221 | C1226 | . | . | . | 122.2(7) | ? |
| C1222 | C1221 | C1226 | . | . | . | 118.5(7) | ? |
| C1221 | C1222 | C1223 | . | . | . | 120.3(7) | ? |
| C1221 | C1222 | H1222 | . | . | . | 121.7 | ? |
| C1223 | C1222 | H1222 | . | . | . | 117.9 | ? |
| C1222 | C1223 | C1224 | . | . | . | 121.4(8) | ? |
| C1222 | C1223 | H1223 | . | . | . | 119.6 | ? |
| C1224 | C1223 | H1223 | . | . | . | 119.0 | ? |
| C1223 | C1224 | C1225 | . | . | . | 118.7(8) | ? |
| C1223 | C1224 | H1224 | . | . | . | 121.4 | ? |

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|-------|-------|-------|---|---|---|-----------|---|
| C1225 | C1224 | H1224 | . | . | . | 119.9 | ? |
| C1224 | C1225 | C1226 | . | . | . | 121.7(8) | ? |
| C1224 | C1225 | H1225 | . | . | . | 119.3 | ? |
| C1226 | C1225 | H1225 | . | . | . | 119.0 | ? |
| C1221 | C1226 | C1225 | . | . | . | 119.4(8) | ? |
| C1221 | C1226 | H1226 | . | . | . | 121.0 | ? |
| C1225 | C1226 | H1226 | . | . | . | 119.5 | ? |
| Ir2 | C221 | Cu2 | . | . | . | 90.4(2) | ? |
| Ir2 | C221 | C222 | . | . | . | 170.0(6) | ? |
| Cu2 | C221 | C222 | . | . | . | 79.6(4) | ? |
| Cu2 | C222 | C221 | . | . | . | 66.2(4) | ? |
| Cu2 | C222 | C2221 | . | . | . | 123.2(5) | ? |
| C221 | C222 | C2221 | . | . | . | 169.9(7) | ? |
| C222 | C2221 | C2222 | . | . | . | 119.1(7) | ? |
| C222 | C2221 | C2226 | . | . | . | 122.1(7) | ? |
| C2222 | C2221 | C2226 | . | . | . | 118.7(8) | ? |
| C2221 | C2222 | C2223 | . | . | . | 123.6(10) | ? |
| C2221 | C2222 | H2222 | . | . | . | 116.1 | ? |
| C2223 | C2222 | H2222 | . | . | . | 120.3 | ? |
| C2222 | C2223 | C2224 | . | . | . | 115.8(11) | ? |
| C2222 | C2223 | H2223 | . | . | . | 121.9 | ? |
| C2224 | C2223 | H2223 | . | . | . | 122.3 | ? |
| C2223 | C2224 | C2225 | . | . | . | 125.3(11) | ? |
| C2223 | C2224 | H2224 | . | . | . | 114.8 | ? |
| C2225 | C2224 | H2224 | . | . | . | 119.9 | ? |
| C2224 | C2225 | C2226 | . | . | . | 117.7(11) | ? |
| C2224 | C2225 | H2225 | . | . | . | 122.7 | ? |
| C2226 | C2225 | H2225 | . | . | . | 119.5 | ? |
| C2221 | C2226 | C2225 | . | . | . | 118.8(9) | ? |
| C2221 | C2226 | H2226 | . | . | . | 119.8 | ? |
| C2225 | C2226 | H2226 | . | . | . | 121.3 | ? |
| Ir1 | C131 | Cu3 | . | . | . | 89.1(3) | ? |
| Ir1 | C131 | C132 | . | . | . | 169.2(6) | ? |
| Cu3 | C131 | C132 | . | . | . | 80.4(5) | ? |
| Cu3 | C132 | C131 | . | . | . | 65.8(4) | ? |
| Cu3 | C132 | C1321 | . | . | . | 122.8(5) | ? |
| C131 | C132 | C1321 | . | . | . | 171.4(7) | ? |
| C132 | C1321 | C1322 | . | . | . | 120.5(7) | ? |
| C132 | C1321 | C1326 | . | . | . | 120.0(7) | ? |
| C1322 | C1321 | C1326 | . | . | . | 119.5(7) | ? |
| C1321 | C1322 | C1323 | . | . | . | 120.2(8) | ? |
| C1321 | C1322 | H1322 | . | . | . | 120.0 | ? |
| C1323 | C1322 | H1322 | . | . | . | 119.7 | ? |
| C1322 | C1323 | C1324 | . | . | . | 120.1(9) | ? |
| C1322 | C1323 | H1323 | . | . | . | 121.1 | ? |
| C1324 | C1323 | H1323 | . | . | . | 118.8 | ? |
| C1323 | C1324 | C1325 | . | . | . | 120.2(8) | ? |
| C1323 | C1324 | H1324 | . | . | . | 119.7 | ? |
| C1325 | C1324 | H1324 | . | . | . | 120.2 | ? |
| C1324 | C1325 | C1326 | . | . | . | 121.1(9) | ? |
| C1324 | C1325 | H1325 | . | . | . | 120.1 | ? |
| C1326 | C1325 | H1325 | . | . | . | 118.8 | ? |
| C1321 | C1326 | C1325 | . | . | . | 118.9(8) | ? |
| C1321 | C1326 | H1326 | . | . | . | 119.9 | ? |
| C1325 | C1326 | H1326 | . | . | . | 121.2 | ? |
| Ir2 | C231 | Cu3 | . | . | . | 91.6(3) | ? |
| Ir2 | C231 | C232 | . | . | . | 170.4(6) | ? |
| Cu3 | C231 | C232 | . | . | . | 78.8(4) | ? |
| Cu3 | C232 | C231 | . | . | . | 66.8(4) | ? |
| Cu3 | C232 | C2321 | . | . | . | 132.0(5) | ? |
| C231 | C232 | C2321 | . | . | . | 161.1(7) | ? |

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|-------|-------|-------|---|---|---|----------|---|
| C232 | C2321 | C2322 | . | . | . | 119.7(6) | ? |
| C232 | C2321 | C2326 | . | . | . | 121.9(6) | ? |
| C2322 | C2321 | C2326 | . | . | . | 118.4(6) | ? |
| C2321 | C2322 | C2323 | . | . | . | 120.7(7) | ? |
| C2321 | C2322 | H2322 | . | . | . | 119.1 | ? |
| C2323 | C2322 | H2322 | . | . | . | 120.0 | ? |
| C2322 | C2323 | C2324 | . | . | . | 120.2(7) | ? |
| C2322 | C2323 | H2323 | . | . | . | 118.5 | ? |
| C2324 | C2323 | H2323 | . | . | . | 121.2 | ? |
| C2323 | C2324 | C2325 | . | . | . | 119.0(7) | ? |
| C2323 | C2324 | H2324 | . | . | . | 121.0 | ? |
| C2325 | C2324 | H2324 | . | . | . | 120.0 | ? |
| C2324 | C2325 | C2326 | . | . | . | 120.9(7) | ? |
| C2324 | C2325 | H2325 | . | . | . | 118.9 | ? |
| C2326 | C2325 | H2325 | . | . | . | 120.2 | ? |
| C2321 | C2326 | C2325 | . | . | . | 120.9(7) | ? |
| C2321 | C2326 | H2326 | . | . | . | 119.4 | ? |
| C2325 | C2326 | H2326 | . | . | . | 119.7 | ? |
| Ir1 | C141 | Cu4 | . | . | . | 86.8(3) | ? |
| Ir1 | C141 | C142 | . | . | . | 168.8(6) | ? |
| Cu4 | C141 | C142 | . | . | . | 82.8(5) | ? |
| Cu4 | C142 | C141 | . | . | . | 63.7(4) | ? |
| Cu4 | C142 | C1421 | . | . | . | 130.0(5) | ? |
| C141 | C142 | C1421 | . | . | . | 166.3(7) | ? |
| C142 | C1421 | C1422 | . | . | . | 121.2(7) | ? |
| C142 | C1421 | C1426 | . | . | . | 120.3(7) | ? |
| C1422 | C1421 | C1426 | . | . | . | 118.4(7) | ? |
| C1421 | C1422 | C1423 | . | . | . | 120.0(8) | ? |
| C1421 | C1422 | H1422 | . | . | . | 118.1 | ? |
| C1423 | C1422 | H1422 | . | . | . | 121.9 | ? |
| C1422 | C1423 | C1424 | . | . | . | 121.0(9) | ? |
| C1422 | C1423 | H1423 | . | . | . | 119.0 | ? |
| C1424 | C1423 | H1423 | . | . | . | 120.0 | ? |
| C1423 | C1424 | C1425 | . | . | . | 120.9(8) | ? |
| C1423 | C1424 | H1424 | . | . | . | 119.8 | ? |
| C1425 | C1424 | H1424 | . | . | . | 119.3 | ? |
| C1424 | C1425 | C1426 | . | . | . | 119.4(9) | ? |
| C1424 | C1425 | H1425 | . | . | . | 120.0 | ? |
| C1426 | C1425 | H1425 | . | . | . | 120.5 | ? |
| C1421 | C1426 | C1425 | . | . | . | 120.2(8) | ? |
| C1421 | C1426 | H1426 | . | . | . | 119.1 | ? |
| C1425 | C1426 | H1426 | . | . | . | 120.7 | ? |
| Ir2 | C241 | Cu4 | . | . | . | 87.5(2) | ? |
| Ir2 | C241 | C242 | . | . | . | 166.3(6) | ? |
| Cu4 | C241 | C242 | . | . | . | 79.3(5) | ? |
| Cu4 | C242 | C241 | . | . | . | 66.7(4) | ? |
| Cu4 | C242 | C2421 | . | . | . | 122.1(5) | ? |
| C241 | C242 | C2421 | . | . | . | 170.9(7) | ? |
| C242 | C2421 | C2422 | . | . | . | 121.5(6) | ? |
| C242 | C2421 | C2426 | . | . | . | 119.8(7) | ? |
| C2422 | C2421 | C2426 | . | . | . | 118.6(6) | ? |
| C2421 | C2422 | C2423 | . | . | . | 120.0(7) | ? |
| C2421 | C2422 | H2422 | . | . | . | 120.1 | ? |
| C2423 | C2422 | H2422 | . | . | . | 119.9 | ? |
| C2422 | C2423 | C2424 | . | . | . | 121.2(7) | ? |
| C2422 | C2423 | H2423 | . | . | . | 118.5 | ? |
| C2424 | C2423 | H2423 | . | . | . | 120.4 | ? |
| C2423 | C2424 | C2425 | . | . | . | 119.3(7) | ? |
| C2423 | C2424 | H2424 | . | . | . | 117.7 | ? |
| C2425 | C2424 | H2424 | . | . | . | 123.0 | ? |
| C2424 | C2425 | C2426 | . | . | . | 120.6(8) | ? |

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|-------|-------|-------|---|---|---|-----------|---|
| C2424 | C2425 | H2425 | . | . | . | 120.1 | ? |
| C2426 | C2425 | H2425 | . | . | . | 119.3 | ? |
| C2421 | C2426 | C2425 | . | . | . | 120.3(7) | ? |
| C2421 | C2426 | H2426 | . | . | . | 119.7 | ? |
| C2425 | C2426 | H2426 | . | . | . | 120.0 | ? |
| C12 | C11 | C16 | . | . | . | 120.9(11) | ? |
| C12 | C11 | H11 | . | . | . | 120.0 | ? |
| C16 | C11 | H11 | . | . | . | 119.0 | ? |
| C11 | C12 | C13 | . | . | . | 118.3(13) | ? |
| C11 | C12 | H12 | . | . | . | 124.9 | ? |
| C13 | C12 | H12 | . | . | . | 116.5 | ? |
| C12 | C13 | C14 | . | . | . | 118.2(12) | ? |
| C12 | C13 | H13 | . | . | . | 121 | ? |
| C14 | C13 | H13 | . | . | . | 120.2 | ? |
| C13 | C14 | C15 | . | . | . | 120.5(14) | ? |
| C13 | C14 | H14 | . | . | . | 120.9 | ? |
| C15 | C14 | H14 | . | . | . | 118.6 | ? |
| C14 | C15 | C16 | . | . | . | 121.5(13) | ? |
| C14 | C15 | H15 | . | . | . | 124.3 | ? |
| C16 | C15 | H15 | . | . | . | 114.2 | ? |
| C11 | C16 | C15 | . | . | . | 120.4(11) | ? |
| C11 | C16 | H16 | . | . | . | 120.6 | ? |
| C15 | C16 | H16 | . | . | . | 118.5 | ? |
| C22 | C21 | C26 | . | . | . | 118.6(9) | ? |
| C22 | C21 | H21 | . | . | . | 120.6 | ? |
| C26 | C21 | H21 | . | . | . | 120.8 | ? |
| C21 | C22 | C23 | . | . | . | 121.7(9) | ? |
| C21 | C22 | H22 | . | . | . | 120.1 | ? |
| C23 | C22 | H22 | . | . | . | 118.1 | ? |
| C22 | C23 | C24 | . | . | . | 118.2(9) | ? |
| C22 | C23 | H23 | . | . | . | 122.1 | ? |
| C24 | C23 | H23 | . | . | . | 119.6 | ? |
| C23 | C24 | C25 | . | . | . | 119.9(9) | ? |
| C23 | C24 | H24 | . | . | . | 119.3 | ? |
| C25 | C24 | H24 | . | . | . | 120.4 | ? |
| C24 | C25 | C26 | . | . | . | 119.3(9) | ? |
| C24 | C25 | H25 | . | . | . | 120.7 | ? |
| C26 | C25 | H25 | . | . | . | 120.0 | ? |
| C21 | C26 | C25 | . | . | . | 122.1(10) | ? |
| C21 | C26 | H26 | . | . | . | 120.7 | ? |
| C25 | C26 | H26 | . | . | . | 117.1 | ? |

loop_

_geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion
 _geom_torsion_publ_flag
 ? ? ? ? ? ? ? ? ? ?

#<< enter YES for value to be published

loop_

_geom_hbond_atom_site_label_D
 _geom_hbond_atom_site_label_H
 _geom_hbond_atom_site_label_A
 _geom_hbond_site_symmetry_D
 _geom_hbond_site_symmetry_H

```
_geom_hbond_site_symmetry_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_publ_flag          #<< enter YES for value to be published
    ? ? ? ? ? ? ? ? ? ?
```

```
#-----
#          Special items requested by author for inclusion in paper
#-----
```

```
loop_
  _publ_manuscript_incl_extra_item
  _publ_manuscript_incl_extra_defn
    ? ?
```

```
#-----
#          Items which are non-mandatory for Acta C submissions
#-----
```

```
loop_
  _geom_contact_atom_site_label_1
  _geom_contact_atom_site_label_2
  _geom_contact_distance
  _geom_contact_site_symmetry_1
  _geom_contact_site_symmetry_2
  _geom_contact_publ_flag
    ? ? ? ? ? ?
```

```
_atom_sites_solution_primary      ?
_atom_sites_solution_secondary     ?
_atom_sites_solution_hydrogens     ?
```

```
_geom_special_details             ?
```

```
_cell_special_details
;      ?
;
```

```
_exptl_special_details
;      ?
;
```

```
_diffraction_special_details
;      ?
;
```

```
_chemical_compound_source         ?
_chemical_name_systematic         ?
_chemical_name_common              ?
_chemical_formula_analytical      ?
_chemical_formula_structural      ?
```

```
_exptl_crystal_F_000             4216
```

```
loop_
  _diffraction_standard_refln_index_h
  _diffraction_standard_refln_index_k
```

```

_diffrn_standard_refl_index_l
? ? ?
loop_
_diffrn_attenuator_code
_diffrn_attenuator_scale
? ?

_reflns_limit_h_min          0
_reflns_limit_h_max         21
_reflns_limit_k_min          0
_reflns_limit_k_max         22
_reflns_limit_l_min          0
_reflns_limit_l_max         44
_reflns_number_observed      ?
_reflns_d_resolution_high    .731
_reflns_d_resolution_low    14.845

_diffrn_refl_av_sigmaI/netI  .041
_diffrn_refl_theta_min      1.37
_diffrn_refl_reduction_process ?

_diffrn_ambient_temperature  153
_diffrn_radiation_source     'sealed tube'
_diffrn_radiation_monochromator graphite
_diffrn_radiation_detector   'CCD area detector'

_refine_ls_extinction_expression 'Eq22 p292 "Cryst. Comp." Munksgaard 1970'
_refine_ls_matrix_type       full
_refine_ls_number_restraints  0
_refine_ls_number_constraints 0
_refine_ls_R_factor_all      .041
_refine_ls_wR_factor_all     .043
_refine_ls_goodness_of_fit_all 1.806
_refine_ls_shift/su_mean     .0002

```

```

#=====
#           Structure Factor lists should be submitted as separate files
#=====

```

```

#data_<structure> # but for xtal use the refln data is needed in same block

```

```

loop_
_refln_index_h
_refln_index_k
_refln_index_l
_refln_F_meas
_refln_F_calc
_refln_F_sigma
_refln_F_squared_meas
_refln_F_squared_calc
_refln_F_squared_sigma
_refln_observed_status
_refln_F_meas_friedel
_refln_F_sigma_friedel
_refln_F_squared_meas_friedel
_refln_F_squared_sigma_friedel
? ? ? ? ? ? ? ? ? ? ? ? ? ?

```



```
#####  
#  
#   CIF generated by the Xtal System   #  
#  
#####
```

data_global

```
_audit_creation_method      Xtal3.6  
_audit_creation_date        01-12-07  
_audit_update_record        ?
```

```
#####  
# (Publishing Staff Use Only)
```

```
_journal_date_recd_electronic  ?  
_journal_date_to_coeditor      ?  
_journal_date_from_coeditor    ?  
_journal_date_accepted         ?  
_journal_date_printers_first   ?  
_journal_date_printers_final   ?  
_journal_date_proofs_out       ?  
_journal_date_proofs_in        ?  
_journal_coeditor_name         ?  
_journal_coeditor_code         ?  
_journal_coeditor_notes  
; ?  
;  
_journal_techeditor_code       ?  
_journal_techeditor_notes  
; ?  
;  
_journal_codен_ASTM           ?  
_journal_name_full            ?  
_journal_year                 ?  
_journal_volume               ?  
_journal_issue                ?  
_journal_page_first           ?  
_journal_page_last            ?  
_journal_suppl_publ_number    ?  
_journal_suppl_publ_pages     ?
```

```
#####
```

1. SUBMISSION DETAILS

#-----

```
_publ_contact_author_name  
  'Skelton, B. W.'  
_publ_contact_author_address  
;  
  Department of Chemistry  
  University of Western Australia  
  35 Stirling Highway  
  Crawley  
  Western Australia 6009  
  Australia  
;  
_publ_contact_author_email      bws@crystal.uwa.edu.au  
_publ_contact_author_fax        (+61)_08_9380_1118  
_publ_contact_author_phone      (+61)_08-9380_3481
```

```

_publ_contact_letter
;   ?                               #<< contact letter
;

_publ_requested_journal   ?
_publ_requested_category ?

_publ_section_title
;   ?                               #<< paper title text
;
_publ_section_title_footnote
;   ?                               #<< paper footnote text
;

loop_
_publ_author_name
_publ_author_footnote
_publ_author_address

'Skelton, Brian W.' .
; Department of Chemistry,
University of Western Australia,
35 Stirling Highway,
Crawley,
WA 6009,
Australia.
;

_publ_section_synopsis
;   ?                               #<< synopsis if FI,CI,CM,CO papers
;
_publ_section_abstract
;   ?                               #<< abstract text
;
_publ_section_comment
;   ?                               #<< scientific commentary text
;

_publ_section_exptl_prep
;   ?                               #<< material & crystal preparation text
;

_publ_section_exptl_refinement
;   ?                               #<< crystallographic methods used
;

_publ_section_acknowledgements
;   ?                               #<< acknowledgements text
;

_publ_section_references
;
Sheldrick, G M. (1996). SADABS. Program for Empirical Absorption Correction
of Area Detector Data. University of Gottingen, Germany.

Siemens (1995). SMART and SAINT. Area-Detector Control and Integration

```

Software. Siemens Analytical X-ray Systems Inc., Madison, Wisconsin, USA.

Hall, S.R., King, G.S.D., and Stewart., J.M. (1995).
The Xtal 3.5 User's Manual. University of Western Australia, Lamb: Perth.

```
;  
_publ_section_figure_captions  
;      ?                               #<< figure captions  
;  
  
#=====  
# Data block for single structure (one for each study in the paper)  
#=====
```

data_br691

```
# 2. EXPERIMENTAL DATA  
#-----
```

| | |
|---------------------------------|-----------------------|
| _chemical_formula_sum | 'C100 H70 Ag4 P2 Rh2' |
| _chemical_formula_moiety | ? |
| _chemical_formula_weight | 1970.89 |
| _chemical_melting_point | ? |
| _symmetry_cell_setting | monoclinic |
| _symmetry_space_group_name_H-M | P_1_21/n_1 |
| _symmetry_space_group_name_Hall | -p_2yn |

```
loop_  
_symmetry_equiv_pos_as_xyz  
+x,+y,+z 1/2-x,1/2+y,1/2-z -x,-y,-z 1/2+x,1/2-y,1/2+z
```

| | |
|-------------------------------|--------------|
| _cell_length_a | 17.003(2) |
| _cell_length_b | 26.137(3) |
| _cell_length_c | 35.440(4) |
| _cell_angle_alpha | 90.00000 |
| _cell_angle_beta | 90.160(2) |
| _cell_angle_gamma | 90.00000 |
| _cell_volume | 15750(3) |
| _cell_formula_units_Z | 8 |
| _exptl_crystal_density_diffn | 1.662 |
| _exptl_crystal_density_meas | ? |
| _exptl_crystal_density_method | ? |
| _diffrn_radiation_type | 'Mo K\alpha' |
| _diffrn_radiation_wavelength | .71073 |
| _cell_measurement_reflns_used | 8192 |
| _cell_measurement_theta_min | 1.2 |
| _cell_measurement_theta_max | 22.3 |
| _cell_measurement_temperature | 153 |
| _exptl_absorpt_coefficient_mu | 1.475 |
| _exptl_crystal_description | leaf |
| _exptl_crystal_size_max | .4 |
| _exptl_crystal_size_mid | .3 |
| _exptl_crystal_size_min | .25 |
| _exptl_crystal_size_rad | ? |

```

_exptl_crystal_colour          dark_red

_diffrn_measurement_device_type
;
Bruker SMART CCD diffractometer
;
_diffrn_measurement_method      '\w scans'
_diffrn_detector_area_resol_mean ?

_exptl_absorpt_correction_type  multi-scan
_exptl_absorpt_process_details
;
SADABS; Sheldrick, 1996
;
_exptl_absorpt_correction_T_min .564
_exptl_absorpt_correction_T_max .837

_diffrn_reflns_number          169166
_reflns_number_total           27603
_reflns_Friedel_coverage       0
_reflns_number_gt              18437
_reflns_threshold_expression    'F > 4.00 sig(F )'

_diffrn_reflns_theta_max       24.97
_diffrn_reflns_theta_full      ?
_diffrn_measured_fraction_theta_max ?
_diffrn_measured_fraction_theta_full ?
_diffrn_reflns_av_R_equivalents .081
_diffrn_reflns_limit_h_min     -20
_diffrn_reflns_limit_h_max     20
_diffrn_reflns_limit_k_min     0
_diffrn_reflns_limit_k_max     31
_diffrn_reflns_limit_l_min     0
_diffrn_reflns_limit_l_max     42
_diffrn_standards_number       ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time ?
_diffrn_standards_decay_%      0

_refine_ls_structure_factor_coef F
_refine_ls_R_factor_gt          .068
_refine_ls_wR_factor_ref        .085
_refine_ls_goodness_of_fit_ref  2.372
_refine_ls_number_reflns        18437
_refine_ls_number_parameters    1931
_refine_ls_weighting_scheme     calc
_refine_ls_weighting_details    ?
_refine_ls_hydrogen_treatment  noref
_refine_ls_shift/su_max         .03
_refine_diff_density_min        -1.358
_refine_diff_density_max        2.756

_refine_ls_extinction_method    ?
_refine_ls_extinction_coef      ?
_refine_ls_abs_structure_details ?
_refine_ls_abs_structure_Flack  ?

```

```

# 3. Information for the "methods" section
#-----

```

```

_computing_data_collection      'Siemens SMART (Siemens, 1995)'
_computing_cell_refinement     'Siemens SAINT (Siemens, 1995)'
_computing_data_reduction      'xtal ADDREF SORTRF'
_computing_structure_solution  xtal
_computing_structure_refinement 'xtal CRYLSQ'
_computing_molecular_graphics  xtal
_computing_publication_material 'xtal BONDLA CIFIO'

```

4. Supplementary data for validation and tables

#-----

loop_

```

_atom_type_symbol
_atom_type_description
_atom_type_oxidation_number
_atom_type_number_in_cell
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
  C ? 0 800 .002 .002 'Int Tables Vol IV Tables 2.2B and 2.3.1'
  H ? 0 560 0 0 'Int Tables Vol IV Tables 2.2B and 2.3.1'
  Ag ? 0 32 -1.085 1.101 'Int Tables Vol IV Tables 2.2B and 2.3.1'
  P ? 0 16 .09 .095 'Int Tables Vol IV Tables 2.2B and 2.3.1'
  Rh ? 0 16 -1.287 .919 'Int Tables Vol IV Tables 2.2B and 2.3.1'

```

loop_

```

_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_calc_flag
_atom_site_calc_attached_atom
_atom_site_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
  Rh11 .27514(5) .07871(3) .38297(2) .0160(5) Uani ? ? 1.00000 ? ?
  Rh12 .23192(5) -.09583(3) .39032(2) .0167(5) Uani ? ? 1.00000 ? ?
  Rh21 .76336(5) .10150(3) .14041(3) .0185(5) Uani ? ? 1.00000 ? ?
  Rh22 .74480(5) -.07284(3) .12654(3) .0187(5) Uani ? ? 1.00000 ? ?
  Ag11 .14702(5) -.00098(3) .36379(3) .0227(5) Uani ? ? 1.00000 ? ?
  Ag12 .20600(5) -.00188(3) .43859(3) .0221(5) Uani ? ? 1.00000 ? ?
  Ag13 .35998(5) -.01504(3) .41147(2) .0217(5) Uani ? ? 1.00000 ? ?
  Ag14 .30363(5) -.01467(3) .33680(3) .0223(5) Uani ? ? 1.00000 ? ?
  Ag21 .64630(6) .02161(3) .11481(3) .0252(5) Uani ? ? 1.00000 ? ?
  Ag22 .71759(5) .00925(3) .18669(3) .0242(5) Uani ? ? 1.00000 ? ?
  Ag23 .86582(5) .00649(3) .14914(3) .0252(5) Uani ? ? 1.00000 ? ?
  Ag24 .79320(5) .02169(3) .07757(3) .0242(5) Uani ? ? 1.00000 ? ?
  P11 .28123(17) .16395(12) .37303(8) .0194(16) Uani ? ? 1.00000 ? ?
  C11011 .3813(7) .1882(5) .3692(3) .023(6) Uani ? ? 1.00000 ? ?
  C11012 .4292(8) .1888(5) .4019(4) .034(8) Uani ? ? 1.00000 ? ?
  C11013 .5033(7) .2081(5) .3991(4) .037(8) Uani ? ? 1.00000 ? ?
  C11014 .5329(8) .2255(6) .3661(5) .049(10) Uani ? ? 1.00000 ? ?
  C11015 .4883(8) .2237(5) .3344(4) .044(9) Uani ? ? 1.00000 ? ?
  C11016 .4113(8) .2046(6) .3356(4) .038(8) Uani ? ? 1.00000 ? ?
  C11021 .2315(6) .1900(5) .3306(3) .017(6) Uani ? ? 1.00000 ? ?
  C11022 .2092(7) .1596(4) .3001(3) .020(6) Uani ? ? 1.00000 ? ?
  C11023 .1702(7) .1810(5) .2689(3) .026(7) Uani ? ? 1.00000 ? ?

```

| | | | | | | | | | | |
|--------|------------|-------------|-----------|-----------|------|---|---|---------|---|---|
| C11024 | .1591(7) | .2325(5) | .2670(3) | .029(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11025 | .1820(7) | .2631(5) | .2971(3) | .032(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11026 | .2182(7) | .2419(5) | .3289(3) | .029(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11031 | .2360(8) | .2037(5) | .4088(3) | .026(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11032 | .1630(7) | .1900(4) | .4232(3) | .024(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11033 | .1222(8) | .2210(5) | .4471(4) | .032(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11034 | .1536(8) | .2680(5) | .4578(3) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11035 | .2250(9) | .2830(5) | .4443(4) | .040(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11036 | .2660(7) | .2509(5) | .4208(4) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C1111 | .1642(6) | .0823(4) | .3619(3) | .020(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1112 | .1004(6) | .0840(4) | .3483(3) | .020(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C11121 | .0303(7) | .0994(5) | .3273(4) | .029(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11122 | .0000(7) | .0706(5) | .2985(4) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11123 | -.0644(9) | .0870(6) | .2779(4) | .049(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C11124 | -.0990(8) | .1328(6) | .2862(5) | .052(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C11125 | -.0708(9) | .1625(6) | .3156(5) | .058(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C11126 | -.0051(8) | .1463(6) | .3357(4) | .043(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C1121 | .2314(6) | .0811(5) | .4364(3) | .022(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1122 | .2031(7) | .0817(4) | .4683(3) | .026(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11221 | .1667(6) | .0927(4) | .5030(3) | .018(2) | Uiso | ? | ? | 1.00000 | ? | ? |
| C11222 | .2087(7) | .0894(5) | .5375(3) | .031(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11223 | .1723(8) | .1007(5) | .5714(3) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11224 | .0941(8) | .1147(5) | .5734(3) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11225 | .0515(8) | .1183(5) | .5392(4) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11226 | .0879(7) | .1074(5) | .5051(3) | .026(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C1131 | .3871(7) | .0670(4) | .4024(3) | .017(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1132 | .4545(7) | .0542(5) | .4114(3) | .022(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C11321 | .5382(7) | .0479(5) | .4194(3) | .025(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11322 | .5779(7) | .0066(5) | .4043(3) | .028(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11323 | .6572(8) | -.0009(5) | .4123(4) | .035(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11324 | .6963(7) | .0339(5) | .4353(4) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11325 | .6573(8) | .0741(6) | .4510(4) | .040(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11326 | .5779(7) | .0826(4) | .4429(3) | .026(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C1141 | .3231(6) | .0682(4) | .3304(3) | .014(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1142 | .3577(6) | .0575(4) | .3013(4) | .024(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11421 | .3970(7) | .0572(4) | .2654(3) | .023(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C11422 | .4477(8) | .0174(5) | .2546(4) | .037(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11423 | .4853(8) | .0182(5) | .2199(4) | .038(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C11424 | .4707(9) | .0567(6) | .1945(4) | .048(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C11425 | .4199(9) | .0956(6) | .2046(4) | .047(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C11426 | .3823(7) | .0954(5) | .2392(3) | .028(7) | Uani | ? | ? | 1.00000 | ? | ? |
| P12 | .21645(17) | -.18150(12) | .38803(8) | .0186(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C12011 | .3034(7) | -.2194(4) | .4012(4) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12012 | .3007(8) | -.2636(5) | .4238(4) | .034(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12013 | .3688(9) | -.2909(5) | .4294(4) | .044(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C12014 | .4392(8) | -.2775(6) | .4133(4) | .041(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12015 | .4415(8) | -.2337(6) | .3910(4) | .039(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12016 | .3750(7) | -.2059(5) | .3848(4) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12021 | .1950(6) | -.2085(4) | .3414(3) | .019(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C12022 | .1707(6) | -.1799(4) | .3107(3) | .021(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C12023 | .1582(8) | -.2032(5) | .2761(3) | .031(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12024 | .1686(8) | -.2551(5) | .2717(3) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12025 | .1917(9) | -.2844(5) | .3027(4) | .042(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C12026 | .2053(8) | -.2613(5) | .3369(4) | .035(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12031 | .1355(7) | -.2061(4) | .4165(3) | .019(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C12032 | .0668(7) | -.2227(5) | .4003(4) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12033 | .0050(8) | -.2413(5) | .4219(4) | .040(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12034 | .0141(8) | -.2446(5) | .4607(4) | .039(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12035 | .0838(9) | -.2271(5) | .4776(4) | .039(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12036 | .1437(7) | -.2085(5) | .4554(4) | .031(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C1211 | .1282(6) | -.0838(4) | .3637(3) | .020(6) | Uani | ? | ? | 1.00000 | ? | ? |

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|--------|------------|------------|-----------|-----------|------|---|---|---------|---|---|
| C1212 | .0677(7) | -.0745(5) | .3455(3) | .025(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12121 | .0005(6) | -.0685(4) | .3201(3) | .017(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C12122 | .0107(8) | -.0805(5) | .2817(4) | .036(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12123 | -.0530(9) | -.0750(5) | .2575(4) | .041(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12124 | -.1256(9) | -.0588(5) | .2698(5) | .051(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C12125 | -.1364(8) | -.0497(6) | .3075(4) | .045(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C12126 | -.0726(8) | -.0539(5) | .3327(4) | .034(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C1221 | .1799(6) | -.0851(4) | .4412(3) | .015(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1222 | .1525(6) | -.0756(4) | .4728(3) | .019(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C12221 | .1212(7) | -.0716(5) | .5104(3) | .025(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12222 | .1292(8) | -.1129(5) | .5354(4) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12223 | .0971(9) | -.1100(6) | .5709(4) | .043(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C12224 | .0597(9) | -.0664(6) | .5830(4) | .047(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C12225 | .0522(8) | -.0256(5) | .5585(4) | .038(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12226 | .0821(8) | -.0278(5) | .5224(4) | .034(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C1231 | .3362(7) | -.0988(4) | .4181(3) | .021(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1232 | .3965(6) | -.0960(4) | .4377(3) | .020(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C12321 | .4632(7) | -.1053(4) | .4615(3) | .021(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C12322 | .4808(7) | -.1553(5) | .4725(3) | .025(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12323 | .5471(8) | -.1651(5) | .4950(3) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12324 | .5938(7) | -.1254(5) | .5062(3) | .029(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12325 | .5770(7) | -.0753(5) | .4956(3) | .026(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12326 | .5121(7) | -.0661(4) | .4735(3) | .023(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1241 | .2887(7) | -.0980(4) | .3401(3) | .019(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C1242 | .3217(7) | -.0981(5) | .3095(4) | .031(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12421 | .3607(8) | -.1043(5) | .2739(4) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12422 | .4337(8) | -.1269(5) | .2712(4) | .032(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12423 | .4726(7) | -.1299(5) | .2365(4) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C12424 | .4384(8) | -.1094(5) | .2050(4) | .039(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12425 | .3663(8) | -.0874(5) | .2066(4) | .034(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C12426 | .3269(7) | -.0864(5) | .2407(4) | .031(7) | Uani | ? | ? | 1.00000 | ? | ? |
| P21 | .76353(17) | .18671(11) | .14899(8) | .0181(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C21011 | .7782(7) | .2244(5) | .1069(3) | .022(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C21012 | .7250(7) | .2169(5) | .0776(3) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21013 | .7240(8) | .2502(5) | .0465(3) | .032(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C21014 | .7778(9) | .2882(5) | .0447(4) | .041(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C21015 | .8334(8) | .2963(5) | .0730(4) | .038(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C21016 | .8322(7) | .2649(5) | .1045(3) | .028(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21021 | .6726(7) | .2174(4) | .1657(3) | .019(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C21022 | .6679(7) | .2702(5) | .1643(3) | .027(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21023 | .6020(8) | .2959(5) | .1765(4) | .035(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C21024 | .5383(8) | .2683(5) | .1909(3) | .035(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C21025 | .5434(7) | .2158(5) | .1917(4) | .032(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21026 | .6094(7) | .1905(4) | .1794(3) | .018(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C21031 | .8393(6) | .2086(4) | .1817(3) | .019(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C21032 | .8168(7) | .2278(5) | .2171(3) | .027(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21033 | .8744(8) | .2438(5) | .2425(3) | .031(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21034 | .9529(7) | .2398(5) | .2326(3) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21035 | .9746(7) | .2199(5) | .1981(4) | .032(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C21036 | .9177(7) | .2042(5) | .1730(4) | .030(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C2111 | .6540(7) | .1049(4) | .1178(3) | .021(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C2112 | .5921(7) | .1075(5) | .0993(3) | .028(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21121 | .5240(8) | .1158(5) | .0756(4) | .036(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C21122 | .5326(9) | .1150(5) | .0356(4) | .047(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C21123 | .4685(10) | .1225(6) | .0124(4) | .053(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C21124 | .3968(10) | .1326(6) | .0281(5) | .063(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C21125 | .3872(9) | .1344(6) | .0667(5) | .059(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C21126 | .4507(8) | .1257(6) | .0904(4) | .048(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C2121 | .7231(6) | .0921(4) | .1943(3) | .017(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C2122 | .7033(7) | .0873(5) | .2268(3) | .025(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21221 | .6755(8) | .0886(4) | .2656(4) | .034(8) | Uani | ? | ? | 1.00000 | ? | ? |

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|--------|------------|-------------|-----------|-----------|------|---|---|---------|---|---|
| C21222 | .6007(8) | .1050(5) | .2752(4) | .039(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C21223 | .5781(9) | .1088(6) | .3128(5) | .056(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C21224 | .6320(12) | .0973(6) | .3401(4) | .061(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C21225 | .7047(11) | .0806(6) | .3314(5) | .061(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C21226 | .7291(9) | .0760(5) | .2944(4) | .041(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C2131 | .8740(6) | .0901(4) | .1592(3) | .019(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C2132 | .9413(7) | .0793(5) | .1683(3) | .026(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21321 | 1.0253(8) | .0774(4) | .1787(3) | .029(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21322 | 1.0522(9) | .0434(6) | .2055(4) | .047(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C21323 | 1.1324(10) | .0411(8) | .2139(5) | .077(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C21324 | 1.1848(9) | .0692(7) | .1973(6) | .077(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C21325 | 1.1580(8) | .1055(8) | .1704(5) | .068(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C21326 | 1.0792(8) | .1088(6) | .1616(4) | .042(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C2141 | .8048(6) | .1051(4) | .0869(3) | .017(2) | Uiso | ? | ? | 1.00000 | ? | ? |
| C2142 | .8290(7) | .1056(5) | .0545(4) | .029(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21421 | .8568(7) | .1186(4) | .0178(3) | .019(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C21422 | .8835(7) | .1688(5) | .0102(3) | .027(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21423 | .9096(7) | .1821(5) | -.0252(3) | .029(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C21424 | .9134(9) | .1452(6) | -.0536(4) | .039(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C21425 | .8900(8) | .0964(6) | -.0473(4) | .038(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C21426 | .8611(8) | .0824(5) | -.0116(4) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| P22 | .73504(18) | -.15872(11) | .12467(8) | .0193(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C22011 | .7812(6) | -.1927(4) | .0850(3) | .018(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C22012 | .7535(8) | -.2383(5) | .0708(4) | .034(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C22013 | .7904(9) | -.2640(5) | .0419(4) | .044(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C22014 | .8548(9) | -.2422(5) | .0251(4) | .039(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C22015 | .8839(8) | -.1963(6) | .0389(4) | .040(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C22016 | .8464(7) | -.1711(5) | .0693(3) | .027(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22021 | .6331(7) | -.1811(5) | .1230(4) | .031(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22022 | .5946(7) | -.1805(5) | .0886(3) | .029(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22023 | .5173(8) | -.1966(5) | .0872(3) | .037(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C22024 | .4776(7) | -.2117(5) | .1194(4) | .032(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22025 | .5158(8) | -.2100(5) | .1534(4) | .032(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22026 | .5923(7) | -.1938(5) | .1558(3) | .026(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22031 | .7748(7) | -.1948(4) | .1648(3) | .023(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C22032 | .7627(7) | -.2477(5) | .1667(4) | .026(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22033 | .7954(8) | -.2766(5) | .1955(4) | .032(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22034 | .8428(8) | -.2543(5) | .2221(4) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C22035 | .8547(7) | -.2024(5) | .2209(3) | .028(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22036 | .8216(7) | -.1722(5) | .1927(3) | .025(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C2211 | .6313(7) | -.0613(4) | .1113(3) | .020(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C2212 | .5642(8) | -.0527(5) | .0990(3) | .032(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22121 | .4866(7) | -.0500(5) | .0832(4) | .033(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C22122 | .4710(9) | -.0179(6) | .0520(4) | .049(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C22123 | .3965(10) | -.0181(6) | .0359(5) | .065(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C22124 | .3373(10) | -.0479(7) | .0497(6) | .073(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C22125 | .3522(9) | -.0791(6) | .0799(5) | .060(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C22126 | .4277(8) | -.0801(6) | .0964(4) | .043(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C2221 | .7117(6) | -.0744(4) | .1818(3) | .012(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2222 | .6907(7) | -.0734(4) | .2146(3) | .022(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C22221 | .6677(7) | -.0805(5) | .2539(3) | .025(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22222 | .6355(8) | -.0414(5) | .2747(3) | .034(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C22223 | .6138(9) | -.0512(6) | .3122(4) | .045(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C22224 | .6254(9) | -.0978(5) | .3283(4) | .044(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C22225 | .6580(9) | -.1367(5) | .3074(5) | .047(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C22226 | .6800(8) | -.1286(5) | .2703(4) | .036(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C2231 | .8609(6) | -.0762(4) | .1408(3) | .015(2) | Uiso | ? | ? | 1.00000 | ? | ? |
| C2232 | .9327(7) | -.0775(4) | .1443(3) | .023(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C22321 | 1.0136(7) | -.0896(5) | .1509(3) | .023(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C22322 | 1.0338(8) | -.1398(5) | .1621(4) | .038(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C22323 | 1.1115(8) | -.1541(6) | .1664(4) | .048(9) | Uani | ? | ? | 1.00000 | ? | ? |

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|--------|-----------|-----------|-----------|----------|------|---|---|---------|---|---|
| C22324 | 1.1714(7) | -.1194(6) | .1604(4) | .044(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C22325 | 1.1533(8) | -.0709(6) | .1505(4) | .043(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C22326 | 1.0741(8) | -.0555(5) | .1453(4) | .031(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C2241 | .7775(7) | -.0614(4) | .0720(3) | .023(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C2242 | .8048(7) | -.0560(5) | .0404(3) | .028(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22421 | .8374(7) | -.0569(4) | .0035(3) | .025(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C22422 | .9203(9) | -.0570(6) | -.0002(4) | .043(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C22423 | .9537(9) | -.0588(7) | -.0358(4) | .052(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C22424 | .9081(10) | -.0584(6) | -.0681(4) | .053(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C22425 | .8271(10) | -.0578(6) | -.0648(4) | .049(10) | Uani | ? | ? | 1.00000 | ? | ? |
| C22426 | .7923(8) | -.0571(6) | -.0296(4) | .040(8) | Uani | ? | ? | 1.00000 | ? | ? |
| H11012 | .40885 | .17634 | .42555 | .04700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11013 | .53592 | .20946 | .42177 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11014 | .58610 | .23883 | .36468 | .06500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11015 | .50962 | .23568 | .31039 | .05600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11016 | .37916 | .20293 | .31308 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11022 | .22089 | .12376 | .30032 | .02400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11023 | .15194 | .15931 | .24873 | .03400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11024 | .13438 | .24695 | .24474 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11025 | .17510 | .30008 | .29544 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11026 | .23193 | .26351 | .35030 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11032 | .13968 | .15733 | .41648 | .03200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11033 | .07278 | .21019 | .45781 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11034 | .12287 | .29026 | .47342 | .04500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11035 | .24800 | .31544 | .45141 | .05500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11036 | .31653 | .26120 | .41191 | .04000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11122 | .02595 | .03870 | .29215 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11123 | -.08479 | .06682 | .25719 | .05700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11124 | -.14434 | .14425 | .27280 | .07100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11125 | -.09659 | .19401 | .32218 | .06100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11126 | .01667 | .16833 | .35545 | .05300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11222 | .26325 | .07932 | .53814 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11223 | .20208 | .09894 | .59425 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11224 | .06999 | .12165 | .59743 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11225 | -.00306 | .12736 | .53996 | .04000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11226 | .05696 | .11007 | .48250 | .03700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11322 | .54945 | -.01680 | .38873 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11323 | .68607 | -.02974 | .40152 | .04500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11324 | .75068 | .02897 | .44096 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11325 | .68631 | .09797 | .46670 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11326 | .55123 | .11083 | .45376 | .03200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11422 | .45578 | -.01107 | .27183 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11423 | .52316 | -.00826 | .21379 | .05400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11424 | .49333 | .05714 | .16992 | .06300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11425 | .41231 | .12398 | .18811 | .06000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H11426 | .34360 | .12134 | .24506 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12012 | .25116 | -.27528 | .43436 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12013 | .36615 | -.32164 | .44496 | .05200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12014 | .48561 | -.29743 | .41810 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12015 | .49079 | -.22404 | .38011 | .05700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12016 | .37736 | -.17568 | .36869 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12022 | .16196 | -.14332 | .31350 | .03200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12023 | .14185 | -.18314 | .25494 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12024 | .16240 | -.26996 | .24731 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12025 | .19470 | -.32137 | .30052 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12026 | .22374 | -.28200 | .35780 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12032 | .06346 | -.22232 | .37273 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12033 | -.04337 | -.25140 | .41003 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12034 | -.02884 | -.25770 | .47553 | .05200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12035 | .09177 | -.22899 | .50494 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12036 | .19089 | -.19647 | .46657 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |

| | | | | | | | | | | |
|--------|---------|---------|---------|--------|------|---|---|---------|---|---|
| H12122 | .05964 | -.09315 | .27232 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12123 | -.04655 | -.08139 | .23107 | .05500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12124 | -.16828 | -.05574 | .25232 | .06200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12125 | -.18780 | -.03882 | .31716 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12126 | -.08018 | -.04590 | .35899 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12222 | .15636 | -.14363 | .52734 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12223 | .10300 | -.13866 | .58767 | .05400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12224 | .03688 | -.06497 | .60789 | .05700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12225 | .02828 | .00558 | .56648 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12226 | .07548 | .00065 | .50523 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12232 | .44612 | -.18248 | .46437 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12233 | .56065 | -.20004 | .50175 | .03700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12234 | .63859 | -.13177 | .52186 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12235 | .61086 | -.04821 | .50387 | .03500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12236 | .49993 | -.03151 | .46659 | .02900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12422 | .45769 | -.14018 | .29394 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12423 | .52284 | -.14669 | .23452 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12424 | .46579 | -.11016 | .18123 | .05200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12425 | .34176 | -.07257 | .18403 | .04500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H12426 | .27426 | -.07358 | .24209 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21012 | .68761 | .18943 | .07870 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21013 | .68526 | .24653 | .02736 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21014 | .77838 | .31111 | .02315 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21015 | .87179 | .32257 | .07091 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21016 | .86687 | .27137 | .12535 | .03500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21022 | .71206 | .28953 | .15442 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21023 | .59975 | .33309 | .17479 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21024 | .49110 | .28505 | .20006 | .04700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21025 | .49913 | .19560 | .20082 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21026 | .61316 | .15361 | .18065 | .02400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21032 | .76223 | .22909 | .22401 | .03500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21033 | .86018 | .25902 | .26669 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21034 | .99233 | .24963 | .25064 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21035 | 1.03070 | .21891 | .19165 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21036 | .93330 | .18936 | .14902 | .03700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21122 | .58353 | .10888 | .02417 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21123 | .47253 | .11921 | -.01479 | .07000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21124 | .35191 | .13918 | .01161 | .07400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21125 | .33534 | .14257 | .07783 | .07900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21126 | .44455 | .12551 | .11765 | .06100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21222 | .56358 | .11367 | .25575 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21223 | .52574 | .11849 | .32000 | .07200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21224 | .61767 | .10129 | .36613 | .07100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21225 | .74156 | .07372 | .35113 | .07600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21226 | .78129 | .06250 | .28875 | .05400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21322 | 1.01469 | .01982 | .21733 | .06900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21323 | 1.15203 | .01689 | .23309 | .09900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21324 | 1.24022 | .06646 | .20163 | .08900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21325 | 1.19528 | .12832 | .15848 | .08500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21326 | 1.06067 | .13368 | .14290 | .05600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21422 | .88383 | .19390 | .03091 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21423 | .92496 | .21709 | -.03047 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21424 | .93186 | .15374 | -.07822 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21425 | .89500 | .07179 | -.06659 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H21426 | .84420 | .04782 | -.00761 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22012 | .70480 | -.25183 | .08095 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22013 | .77239 | -.29815 | .03444 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22014 | .87900 | -.25827 | .00389 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22015 | .93072 | -.18135 | .02867 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22016 | .86445 | -.13859 | .07787 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22022 | .62134 | -.16962 | .06578 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |

| | | | | | | | | | | |
|--------|---------|---------|---------|--------|------|---|---|---------|---|---|
| H22023 | .48979 | -.19675 | .06339 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22024 | .42263 | -.22279 | .11756 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22025 | .48873 | -.22053 | .17600 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22026 | .61846 | -.19243 | .18026 | .03500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22032 | .72947 | -.26368 | .14801 | .03400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22033 | .78577 | -.31284 | .19643 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22034 | .86821 | -.27473 | .24123 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22035 | .88688 | -.18645 | .24010 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22036 | .83009 | -.13589 | .19264 | .03300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22122 | .51221 | .00446 | .04249 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22123 | .38482 | .00530 | .01545 | .08400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22124 | .28746 | -.04912 | .03651 | .08800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22125 | .30992 | -.09962 | .09098 | .07700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22126 | .43875 | -.10257 | .11748 | .05400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22222 | .62818 | -.00806 | .26361 | .04500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22223 | .59085 | -.02376 | .32706 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22224 | .60864 | -.10340 | .35397 | .05500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22225 | .66672 | -.16934 | .31957 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22226 | .70219 | -.15630 | .25651 | .04500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22322 | .99395 | -.16592 | .16556 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22323 | 1.12487 | -.18769 | .17496 | .05900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22324 | 1.22497 | -.12941 | .16317 | .05700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22325 | 1.19545 | -.04636 | .14653 | .05500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22326 | 1.06169 | -.02093 | .13713 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22422 | .95355 | -.05606 | .02138 | .05500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22423 | 1.01108 | -.05835 | -.03897 | .07000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22424 | .93123 | -.05882 | -.09240 | .06400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22425 | .79609 | -.05749 | -.08793 | .06600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H22426 | .73514 | -.05749 | -.02784 | .05300 | Uiso | ? | ? | 1.00000 | ? | ? |

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

| | | | | | | |
|--------|-----------|-----------|-----------|------------|------------|------------|
| Rh11 | .0145(5) | .0193(5) | .0141(5) | .0004(4) | -.0026(4) | .0003(4) |
| Rh12 | .0152(5) | .0205(5) | .0143(5) | -.0015(4) | -.0042(4) | -.0014(4) |
| Rh21 | .0180(5) | .0199(5) | .0175(5) | -.0011(4) | -.0028(4) | -.0007(4) |
| Rh22 | .0164(5) | .0205(5) | .0193(5) | -.0006(4) | -.0055(4) | .0012(4) |
| Ag11 | .0215(5) | .0236(5) | .0231(5) | -.0015(4) | -.0027(4) | -.0004(4) |
| Ag12 | .0207(5) | .0223(5) | .0234(5) | -.0021(4) | -.0044(4) | -.0010(4) |
| Ag13 | .0199(5) | .0236(5) | .0215(5) | -.0006(4) | -.0033(4) | -.0013(4) |
| Ag14 | .0217(5) | .0224(5) | .0229(5) | -.0021(4) | -.0044(4) | -.0013(4) |
| Ag21 | .0260(5) | .0236(5) | .0259(5) | -.0022(4) | -.0031(4) | .0009(4) |
| Ag22 | .0239(5) | .0226(5) | .0261(5) | -.0024(4) | -.0053(4) | .0002(4) |
| Ag23 | .0260(5) | .0238(5) | .0259(5) | -.0021(4) | -.0039(4) | -.0002(4) |
| Ag24 | .0242(5) | .0217(5) | .0267(5) | -.0004(4) | -.0045(4) | -.0003(4) |
| P11 | .0164(16) | .0253(16) | .0166(16) | -.0030(13) | -.0035(12) | -.0011(13) |
| C11011 | .016(6) | .031(7) | .023(7) | .003(5) | -.000(5) | .007(5) |
| C11012 | .035(8) | .031(7) | .034(8) | .005(6) | -.015(6) | -.007(6) |
| C11013 | .018(7) | .042(8) | .049(9) | -.006(6) | -.018(6) | .005(7) |
| C11014 | .026(8) | .043(9) | .080(12) | -.004(7) | -.008(8) | .006(8) |
| C11015 | .036(9) | .041(9) | .056(10) | .004(7) | .021(7) | .012(7) |
| C11016 | .022(7) | .051(9) | .039(8) | -.001(6) | -.002(6) | .012(7) |
| C11021 | .003(5) | .037(7) | .012(6) | -.001(5) | -.001(4) | .003(5) |
| C11022 | .039(7) | .007(5) | .014(6) | -.003(5) | .002(5) | -.002(4) |
| C11023 | .016(6) | .033(7) | .029(7) | .002(5) | -.003(5) | .001(6) |
| C11024 | .016(6) | .048(8) | .024(7) | .009(6) | .010(5) | .008(6) |

| | | | | | | |
|--------|-----------|-----------|-----------|------------|------------|------------|
| C11025 | .027(7) | .048(9) | .022(7) | .007(6) | .001(6) | .004(6) |
| C11026 | .016(6) | .045(8) | .025(7) | .008(6) | -.000(5) | .012(6) |
| C11031 | .040(8) | .035(7) | .003(5) | .010(6) | -.000(5) | .009(5) |
| C11032 | .030(7) | .017(6) | .025(7) | .001(5) | -.006(6) | .009(5) |
| C11033 | .029(7) | .039(8) | .028(7) | .011(6) | -.002(6) | .011(6) |
| C11034 | .037(8) | .046(8) | .017(7) | .021(7) | .001(6) | -.002(6) |
| C11035 | .052(9) | .040(8) | .027(8) | .016(7) | -.015(7) | -.014(6) |
| C11036 | .021(7) | .035(7) | .034(8) | -.008(6) | .002(6) | -.000(6) |
| C1111 | .009(6) | .023(6) | .027(7) | -.004(5) | .003(5) | .002(5) |
| C1112 | .012(6) | .019(6) | .030(7) | -.001(5) | .015(5) | -.000(5) |
| C11121 | .018(6) | .026(7) | .042(8) | .001(5) | -.004(6) | -.000(6) |
| C11122 | .016(6) | .037(8) | .037(8) | -.011(6) | -.009(6) | .000(6) |
| C11123 | .040(9) | .043(9) | .064(11) | .004(7) | -.031(8) | -.010(8) |
| C11124 | .031(9) | .039(9) | .085(13) | -.004(7) | -.029(8) | .013(8) |
| C11125 | .039(9) | .035(9) | .099(14) | .015(7) | -.033(9) | -.011(9) |
| C11126 | .030(8) | .052(9) | .048(9) | -.006(7) | -.021(7) | .001(8) |
| C1121 | .014(6) | .044(8) | .009(6) | -.004(5) | -.004(5) | .003(5) |
| C1122 | .020(6) | .025(7) | .031(7) | -.006(5) | -.021(5) | .006(6) |
| C11222 | .028(7) | .048(8) | .016(6) | .013(6) | -.001(5) | .006(6) |
| C11223 | .040(8) | .046(8) | .013(6) | .006(7) | -.009(6) | -.008(6) |
| C11224 | .045(8) | .040(8) | .016(7) | .004(7) | .012(6) | -.004(6) |
| C11225 | .029(7) | .027(7) | .042(8) | .003(6) | .007(6) | .009(6) |
| C11226 | .030(7) | .025(7) | .022(7) | .000(6) | -.002(5) | -.002(5) |
| C1131 | .032(7) | .008(5) | .010(6) | -.005(5) | -.001(5) | .006(4) |
| C1132 | .016(6) | .030(7) | .022(6) | .001(5) | -.006(5) | .003(5) |
| C11321 | .023(7) | .031(7) | .021(7) | .006(6) | .004(5) | .004(5) |
| C11322 | .030(7) | .028(7) | .024(7) | -.005(6) | -.002(6) | .005(6) |
| C11323 | .027(7) | .047(8) | .030(7) | .008(6) | .002(6) | .008(7) |
| C11324 | .017(7) | .039(8) | .035(8) | -.004(6) | -.012(6) | .007(6) |
| C11325 | .026(8) | .060(10) | .034(8) | -.013(7) | .003(6) | -.018(7) |
| C11326 | .025(7) | .022(6) | .031(7) | -.006(5) | -.010(6) | -.008(5) |
| C1141 | .011(5) | .021(6) | .010(5) | .007(5) | -.008(4) | -.005(5) |
| C1142 | .007(6) | .022(6) | .041(8) | .001(5) | -.007(5) | -.005(6) |
| C11421 | .023(7) | .026(7) | .021(6) | -.000(5) | .006(5) | -.007(5) |
| C11422 | .041(8) | .036(8) | .033(8) | -.004(7) | -.003(6) | -.015(6) |
| C11423 | .033(8) | .035(8) | .046(9) | -.013(6) | .014(7) | -.008(7) |
| C11424 | .047(10) | .065(11) | .031(8) | -.011(8) | .009(7) | -.006(8) |
| C11425 | .045(9) | .062(10) | .034(8) | .004(8) | -.000(7) | .023(8) |
| C11426 | .020(6) | .042(8) | .023(7) | .009(6) | .004(5) | .004(6) |
| P12 | .0125(15) | .0240(16) | .0192(16) | -.0010(13) | -.0034(12) | -.0001(13) |
| C12011 | .033(8) | .016(6) | .041(8) | .008(5) | -.018(6) | -.012(6) |
| C12012 | .034(8) | .033(8) | .034(8) | .009(6) | -.004(6) | -.002(6) |
| C12013 | .050(10) | .032(8) | .049(9) | .017(7) | -.029(8) | .002(7) |
| C12014 | .026(8) | .057(9) | .039(8) | .014(7) | -.019(6) | -.021(7) |
| C12015 | .026(8) | .054(9) | .037(8) | .002(7) | .001(6) | -.011(7) |
| C12016 | .017(6) | .040(8) | .033(7) | .001(6) | .000(6) | -.025(6) |
| C12021 | .014(6) | .025(6) | .017(6) | -.002(5) | -.000(5) | -.009(5) |
| C12022 | .013(6) | .029(7) | .023(6) | .006(5) | -.002(5) | .004(5) |
| C12023 | .031(7) | .047(8) | .015(6) | .002(6) | -.003(5) | -.004(6) |
| C12024 | .037(8) | .051(9) | .011(6) | .000(7) | -.008(6) | -.011(6) |
| C12025 | .044(9) | .034(8) | .047(9) | -.005(7) | -.019(7) | -.018(7) |
| C12026 | .047(9) | .018(7) | .040(8) | -.019(6) | .008(7) | -.014(6) |
| C12031 | .024(6) | .019(6) | .013(6) | -.006(5) | .007(5) | -.005(5) |
| C12032 | .023(7) | .038(8) | .037(8) | .001(6) | -.007(6) | .001(6) |
| C12033 | .028(8) | .040(8) | .051(9) | -.001(6) | .000(7) | -.003(7) |
| C12034 | .032(8) | .037(8) | .049(9) | -.009(7) | .016(7) | -.002(7) |
| C12035 | .047(9) | .036(8) | .036(8) | -.002(7) | .010(7) | -.001(6) |
| C12036 | .026(7) | .040(8) | .028(7) | -.004(6) | -.005(6) | -.006(6) |
| C1211 | .015(6) | .009(5) | .036(7) | .006(5) | -.005(5) | .001(5) |
| C1212 | .028(7) | .026(7) | .021(7) | -.002(6) | -.001(5) | .001(5) |
| C12121 | .011(6) | .021(6) | .020(6) | -.010(5) | -.006(5) | .002(5) |

| | | | | | | |
|--------|-----------|-----------|-----------|------------|------------|------------|
| C12122 | .036(8) | .040(8) | .033(8) | -.001(7) | -.010(6) | -.010(6) |
| C12123 | .061(10) | .038(8) | .024(7) | -.009(7) | -.029(7) | -.000(6) |
| C12124 | .043(9) | .037(8) | .072(11) | -.012(7) | -.040(8) | .008(8) |
| C12125 | .023(8) | .060(10) | .052(10) | .000(7) | -.005(7) | .011(8) |
| C12126 | .034(8) | .037(8) | .030(8) | -.003(6) | -.000(6) | .004(6) |
| C1221 | .009(5) | .011(5) | .026(6) | .004(4) | -.004(5) | .005(5) |
| C1222 | .020(6) | .020(6) | .015(6) | -.004(5) | -.008(5) | -.006(5) |
| C12221 | .025(7) | .031(7) | .020(6) | -.014(6) | -.003(5) | -.004(5) |
| C12222 | .028(7) | .039(8) | .032(8) | .002(6) | .007(6) | .001(6) |
| C12223 | .055(10) | .051(9) | .023(7) | .006(8) | .009(7) | .011(7) |
| C12224 | .061(10) | .049(9) | .031(8) | -.010(8) | .022(7) | -.007(7) |
| C12225 | .046(9) | .027(7) | .041(8) | -.001(7) | .013(7) | -.007(6) |
| C12226 | .039(8) | .028(7) | .037(8) | -.010(6) | .018(6) | -.005(6) |
| C1231 | .017(6) | .023(6) | .024(6) | .007(5) | .005(5) | -.006(5) |
| C1232 | .017(6) | .025(6) | .018(6) | -.003(5) | -.008(5) | -.002(5) |
| C12321 | .015(6) | .026(6) | .023(6) | -.005(5) | .003(5) | .003(5) |
| C12322 | .031(7) | .029(7) | .015(6) | -.002(6) | -.001(5) | -.004(5) |
| C12323 | .039(8) | .028(7) | .022(7) | .011(6) | -.010(6) | -.001(5) |
| C12324 | .022(7) | .046(8) | .018(7) | .013(6) | -.006(5) | -.004(6) |
| C12325 | .014(6) | .049(8) | .016(6) | -.007(6) | -.006(5) | -.004(6) |
| C12326 | .036(7) | .012(6) | .022(6) | -.000(5) | .001(6) | .008(5) |
| C1241 | .025(6) | .028(6) | .005(5) | .003(5) | -.008(5) | .002(5) |
| C1242 | .027(7) | .033(7) | .034(8) | .006(6) | -.015(6) | -.002(6) |
| C12421 | .032(8) | .037(8) | .031(8) | -.008(6) | -.009(6) | -.007(6) |
| C12422 | .032(8) | .031(7) | .031(8) | .010(6) | -.008(6) | -.000(6) |
| C12423 | .030(7) | .020(7) | .040(8) | -.000(6) | .011(6) | -.011(6) |
| C12424 | .046(9) | .047(9) | .025(7) | -.016(7) | .017(7) | -.004(6) |
| C12425 | .038(8) | .038(8) | .024(7) | .000(6) | -.007(6) | -.008(6) |
| C12426 | .020(7) | .039(8) | .033(7) | -.006(6) | .005(6) | -.012(6) |
| P21 | .0161(15) | .0230(16) | .0153(15) | -.0027(13) | -.0038(12) | -.0009(13) |
| C21011 | .025(7) | .036(7) | .004(5) | .001(6) | -.006(5) | .001(5) |
| C21012 | .030(7) | .040(8) | .019(7) | .007(6) | .003(6) | .001(6) |
| C21013 | .034(8) | .047(8) | .016(7) | -.005(6) | -.006(6) | .004(6) |
| C21014 | .048(9) | .044(9) | .031(8) | .019(7) | .005(7) | .019(7) |
| C21015 | .045(9) | .036(8) | .032(8) | -.011(7) | .002(7) | .002(6) |
| C21016 | .035(8) | .027(7) | .021(7) | -.002(6) | .005(6) | .002(5) |
| C21021 | .020(6) | .025(6) | .012(6) | -.004(5) | -.015(5) | -.001(5) |
| C21022 | .024(7) | .028(7) | .028(7) | -.001(6) | .000(6) | .004(6) |
| C21023 | .040(8) | .044(8) | .021(7) | .005(7) | -.009(6) | .001(6) |
| C21024 | .034(8) | .053(9) | .018(7) | .004(7) | -.005(6) | -.003(6) |
| C21025 | .017(7) | .035(8) | .043(8) | -.004(6) | -.008(6) | -.003(6) |
| C21026 | .027(7) | .024(6) | .003(5) | .002(5) | -.005(5) | -.003(5) |
| C21031 | .013(6) | .017(6) | .026(7) | .002(5) | .001(5) | .004(5) |
| C21032 | .021(7) | .035(7) | .024(7) | -.001(6) | -.005(5) | -.003(6) |
| C21033 | .037(8) | .042(8) | .014(6) | .003(6) | .002(6) | -.013(6) |
| C21034 | .028(7) | .040(8) | .023(7) | -.002(6) | -.007(6) | -.013(6) |
| C21035 | .021(7) | .046(8) | .029(7) | -.001(6) | -.001(6) | -.004(6) |
| C21036 | .016(6) | .039(8) | .034(8) | -.000(6) | -.010(6) | .001(6) |
| C2111 | .018(6) | .017(6) | .027(7) | -.010(5) | -.004(5) | -.004(5) |
| C2112 | .033(7) | .026(7) | .025(7) | -.010(6) | .005(6) | .005(5) |
| C21121 | .038(8) | .017(6) | .053(9) | -.000(6) | -.024(7) | -.013(6) |
| C21122 | .058(10) | .037(8) | .045(9) | -.007(7) | -.012(8) | .007(7) |
| C21123 | .063(11) | .053(10) | .042(9) | -.002(8) | -.035(8) | .005(8) |
| C21124 | .066(12) | .054(10) | .068(12) | -.014(9) | -.040(10) | .019(9) |
| C21125 | .024(8) | .055(10) | .100(14) | .003(7) | -.003(9) | .023(10) |
| C21126 | .031(8) | .064(11) | .050(10) | -.004(8) | -.007(7) | .020(8) |
| C2121 | .007(5) | .009(5) | .034(7) | -.000(4) | -.013(5) | -.006(5) |
| C2122 | .033(7) | .025(7) | .019(6) | -.006(6) | .001(5) | -.004(5) |
| C21221 | .049(9) | .004(6) | .049(9) | -.014(6) | .001(7) | -.005(6) |
| C21222 | .039(8) | .026(7) | .051(9) | -.005(6) | .010(7) | -.013(7) |
| C21223 | .046(10) | .047(10) | .076(12) | -.019(8) | .048(9) | -.023(9) |

| | | | | | | |
|--------|-----------|-----------|-----------|------------|------------|------------|
| C21224 | .114(15) | .033(9) | .035(9) | -.028(9) | .026(9) | -.000(7) |
| C21225 | .083(13) | .045(10) | .055(11) | -.015(9) | .018(10) | .005(8) |
| C21226 | .059(10) | .034(8) | .030(8) | -.005(7) | -.005(7) | .004(6) |
| C2131 | .016(6) | .012(6) | .030(7) | -.002(5) | -.006(5) | -.005(5) |
| C2132 | .028(7) | .027(7) | .023(7) | -.001(6) | .005(5) | -.010(5) |
| C21321 | .042(8) | .018(6) | .027(7) | -.003(6) | .004(6) | -.005(5) |
| C21322 | .043(9) | .049(9) | .048(9) | .002(7) | -.027(8) | .002(8) |
| C21323 | .051(11) | .100(15) | .080(13) | .036(10) | -.056(10) | -.033(11) |
| C21324 | .035(10) | .084(13) | .113(16) | .012(9) | -.030(10) | -.069(12) |
| C21325 | .019(8) | .110(15) | .075(12) | -.016(9) | .012(8) | -.050(11) |
| C21326 | .026(8) | .061(10) | .038(8) | -.003(7) | .003(6) | -.026(7) |
| C2142 | .024(7) | .026(7) | .038(8) | .001(6) | .008(6) | -.012(6) |
| C21421 | .020(6) | .016(6) | .022(6) | .007(5) | -.008(5) | -.000(5) |
| C21422 | .031(7) | .035(7) | .014(6) | -.002(6) | -.015(5) | -.001(5) |
| C21423 | .023(7) | .036(7) | .029(7) | -.009(6) | -.001(6) | .011(6) |
| C21424 | .048(9) | .052(9) | .018(7) | .002(7) | .002(6) | .003(6) |
| C21425 | .036(8) | .053(9) | .025(7) | -.007(7) | .003(6) | -.011(7) |
| C21426 | .043(8) | .029(7) | .028(7) | .010(6) | -.008(6) | -.004(6) |
| P22 | .0203(16) | .0197(15) | .0177(16) | -.0042(13) | -.0069(13) | -.0020(13) |
| C22011 | .009(6) | .026(6) | .019(6) | -.004(5) | -.006(5) | .003(5) |
| C22012 | .038(8) | .033(8) | .031(8) | -.002(6) | -.005(6) | -.007(6) |
| C22013 | .057(10) | .041(9) | .035(8) | .005(8) | -.001(7) | -.014(7) |
| C22014 | .050(9) | .041(8) | .026(7) | .009(7) | -.000(7) | -.005(6) |
| C22015 | .027(8) | .048(9) | .045(9) | .003(7) | -.001(7) | .006(7) |
| C22016 | .030(7) | .044(8) | .008(6) | -.006(6) | -.009(5) | -.002(5) |
| C22021 | .017(7) | .031(7) | .043(8) | -.008(6) | -.005(6) | -.001(6) |
| C22022 | .030(7) | .040(8) | .016(6) | -.006(6) | -.003(5) | .009(6) |
| C22023 | .038(8) | .051(9) | .020(7) | -.015(7) | -.009(6) | .004(6) |
| C22024 | .021(7) | .040(8) | .034(8) | -.006(6) | -.005(6) | -.004(6) |
| C22025 | .028(7) | .030(7) | .037(8) | -.004(6) | -.002(6) | .004(6) |
| C22026 | .024(7) | .045(8) | .008(6) | .004(6) | -.007(5) | -.009(5) |
| C22031 | .024(7) | .026(7) | .018(6) | .016(5) | -.005(5) | .008(5) |
| C22032 | .021(7) | .022(6) | .036(8) | .001(5) | -.000(6) | .010(6) |
| C22033 | .036(8) | .024(7) | .037(8) | .013(6) | .003(6) | .014(6) |
| C22034 | .032(8) | .042(8) | .026(7) | .009(6) | .000(6) | .009(6) |
| C22035 | .022(7) | .042(8) | .020(7) | .007(6) | -.003(5) | .002(6) |
| C22036 | .033(7) | .033(7) | .009(6) | .005(6) | -.000(5) | .012(5) |
| C2211 | .034(7) | .010(5) | .017(6) | .007(5) | -.009(5) | .000(5) |
| C2212 | .040(8) | .037(8) | .019(7) | -.002(6) | .003(6) | .001(6) |
| C22121 | .023(7) | .027(7) | .050(9) | .002(6) | -.008(6) | -.004(6) |
| C22122 | .043(9) | .048(9) | .057(10) | -.000(7) | -.026(8) | .026(8) |
| C22123 | .056(11) | .049(10) | .088(14) | .000(8) | -.039(10) | .021(9) |
| C22124 | .038(10) | .065(12) | .116(17) | -.005(9) | -.043(10) | .011(11) |
| C22125 | .032(9) | .050(10) | .099(14) | -.001(8) | -.011(9) | -.009(10) |
| C22126 | .031(8) | .059(10) | .039(9) | .002(7) | .005(7) | -.002(7) |
| C2221 | .008(5) | .001(5) | .027(6) | -.001(4) | -.005(5) | -.002(4) |
| C2222 | .024(7) | .013(6) | .028(7) | -.002(5) | -.003(5) | -.008(5) |
| C22221 | .023(7) | .032(7) | .021(6) | -.001(6) | .004(5) | -.001(5) |
| C22222 | .047(9) | .037(8) | .019(7) | -.007(7) | -.007(6) | .002(6) |
| C22223 | .067(11) | .044(9) | .024(7) | .004(8) | .022(7) | -.002(7) |
| C22224 | .061(10) | .035(8) | .035(8) | .004(7) | .000(7) | .006(7) |
| C22225 | .041(9) | .030(8) | .070(11) | .010(7) | .003(8) | .012(8) |
| C22226 | .035(8) | .040(8) | .034(8) | .001(7) | .013(6) | .002(6) |
| C2232 | .027(7) | .015(6) | .026(7) | -.006(5) | .007(5) | -.009(5) |
| C22321 | .020(6) | .039(7) | .009(6) | .005(6) | .002(5) | .000(5) |
| C22322 | .022(7) | .042(8) | .051(9) | .007(6) | .001(6) | -.006(7) |
| C22323 | .028(8) | .058(10) | .059(10) | .023(7) | -.007(7) | .007(8) |
| C22324 | .011(7) | .058(10) | .061(10) | .010(6) | .001(6) | -.013(8) |
| C22325 | .024(8) | .046(9) | .058(10) | -.007(7) | -.002(7) | .000(8) |
| C22326 | .028(7) | .040(8) | .026(7) | .002(6) | .001(6) | .003(6) |
| C2241 | .021(7) | .027(7) | .022(7) | -.003(5) | -.011(5) | -.008(5) |

| | | | | | | |
|--------|----------|----------|---------|----------|----------|----------|
| C2242 | .024(7) | .035(7) | .025(7) | -.001(6) | -.013(6) | -.003(6) |
| C22421 | .038(8) | .007(5) | .031(7) | -.004(5) | -.006(6) | -.000(5) |
| C22422 | .045(9) | .056(9) | .029(8) | .024(8) | -.006(7) | .004(7) |
| C22423 | .036(9) | .079(12) | .042(9) | .020(8) | .008(7) | .023(8) |
| C22424 | .073(12) | .051(10) | .034(9) | .003(9) | .028(8) | -.007(7) |
| C22425 | .068(11) | .046(9) | .032(8) | .001(8) | .003(8) | -.004(7) |
| C22426 | .038(8) | .062(10) | .019(7) | .005(7) | -.014(6) | -.005(7) |

5. Molecular Geometry

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loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_distance

_geom_bond_publ_flag

#<< enter YES for value to be published

| | | | | | |
|------|-------|---|---|-----------|---|
| Rh11 | P11 | . | . | 2.258(3) | ? |
| Rh11 | C1111 | . | . | 2.030(11) | ? |
| Rh11 | C1121 | . | . | 2.037(11) | ? |
| Rh11 | C1131 | . | . | 2.046(11) | ? |
| Rh11 | C1141 | . | . | 2.056(10) | ? |
| Rh12 | P12 | . | . | 2.256(3) | ? |
| Rh12 | C1211 | . | . | 2.021(11) | ? |
| Rh12 | C1221 | . | . | 2.031(11) | ? |
| Rh12 | C1231 | . | . | 2.027(11) | ? |
| Rh12 | C1241 | . | . | 2.029(10) | ? |
| Rh21 | P21 | . | . | 2.248(3) | ? |
| Rh21 | C2111 | . | . | 2.025(11) | ? |
| Rh21 | C2121 | . | . | 2.046(11) | ? |
| Rh21 | C2131 | . | . | 2.015(11) | ? |
| Rh21 | C2141 | . | . | 2.026(11) | ? |
| Rh22 | P22 | . | . | 2.252(3) | ? |
| Rh22 | C2211 | . | . | 2.025(12) | ? |
| Rh22 | C2221 | . | . | 2.040(11) | ? |
| Rh22 | C2231 | . | . | 2.037(10) | ? |
| Rh22 | C2241 | . | . | 2.037(11) | ? |
| Ag11 | C1111 | . | . | 2.197(11) | ? |
| Ag11 | C1112 | . | . | 2.422(11) | ? |
| Ag11 | C1211 | . | . | 2.188(10) | ? |
| Ag11 | C1212 | . | . | 2.433(12) | ? |
| Ag12 | C1121 | . | . | 2.213(12) | ? |
| Ag12 | C1122 | . | . | 2.425(12) | ? |
| Ag12 | C1221 | . | . | 2.223(10) | ? |
| Ag12 | C1222 | . | . | 2.452(11) | ? |
| Ag13 | C1131 | . | . | 2.216(10) | ? |
| Ag13 | C1132 | . | . | 2.422(12) | ? |
| Ag13 | C1231 | . | . | 2.240(11) | ? |
| Ag13 | C1232 | . | . | 2.393(11) | ? |
| Ag14 | C1141 | . | . | 2.202(11) | ? |
| Ag14 | C1142 | . | . | 2.447(12) | ? |
| Ag14 | C1241 | . | . | 2.196(11) | ? |
| Ag14 | C1242 | . | . | 2.406(13) | ? |
| Ag21 | C2111 | . | . | 2.184(11) | ? |
| Ag21 | C2112 | . | . | 2.487(12) | ? |
| Ag21 | C2211 | . | . | 2.184(10) | ? |
| Ag21 | C2212 | . | . | 2.455(13) | ? |
| Ag22 | C2121 | . | . | 2.185(10) | ? |
| Ag22 | C2122 | . | . | 2.499(12) | ? |

| | | | | | |
|--------|--------|---|---|-----------|---|
| Ag22 | C2221 | . | . | 2.195(9) | ? |
| Ag22 | C2222 | . | . | 2.420(11) | ? |
| Ag23 | C2131 | . | . | 2.217(11) | ? |
| Ag23 | C2132 | . | . | 2.393(12) | ? |
| Ag23 | C2231 | . | . | 2.182(10) | ? |
| Ag23 | C2232 | . | . | 2.478(11) | ? |
| Ag24 | C2141 | . | . | 2.213(11) | ? |
| Ag24 | C2142 | . | . | 2.418(12) | ? |
| Ag24 | C2241 | . | . | 2.197(12) | ? |
| Ag24 | C2242 | . | . | 2.428(12) | ? |
| P11 | C11011 | . | . | 1.821(12) | ? |
| P11 | C11021 | . | . | 1.853(11) | ? |
| P11 | C11031 | . | . | 1.811(12) | ? |
| C11011 | C11012 | . | . | 1.416(17) | ? |
| C11011 | C11016 | . | . | 1.366(18) | ? |
| C11012 | C11013 | . | . | 1.361(18) | ? |
| C11012 | H11012 | . | . | .965 | ? |
| C11013 | C11014 | . | . | 1.35(2) | ? |
| C11013 | H11013 | . | . | .974 | ? |
| C11014 | C11015 | . | . | 1.35(2) | ? |
| C11014 | H11014 | . | . | .970 | ? |
| C11015 | C11016 | . | . | 1.40(2) | ? |
| C11015 | H11015 | . | . | .979 | ? |
| C11016 | H11016 | . | . | .966 | ? |
| C11021 | C11022 | . | . | 1.393(15) | ? |
| C11021 | C11026 | . | . | 1.377(18) | ? |
| C11022 | C11023 | . | . | 1.404(16) | ? |
| C11022 | H11022 | . | . | .957 | ? |
| C11023 | C11024 | . | . | 1.361(18) | ? |
| C11023 | H11023 | . | . | .964 | ? |
| C11024 | C11025 | . | . | 1.388(18) | ? |
| C11024 | H11024 | . | . | .970 | ? |
| C11025 | C11026 | . | . | 1.395(17) | ? |
| C11025 | H11025 | . | . | .976 | ? |
| C11026 | H11026 | . | . | .974 | ? |
| C11031 | C11032 | . | . | 1.390(17) | ? |
| C11031 | C11036 | . | . | 1.399(18) | ? |
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C2121 Rh21 C2131 . . . 89.3(4) ?
C2121 Rh21 C2141 . . . 175.7(4) ?
C2131 Rh21 C2141 . . . 89.4(4) ?
P22 Rh22 C2211 . . . 94.1(3) ?
P22 Rh22 C2221 . . . 89.3(3) ?
P22 Rh22 C2231 . . . 92.1(3) ?
P22 Rh22 C2241 . . . 98.0(3) ?
C2211 Rh22 C2221 . . . 89.6(4) ?
C2211 Rh22 C2231 . . . 173.7(4) ?
C2211 Rh22 C2241 . . . 89.3(5) ?
C2221 Rh22 C2231 . . . 91.8(4) ?
C2221 Rh22 C2241 . . . 172.7(4) ?
C2231 Rh22 C2241 . . . 88.5(4) ?
C1111 Ag11 C1112 . . . 29.2(4) ?
C1111 Ag11 C1211 . . . 178.0(4) ?
C1111 Ag11 C1212 . . . 147.9(4) ?
C1112 Ag11 C1211 . . . 149.3(4) ?
C1112 Ag11 C1212 . . . 118.9(4) ?
C1211 Ag11 C1212 . . . 30.5(4) ?
C1121 Ag12 C1122 . . . 30.4(4) ?
C1121 Ag12 C1221 . . . 179.5(4) ?
C1121 Ag12 C1222 . . . 149.3(4) ?
C1122 Ag12 C1221 . . . 149.2(4) ?
C1122 Ag12 C1222 . . . 118.9(4) ?
C1221 Ag12 C1222 . . . 30.2(4) ?
C1131 Ag13 C1132 . . . 30.5(4) ?
C1131 Ag13 C1231 . . . 177.1(4) ?
C1131 Ag13 C1232 . . . 149.1(4) ?

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| C1132 | Ag13 | C1231 | . | . | . | 148.4(4) | ? |
| C1132 | Ag13 | C1232 | . | . | . | 119.4(4) | ? |
| C1231 | Ag13 | C1232 | . | . | . | 30.8(4) | ? |
| C1141 | Ag14 | C1142 | . | . | . | 29.8(4) | ? |
| C1141 | Ag14 | C1241 | . | . | . | 176.4(4) | ? |
| C1141 | Ag14 | C1242 | . | . | . | 146.1(4) | ? |
| C1142 | Ag14 | C1241 | . | . | . | 146.6(4) | ? |
| C1142 | Ag14 | C1242 | . | . | . | 116.3(4) | ? |
| C1241 | Ag14 | C1242 | . | . | . | 30.3(4) | ? |
| C2111 | Ag21 | C2112 | . | . | . | 29.9(4) | ? |
| C2111 | Ag21 | C2211 | . | . | . | 176.7(4) | ? |
| C2111 | Ag21 | C2212 | . | . | . | 146.5(4) | ? |
| C2112 | Ag21 | C2211 | . | . | . | 147.1(4) | ? |
| C2112 | Ag21 | C2212 | . | . | . | 116.9(4) | ? |
| C2211 | Ag21 | C2212 | . | . | . | 30.3(4) | ? |
| C2121 | Ag22 | C2122 | . | . | . | 28.9(4) | ? |
| C2121 | Ag22 | C2221 | . | . | . | 177.4(4) | ? |
| C2121 | Ag22 | C2222 | . | . | . | 147.4(4) | ? |
| C2122 | Ag22 | C2221 | . | . | . | 148.6(4) | ? |
| C2122 | Ag22 | C2222 | . | . | . | 118.5(4) | ? |
| C2221 | Ag22 | C2222 | . | . | . | 30.1(4) | ? |
| C2131 | Ag23 | C2132 | . | . | . | 30.4(4) | ? |
| C2131 | Ag23 | C2231 | . | . | . | 178.0(4) | ? |
| C2131 | Ag23 | C2232 | . | . | . | 148.8(4) | ? |
| C2132 | Ag23 | C2231 | . | . | . | 147.9(4) | ? |
| C2132 | Ag23 | C2232 | . | . | . | 118.6(4) | ? |
| C2231 | Ag23 | C2232 | . | . | . | 29.7(4) | ? |
| C2141 | Ag24 | C2142 | . | . | . | 30.2(4) | ? |
| C2141 | Ag24 | C2241 | . | . | . | 176.1(4) | ? |
| C2141 | Ag24 | C2242 | . | . | . | 153.8(4) | ? |
| C2142 | Ag24 | C2241 | . | . | . | 153.7(4) | ? |
| C2142 | Ag24 | C2242 | . | . | . | 123.6(4) | ? |
| C2241 | Ag24 | C2242 | . | . | . | 30.1(4) | ? |
| Rh11 | P11 | C11011 | . | . | . | 113.5(4) | ? |
| Rh11 | P11 | C11021 | . | . | . | 117.9(4) | ? |
| Rh11 | P11 | C11031 | . | . | . | 115.9(4) | ? |
| C11011 | P11 | C11021 | . | . | . | 103.6(5) | ? |
| C11011 | P11 | C11031 | . | . | . | 104.5(6) | ? |
| C11021 | P11 | C11031 | . | . | . | 99.4(5) | ? |
| P11 | C11011 | C11012 | . | . | . | 118.6(9) | ? |
| P11 | C11011 | C11016 | . | . | . | 121.8(9) | ? |
| C11012 | C11011 | C11016 | . | . | . | 119.7(11) | ? |
| C11011 | C11012 | C11013 | . | . | . | 118.4(12) | ? |
| C11011 | C11012 | H11012 | . | . | . | 120.0 | ? |
| C11013 | C11012 | H11012 | . | . | . | 121.5 | ? |
| C11012 | C11013 | C11014 | . | . | . | 122.2(13) | ? |
| C11012 | C11013 | H11013 | . | . | . | 118.6 | ? |
| C11014 | C11013 | H11013 | . | . | . | 119.2 | ? |
| C11013 | C11014 | C11015 | . | . | . | 119.8(13) | ? |
| C11013 | C11014 | H11014 | . | . | . | 121.0 | ? |
| C11015 | C11014 | H11014 | . | . | . | 119.2 | ? |
| C11014 | C11015 | C11016 | . | . | . | 120.6(14) | ? |
| C11014 | C11015 | H11015 | . | . | . | 120.2 | ? |
| C11016 | C11015 | H11015 | . | . | . | 119.1 | ? |
| C11011 | C11016 | C11015 | . | . | . | 119.2(12) | ? |
| C11011 | C11016 | H11016 | . | . | . | 119.5 | ? |
| C11015 | C11016 | H11016 | . | . | . | 121.3 | ? |
| P11 | C11021 | C11022 | . | . | . | 122.9(9) | ? |
| P11 | C11021 | C11026 | . | . | . | 118.1(8) | ? |
| C11022 | C11021 | C11026 | . | . | . | 118.9(10) | ? |
| C11021 | C11022 | C11023 | . | . | . | 120.6(10) | ? |

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| C11021 | C11022 | H11022 | . | . | . | 119.7 | ? |
| C11023 | C11022 | H11022 | . | . | . | 119.6 | ? |
| C11022 | C11023 | C11024 | . | . | . | 119.9(11) | ? |
| C11022 | C11023 | H11023 | . | . | . | 120.0 | ? |
| C11024 | C11023 | H11023 | . | . | . | 120.1 | ? |
| C11023 | C11024 | C11025 | . | . | . | 119.5(11) | ? |
| C11023 | C11024 | H11024 | . | . | . | 119.0 | ? |
| C11025 | C11024 | H11024 | . | . | . | 121.5 | ? |
| C11024 | C11025 | C11026 | . | . | . | 120.9(12) | ? |
| C11024 | C11025 | H11025 | . | . | . | 119.3 | ? |
| C11026 | C11025 | H11025 | . | . | . | 119.8 | ? |
| C11021 | C11026 | C11025 | . | . | . | 119.9(11) | ? |
| C11021 | C11026 | H11026 | . | . | . | 119.9 | ? |
| C11025 | C11026 | H11026 | . | . | . | 120.1 | ? |
| P11 | C11031 | C11032 | . | . | . | 119.3(9) | ? |
| P11 | C11031 | C11036 | . | . | . | 124.3(9) | ? |
| C11032 | C11031 | C11036 | . | . | . | 116.1(11) | ? |
| C11031 | C11032 | C11033 | . | . | . | 122.0(11) | ? |
| C11031 | C11032 | H11032 | . | . | . | 120.2 | ? |
| C11033 | C11032 | H11032 | . | . | . | 117.8 | ? |
| C11032 | C11033 | C11034 | . | . | . | 119.9(12) | ? |
| C11032 | C11033 | H11033 | . | . | . | 120.9 | ? |
| C11034 | C11033 | H11033 | . | . | . | 119.1 | ? |
| C11033 | C11034 | C11035 | . | . | . | 119.9(12) | ? |
| C11033 | C11034 | H11034 | . | . | . | 118.9 | ? |
| C11035 | C11034 | H11034 | . | . | . | 121.1 | ? |
| C11034 | C11035 | C11036 | . | . | . | 119.5(13) | ? |
| C11034 | C11035 | H11035 | . | . | . | 121.3 | ? |
| C11036 | C11035 | H11035 | . | . | . | 119.2 | ? |
| C11031 | C11036 | C11035 | . | . | . | 122.5(12) | ? |
| C11031 | C11036 | H11036 | . | . | . | 118.4 | ? |
| C11035 | C11036 | H11036 | . | . | . | 119.1 | ? |
| Rh11 | C1111 | Ag11 | . | . | . | 93.8(4) | ? |
| Rh11 | C1111 | C1112 | . | . | . | 177.7(10) | ? |
| Ag11 | C1111 | C1112 | . | . | . | 86.0(8) | ? |
| Ag11 | C1112 | C1111 | . | . | . | 64.8(7) | ? |
| Ag11 | C1112 | C11121 | . | . | . | 129.4(8) | ? |
| C1111 | C1112 | C11121 | . | . | . | 164.1(12) | ? |
| C1112 | C11121 | C11122 | . | . | . | 122.3(11) | ? |
| C1112 | C11121 | C11126 | . | . | . | 119.0(11) | ? |
| C11122 | C11121 | C11126 | . | . | . | 118.6(12) | ? |
| C11121 | C11122 | C11123 | . | . | . | 121.3(12) | ? |
| C11121 | C11122 | H11122 | . | . | . | 118.4 | ? |
| C11123 | C11122 | H11122 | . | . | . | 120.3 | ? |
| C11122 | C11123 | C11124 | . | . | . | 119.9(14) | ? |
| C11122 | C11123 | H11123 | . | . | . | 120.9 | ? |
| C11124 | C11123 | H11123 | . | . | . | 119.2 | ? |
| C11123 | C11124 | C11125 | . | . | . | 120.4(14) | ? |
| C11123 | C11124 | H11124 | . | . | . | 121.0 | ? |
| C11125 | C11124 | H11124 | . | . | . | 118.6 | ? |
| C11124 | C11125 | C11126 | . | . | . | 119.5(14) | ? |
| C11124 | C11125 | H11125 | . | . | . | 120.4 | ? |
| C11126 | C11125 | H11125 | . | . | . | 120.1 | ? |
| C11121 | C11126 | C11125 | . | . | . | 120.3(13) | ? |
| C11121 | C11126 | H11126 | . | . | . | 120.3 | ? |
| C11125 | C11126 | H11126 | . | . | . | 119.4 | ? |
| Rh11 | C1121 | Ag12 | . | . | . | 94.3(5) | ? |
| Rh11 | C1121 | C1122 | . | . | . | 178.1(10) | ? |
| Ag12 | C1121 | C1122 | . | . | . | 84.4(8) | ? |
| Ag12 | C1122 | C1121 | . | . | . | 65.2(8) | ? |
| Ag12 | C1122 | C11221 | . | . | . | 125.0(8) | ? |

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| C1121 | C1122 | C11221 | . . . | 168.3(12) | ? |
| C1122 | C11221 | C11222 | . . . | 121.3(10) | ? |
| C1122 | C11221 | C11226 | . . . | 121.8(10) | ? |
| C11222 | C11221 | C11226 | . . . | 116.9(10) | ? |
| C11221 | C11222 | C11223 | . . . | 120.7(11) | ? |
| C11221 | C11222 | H11222 | . . . | 121.3 | ? |
| C11223 | C11222 | H11222 | . . . | 118.1 | ? |
| C11222 | C11223 | C11224 | . . . | 122.3(11) | ? |
| C11222 | C11223 | H11223 | . . . | 119.2 | ? |
| C11224 | C11223 | H11223 | . . . | 118.4 | ? |
| C11223 | C11224 | C11225 | . . . | 117.7(11) | ? |
| C11223 | C11224 | H11224 | . . . | 120.6 | ? |
| C11225 | C11224 | H11224 | . . . | 121.7 | ? |
| C11224 | C11225 | C11226 | . . . | 120.3(12) | ? |
| C11224 | C11225 | H11225 | . . . | 119.3 | ? |
| C11226 | C11225 | H11225 | . . . | 120.5 | ? |
| C11221 | C11226 | C11225 | . . . | 122.1(11) | ? |
| C11221 | C11226 | H11226 | . . . | 120.0 | ? |
| C11225 | C11226 | H11226 | . . . | 117.9 | ? |
| Rh11 | C1131 | Ag13 | . . . | 90.0(4) | ? |
| Rh11 | C1131 | C1132 | . . . | 171.9(9) | ? |
| Ag13 | C1131 | C1132 | . . . | 84.0(7) | ? |
| Ag13 | C1132 | C1131 | . . . | 65.5(7) | ? |
| Ag13 | C1132 | C11321 | . . . | 124.2(8) | ? |
| C1131 | C1132 | C11321 | . . . | 170.0(12) | ? |
| C1132 | C11321 | C11322 | . . . | 119.5(11) | ? |
| C1132 | C11321 | C11326 | . . . | 120.5(11) | ? |
| C11322 | C11321 | C11326 | . . . | 120.0(11) | ? |
| C11321 | C11322 | C11323 | . . . | 120.4(11) | ? |
| C11321 | C11322 | H11322 | . . . | 118.5 | ? |
| C11323 | C11322 | H11322 | . . . | 121.2 | ? |
| C11322 | C11323 | C11324 | . . . | 119.3(12) | ? |
| C11322 | C11323 | H11323 | . . . | 121.1 | ? |
| C11324 | C11323 | H11323 | . . . | 119.6 | ? |
| C11323 | C11324 | C11325 | . . . | 120.7(12) | ? |
| C11323 | C11324 | H11324 | . . . | 119.8 | ? |
| C11325 | C11324 | H11324 | . . . | 119.4 | ? |
| C11324 | C11325 | C11326 | . . . | 120.6(12) | ? |
| C11324 | C11325 | H11325 | . . . | 118.8 | ? |
| C11326 | C11325 | H11325 | . . . | 120.4 | ? |
| C11321 | C11326 | C11325 | . . . | 118.9(11) | ? |
| C11321 | C11326 | H11326 | . . . | 121.0 | ? |
| C11325 | C11326 | H11326 | . . . | 120.1 | ? |
| Rh11 | C1141 | Ag14 | . . . | 88.7(4) | ? |
| Rh11 | C1141 | C1142 | . . . | 171.8(9) | ? |
| Ag14 | C1141 | C1142 | . . . | 86.3(8) | ? |
| Ag14 | C1142 | C1141 | . . . | 63.9(7) | ? |
| Ag14 | C1142 | C11421 | . . . | 128.8(8) | ? |
| C1141 | C1142 | C11421 | . . . | 166.9(12) | ? |
| C1142 | C11421 | C11422 | . . . | 122.0(11) | ? |
| C1142 | C11421 | C11426 | . . . | 120.4(11) | ? |
| C11422 | C11421 | C11426 | . . . | 117.5(11) | ? |
| C11421 | C11422 | C11423 | . . . | 120.9(12) | ? |
| C11421 | C11422 | H11422 | . . . | 118.9 | ? |
| C11423 | C11422 | H11422 | . . . | 120.1 | ? |
| C11422 | C11423 | C11424 | . . . | 120.6(13) | ? |
| C11422 | C11423 | H11423 | . . . | 119.7 | ? |
| C11424 | C11423 | H11423 | . . . | 119.6 | ? |
| C11423 | C11424 | C11425 | . . . | 118.7(13) | ? |
| C11423 | C11424 | H11424 | . . . | 122.4 | ? |
| C11425 | C11424 | H11424 | . . . | 118.9 | ? |

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| C11424 | C11425 | C11426 | . | . | . | 121.3(14) | ? |
| C11424 | C11425 | H11425 | . | . | . | 119.7 | ? |
| C11426 | C11425 | H11425 | . | . | . | 119.0 | ? |
| C11421 | C11426 | C11425 | . | . | . | 120.8(12) | ? |
| C11421 | C11426 | H11426 | . | . | . | 118.8 | ? |
| C11425 | C11426 | H11426 | . | . | . | 120.3 | ? |
| Rh12 | P12 | C12011 | . | . | . | 115.6(4) | ? |
| Rh12 | P12 | C12021 | . | . | . | 115.9(4) | ? |
| Rh12 | P12 | C12031 | . | . | . | 114.7(4) | ? |
| C12011 | P12 | C12021 | . | . | . | 100.3(5) | ? |
| C12011 | P12 | C12031 | . | . | . | 106.1(5) | ? |
| C12021 | P12 | C12031 | . | . | . | 102.4(5) | ? |
| P12 | C12011 | C12012 | . | . | . | 124.0(10) | ? |
| P12 | C12011 | C12016 | . | . | . | 117.3(9) | ? |
| C12012 | C12011 | C12016 | . | . | . | 118.4(11) | ? |
| C12011 | C12012 | C12013 | . | . | . | 118.7(12) | ? |
| C12011 | C12012 | H12012 | . | . | . | 120.5 | ? |
| C12013 | C12012 | H12012 | . | . | . | 120.8 | ? |
| C12012 | C12013 | C12014 | . | . | . | 122.9(13) | ? |
| C12012 | C12013 | H12013 | . | . | . | 117.9 | ? |
| C12014 | C12013 | H12013 | . | . | . | 119.2 | ? |
| C12013 | C12014 | C12015 | . | . | . | 118.1(13) | ? |
| C12013 | C12014 | H12014 | . | . | . | 120.3 | ? |
| C12015 | C12014 | H12014 | . | . | . | 121.5 | ? |
| C12014 | C12015 | C12016 | . | . | . | 120.5(12) | ? |
| C12014 | C12015 | H12015 | . | . | . | 118.2 | ? |
| C12016 | C12015 | H12015 | . | . | . | 121.3 | ? |
| C12011 | C12016 | C12015 | . | . | . | 121.4(12) | ? |
| C12011 | C12016 | H12016 | . | . | . | 119.1 | ? |
| C12015 | C12016 | H12016 | . | . | . | 119.5 | ? |
| P12 | C12021 | C12022 | . | . | . | 124.1(9) | ? |
| P12 | C12021 | C12026 | . | . | . | 117.1(9) | ? |
| C12022 | C12021 | C12026 | . | . | . | 118.8(11) | ? |
| C12021 | C12022 | C12023 | . | . | . | 120.2(11) | ? |
| C12021 | C12022 | H12022 | . | . | . | 119.7 | ? |
| C12023 | C12022 | H12022 | . | . | . | 120.0 | ? |
| C12022 | C12023 | C12024 | . | . | . | 121.0(11) | ? |
| C12022 | C12023 | H12023 | . | . | . | 119.8 | ? |
| C12024 | C12023 | H12023 | . | . | . | 119.1 | ? |
| C12023 | C12024 | C12025 | . | . | . | 119.0(11) | ? |
| C12023 | C12024 | H12024 | . | . | . | 119.4 | ? |
| C12025 | C12024 | H12024 | . | . | . | 121.5 | ? |
| C12024 | C12025 | C12026 | . | . | . | 120.2(12) | ? |
| C12024 | C12025 | H12025 | . | . | . | 119.9 | ? |
| C12026 | C12025 | H12025 | . | . | . | 119.7 | ? |
| C12021 | C12026 | C12025 | . | . | . | 120.7(12) | ? |
| C12021 | C12026 | H12026 | . | . | . | 120.3 | ? |
| C12025 | C12026 | H12026 | . | . | . | 119.0 | ? |
| P12 | C12031 | C12032 | . | . | . | 121.6(9) | ? |
| P12 | C12031 | C12036 | . | . | . | 119.4(9) | ? |
| C12032 | C12031 | C12036 | . | . | . | 119.0(11) | ? |
| C12031 | C12032 | C12033 | . | . | . | 121.7(12) | ? |
| C12031 | C12032 | H12032 | . | . | . | 117.5 | ? |
| C12033 | C12032 | H12032 | . | . | . | 120.8 | ? |
| C12032 | C12033 | C12034 | . | . | . | 119.1(12) | ? |
| C12032 | C12033 | H12033 | . | . | . | 120.2 | ? |
| C12034 | C12033 | H12033 | . | . | . | 120.6 | ? |
| C12033 | C12034 | C12035 | . | . | . | 119.6(13) | ? |
| C12033 | C12034 | H12034 | . | . | . | 118.7 | ? |
| C12035 | C12034 | H12034 | . | . | . | 121.7 | ? |
| C12034 | C12035 | C12036 | . | . | . | 119.7(12) | ? |

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| C12034 | C12035 | H12035 | . | . | . | 121.3 | ? |
| C12036 | C12035 | H12035 | . | . | . | 119.0 | ? |
| C12031 | C12036 | C12035 | . | . | . | 120.9(12) | ? |
| C12031 | C12036 | H12036 | . | . | . | 118.9 | ? |
| C12035 | C12036 | H12036 | . | . | . | 120.2 | ? |
| Rh12 | C1211 | Ag11 | . | . | . | 91.5(4) | ? |
| Rh12 | C1211 | C1212 | . | . | . | 175.3(10) | ? |
| Ag11 | C1211 | C1212 | . | . | . | 85.8(8) | ? |
| Ag11 | C1212 | C1211 | . | . | . | 63.7(7) | ? |
| Ag11 | C1212 | C12121 | . | . | . | 120.8(8) | ? |
| C1211 | C1212 | C12121 | . | . | . | 172.0(12) | ? |
| C1212 | C12121 | C12122 | . | . | . | 118.2(10) | ? |
| C1212 | C12121 | C12126 | . | . | . | 122.4(10) | ? |
| C12122 | C12121 | C12126 | . | . | . | 119.3(11) | ? |
| C12121 | C12122 | C12123 | . | . | . | 118.4(12) | ? |
| C12121 | C12122 | H12122 | . | . | . | 121.6 | ? |
| C12123 | C12122 | H12122 | . | . | . | 119.9 | ? |
| C12122 | C12123 | C12124 | . | . | . | 122.3(13) | ? |
| C12122 | C12123 | H12123 | . | . | . | 119.6 | ? |
| C12124 | C12123 | H12123 | . | . | . | 118.0 | ? |
| C12123 | C12124 | C12125 | . | . | . | 119.0(14) | ? |
| C12123 | C12124 | H12124 | . | . | . | 119.9 | ? |
| C12125 | C12124 | H12124 | . | . | . | 121.0 | ? |
| C12124 | C12125 | C12126 | . | . | . | 120.0(13) | ? |
| C12124 | C12125 | H12125 | . | . | . | 120.7 | ? |
| C12126 | C12125 | H12125 | . | . | . | 119.2 | ? |
| C12121 | C12126 | C12125 | . | . | . | 120.8(12) | ? |
| C12121 | C12126 | H12126 | . | . | . | 119.8 | ? |
| C12125 | C12126 | H12126 | . | . | . | 119.4 | ? |
| Rh12 | C1221 | Ag12 | . | . | . | 90.6(4) | ? |
| Rh12 | C1221 | C1222 | . | . | . | 174.8(9) | ? |
| Ag12 | C1221 | C1222 | . | . | . | 85.2(7) | ? |
| Ag12 | C1222 | C1221 | . | . | . | 64.6(7) | ? |
| Ag12 | C1222 | C12221 | . | . | . | 122.7(8) | ? |
| C1221 | C1222 | C12221 | . | . | . | 172.4(12) | ? |
| C1222 | C12221 | C12222 | . | . | . | 119.7(11) | ? |
| C1222 | C12221 | C12226 | . | . | . | 121.4(11) | ? |
| C12222 | C12221 | C12226 | . | . | . | 118.9(11) | ? |
| C12221 | C12222 | C12223 | . | . | . | 119.8(12) | ? |
| C12221 | C12222 | H12222 | . | . | . | 119.6 | ? |
| C12223 | C12222 | H12222 | . | . | . | 120.5 | ? |
| C12222 | C12223 | C12224 | . | . | . | 121.2(13) | ? |
| C12222 | C12223 | H12223 | . | . | . | 118.7 | ? |
| C12224 | C12223 | H12223 | . | . | . | 120.0 | ? |
| C12223 | C12224 | C12225 | . | . | . | 119.1(13) | ? |
| C12223 | C12224 | H12224 | . | . | . | 120.3 | ? |
| C12225 | C12224 | H12224 | . | . | . | 120.5 | ? |
| C12224 | C12225 | C12226 | . | . | . | 121.1(13) | ? |
| C12224 | C12225 | H12225 | . | . | . | 120.8 | ? |
| C12226 | C12225 | H12225 | . | . | . | 118.0 | ? |
| C12221 | C12226 | C12225 | . | . | . | 119.8(12) | ? |
| C12221 | C12226 | H12226 | . | . | . | 119.6 | ? |
| C12225 | C12226 | H12226 | . | . | . | 120.6 | ? |
| Rh12 | C1231 | Ag13 | . | . | . | 94.0(4) | ? |
| Rh12 | C1231 | C1232 | . | . | . | 172.3(10) | ? |
| Ag13 | C1231 | C1232 | . | . | . | 81.4(8) | ? |
| Ag13 | C1232 | C1231 | . | . | . | 67.7(7) | ? |
| Ag13 | C1232 | C12321 | . | . | . | 125.7(8) | ? |
| C1231 | C1232 | C12321 | . | . | . | 166.6(12) | ? |
| C1232 | C12321 | C12322 | . | . | . | 119.6(10) | ? |
| C1232 | C12321 | C12326 | . | . | . | 121.9(10) | ? |

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|--------|--------|--------|---|---|---|-----------|---|
| C12322 | C12321 | C12326 | . | . | . | 118.5(10) | ? |
| C12321 | C12322 | C12323 | . | . | . | 120.2(11) | ? |
| C12321 | C12322 | H12232 | . | . | . | 118.2 | ? |
| C12323 | C12322 | H12232 | . | . | . | 121.6 | ? |
| C12322 | C12323 | C12324 | . | . | . | 119.5(11) | ? |
| C12322 | C12323 | H12233 | . | . | . | 120.1 | ? |
| C12324 | C12323 | H12233 | . | . | . | 120.4 | ? |
| C12323 | C12324 | C12325 | . | . | . | 121.2(11) | ? |
| C12323 | C12324 | H12234 | . | . | . | 119.8 | ? |
| C12325 | C12324 | H12234 | . | . | . | 119.0 | ? |
| C12324 | C12325 | C12326 | . | . | . | 118.9(11) | ? |
| C12324 | C12325 | H12235 | . | . | . | 119.4 | ? |
| C12326 | C12325 | H12235 | . | . | . | 121.7 | ? |
| C12321 | C12326 | C12325 | . | . | . | 121.7(11) | ? |
| C12321 | C12326 | H12236 | . | . | . | 119.3 | ? |
| C12325 | C12326 | H12236 | . | . | . | 119.0 | ? |
| Rh12 | C1241 | Ag14 | . | . | . | 94.2(4) | ? |
| Rh12 | C1241 | C1242 | . | . | . | 178.2(10) | ? |
| Ag14 | C1241 | C1242 | . | . | . | 84.4(8) | ? |
| Ag14 | C1242 | C1241 | . | . | . | 65.3(8) | ? |
| Ag14 | C1242 | C12421 | . | . | . | 120.9(9) | ? |
| C1241 | C1242 | C12421 | . | . | . | 173.7(13) | ? |
| C1242 | C12421 | C12422 | . | . | . | 121.7(12) | ? |
| C1242 | C12421 | C12426 | . | . | . | 121.1(12) | ? |
| C12422 | C12421 | C12426 | . | . | . | 117.2(12) | ? |
| C12421 | C12422 | C12423 | . | . | . | 120.8(12) | ? |
| C12421 | C12422 | H12422 | . | . | . | 118.4 | ? |
| C12423 | C12422 | H12422 | . | . | . | 120.7 | ? |
| C12422 | C12423 | C12424 | . | . | . | 119.6(12) | ? |
| C12422 | C12423 | H12423 | . | . | . | 120.9 | ? |
| C12424 | C12423 | H12423 | . | . | . | 119.5 | ? |
| C12423 | C12424 | C12425 | . | . | . | 120.9(12) | ? |
| C12423 | C12424 | H12424 | . | . | . | 120.0 | ? |
| C12425 | C12424 | H12424 | . | . | . | 119.1 | ? |
| C12424 | C12425 | C12426 | . | . | . | 119.0(12) | ? |
| C12424 | C12425 | H12425 | . | . | . | 120.9 | ? |
| C12426 | C12425 | H12425 | . | . | . | 120.0 | ? |
| C12421 | C12426 | C12425 | . | . | . | 122.3(12) | ? |
| C12421 | C12426 | H12426 | . | . | . | 117.3 | ? |
| C12425 | C12426 | H12426 | . | . | . | 120.4 | ? |
| Rh21 | P21 | C21011 | . | . | . | 115.4(4) | ? |
| Rh21 | P21 | C21021 | . | . | . | 118.3(4) | ? |
| Rh21 | P21 | C21031 | . | . | . | 113.4(4) | ? |
| C21011 | P21 | C21021 | . | . | . | 98.4(5) | ? |
| C21011 | P21 | C21031 | . | . | . | 104.8(5) | ? |
| C21021 | P21 | C21031 | . | . | . | 104.6(5) | ? |
| P21 | C21011 | C21012 | . | . | . | 116.8(9) | ? |
| P21 | C21011 | C21016 | . | . | . | 123.6(8) | ? |
| C21012 | C21011 | C21016 | . | . | . | 119.0(11) | ? |
| C21011 | C21012 | C21013 | . | . | . | 120.4(12) | ? |
| C21011 | C21012 | H21012 | . | . | . | 120.3 | ? |
| C21013 | C21012 | H21012 | . | . | . | 119.3 | ? |
| C21012 | C21013 | C21014 | . | . | . | 119.1(12) | ? |
| C21012 | C21013 | H21013 | . | . | . | 120.4 | ? |
| C21014 | C21013 | H21013 | . | . | . | 120.5 | ? |
| C21013 | C21014 | C21015 | . | . | . | 122.3(13) | ? |
| C21013 | C21014 | H21014 | . | . | . | 119.9 | ? |
| C21015 | C21014 | H21014 | . | . | . | 117.8 | ? |
| C21014 | C21015 | C21016 | . | . | . | 118.6(13) | ? |
| C21014 | C21015 | H21015 | . | . | . | 121.1 | ? |
| C21016 | C21015 | H21015 | . | . | . | 120.2 | ? |

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|--------|--------|--------|---|---|---|-----------|---|
| C21011 | C21016 | C21015 | . | . | . | 120.5(11) | ? |
| C21011 | C21016 | H21016 | . | . | . | 119.1 | ? |
| C21015 | C21016 | H21016 | . | . | . | 120.4 | ? |
| P21 | C21021 | C21022 | . | . | . | 118.2(9) | ? |
| P21 | C21021 | C21026 | . | . | . | 123.3(9) | ? |
| C21022 | C21021 | C21026 | . | . | . | 118.5(10) | ? |
| C21021 | C21022 | C21023 | . | . | . | 121.6(11) | ? |
| C21021 | C21022 | H21022 | . | . | . | 119.1 | ? |
| C21023 | C21022 | H21022 | . | . | . | 119.3 | ? |
| C21022 | C21023 | C21024 | . | . | . | 119.6(12) | ? |
| C21022 | C21023 | H21023 | . | . | . | 120.0 | ? |
| C21024 | C21023 | H21023 | . | . | . | 120.5 | ? |
| C21023 | C21024 | C21025 | . | . | . | 118.3(12) | ? |
| C21023 | C21024 | H21024 | . | . | . | 122.0 | ? |
| C21025 | C21024 | H21024 | . | . | . | 119.7 | ? |
| C21024 | C21025 | C21026 | . | . | . | 121.7(12) | ? |
| C21024 | C21025 | H21025 | . | . | . | 119.8 | ? |
| C21026 | C21025 | H21025 | . | . | . | 118.5 | ? |
| C21021 | C21026 | C21025 | . | . | . | 120.4(11) | ? |
| C21021 | C21026 | H21026 | . | . | . | 118.3 | ? |
| C21025 | C21026 | H21026 | . | . | . | 121.4 | ? |
| P21 | C21031 | C21032 | . | . | . | 119.0(8) | ? |
| P21 | C21031 | C21036 | . | . | . | 121.0(9) | ? |
| C21032 | C21031 | C21036 | . | . | . | 119.9(11) | ? |
| C21031 | C21032 | C21033 | . | . | . | 119.3(11) | ? |
| C21031 | C21032 | H21032 | . | . | . | 120.4 | ? |
| C21033 | C21032 | H21032 | . | . | . | 120.2 | ? |
| C21032 | C21033 | C21034 | . | . | . | 119.5(11) | ? |
| C21032 | C21033 | H21033 | . | . | . | 120.9 | ? |
| C21034 | C21033 | H21033 | . | . | . | 119.6 | ? |
| C21033 | C21034 | C21035 | . | . | . | 120.8(11) | ? |
| C21033 | C21034 | H21034 | . | . | . | 119.0 | ? |
| C21035 | C21034 | H21034 | . | . | . | 120.2 | ? |
| C21034 | C21035 | C21036 | . | . | . | 119.7(12) | ? |
| C21034 | C21035 | H21035 | . | . | . | 118.5 | ? |
| C21036 | C21035 | H21035 | . | . | . | 121.7 | ? |
| C21031 | C21036 | C21035 | . | . | . | 120.8(12) | ? |
| C21031 | C21036 | H21036 | . | . | . | 119.8 | ? |
| C21035 | C21036 | H21036 | . | . | . | 119.4 | ? |
| Rh21 | C2111 | Ag21 | . | . | . | 91.7(4) | ? |
| Rh21 | C2111 | C2112 | . | . | . | 171.4(10) | ? |
| Ag21 | C2111 | C2112 | . | . | . | 88.7(8) | ? |
| Ag21 | C2112 | C2111 | . | . | . | 61.4(7) | ? |
| Ag21 | C2112 | C21121 | . | . | . | 124.0(8) | ? |
| C2111 | C2112 | C21121 | . | . | . | 173.1(13) | ? |
| C2112 | C21121 | C21122 | . | . | . | 119.6(12) | ? |
| C2112 | C21121 | C21126 | . | . | . | 121.9(13) | ? |
| C21122 | C21121 | C21126 | . | . | . | 118.5(13) | ? |
| C21121 | C21122 | C21123 | . | . | . | 120.5(14) | ? |
| C21121 | C21122 | H21122 | . | . | . | 120.7 | ? |
| C21123 | C21122 | H21122 | . | . | . | 118.8 | ? |
| C21122 | C21123 | C21124 | . | . | . | 119.4(15) | ? |
| C21122 | C21123 | H21123 | . | . | . | 121.4 | ? |
| C21124 | C21123 | H21123 | . | . | . | 119.1 | ? |
| C21123 | C21124 | C21125 | . | . | . | 121.2(15) | ? |
| C21123 | C21124 | H21124 | . | . | . | 119.2 | ? |
| C21125 | C21124 | H21124 | . | . | . | 119.6 | ? |
| C21124 | C21125 | C21126 | . | . | . | 120.2(15) | ? |
| C21124 | C21125 | H21125 | . | . | . | 120.7 | ? |
| C21126 | C21125 | H21125 | . | . | . | 119.1 | ? |
| C21121 | C21126 | C21125 | . | . | . | 120.2(14) | ? |

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|--------|--------|--------|---|---|---|-----------|---|
| C21121 | C21126 | H21126 | . | . | . | 118.6 | ? |
| C21125 | C21126 | H21126 | . | . | . | 121.2 | ? |
| Rh21 | C2121 | Ag22 | . | . | . | 91.0(4) | ? |
| Rh21 | C2121 | C2122 | . | . | . | 176.6(10) | ? |
| Ag22 | C2121 | C2122 | . | . | . | 90.2(8) | ? |
| Ag22 | C2122 | C2121 | . | . | . | 61.0(7) | ? |
| Ag22 | C2122 | C21221 | . | . | . | 126.0(8) | ? |
| C2121 | C2122 | C21221 | . | . | . | 172.3(12) | ? |
| C2122 | C21221 | C21222 | . | . | . | 122.7(12) | ? |
| C2122 | C21221 | C21226 | . | . | . | 118.0(12) | ? |
| C21222 | C21221 | C21226 | . | . | . | 119.2(13) | ? |
| C21221 | C21222 | C21223 | . | . | . | 120.9(13) | ? |
| C21221 | C21222 | H21222 | . | . | . | 119.9 | ? |
| C21223 | C21222 | H21222 | . | . | . | 119.2 | ? |
| C21222 | C21223 | C21224 | . | . | . | 118.4(14) | ? |
| C21222 | C21223 | H21223 | . | . | . | 122.1 | ? |
| C21224 | C21223 | H21223 | . | . | . | 119.5 | ? |
| C21223 | C21224 | C21225 | . | . | . | 121.7(15) | ? |
| C21223 | C21224 | H21224 | . | . | . | 119.0 | ? |
| C21225 | C21224 | H21224 | . | . | . | 119.3 | ? |
| C21224 | C21225 | C21226 | . | . | . | 121.5(15) | ? |
| C21224 | C21225 | H21225 | . | . | . | 119.7 | ? |
| C21226 | C21225 | H21225 | . | . | . | 118.7 | ? |
| C21221 | C21226 | C21225 | . | . | . | 118.2(14) | ? |
| C21221 | C21226 | H21226 | . | . | . | 121.5 | ? |
| C21225 | C21226 | H21226 | . | . | . | 120.1 | ? |
| Rh21 | C2131 | Ag23 | . | . | . | 92.0(4) | ? |
| Rh21 | C2131 | C2132 | . | . | . | 174.0(10) | ? |
| Ag23 | C2131 | C2132 | . | . | . | 82.8(8) | ? |
| Ag23 | C2132 | C2131 | . | . | . | 66.8(7) | ? |
| Ag23 | C2132 | C21321 | . | . | . | 124.1(8) | ? |
| C2131 | C2132 | C21321 | . | . | . | 168.6(12) | ? |
| C2132 | C21321 | C21322 | . | . | . | 120.9(12) | ? |
| C2132 | C21321 | C21326 | . | . | . | 121.1(11) | ? |
| C21322 | C21321 | C21326 | . | . | . | 118.0(13) | ? |
| C21321 | C21322 | C21323 | . | . | . | 119.7(14) | ? |
| C21321 | C21322 | H21322 | . | . | . | 119.0 | ? |
| C21323 | C21322 | H21322 | . | . | . | 121.2 | ? |
| C21322 | C21323 | C21324 | . | . | . | 123.5(17) | ? |
| C21322 | C21323 | H21323 | . | . | . | 120.1 | ? |
| C21324 | C21323 | H21323 | . | . | . | 116.4 | ? |
| C21323 | C21324 | C21325 | . | . | . | 117.7(15) | ? |
| C21323 | C21324 | H21324 | . | . | . | 124 | ? |
| C21325 | C21324 | H21324 | . | . | . | 118.2 | ? |
| C21324 | C21325 | C21326 | . | . | . | 120.2(15) | ? |
| C21324 | C21325 | H21325 | . | . | . | 119.8 | ? |
| C21326 | C21325 | H21325 | . | . | . | 120.0 | ? |
| C21321 | C21326 | C21325 | . | . | . | 120.9(14) | ? |
| C21321 | C21326 | H21326 | . | . | . | 118.8 | ? |
| C21325 | C21326 | H21326 | . | . | . | 120.3 | ? |
| Rh21 | C2141 | Ag24 | . | . | . | 93.7(4) | ? |
| Rh21 | C2141 | C2142 | . | . | . | 177.9(10) | ? |
| Ag24 | C2141 | C2142 | . | . | . | 84.3(8) | ? |
| Ag24 | C2142 | C2141 | . | . | . | 65.6(7) | ? |
| Ag24 | C2142 | C21421 | . | . | . | 127.5(8) | ? |
| C2141 | C2142 | C21421 | . | . | . | 166.8(12) | ? |
| C2142 | C21421 | C21422 | . | . | . | 120.2(10) | ? |
| C2142 | C21421 | C21426 | . | . | . | 122.1(10) | ? |
| C21422 | C21421 | C21426 | . | . | . | 117.7(10) | ? |
| C21421 | C21422 | C21423 | . | . | . | 120.9(11) | ? |
| C21421 | C21422 | H21422 | . | . | . | 118.6 | ? |

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|--------|--------|--------|---|---|---|-----------|---|
| C21423 | C21422 | H21422 | . | . | . | 120.5 | ? |
| C21422 | C21423 | C21424 | . | . | . | 119.8(12) | ? |
| C21422 | C21423 | H21423 | . | . | . | 120.1 | ? |
| C21424 | C21423 | H21423 | . | . | . | 120.1 | ? |
| C21423 | C21424 | C21425 | . | . | . | 121.2(12) | ? |
| C21423 | C21424 | H21424 | . | . | . | 120.9 | ? |
| C21425 | C21424 | H21424 | . | . | . | 118.0 | ? |
| C21424 | C21425 | C21426 | . | . | . | 119.8(12) | ? |
| C21424 | C21425 | H21425 | . | . | . | 119.6 | ? |
| C21426 | C21425 | H21425 | . | . | . | 120.6 | ? |
| C21421 | C21426 | C21425 | . | . | . | 120.6(12) | ? |
| C21421 | C21426 | H21426 | . | . | . | 120.6 | ? |
| C21425 | C21426 | H21426 | . | . | . | 118.8 | ? |
| Rh22 | P22 | C22011 | . | . | . | 118.2(4) | ? |
| Rh22 | P22 | C22021 | . | . | . | 112.9(4) | ? |
| Rh22 | P22 | C22031 | . | . | . | 117.6(4) | ? |
| C22011 | P22 | C22021 | . | . | . | 103.1(5) | ? |
| C22011 | P22 | C22031 | . | . | . | 100.8(5) | ? |
| C22021 | P22 | C22031 | . | . | . | 102.0(6) | ? |
| P22 | C22011 | C22012 | . | . | . | 123.4(9) | ? |
| P22 | C22011 | C22016 | . | . | . | 117.4(9) | ? |
| C22012 | C22011 | C22016 | . | . | . | 119.2(11) | ? |
| C22011 | C22012 | C22013 | . | . | . | 122.6(12) | ? |
| C22011 | C22012 | H22012 | . | . | . | 118.1 | ? |
| C22013 | C22012 | H22012 | . | . | . | 119.3 | ? |
| C22012 | C22013 | C22014 | . | . | . | 119.0(13) | ? |
| C22012 | C22013 | H22013 | . | . | . | 120.2 | ? |
| C22014 | C22013 | H22013 | . | . | . | 120.7 | ? |
| C22013 | C22014 | C22015 | . | . | . | 119.4(13) | ? |
| C22013 | C22014 | H22014 | . | . | . | 120.3 | ? |
| C22015 | C22014 | H22014 | . | . | . | 120.2 | ? |
| C22014 | C22015 | C22016 | . | . | . | 120.6(12) | ? |
| C22014 | C22015 | H22015 | . | . | . | 120.9 | ? |
| C22016 | C22015 | H22015 | . | . | . | 118.4 | ? |
| C22011 | C22016 | C22015 | . | . | . | 119.0(12) | ? |
| C22011 | C22016 | H22016 | . | . | . | 120.2 | ? |
| C22015 | C22016 | H22016 | . | . | . | 120.7 | ? |
| P22 | C22021 | C22022 | . | . | . | 118.2(10) | ? |
| P22 | C22021 | C22026 | . | . | . | 121.5(9) | ? |
| C22022 | C22021 | C22026 | . | . | . | 120.0(11) | ? |
| C22021 | C22022 | C22023 | . | . | . | 118.5(11) | ? |
| C22021 | C22022 | H22022 | . | . | . | 120.9 | ? |
| C22023 | C22022 | H22022 | . | . | . | 120.5 | ? |
| C22022 | C22023 | C22024 | . | . | . | 121.6(12) | ? |
| C22022 | C22023 | H22023 | . | . | . | 119.4 | ? |
| C22024 | C22023 | H22023 | . | . | . | 119.0 | ? |
| C22023 | C22024 | C22025 | . | . | . | 119.0(12) | ? |
| C22023 | C22024 | H22024 | . | . | . | 119.6 | ? |
| C22025 | C22024 | H22024 | . | . | . | 121.4 | ? |
| C22024 | C22025 | C22026 | . | . | . | 120.9(12) | ? |
| C22024 | C22025 | H22025 | . | . | . | 119.7 | ? |
| C22026 | C22025 | H22025 | . | . | . | 119.4 | ? |
| C22021 | C22026 | C22025 | . | . | . | 119.7(11) | ? |
| C22021 | C22026 | H22026 | . | . | . | 120.3 | ? |
| C22025 | C22026 | H22026 | . | . | . | 119.9 | ? |
| P22 | C22031 | C22032 | . | . | . | 119.5(9) | ? |
| P22 | C22031 | C22036 | . | . | . | 122.6(9) | ? |
| C22032 | C22031 | C22036 | . | . | . | 117.8(11) | ? |
| C22031 | C22032 | C22033 | . | . | . | 121.0(11) | ? |
| C22031 | C22032 | H22032 | . | . | . | 118.8 | ? |
| C22033 | C22032 | H22032 | . | . | . | 120.2 | ? |

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|--------|--------|--------|-------|-----------|---|
| C22032 | C22033 | C22034 | . . . | 120.6(12) | ? |
| C22032 | C22033 | H22033 | . . . | 119.6 | ? |
| C22034 | C22033 | H22033 | . . . | 119.7 | ? |
| C22033 | C22034 | C22035 | . . . | 119.2(12) | ? |
| C22033 | C22034 | H22034 | . . . | 120.7 | ? |
| C22035 | C22034 | H22034 | . . . | 120.1 | ? |
| C22034 | C22035 | C22036 | . . . | 121.5(11) | ? |
| C22034 | C22035 | H22035 | . . . | 119.3 | ? |
| C22036 | C22035 | H22035 | . . . | 119.3 | ? |
| C22031 | C22036 | C22035 | . . . | 119.8(11) | ? |
| C22031 | C22036 | H22036 | . . . | 120.0 | ? |
| C22035 | C22036 | H22036 | . . . | 120.2 | ? |
| Rh22 | C2211 | Ag21 | . . . | 91.3(4) | ? |
| Rh22 | C2211 | C2212 | . . . | 174.4(10) | ? |
| Ag21 | C2211 | C2212 | . . . | 87.0(8) | ? |
| Ag21 | C2212 | C2211 | . . . | 62.7(7) | ? |
| Ag21 | C2212 | C22121 | . . . | 124.9(9) | ? |
| C2211 | C2212 | C22121 | . . . | 172.1(13) | ? |
| C2212 | C22121 | C22122 | . . . | 120.5(12) | ? |
| C2212 | C22121 | C22126 | . . . | 120.9(12) | ? |
| C22122 | C22121 | C22126 | . . . | 118.5(13) | ? |
| C22121 | C22122 | C22123 | . . . | 119.4(14) | ? |
| C22121 | C22122 | H22122 | . . . | 119.6 | ? |
| C22123 | C22122 | H22122 | . . . | 121.0 | ? |
| C22122 | C22123 | C22124 | . . . | 121.8(17) | ? |
| C22122 | C22123 | H22123 | . . . | 119.5 | ? |
| C22124 | C22123 | H22123 | . . . | 118.6 | ? |
| C22123 | C22124 | C22125 | . . . | 119.1(16) | ? |
| C22123 | C22124 | H22124 | . . . | 119 | ? |
| C22125 | C22124 | H22124 | . . . | 121.2 | ? |
| C22124 | C22125 | C22126 | . . . | 120.1(15) | ? |
| C22124 | C22125 | H22125 | . . . | 120.3 | ? |
| C22126 | C22125 | H22125 | . . . | 119.6 | ? |
| C22121 | C22126 | C22125 | . . . | 121.1(14) | ? |
| C22121 | C22126 | H22126 | . . . | 118.5 | ? |
| C22125 | C22126 | H22126 | . . . | 120.4 | ? |
| Rh22 | C2221 | Ag22 | . . . | 92.5(4) | ? |
| Rh22 | C2221 | C2222 | . . . | 177.4(9) | ? |
| Ag22 | C2221 | C2222 | . . . | 85.2(7) | ? |
| Ag22 | C2222 | C2221 | . . . | 64.7(6) | ? |
| Ag22 | C2222 | C22221 | . . . | 123.6(8) | ? |
| C2221 | C2222 | C22221 | . . . | 171.4(11) | ? |
| C2222 | C22221 | C22222 | . . . | 121.7(11) | ? |
| C2222 | C22221 | C22226 | . . . | 117.9(11) | ? |
| C22222 | C22221 | C22226 | . . . | 120.4(11) | ? |
| C22221 | C22222 | C22223 | . . . | 118.5(12) | ? |
| C22221 | C22222 | H22222 | . . . | 120.3 | ? |
| C22223 | C22222 | H22222 | . . . | 121.2 | ? |
| C22222 | C22223 | C22224 | . . . | 121.5(13) | ? |
| C22222 | C22223 | H22223 | . . . | 119.0 | ? |
| C22224 | C22223 | H22223 | . . . | 119.5 | ? |
| C22223 | C22224 | C22225 | . . . | 119.6(13) | ? |
| C22223 | C22224 | H22224 | . . . | 119.3 | ? |
| C22225 | C22224 | H22224 | . . . | 121.1 | ? |
| C22224 | C22225 | C22226 | . . . | 120.7(13) | ? |
| C22224 | C22225 | H22225 | . . . | 118.3 | ? |
| C22226 | C22225 | H22225 | . . . | 121.0 | ? |
| C22221 | C22226 | C22225 | . . . | 119.2(12) | ? |
| C22221 | C22226 | H22226 | . . . | 122.0 | ? |
| C22225 | C22226 | H22226 | . . . | 118.7 | ? |
| Rh22 | C2231 | Ag23 | . . . | 91.6(4) | ? |

| | | | | | | | |
|--------|--------|--------|---|---|---|-----------|---|
| Rh22 | C2231 | C2232 | . | . | . | 171.5(9) | ? |
| Ag23 | C2231 | C2232 | . | . | . | 88.6(7) | ? |
| Ag23 | C2232 | C2231 | . | . | . | 61.7(7) | ? |
| Ag23 | C2232 | C22321 | . | . | . | 128.8(8) | ? |
| C2231 | C2232 | C22321 | . | . | . | 168.2(12) | ? |
| C2232 | C22321 | C22322 | . | . | . | 119.0(11) | ? |
| C2232 | C22321 | C22326 | . | . | . | 123.5(11) | ? |
| C22322 | C22321 | C22326 | . | . | . | 117.4(11) | ? |
| C22321 | C22322 | C22323 | . | . | . | 121.0(12) | ? |
| C22321 | C22322 | H22322 | . | . | . | 121.3 | ? |
| C22323 | C22322 | H22322 | . | . | . | 117.7 | ? |
| C22322 | C22323 | C22324 | . | . | . | 120.6(14) | ? |
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| C22324 | C22323 | H22323 | . | . | . | 118.6 | ? |
| C22323 | C22324 | C22325 | . | . | . | 119.3(12) | ? |
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| C22326 | C22325 | H22325 | . | . | . | 119.6 | ? |
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| C22321 | C22326 | H22326 | . | . | . | 118.9 | ? |
| C22325 | C22326 | H22326 | . | . | . | 120.6 | ? |
| Rh22 | C2241 | Ag24 | . | . | . | 95.3(5) | ? |
| Rh22 | C2241 | C2242 | . | . | . | 173.4(10) | ? |
| Ag24 | C2241 | C2242 | . | . | . | 85.5(8) | ? |
| Ag24 | C2242 | C2241 | . | . | . | 64.4(8) | ? |
| Ag24 | C2242 | C22421 | . | . | . | 123.0(8) | ? |
| C2241 | C2242 | C22421 | . | . | . | 172.4(13) | ? |
| C2242 | C22421 | C22422 | . | . | . | 118.5(11) | ? |
| C2242 | C22421 | C22426 | . | . | . | 123.8(12) | ? |
| C22422 | C22421 | C22426 | . | . | . | 117.7(12) | ? |
| C22421 | C22422 | C22423 | . | . | . | 119.8(13) | ? |
| C22421 | C22422 | H22422 | . | . | . | 121.0 | ? |
| C22423 | C22422 | H22422 | . | . | . | 119.2 | ? |
| C22422 | C22423 | C22424 | . | . | . | 121.6(14) | ? |
| C22422 | C22423 | H22423 | . | . | . | 121.1 | ? |
| C22424 | C22423 | H22423 | . | . | . | 117.2 | ? |
| C22423 | C22424 | C22425 | . | . | . | 119.1(14) | ? |
| C22423 | C22424 | H22424 | . | . | . | 121.4 | ? |
| C22425 | C22424 | H22424 | . | . | . | 119.5 | ? |
| C22424 | C22425 | C22426 | . | . | . | 120.4(14) | ? |
| C22424 | C22425 | H22425 | . | . | . | 117.9 | ? |
| C22426 | C22425 | H22425 | . | . | . | 121.7 | ? |
| C22421 | C22426 | C22425 | . | . | . | 121.4(13) | ? |
| C22421 | C22426 | H22426 | . | . | . | 119.5 | ? |
| C22425 | C22426 | H22426 | . | . | . | 119.1 | ? |

loop_

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_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

_geom_torsion_atom_site_label_4

_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion

_geom_torsion_publ_flag

#<< enter YES for value to be published

? ? ? ? ? ? ? ? ? ?

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_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_site_symmetry_D
_geom_hbond_site_symmetry_H
_geom_hbond_site_symmetry_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_publ_flag          #<< enter YES for value to be published
    ? ? ? ? ? ? ? ? ? ?
```

```
#-----
#      Special items requested by author for inclusion in paper
#-----
```

```
loop_
_publ_manuscript_incl_extra_item
_publ_manuscript_incl_extra_defn
    ? ?
```

```
#-----
#      Items which are non-mandatory for Acta C submissions
#-----
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_atom_sites_solution_primary      ?
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_atom_sites_solution_hydrogens     ?

_geom_special_details              ?
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_cell_special_details
;      ?
;
```

```
_exptl_special_details
;      ?
;
```

```
_diffrn_special_details
;      ?
;
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_chemical_compound_source          ?
_chemical_name_systematic           ?
_chemical_name_common               ?
_chemical_formula_analytical        ?
_chemical_formula_structural        ?
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```
_exptl_crystal_F_000              7824
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```
loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
    ? ? ?
```



```
#####
#
#   CIF generated by the Xtal System   #
#
#####
```

data_global

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_audit_creation_method      Xtal3.6
_audit_creation_date        01-12-06
_audit_update_record        ?
```

```
#####
# (Publishing Staff Use Only)
```

```
_journal_date_recd_electronic  ?
_journal_date_to_coeditor      ?
_journal_date_from_coeditor    ?
_journal_date_accepted         ?
_journal_date_printers_first   ?
_journal_date_printers_final   ?
_journal_date_proofs_out       ?
_journal_date_proofs_in        ?
_journal_coeditor_name         ?
_journal_coeditor_code         ?
_journal_coeditor_notes        ?
; ?
;
_journal_techeditor_code       ?
_journal_techeditor_notes      ?
; ?
;
_journal_coden_ASTM            ?
_journal_name_full             ?
_journal_year                  ?
_journal_volume                ?
_journal_issue                 ?
_journal_page_first            ?
_journal_page_last             ?
_journal_suppl_publ_number     ?
_journal_suppl_publ_pages      ?
```

```
#####
```

```
# 1. SUBMISSION DETAILS
```

```
#-----
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```
_publ_contact_author_name
  'Skelton, B. W.'
_publ_contact_author_address
;
  Department of Chemistry
  University of Western Australia
  35 Stirling Highway
  Crawley
  Western Australia 6009
  Australia
;
_publ_contact_author_email      bws@crystal.uwa.edu.au
_publ_contact_author_fax        (+61)_08_9380_1118
_publ_contact_author_phone      (+61)_08-9380_3481
```

```

_publ_contact_letter
;   ?                               #<< contact letter
;

_publ_requested_journal   ?
_publ_requested_category ?

_publ_section_title
;   ?                               #<< paper title text
;
_publ_section_title_footnote
;   ?                               #<< paper footnote text
;

loop_
_publ_author_name
_publ_author_footnote
_publ_author_address

'Skelton, Brian W.' .
; Department of Chemistry,
University of Western Australia,
35 Stirling Highway,
Crawley,
WA 6009,
Australia.
;

_publ_section_synopsis
;   ?                               #<< synopsis if FI,CI,CM,CO papers
;
_publ_section_abstract
;   ?                               #<< abstract text
;
_publ_section_comment
;   ?                               #<< scientific commentary text
;

_publ_section_exptl_prep
;   ?                               #<< material & crystal preparation text
;

_publ_section_exptl_refinement
;   ?                               #<< crystallographic methods used
;

_publ_section_acknowledgements
;   ?                               #<< acknowledgements text
;

_publ_section_references
;
Sheldrick, G M. (1996). SADABS. Program for Empirical Absorption Correction
of Area Detector Data. University of Gottingen, Germany.

Siemens (1995). SMART and SAINT. Area-Detector Control and Integration

```

Software. Siemens Analytical X-ray Systems Inc., Madison, Wisconsin, USA.

Hall, S.R., King, G.S.D., and Stewart., J.M. (1995).
The Xtal 3.5 User's Manual. University of Western Australia, Lamb: Perth.

```
;  
_publ_section_figure_captions  
;      ?                               #<< figure captions  
;  
  
#=====  
# Data block for single structure (one for each study in the paper)  
#=====
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data_br692

```
# 2. EXPERIMENTAL DATA  
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|---------------------------------|-----------------------|
| _chemical_formula_sum | 'C112 H82 Cu4 P2 Rh2' |
| _chemical_formula_moiety | ? |
| _chemical_formula_weight | 1949.83 |
| _chemical_melting_point | ? |
| _symmetry_cell_setting | triclinic |
| _symmetry_space_group_name_H-M | P_-1 |
| _symmetry_space_group_name_Hall | -p_1 |
| loop_ | |
| _symmetry_equiv_pos_as_xyz | +x,+y,+z -x,-y,-z |
| _cell_length_a | 11.480(2) |
| _cell_length_b | 13.581(2) |
| _cell_length_c | 15.164(2) |
| _cell_angle_alpha | 111.888(3) |
| _cell_angle_beta | 93.229(3) |
| _cell_angle_gamma | 101.666(3) |
| _cell_volume | 2125.8(6) |
| _cell_formula_units_Z | 1 |
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| _exptl_crystal_density_meas | ? |
| _exptl_crystal_density_method | ? |
| _diffrn_radiation_type | 'Mo K\alpha' |
| _diffrn_radiation_wavelength | .71073 |
| _cell_measurement_reflms_used | 2991 |
| _cell_measurement_theta_min | 1.7 |
| _cell_measurement_theta_max | 20.3 |
| _cell_measurement_temperature | 153 |
| _exptl_absorpt_coefficient_mu | 1.452 |
| _exptl_crystal_description | plate |
| _exptl_crystal_size_max | .2 |
| _exptl_crystal_size_mid | .1 |
| _exptl_crystal_size_min | .05 |
| _exptl_crystal_size_rad | ? |

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_exptl_crystal_colour          colourless

_diffrn_measurement_device_type
;
Bruker SMART CCD diffractometer
;
_diffrn_measurement_method      '\w scans'
_diffrn_detector_area_resol_mean ?

_exptl_absorpt_correction_type  multi-scan
_exptl_absorpt_process_details
;
SADABS; Sheldrick, 1996
;
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_exptl_absorpt_correction_T_max .86

_diffrn_reflns_number           25502
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_reflns_number_gt               5514
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_diffrn_measured_fraction_theta_full ?
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_diffrn_reflns_limit_h_max      15
_diffrn_reflns_limit_k_min      -18
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_diffrn_reflns_limit_l_min      0
_diffrn_reflns_limit_l_max      20
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_diffrn_standards_interval_count ?
_diffrn_standards_interval_time ?
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_refine_ls_number_reflns        5514
_refine_ls_number_parameters     536
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_refine_ls_weighting_details     ?
_refine_ls_hydrogen_treatment    noref
_refine_ls_shift/su_max          .068
_refine_diff_density_min         -.831
_refine_diff_density_max         1.454

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_refine_ls_abs_structure_Flack   ?

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# 3. Information for the "methods" section
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_computing_cell_refinement     'Siemens SAINT (Siemens, 1995)'
_computing_data_reduction      'xtal ADDREF SORTRF'
_computing_structure_solution  xtal
_computing_structure_refinement 'xtal CRYLSQ'
_computing_molecular_graphics  xtal
_computing_publication_material 'xtal BONDLA CIFIO'

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4. Supplementary data for validation and tables

#-----

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_atom_type_number_in_cell
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
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  H ? 0 82 0 0 'Int Tables Vol IV Tables 2.2B and 2.3.1'
  Cu ? 0 4 .263 1.266 'Int Tables Vol IV Tables 2.2B and 2.3.1'
  P ? 0 2 .09 .095 'Int Tables Vol IV Tables 2.2B and 2.3.1'
  Rh ? 0 2 -1.287 .919 'Int Tables Vol IV Tables 2.2B and 2.3.1'

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loop_

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_atom_site_fract_y
_atom_site_fract_z
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_atom_site_adp_type
_atom_site_calc_flag
_atom_site_calc_attached_atom
_atom_site_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
  Rh .99469(5) .86887(5) .37201(4) .0358(3) Uani ? ? 1.00000 ? ?
  Cu1 .83689(9) 1.01461(7) .44796(6) .0435(4) Uani ? ? 1.00000 ? ?
  Cu2 .92173(8) .89470(8) .55264(6) .0446(4) Uani ? ? 1.00000 ? ?
  P1 .97710(17) .72965(15) .22537(13) .0335(8) Uani ? ? 1.00000 ? ?
  C0111 .8298(6) .6335(5) .1792(5) .035(3) Uani ? ? 1.00000 ? ?
  C0112 .8037(7) .5634(6) .0826(5) .046(4) Uani ? ? 1.00000 ? ?
  C0113 .6908(8) .4941(7) .0456(5) .057(4) Uani ? ? 1.00000 ? ?
  C0114 .6018(7) .4924(6) .1029(6) .051(4) Uani ? ? 1.00000 ? ?
  C0115 .6273(7) .5605(6) .1991(6) .048(4) Uani ? ? 1.00000 ? ?
  C0116 .7392(6) .6300(6) .2370(5) .039(3) Uani ? ? 1.00000 ? ?
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  C0122 1.2064(6) .6987(6) .2331(5) .039(3) Uani ? ? 1.00000 ? ?
  C0123 1.2944(7) .6415(6) .2238(5) .044(4) Uani ? ? 1.00000 ? ?
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  C0125 1.1408(8) .4783(6) .1859(6) .055(4) Uani ? ? 1.00000 ? ?
  C0126 1.0522(7) .5365(6) .1944(5) .044(4) Uani ? ? 1.00000 ? ?
  C0131 .9987(6) .7734(5) .1261(5) .035(3) Uani ? ? 1.00000 ? ?
  C0132 1.0697(6) .7326(6) .0561(5) .040(3) Uani ? ? 1.00000 ? ?
  C0133 1.0748(7) .7635(6) -.0216(5) .048(4) Uani ? ? 1.00000 ? ?
  C0134 1.0098(7) .8348(6) -.0304(5) .049(4) Uani ? ? 1.00000 ? ?
  C0135 .9393(7) .8771(6) .0391(5) .045(4) Uani ? ? 1.00000 ? ?
  C0136 .9338(7) .8480(6) .1170(5) .042(3) Uani ? ? 1.00000 ? ?

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| C11 | .8329(7) | .8895(5) | .3294(5) | .037(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C12 | .7423(7) | .9004(6) | .3067(5) | .044(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C121 | .6287(7) | .8859(6) | .2460(6) | .048(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C122 | .6048(8) | .8109(7) | .1477(6) | .060(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C123 | .5044(8) | .7991(7) | .0898(7) | .071(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C124 | .4203(8) | .8572(8) | .1231(6) | .065(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C125 | .4371(8) | .9273(8) | .2179(6) | .067(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C126 | .5406(8) | .9402(7) | .2784(6) | .061(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C21 | .9149(7) | .7627(6) | .4356(5) | .048(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C22 | .8863(7) | .7179(7) | .4659(5) | .052(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C221 | .8153(12) | .6206(11) | .4947(11) | .059(5) | Uiso | ? | ? | .50000 | ? | ? |
| C222 | .6886(15) | .5742(18) | .4677(16) | .112(8) | Uiso | ? | ? | .50000 | ? | ? |
| C223 | .6312(10) | .494(2) | .5007(17) | .118(9) | Uiso | ? | ? | .50000 | ? | ? |
| C224 | .6984(16) | .4545(17) | .5510(17) | .125(9) | Uiso | ? | ? | .50000 | ? | ? |
| C225 | .8186(13) | .4813(14) | .5613(13) | .079(6) | Uiso | ? | ? | .50000 | ? | ? |
| C226 | .8805(9) | .5748(14) | .5412(14) | .085(6) | Uiso | ? | ? | .50000 | ? | ? |
| C221' | .8686(17) | .6134(15) | .4906(18) | .119(9) | Uiso | ? | ? | .50000 | ? | ? |
| C222' | .7457(15) | .5669(19) | .493(2) | .149(11) | Uiso | ? | ? | .50000 | ? | ? |
| C223' | .7153(12) | .472(2) | .519(2) | .213(17) | Uiso | ? | ? | .50000 | ? | ? |
| C224' | .803(2) | .446(3) | .566(3) | .39(4) | Uiso | ? | ? | .50000 | ? | ? |
| C225' | .9259(17) | .483(3) | .558(2) | .202(16) | Uiso | ? | ? | .50000 | ? | ? |
| C226' | .9610(12) | .568(2) | .518(2) | .181(14) | Uiso | ? | ? | .50000 | ? | ? |
| C31 | 1.1578(7) | .8605(5) | .4263(5) | .041(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C32 | 1.2425(7) | .8563(6) | .4682(5) | .048(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C321 | 1.3545(7) | .8335(6) | .4978(6) | .049(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C322 | 1.3712(8) | .8022(9) | .5740(7) | .075(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C323 | 1.4814(9) | .7837(9) | .5998(7) | .085(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C324 | 1.5736(8) | .7979(10) | .5491(8) | .087(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C325 | 1.5578(8) | .8235(10) | .4733(7) | .088(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C326 | 1.4502(8) | .8433(8) | .4501(7) | .070(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C41 | 1.0846(7) | .9854(5) | .3238(4) | .039(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C42 | 1.1250(7) | 1.0494(6) | .3043(5) | .049(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C421 | 1.1898(7) | 1.1120(7) | .2509(6) | .056(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C422 | 1.2194(10) | 1.2252(8) | .2841(8) | .084(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C423 | 1.2885(11) | 1.2762(8) | .2314(9) | .098(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C424 | 1.3236(11) | 1.2164(10) | .1471(8) | .100(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C425 | 1.2919(9) | 1.1054(10) | .1133(7) | .086(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C426 | 1.2238(8) | 1.0554(8) | .1624(6) | .065(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C1 | .8344(12) | 1.3187(9) | .2710(8) | .112(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C2 | .8774(10) | 1.2340(10) | .2664(8) | .093(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C3 | .8145(12) | 1.1348(9) | .2183(8) | .104(7) | Uani | ? | ? | 1.00000 | ? | ? |
| C4 | .7075(12) | 1.1157(10) | .1695(7) | .130(8) | Uani | ? | ? | 1.00000 | ? | ? |
| C5 | .6612(11) | 1.2018(16) | .1723(9) | .161(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C6 | .7260(14) | 1.3045(11) | .2249(9) | .137(10) | Uani | ? | ? | 1.00000 | ? | ? |
| H0112 | .86561 | .56328 | .04054 | .06000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0113 | .67385 | .44545 | -.02192 | .07200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0114 | .52320 | .44284 | .07570 | .06500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0115 | .56443 | .55896 | .23960 | .06300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0116 | .75555 | .67755 | .30499 | .05200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0122 | 1.22896 | .77772 | .25170 | .05200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0123 | 1.37862 | .67858 | .23316 | .06100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0124 | 1.32136 | .48752 | .19397 | .06400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0125 | 1.11822 | .40001 | .16927 | .06900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0126 | .96776 | .49814 | .18360 | .05700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0132 | 1.11560 | .68187 | .06137 | .05200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0133 | 1.12429 | .73595 | -.07000 | .06400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0134 | 1.01306 | .85688 | -.08461 | .06200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0135 | .89360 | .92847 | .03338 | .05700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0136 | .88578 | .87858 | .16635 | .05500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H112 | .66141 | .76632 | .12210 | .07300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H113 | .49240 | .74929 | .02279 | .08900 | Uiso | ? | ? | 1.00000 | ? | ? |

| | | | | | | | | | | |
|-------|---------|---------|--------|--------|------|---|---|---------|---|---|
| H114 | .34983 | .85026 | .07981 | .08000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H115 | .37714 | .96624 | .24286 | .08200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H116 | .55083 | .99022 | .34471 | .07600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H222 | .63854 | .60343 | .43278 | .13100 | Uiso | ? | ? | .50000 | ? | ? |
| H223 | .54016 | .46609 | .48745 | .15700 | Uiso | ? | ? | .50000 | ? | ? |
| H224 | .65414 | .40239 | .57604 | .15900 | Uiso | ? | ? | .50000 | ? | ? |
| H225 | .86368 | .44089 | .58254 | .36500 | Uiso | ? | ? | .50000 | ? | ? |
| H226 | .96483 | .60329 | .55991 | .10500 | Uiso | ? | ? | .50000 | ? | ? |
| H222' | .68415 | .60210 | .47476 | .13100 | Uiso | ? | ? | .50000 | ? | ? |
| H223' | .62577 | .43306 | .50113 | .15700 | Uiso | ? | ? | .50000 | ? | ? |
| H224' | .76645 | .40508 | .60235 | .36500 | Uiso | ? | ? | .50000 | ? | ? |
| H225' | .97601 | .44134 | .57364 | .22200 | Uiso | ? | ? | .50000 | ? | ? |
| H226' | 1.04734 | .59161 | .51995 | .19600 | Uiso | ? | ? | .50000 | ? | ? |
| H312 | 1.30513 | .79132 | .61049 | .08700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H313 | 1.49438 | .76358 | .65551 | .10100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H314 | 1.65136 | .78712 | .56871 | .10300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H315 | 1.62342 | .82865 | .43686 | .10300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H316 | 1.44133 | .86499 | .39586 | .08300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H412 | 1.19739 | 1.26953 | .34496 | .10000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H413 | 1.30920 | 1.35502 | .25444 | .11900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H414 | 1.37300 | 1.25239 | .11328 | .12700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H415 | 1.31525 | 1.06186 | .05177 | .10600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H416 | 1.19767 | .97410 | .13565 | .08200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1 | .86988 | 1.39733 | .30230 | .13500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2 | .95761 | 1.25374 | .30181 | .12000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H3 | .85418 | 1.07792 | .22152 | .12500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H4 | .67343 | 1.03376 | .13562 | .13700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H5 | .57909 | 1.16587 | .13127 | .15800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H6 | .67490 | 1.35318 | .21955 | .14100 | Uiso | ? | ? | 1.00000 | ? | ? |

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

| | | | | | | |
|-------|-----------|-----------|-----------|----------|----------|----------|
| Rh | .0415(4) | .0267(3) | .0343(3) | .0112(3) | .0020(3) | .0057(3) |
| Cu1 | .0527(6) | .0297(5) | .0434(6) | .0123(5) | .0106(5) | .0076(4) |
| Cu2 | .0440(6) | .0414(6) | .0379(5) | .0117(5) | .0030(4) | .0037(5) |
| P1 | .0383(11) | .0267(10) | .0321(10) | .0089(9) | .0044(8) | .0074(8) |
| C0111 | .047(5) | .026(4) | .028(4) | .012(3) | .003(3) | .006(3) |
| C0112 | .045(5) | .045(5) | .036(4) | .001(4) | .003(4) | .007(4) |
| C0113 | .064(6) | .051(6) | .043(5) | .005(5) | -.003(4) | .009(4) |
| C0114 | .048(5) | .034(5) | .058(5) | -.004(4) | -.001(4) | .010(4) |
| C0115 | .042(5) | .040(5) | .060(5) | .006(4) | .009(4) | .019(4) |
| C0116 | .039(5) | .027(4) | .041(4) | .005(3) | .002(3) | .006(3) |
| C0121 | .036(4) | .027(4) | .025(4) | .010(3) | .008(3) | .004(3) |
| C0122 | .044(5) | .034(4) | .035(4) | .008(4) | .006(3) | .007(3) |
| C0123 | .047(5) | .044(5) | .041(4) | .016(4) | .006(4) | .014(4) |
| C0124 | .055(5) | .043(5) | .054(5) | .021(4) | .005(4) | .014(4) |
| C0125 | .062(6) | .032(5) | .071(6) | .015(4) | .000(5) | .020(4) |
| C0126 | .047(5) | .034(4) | .051(5) | .010(4) | .002(4) | .016(4) |
| C0131 | .041(4) | .022(4) | .032(4) | .001(3) | .003(3) | .004(3) |
| C0132 | .040(5) | .034(4) | .040(4) | .005(4) | .008(3) | .010(4) |
| C0133 | .051(5) | .043(5) | .041(4) | .001(4) | .012(4) | .011(4) |
| C0134 | .057(5) | .043(5) | .042(5) | -.000(4) | -.002(4) | .018(4) |
| C0135 | .054(5) | .040(5) | .038(4) | .008(4) | -.003(4) | .014(4) |
| C0136 | .050(5) | .033(4) | .033(4) | .006(4) | -.001(3) | .006(3) |
| C11 | .052(5) | .021(4) | .025(4) | -.003(3) | .014(3) | -.000(3) |

| | | | | | | |
|------|----------|----------|----------|----------|----------|----------|
| C12 | .067(6) | .023(4) | .039(4) | .013(4) | .024(4) | .007(3) |
| C121 | .051(5) | .047(5) | .052(5) | .016(4) | .012(4) | .022(4) |
| C122 | .067(6) | .039(5) | .061(6) | .007(4) | -.005(5) | .011(4) |
| C123 | .063(6) | .056(6) | .077(7) | .003(5) | -.006(5) | .017(5) |
| C124 | .058(6) | .069(7) | .068(6) | .006(5) | -.001(5) | .033(5) |
| C125 | .058(6) | .079(7) | .074(6) | .030(5) | .014(5) | .036(6) |
| C126 | .067(6) | .068(6) | .053(5) | .025(5) | .010(5) | .024(5) |
| C21 | .046(5) | .044(5) | .038(4) | .026(4) | -.009(4) | -.008(4) |
| C22 | .064(6) | .050(5) | .023(4) | .010(4) | .001(4) | -.004(4) |
| C31 | .067(5) | .022(4) | .022(4) | .012(4) | .000(4) | -.005(3) |
| C32 | .048(5) | .033(4) | .051(5) | .009(4) | .013(4) | .003(4) |
| C321 | .056(5) | .042(5) | .052(5) | .017(4) | .010(4) | .017(4) |
| C322 | .068(7) | .101(8) | .083(7) | .043(6) | .031(5) | .050(6) |
| C323 | .085(8) | .106(9) | .082(7) | .043(7) | .012(6) | .048(7) |
| C324 | .055(6) | .124(10) | .096(8) | .039(6) | .021(6) | .049(7) |
| C325 | .049(6) | .148(11) | .084(7) | .019(6) | .017(5) | .067(8) |
| C326 | .058(6) | .093(8) | .067(6) | .015(6) | .013(5) | .042(6) |
| C41 | .060(5) | .026(4) | .022(4) | .020(4) | -.012(3) | -.002(3) |
| C42 | .043(5) | .051(5) | .032(4) | .012(4) | .001(4) | -.005(4) |
| C421 | .055(6) | .053(5) | .056(5) | .025(4) | .002(4) | .013(4) |
| C422 | .108(9) | .055(6) | .098(8) | .024(6) | .024(7) | .038(6) |
| C423 | .121(10) | .067(7) | .126(10) | .026(7) | .009(8) | .061(7) |
| C424 | .112(10) | .132(11) | .094(8) | .050(8) | .024(7) | .076(8) |
| C425 | .067(7) | .142(10) | .069(7) | .042(7) | .010(5) | .056(7) |
| C426 | .054(6) | .080(7) | .055(6) | .021(5) | .001(4) | .017(5) |
| C1 | .172(13) | .071(8) | .078(8) | .000(8) | .048(8) | .022(6) |
| C2 | .079(8) | .131(11) | .085(8) | .030(7) | .033(6) | .054(8) |
| C3 | .192(13) | .072(7) | .089(8) | .070(8) | .085(8) | .048(7) |
| C4 | .153(12) | .118(11) | .056(7) | -.064(9) | .029(7) | .012(7) |
| C5 | .089(10) | .34(2) | .111(11) | .092(12) | .045(8) | .132(14) |
| C6 | .254(17) | .140(12) | .113(10) | .148(12) | .117(11) | .090(9) |

5. Molecular Geometry

#-----

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_distance

_geom_bond_publ_flag

#<< enter YES for value to be published

| | | | | | |
|-------|-------|---|---------|------------|---|
| Rh | P1 | . | . | 2.2849(17) | ? |
| Rh | C11 | . | . | 2.038(8) | ? |
| Rh | C21 | . | . | 2.109(9) | ? |
| Rh | C31 | . | . | 2.044(8) | ? |
| Rh | C41 | . | . | 2.096(8) | ? |
| Cu1 | C11 | . | . | 1.950(6) | ? |
| Cu1 | C12 | . | . | 2.180(6) | ? |
| Cu1 | C31 | . | '2 776' | 2.012(6) | ? |
| Cu1 | C32 | . | '2 776' | 2.153(8) | ? |
| Cu2 | C21 | . | . | 1.981(7) | ? |
| Cu2 | C22 | . | . | 2.203(8) | ? |
| Cu2 | C41 | . | '2 776' | 1.988(6) | ? |
| Cu2 | C42 | . | '2 776' | 2.153(7) | ? |
| P1 | C0111 | . | . | 1.829(6) | ? |
| P1 | C0121 | . | . | 1.814(8) | ? |
| P1 | C0131 | . | . | 1.825(8) | ? |
| C0111 | C0112 | . | . | 1.392(9) | ? |
| C0111 | C0116 | . | . | 1.402(11) | ? |

| | | | | | |
|-------|-------|---|---|-----------|---|
| C0112 | C0113 | . | . | 1.383(10) | ? |
| C0112 | H0112 | . | . | .981 | ? |
| C0113 | C0114 | . | . | 1.381(12) | ? |
| C0113 | H0113 | . | . | .972 | ? |
| C0114 | C0115 | . | . | 1.380(10) | ? |
| C0114 | H0114 | . | . | .971 | ? |
| C0115 | C0116 | . | . | 1.375(9) | ? |
| C0115 | H0115 | . | . | .976 | ? |
| C0116 | H0116 | . | . | .974 | ? |
| C0121 | C0122 | . | . | 1.388(9) | ? |
| C0121 | C0126 | . | . | 1.374(10) | ? |
| C0122 | C0123 | . | . | 1.376(12) | ? |
| C0122 | H0122 | . | . | .976 | ? |
| C0123 | C0124 | . | . | 1.395(11) | ? |
| C0123 | H0123 | . | . | .971 | ? |
| C0124 | C0125 | . | . | 1.372(11) | ? |
| C0124 | H0124 | . | . | .972 | ? |
| C0125 | C0126 | . | . | 1.392(13) | ? |
| C0125 | H0125 | . | . | .971 | ? |
| C0126 | H0126 | . | . | .976 | ? |
| C0131 | C0132 | . | . | 1.393(10) | ? |
| C0131 | C0136 | . | . | 1.415(12) | ? |
| C0132 | C0133 | . | . | 1.390(13) | ? |
| C0132 | H0132 | . | . | .970 | ? |
| C0133 | C0134 | . | . | 1.376(14) | ? |
| C0133 | H0133 | . | . | .964 | ? |
| C0134 | C0135 | . | . | 1.389(11) | ? |
| C0134 | H0134 | . | . | .974 | ? |
| C0135 | C0136 | . | . | 1.378(12) | ? |
| C0135 | H0135 | . | . | .978 | ? |
| C0136 | H0136 | . | . | .972 | ? |
| C11 | C12 | . | . | 1.133(12) | ? |
| C12 | C121 | . | . | 1.488(12) | ? |
| C121 | C122 | . | . | 1.430(10) | ? |
| C121 | C126 | . | . | 1.376(13) | ? |
| C122 | C123 | . | . | 1.354(13) | ? |
| C122 | H112 | . | . | .975 | ? |
| C123 | C124 | . | . | 1.370(14) | ? |
| C123 | H113 | . | . | .971 | ? |
| C124 | C125 | . | . | 1.372(12) | ? |
| C124 | H114 | . | . | .979 | ? |
| C125 | C126 | . | . | 1.399(13) | ? |
| C125 | H115 | . | . | .962 | ? |
| C126 | H116 | . | . | .965 | ? |
| C21 | C22 | . | . | .913(13) | ? |
| C22 | C221 | . | . | 1.624(19) | ? |
| C22 | C221' | . | . | 1.58(3) | ? |
| C221 | C222 | . | . | 1.43(2) | ? |
| C221 | C226 | . | . | 1.38(3) | ? |
| C222 | C223 | . | . | 1.42(4) | ? |
| C222 | H222 | . | . | .99 | ? |
| C223 | C224 | . | . | 1.37(4) | ? |
| C223 | H223 | . | . | 1.018 | ? |
| C224 | C225 | . | . | 1.34(2) | ? |
| C224 | H224 | . | . | .99 | ? |
| C225 | C226 | . | . | 1.47(3) | ? |
| C225 | H225 | . | . | .95 | ? |
| C226 | H226 | . | . | .951 | ? |
| C221' | C222' | . | . | 1.43(3) | ? |
| C221' | C226' | . | . | 1.45(4) | ? |
| C222' | C223' | . | . | 1.47(5) | ? |

C222' H222' . . 1.01 ?
 C223' C224' . . 1.37(5) ?
 C223' H223' . . 1.025 ?
 C224' C225' . . 1.42(3) ?
 C224' H224' . . .98 ?
 C225' C226' . . 1.49(6) ?
 C225' H225' . . .96 ?
 C226' H226' . . .974 ?
 C31 C32 . . 1.154(12) ?
 C32 C321 . . 1.467(13) ?
 C321 C322 . . 1.388(16) ?
 C321 C326 . . 1.360(13) ?
 C322 C323 . . 1.401(16) ?
 C322 H312 . . .983 ?
 C323 C324 . . 1.368(16) ?
 C323 H313 . . .992 ?
 C324 C325 . . 1.33(2) ?
 C324 H314 . . .980 ?
 C325 C326 . . 1.371(15) ?
 C325 H315 . . .965 ?
 C326 H316 . . .978 ?
 C41 C42 . . 1.049(12) ?
 C42 C421 . . 1.502(13) ?
 C421 C422 . . 1.388(13) ?
 C421 C426 . . 1.399(12) ?
 C422 C423 . . 1.417(18) ?
 C422 H412 . . .976 ?
 C423 C424 . . 1.368(16) ?
 C423 H413 . . .966 ?
 C424 C425 . . 1.361(18) ?
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 C425 H415 . . .987 ?
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 C1 C2 . . 1.32(2) ?
 C1 C6 . . 1.33(2) ?
 C1 H1 . . .977 ?
 C2 C3 . . 1.297(14) ?
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 C3 C4 . . 1.323(19) ?
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 C11 Rh C21 . . . 92.6(3) ?

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| C21 | Rh | C31 | . | . | . | 87.4(3) | ? |
| C21 | Rh | C41 | . | . | . | 173.7(2) | ? |
| C21 | Rh | Cu1 | . | . | '2 776' | 86.57(18) | ? |
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| C31 | Rh | C41 | . | . | . | 88.8(3) | ? |
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| C12 | Cu1 | C31 | . | . | '2 776' | 150.2(3) | ? |
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| C31 | Cu1 | C32 | '2 776' | . | '2 776' | 31.9(3) | ? |
| C21 | Cu2 | C22 | . | . | . | 24.5(3) | ? |
| C21 | Cu2 | C41 | . | . | '2 776' | 172.7(3) | ? |
| C21 | Cu2 | C42 | . | . | '2 776' | 143.8(3) | ? |
| C22 | Cu2 | C41 | . | . | '2 776' | 148.5(3) | ? |
| C22 | Cu2 | C42 | . | . | '2 776' | 119.5(3) | ? |
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| Rh | C21 | C22 | . | . | . | 175.4(8) | ? |
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| C223 | C224 | C225 | . | . | . | 121(2) | ? |

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| C32 | C31 | Cu1 | . | . | '2 776' | 80.8(5) | ? |
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1. SUBMISSION DETAILS

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_publ_contact_author_address  
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  Department of Chemistry  
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Sheldrick, G M. (1996). SADABS. Pogram for Empirical Absorption Correction
of Area Detector Data. University of Gottingen, Germany.

Siemens (1995). SMART and SAINT. Area-Detector Control and Integration
Software. Siemens Analytical X-ray Systems Inc., Madison, Wisconsin, USA.

Hall, S.R., King, G.S.D., and Stewart., J.M. (1995).

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The Xtal 3.5 User's Manual. University of Western Australia, Lamb: Perth.
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# Data block for single structure (one for each study in the paper)
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# 2. EXPERIMENTAL DATA
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  +x,+y,+z  -x,-y,-z

_cell_length_a            11.020(2)
_cell_length_b            11.907(3)
_cell_length_c            15.920(4)
_cell_angle_alpha        100.906(3)
_cell_angle_beta         96.047(4)
_cell_angle_gamma        95.275(4)
_cell_volume              2026.4(8)
_cell_formula_units_Z    1

_exptl_crystal_density_diffn  1.786
_exptl_crystal_density_meas  ?
_exptl_crystal_density_method ?
_diffn_radiation_type      'Mo K\alpha'
_diffn_radiation_wavelength .71073

_cell_measurement_reflns_used  8192
_cell_measurement_theta_min    1.8
_cell_measurement_theta_max    24.4
_cell_measurement_temperature  153

_exptl_absorpt_coefficient_mu  4.33
_exptl_crystal_description    prism
_exptl_crystal_size_max       .18
_exptl_crystal_size_mid       .16
_exptl_crystal_size_min       .13
_exptl_crystal_size_rad       ?
_exptl_crystal_colour         dark

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_diffrn_measurement_device_type
;
Bruker SMART CCD diffractometer
;
_diffrn_measurement_method          '\w scans'
_diffrn_detector_area_resol_mean    ?

_exptl_absorpt_correction_type      multi-scan
_exptl_absorpt_process_details
;
SADABS; Sheldrick, 1996
;
_exptl_absorpt_correction_T_min     .438
_exptl_absorpt_correction_T_max     .914

_diffrn_reflns_number                23349
_reflns_number_total                 9837
_reflns_Friedel_coverage              0
_reflns_number_gt                    7592
_reflns_threshold_expression          'F      > 4.00 sig(F      )'

_diffrn_reflns_theta_max             29.16
_diffrn_reflns_theta_full            ?
_diffrn_measured_fraction_theta_max  ?
_diffrn_measured_fraction_theta_full ?
_diffrn_reflns_av_R_equivalents      .057
_diffrn_reflns_limit_h_min           -15
_diffrn_reflns_limit_h_max           14
_diffrn_reflns_limit_k_min           -15
_diffrn_reflns_limit_k_max           15
_diffrn_reflns_limit_l_min           0
_diffrn_reflns_limit_l_max           20
_diffrn_standards_number              ?
_diffrn_standards_interval_count      ?
_diffrn_standards_interval_time      ?
_diffrn_standards_decay_%            0

_refine_ls_structure_factor_coef      F
_refine_ls_R_factor_gt                .055
_refine_ls_wR_factor_ref               .06
_refine_ls_goodness_of_fit_ref        1.527
_refine_ls_number_reflns              7592
_refine_ls_number_parameters           501
_refine_ls_weighting_scheme            calc
_refine_ls_weighting_details           ?
_refine_ls_hydrogen_treatment         noref
_refine_ls_shift/su_max                .031
_refine_diff_density_min               -2.751
_refine_diff_density_max               4.212

_refine_ls_extinction_method           ?
_refine_ls_extinction_coef             ?
_refine_ls_abs_structure_details       ?
_refine_ls_abs_structure_Flack         ?

# 3. Information for the "methods" section
#-----

_computing_data_collection             'Siemens SMART (Siemens, 1995)'

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_computing_cell_refinement      'Siemens SAINT (Siemens, 1995)'
_computing_data_reduction      'xtal ADDREF SORTRF'
_computing_structure_solution  'xtal'
_computing_structure_refinement 'xtal CRYLSQ'
_computing_molecular_graphics  'xtal'
_computing_publication_material 'xtal BONDLA CIFIO'

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4. Supplementary data for validation and tables

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loop_
_atom_type_symbol
_atom_type_description
_atom_type_oxidation_number
_atom_type_number_in_cell
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
C ? 0 100.36 .002 .002 'Int Tables Vol IV Tables 2.2B and 2.3.1'
H ? 0 70.72 0 0 'Int Tables Vol IV Tables 2.2B and 2.3.1'
Cl ? 0 .72 .132 .159 'Int Tables Vol IV Tables 2.2B and 2.3.1'
Ag ? 0 4 -1.085 1.101 'Int Tables Vol IV Tables 2.2B and 2.3.1'
P ? 0 2 .09 .095 'Int Tables Vol IV Tables 2.2B and 2.3.1'
Ir ? 0 2 -2.066 7.99 'Int Tables Vol IV Tables 2.2B and 2.3.1'

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loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_calc_flag
_atom_site_calc_attached_atom
_atom_site_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
Ir -.01428(3) -.00442(3) .14417(2) .02339(14) Uani ? ? 1.00000 ? ?
Ag1 -.07530(6) -.15718(5) -.03500(4) .0279(3) Uani ? ? 1.00000 ? ?
Ag2 .17608(6) -.05950(5) .00705(4) .0280(3) Uani ? ? 1.00000 ? ?
P -.0063(2) -.00982(18) .28614(13) .0248(9) Uani ? ? 1.00000 ? ?
C011 -.0964(8) .0934(7) .3440(5) .027(3) Uani ? ? 1.00000 ? ?
C012 -.2213(8) .0810(8) .3183(6) .036(4) Uani ? ? 1.00000 ? ?
C013 -.2950(8) .1623(8) .3589(5) .037(4) Uani ? ? 1.00000 ? ?
C014 -.2394(10) .2533(9) .4250(6) .044(5) Uani ? ? 1.00000 ? ?
C015 -.1159(10) .2646(8) .4497(6) .044(5) Uani ? ? 1.00000 ? ?
C016 -.0421(8) .1838(8) .4101(5) .034(4) Uani ? ? 1.00000 ? ?
C021 .1482(7) .0230(7) .3471(5) .026(3) Uani ? ? 1.00000 ? ?
C022 .2328(8) .1058(8) .3281(5) .032(4) Uani ? ? 1.00000 ? ?
C023 .3486(8) .1357(8) .3774(6) .037(4) Uani ? ? 1.00000 ? ?
C024 .3800(8) .0823(9) .4449(6) .041(4) Uani ? ? 1.00000 ? ?
C025 .2973(8) -.0019(10) .4630(6) .042(5) Uani ? ? 1.00000 ? ?
C026 .1807(8) -.0317(9) .4157(5) .036(4) Uani ? ? 1.00000 ? ?
C031 -.0616(7) -.1469(7) .3132(5) .029(4) Uani ? ? 1.00000 ? ?
C032 -.0171(9) -.2484(8) .2724(5) .037(4) Uani ? ? 1.00000 ? ?
C033 -.0567(10) -.3522(8) .2935(6) .041(4) Uani ? ? 1.00000 ? ?
C034 -.1369(9) -.3576(8) .3546(6) .040(4) Uani ? ? 1.00000 ? ?
C035 -.1789(8) -.2582(8) .3951(5) .037(4) Uani ? ? 1.00000 ? ?
C036 -.1409(8) -.1532(8) .3749(5) .033(4) Uani ? ? 1.00000 ? ?
C11 -.0928(7) -.1681(7) .1018(5) .026(3) Uani ? ? 1.00000 ? ?

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| | | | | | | | | | | |
|------|------------|-----------|-----------|----------|------|---|---|----------|---|---|
| C12 | -.1420(7) | -.2685(7) | .0703(5) | .028(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C121 | -.1841(7) | -.3893(7) | .0504(5) | .027(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C122 | -.3042(8) | -.4328(7) | .0093(6) | .033(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C123 | -.3391(8) | -.5503(8) | -.0127(6) | .038(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C124 | -.2581(9) | -.6249(8) | .0073(6) | .041(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C125 | -.1417(9) | -.5841(8) | .0489(6) | .040(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C126 | -.1048(8) | -.4672(7) | .0698(5) | .032(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C21 | .1570(7) | -.0587(6) | .1453(5) | .024(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C22 | .2596(9) | -.0891(7) | .1444(5) | .031(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C221 | .3766(7) | -.1248(6) | .1661(5) | .025(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C222 | .4111(8) | -.1463(8) | .2494(5) | .035(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C223 | .5231(9) | -.1862(9) | .2692(6) | .043(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C224 | .6058(8) | -.2037(8) | .2088(7) | .043(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C225 | .5757(8) | -.1794(8) | .1277(6) | .040(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C226 | .4634(8) | -.1414(7) | .1065(5) | .033(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C31 | .0586(7) | .1634(7) | .1727(5) | .026(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C32 | .0964(7) | .2681(7) | .1880(5) | .025(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C321 | .1454(8) | .3824(7) | .2309(5) | .031(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C322 | .1664(10) | .4089(8) | .3210(6) | .044(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C323 | .2191(12) | .5170(9) | .3641(6) | .058(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C324 | .2540(10) | .5993(8) | .3183(7) | .049(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C325 | .2336(9) | .5765(8) | .2289(6) | .039(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C326 | .1795(8) | .4680(7) | .1852(5) | .032(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C41 | -.1766(7) | .0595(7) | .1320(5) | .026(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C42 | -.2677(8) | .1169(7) | .1276(5) | .030(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C421 | -.3567(8) | .1956(8) | .1488(5) | .033(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C422 | -.3152(9) | .3075(9) | .1935(6) | .043(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C423 | -.3978(10) | .3842(9) | .2175(7) | .050(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C424 | -.5219(10) | .3531(11) | .1999(7) | .056(6) | Uani | ? | ? | 1.00000 | ? | ? |
| C425 | -.5660(9) | .2418(10) | .1560(7) | .048(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C426 | -.4848(8) | .1634(8) | .1296(6) | .041(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C1 | -.4521(12) | .5942(13) | .4651(11) | .143(11) | Uani | ? | ? | .374(14) | ? | ? |
| C0 | -.504(5) | .459(5) | .430(4) | .053(14) | Uiso | ? | ? | .187(7) | ? | ? |
| H012 | -.25881 | .01753 | .27362 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H013 | -.38180 | .15487 | .34076 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H014 | -.28846 | .30787 | .45284 | .05300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H015 | -.07926 | .32852 | .49385 | .05400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H016 | .04415 | .19090 | .42846 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H022 | .21078 | .14286 | .28134 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H023 | .40660 | .19287 | .36345 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H024 | .45856 | .10381 | .47947 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H025 | .31945 | -.04045 | .50943 | .05300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H026 | .12408 | -.08896 | .42999 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H032 | .03994 | -.24475 | .23100 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H033 | -.02858 | -.42221 | .26460 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H034 | -.16366 | -.43082 | .36788 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H035 | -.23468 | -.26174 | .43811 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H036 | -.16986 | -.08351 | .40351 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H122 | -.36094 | -.38022 | -.00386 | .04000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H123 | -.42025 | -.57866 | -.04121 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H124 | -.28408 | -.70672 | -.00772 | .04900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H125 | -.08580 | -.63755 | .06305 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H126 | -.02268 | -.43911 | .09749 | .04000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H222 | .35567 | -.13335 | .29261 | .04500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H223 | .54408 | -.20124 | .32605 | .05300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H224 | .68227 | -.23278 | .22315 | .05500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H225 | .63372 | -.18875 | .08584 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H226 | .44348 | -.12488 | .05016 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H322 | .14312 | .35127 | .35363 | .05300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H323 | .23120 | .53573 | .42571 | .06800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H324 | .29504 | .67294 | .34905 | .06100 | Uiso | ? | ? | 1.00000 | ? | ? |

| | | | | | | | | | | |
|------|---------|--------|--------|--------|------|---|---|---------|---|---|
| H325 | .25687 | .63529 | .19776 | .04900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H326 | .16463 | .45147 | .12329 | .04000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H422 | -.22791 | .33039 | .20691 | .05300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H423 | -.36722 | .46180 | .24843 | .06100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H424 | -.57914 | .40747 | .21682 | .06900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H425 | -.65342 | .21890 | .14383 | .06000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H426 | -.51583 | .08661 | .09816 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0a | -.57392 | .44832 | .38429 | .13000 | Uiso | ? | ? | .187(7) | ? | ? |
| H0b | -.44219 | .41493 | .40194 | .13000 | Uiso | ? | ? | .187(7) | ? | ? |

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

| | | | | | | | | | | |
|------|------------|------------|------------|-------------|------------|------------|--|--|--|--|
| Ir | .02729(17) | .02250(16) | .01855(15) | -.00040(12) | .00249(11) | .00132(11) | | | | |
| Ag1 | .0314(3) | .0324(4) | .0199(3) | .0031(3) | .0039(2) | .0048(3) | | | | |
| Ag2 | .0356(4) | .0273(3) | .0193(3) | -.0011(3) | .0028(2) | .0026(2) | | | | |
| P | .0277(11) | .0238(10) | .0212(10) | .0005(8) | .0030(8) | .0016(8) | | | | |
| C011 | .035(4) | .027(4) | .018(4) | .001(3) | .007(3) | .000(3) | | | | |
| C012 | .026(4) | .038(5) | .045(5) | -.006(4) | -.011(4) | .026(4) | | | | |
| C013 | .039(5) | .047(6) | .026(4) | .012(4) | .008(4) | .004(4) | | | | |
| C014 | .052(6) | .046(6) | .036(5) | .022(5) | .018(4) | .001(4) | | | | |
| C015 | .061(7) | .032(5) | .039(5) | .006(5) | .011(5) | -.000(4) | | | | |
| C016 | .038(5) | .034(5) | .024(4) | .002(4) | .002(3) | -.003(4) | | | | |
| C021 | .027(4) | .030(4) | .018(4) | .003(3) | .003(3) | -.005(3) | | | | |
| C022 | .038(5) | .034(5) | .022(4) | .007(4) | -.000(3) | .003(4) | | | | |
| C023 | .030(5) | .038(5) | .041(5) | -.001(4) | .001(4) | .006(4) | | | | |
| C024 | .030(5) | .054(6) | .035(5) | .004(4) | -.002(4) | .002(4) | | | | |
| C025 | .027(5) | .072(7) | .027(4) | .008(5) | -.000(3) | .011(5) | | | | |
| C026 | .031(5) | .053(6) | .025(4) | .012(4) | .005(3) | .009(4) | | | | |
| C031 | .032(4) | .031(4) | .019(4) | -.003(4) | -.002(3) | .003(3) | | | | |
| C032 | .052(6) | .032(5) | .027(4) | .004(4) | .006(4) | .005(4) | | | | |
| C033 | .064(6) | .029(5) | .029(5) | .007(4) | .004(4) | .005(4) | | | | |
| C034 | .051(6) | .033(5) | .036(5) | -.006(4) | -.004(4) | .013(4) | | | | |
| C035 | .042(5) | .038(5) | .028(4) | -.010(4) | .006(4) | .007(4) | | | | |
| C036 | .038(5) | .031(5) | .027(4) | -.004(4) | .004(4) | .000(4) | | | | |
| C11 | .028(4) | .025(4) | .023(4) | -.001(3) | .005(3) | .004(3) | | | | |
| C12 | .026(4) | .034(5) | .023(4) | .005(3) | .005(3) | .006(3) | | | | |
| C121 | .030(4) | .026(4) | .025(4) | -.001(3) | .008(3) | .003(3) | | | | |
| C122 | .034(5) | .030(5) | .034(5) | -.002(4) | .004(4) | .004(4) | | | | |
| C123 | .034(5) | .040(5) | .033(5) | -.009(4) | .001(4) | .001(4) | | | | |
| C124 | .046(6) | .027(5) | .046(5) | -.005(4) | .009(4) | .004(4) | | | | |
| C125 | .047(6) | .028(5) | .045(5) | .005(4) | .001(4) | .007(4) | | | | |
| C126 | .029(4) | .030(4) | .033(4) | .001(4) | .001(3) | -.000(4) | | | | |
| C21 | .030(4) | .017(4) | .021(4) | -.003(3) | .001(3) | -.001(3) | | | | |
| C22 | .047(5) | .025(4) | .018(4) | -.003(4) | .004(3) | -.001(3) | | | | |
| C221 | .032(4) | .014(4) | .026(4) | -.001(3) | .003(3) | -.003(3) | | | | |
| C222 | .039(5) | .037(5) | .028(4) | -.001(4) | .000(4) | .005(4) | | | | |
| C223 | .045(6) | .043(6) | .038(5) | .003(4) | -.003(4) | .005(4) | | | | |
| C224 | .031(5) | .036(5) | .056(6) | .005(4) | -.006(4) | -.002(5) | | | | |
| C225 | .029(5) | .041(5) | .043(5) | -.002(4) | .006(4) | -.007(4) | | | | |
| C226 | .035(5) | .030(5) | .029(4) | -.004(4) | .004(3) | -.000(4) | | | | |
| C31 | .028(4) | .030(4) | .019(4) | .001(3) | .005(3) | .002(3) | | | | |
| C32 | .030(4) | .024(4) | .022(4) | .008(3) | .004(3) | .003(3) | | | | |
| C321 | .032(4) | .027(4) | .029(4) | -.000(3) | -.002(3) | -.001(3) | | | | |
| C322 | .073(7) | .023(4) | .030(5) | -.001(4) | .003(4) | -.000(4) | | | | |
| C323 | .098(9) | .040(6) | .026(5) | -.005(6) | -.006(5) | -.002(4) | | | | |

| | | | | | | |
|------|----------|----------|----------|----------|----------|----------|
| C324 | .064(7) | .025(5) | .048(6) | -.005(5) | -.006(5) | -.008(4) |
| C325 | .046(6) | .029(5) | .040(5) | -.003(4) | .006(4) | .002(4) |
| C326 | .039(5) | .026(4) | .030(4) | -.001(4) | .006(4) | .001(4) |
| C41 | .024(4) | .028(4) | .025(4) | -.006(3) | .003(3) | .004(3) |
| C42 | .037(5) | .029(4) | .024(4) | .004(4) | .004(3) | .005(3) |
| C421 | .038(5) | .035(5) | .027(4) | .011(4) | .008(3) | .009(4) |
| C422 | .039(5) | .048(6) | .038(5) | .004(5) | .006(4) | .003(4) |
| C423 | .056(7) | .039(6) | .050(6) | .014(5) | .005(5) | -.008(5) |
| C424 | .048(6) | .068(8) | .056(7) | .030(6) | .012(5) | .007(6) |
| C425 | .034(5) | .063(7) | .052(6) | .015(5) | .013(4) | .013(5) |
| C426 | .030(5) | .043(6) | .051(6) | .004(4) | .005(4) | .013(5) |
| C1 | .096(10) | .138(13) | .190(17) | -.053(9) | -.009(9) | .066(12) |

5. Molecular Geometry

#-----

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_distance

_geom_bond_publ_flag

#<< enter YES for value to be published

| | | | | | |
|------|------|---|---|-----------|---|
| Ir | P | . | . | 2.266(2) | ? |
| Ir | C11 | . | . | 2.018(7) | ? |
| Ir | C21 | . | . | 2.050(8) | ? |
| Ir | C31 | . | . | 2.032(8) | ? |
| Ir | C41 | . | . | 2.013(8) | ? |
| Ir | Ag1 | . | 2 | 2.9958(9) | ? |
| Ir | Ag2 | . | 2 | 3.0972(9) | ? |
| Ag1 | C11 | . | . | 2.234(8) | ? |
| Ag1 | C31 | . | 2 | 2.207(8) | ? |
| Ag2 | C21 | . | . | 2.232(8) | ? |
| Ag2 | C22 | . | . | 2.383(8) | ? |
| Ag2 | C41 | . | 2 | 2.214(8) | ? |
| P | C011 | . | . | 1.826(8) | ? |
| P | C021 | . | . | 1.839(8) | ? |
| P | C031 | . | . | 1.833(9) | ? |
| C011 | C012 | . | . | 1.380(11) | ? |
| C011 | C016 | . | . | 1.395(10) | ? |
| C012 | C013 | . | . | 1.425(13) | ? |
| C012 | H012 | . | . | .962 | ? |
| C013 | C014 | . | . | 1.403(12) | ? |
| C013 | H013 | . | . | .961 | ? |
| C014 | C015 | . | . | 1.363(15) | ? |
| C014 | H014 | . | . | .958 | ? |
| C015 | C016 | . | . | 1.417(14) | ? |
| C015 | H015 | . | . | .958 | ? |
| C016 | H016 | . | . | .956 | ? |
| C021 | C022 | . | . | 1.392(12) | ? |
| C021 | C026 | . | . | 1.405(13) | ? |
| C022 | C023 | . | . | 1.404(12) | ? |
| C022 | H022 | . | . | .956 | ? |
| C023 | C024 | . | . | 1.377(15) | ? |
| C023 | H023 | . | . | .964 | ? |
| C024 | C025 | . | . | 1.384(14) | ? |
| C024 | H024 | . | . | .961 | ? |
| C025 | C026 | . | . | 1.398(12) | ? |
| C025 | H025 | . | . | .963 | ? |
| C026 | H026 | . | . | .957 | ? |

| | | | | | |
|------|------|---|---|-----------|---|
| C031 | C032 | . | . | 1.414(12) | ? |
| C031 | C036 | . | . | 1.390(12) | ? |
| C032 | C033 | . | . | 1.386(14) | ? |
| C032 | H032 | . | . | .962 | ? |
| C033 | C034 | . | . | 1.386(15) | ? |
| C033 | H033 | . | . | .967 | ? |
| C034 | C035 | . | . | 1.381(13) | ? |
| C034 | H034 | . | . | .963 | ? |
| C035 | C036 | . | . | 1.387(13) | ? |
| C035 | H035 | . | . | .971 | ? |
| C036 | H036 | . | . | .966 | ? |
| C11 | C12 | . | . | 1.253(11) | ? |
| C12 | C121 | . | . | 1.434(11) | ? |
| C121 | C122 | . | . | 1.418(11) | ? |
| C121 | C126 | . | . | 1.386(13) | ? |
| C122 | C123 | . | . | 1.384(13) | ? |
| C122 | H122 | . | . | .959 | ? |
| C123 | C124 | . | . | 1.371(14) | ? |
| C123 | H123 | . | . | .960 | ? |
| C124 | C125 | . | . | 1.380(13) | ? |
| C124 | H124 | . | . | .967 | ? |
| C125 | C126 | . | . | 1.380(12) | ? |
| C125 | H125 | . | . | .966 | ? |
| C126 | H126 | . | . | .964 | ? |
| C21 | C22 | . | . | 1.220(13) | ? |
| C22 | C221 | . | . | 1.423(12) | ? |
| C221 | C222 | . | . | 1.417(12) | ? |
| C221 | C226 | . | . | 1.418(12) | ? |
| C222 | C223 | . | . | 1.390(14) | ? |
| C222 | H222 | . | . | .967 | ? |
| C223 | C224 | . | . | 1.394(15) | ? |
| C223 | H223 | . | . | .964 | ? |
| C224 | C225 | . | . | 1.389(15) | ? |
| C224 | H224 | . | . | .962 | ? |
| C225 | C226 | . | . | 1.386(13) | ? |
| C225 | H225 | . | . | .969 | ? |
| C226 | H226 | . | . | .962 | ? |
| C31 | C32 | . | . | 1.248(11) | ? |
| C32 | C321 | . | . | 1.431(11) | ? |
| C321 | C322 | . | . | 1.398(12) | ? |
| C321 | C326 | . | . | 1.406(13) | ? |
| C322 | C323 | . | . | 1.382(13) | ? |
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| C323 | C324 | . | . | 1.378(16) | ? |
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| C325 | C326 | . | . | 1.393(11) | ? |
| C325 | H325 | . | . | .963 | ? |
| C326 | H326 | . | . | .961 | ? |
| C41 | C42 | . | . | 1.268(12) | ? |
| C42 | C421 | . | . | 1.439(13) | ? |
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| C423 | H423 | . | . | .972 | ? |
| C424 | C425 | . | . | 1.393(15) | ? |
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| C425 | C426 | . | . | 1.390(15) | ? |

C425 H425 . . .966 ?
C426 H426 . . .968 ?
C1 C0 . . 1.63(6) ?
C1 C0 . '2 466' 1.99(7) ?
C0 H0a . . .98 ?
C0 H0b . . .99 ?

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_geom_angle_site_symmetry_2

_geom_angle_site_symmetry_3

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_geom_angle_publ_flag

#<< enter YES for value to be published

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P Ir C21 . . . 88.9(2) ?
P Ir C31 . . . 91.1(2) ?
P Ir C41 . . . 97.1(2) ?
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C11 Ag1 C31 . . 2 174.9(3) ?
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C22 Ag2 C41 . . 2 154.6(3) ?
Ir P C011 . . . 112.9(3) ?
Ir P C021 . . . 114.9(3) ?
Ir P C031 . . . 116.9(2) ?
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C011 P C031 . . . 103.8(4) ?
C021 P C031 . . . 102.5(4) ?
P C011 C012 . . . 117.5(6) ?
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C022 C023 C024 . . . 120.1(9) ?

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| C025 | C024 | H024 | . | . | . | 120.2 | ? |
| C024 | C025 | C026 | . | . | . | 121.3(10) | ? |
| C024 | C025 | H025 | . | . | . | 119.9 | ? |
| C026 | C025 | H025 | . | . | . | 118.9 | ? |
| C021 | C026 | C025 | . | . | . | 119.3(9) | ? |
| C021 | C026 | H026 | . | . | . | 120.6 | ? |
| C025 | C026 | H026 | . | . | . | 120.1 | ? |
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| P | C031 | C036 | . | . | . | 122.1(6) | ? |
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| C034 | C035 | C036 | . | . | . | 120.1(9) | ? |
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| C031 | C036 | C035 | . | . | . | 120.6(8) | ? |
| C031 | C036 | H036 | . | . | . | 119.2 | ? |
| C035 | C036 | H036 | . | . | . | 120.2 | ? |
| Ir | C11 | Ag1 | . | . | . | 91.5(3) | ? |
| Ir | C11 | C12 | . | . | . | 176.0(7) | ? |
| Ag1 | C11 | C12 | . | . | . | 84.5(5) | ? |
| C11 | C12 | C121 | . | . | . | 167.6(9) | ? |
| C12 | C121 | C122 | . | . | . | 122.2(8) | ? |
| C12 | C121 | C126 | . | . | . | 119.5(7) | ? |
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| C122 | C123 | C124 | . | . | . | 119.8(8) | ? |
| C122 | C123 | H123 | . | . | . | 119.6 | ? |
| C124 | C123 | H123 | . | . | . | 120.7 | ? |
| C123 | C124 | C125 | . | . | . | 120.7(8) | ? |
| C123 | C124 | H124 | . | . | . | 118.9 | ? |
| C125 | C124 | H124 | . | . | . | 120.3 | ? |
| C124 | C125 | C126 | . | . | . | 120.2(9) | ? |
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| C126 | C125 | H125 | . | . | . | 120.0 | ? |
| C121 | C126 | C125 | . | . | . | 120.7(8) | ? |
| C121 | C126 | H126 | . | . | . | 119.3 | ? |
| C125 | C126 | H126 | . | . | . | 120.0 | ? |
| Ir | C21 | Ag2 | . | . | . | 96.8(3) | ? |
| Ir | C21 | C22 | . | . | . | 178.2(8) | ? |
| Ag2 | C21 | C22 | . | . | . | 81.7(6) | ? |
| Ag2 | C22 | C21 | . | . | . | 67.9(5) | ? |
| Ag2 | C22 | C221 | . | . | . | 127.0(6) | ? |
| C21 | C22 | C221 | . | . | . | 165.1(9) | ? |
| C22 | C221 | C222 | . | . | . | 120.8(8) | ? |
| C22 | C221 | C226 | . | . | . | 122.4(8) | ? |
| C222 | C221 | C226 | . | . | . | 116.8(8) | ? |
| C221 | C222 | C223 | . | . | . | 120.7(8) | ? |

| | | | | | | | |
|------|------|------|---|---|---------|-----------|---|
| C221 | C222 | H222 | . | . | . | 119.4 | ? |
| C223 | C222 | H222 | . | . | . | 119.9 | ? |
| C222 | C223 | C224 | . | . | . | 121.2(9) | ? |
| C222 | C223 | H223 | . | . | . | 119.2 | ? |
| C224 | C223 | H223 | . | . | . | 119.6 | ? |
| C223 | C224 | C225 | . | . | . | 119.1(9) | ? |
| C223 | C224 | H224 | . | . | . | 120.2 | ? |
| C225 | C224 | H224 | . | . | . | 120.7 | ? |
| C224 | C225 | C226 | . | . | . | 120.3(9) | ? |
| C224 | C225 | H225 | . | . | . | 119.8 | ? |
| C226 | C225 | H225 | . | . | . | 119.9 | ? |
| C221 | C226 | C225 | . | . | . | 121.9(8) | ? |
| C221 | C226 | H226 | . | . | . | 118.5 | ? |
| C225 | C226 | H226 | . | . | . | 119.6 | ? |
| Ir | C31 | C32 | . | . | . | 176.0(7) | ? |
| Ir | C31 | Ag1 | . | . | 2 | 89.9(3) | ? |
| C32 | C31 | Ag1 | . | . | 2 | 89.0(6) | ? |
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| C321 | C326 | C325 | . | . | . | 120.5(8) | ? |
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| Ir | C41 | Ag2 | . | . | 2 | 94.1(3) | ? |
| C42 | C41 | Ag2 | . | . | 2 | 85.9(6) | ? |
| C41 | C42 | C421 | . | . | . | 163.1(8) | ? |
| C42 | C421 | C422 | . | . | . | 118.7(8) | ? |
| C42 | C421 | C426 | . | . | . | 123.0(8) | ? |
| C422 | C421 | C426 | . | . | . | 118.2(9) | ? |
| C421 | C422 | C423 | . | . | . | 120.5(9) | ? |
| C421 | C422 | H422 | . | . | . | 118.9 | ? |
| C423 | C422 | H422 | . | . | . | 120.6 | ? |
| C422 | C423 | C424 | . | . | . | 121.5(9) | ? |
| C422 | C423 | H423 | . | . | . | 119.3 | ? |
| C424 | C423 | H423 | . | . | . | 119.1 | ? |
| C423 | C424 | C425 | . | . | . | 119.3(11) | ? |
| C423 | C424 | H424 | . | . | . | 121.0 | ? |
| C425 | C424 | H424 | . | . | . | 119.7 | ? |
| C424 | C425 | C426 | . | . | . | 120.4(9) | ? |
| C424 | C425 | H425 | . | . | . | 119.8 | ? |
| C426 | C425 | H425 | . | . | . | 119.8 | ? |
| C421 | C426 | C425 | . | . | . | 120.1(8) | ? |
| C421 | C426 | H426 | . | . | . | 119.8 | ? |
| C425 | C426 | H426 | . | . | . | 120.1 | ? |
| C0 | C1 | C0 | . | . | '2 466' | 76(3) | ? |
| C1 | C0 | H0a | . | . | . | 113 | ? |
| C1 | C0 | H0b | . | . | . | 112 | ? |

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C1 C0 C1 . . '2 466' 104(3) ?
H0a C0 H0b . . . 104 ?
H0a C0 C1 . . '2 466' 113 ?
H0b C0 C1 . . '2 466' 112 ?
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_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion
_geom_torsion_publ_flag #<< enter YES for value to be published
  ? ? ? ? ? ? ? ? ? ?
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_geom_hbond_atom_site_label_A
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_geom_hbond_site_symmetry_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_publ_flag #<< enter YES for value to be published
  ? ? ? ? ? ? ? ? ? ?
```

```
#-----
# Special items requested by author for inclusion in paper
#-----
```

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_publ_manuscript_incl_extra_item
_publ_manuscript_incl_extra_defn
  ? ?
```

```
#-----
# Items which are non-mandatory for Acta C submissions
#-----
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_atom_sites_solution_secondary ?
_atom_sites_solution_hydrogens ?

_geom_special_details ?
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_cell_special_details
; ?
;
```

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_exptl_special_details
; ?
;
```



```
#####  
#  
#   CIF generated by the Xtal System   #  
#  
#####
```

data_global

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_audit_creation_date        01-12-07  
_audit_update_record        ?
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#####  
# (Publishing Staff Use Only)
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_journal_coeditor_notes        ?  
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_journal_page_last             ?  
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1. SUBMISSION DETAILS

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_publ_contact_author_address  
;  
  Department of Chemistry  
  University of Western Australia  
  35 Stirling Highway  
  Crawley  
  Western Australia 6009  
  Australia  
;  
_publ_contact_author_email      bws@crystal.uwa.edu.au  
_publ_contact_author_fax        (+61)_08_9380_1118  
_publ_contact_author_phone      (+61)_08-9380_3481
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;

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_publ_requested_category ?

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;   ?                               #<< paper title text
;
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;   ?                               #<< paper footnote text
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_publ_author_footnote
_publ_author_address

'Skelton, Brian W.' .
; Department of Chemistry,
University of Western Australia,
35 Stirling Highway,
Crawley,
WA 6009,
Australia.
;

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;   ?                               #<< synopsis if FI,CI,CM,CO papers
;
_publ_section_abstract
;   ?                               #<< abstract text
;
_publ_section_comment
;   ?                               #<< scientific commentary text
;

_publ_section_exptl_prep
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;

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;   ?                               #<< crystallographic methods used
;

_publ_section_acknowledgements
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_publ_section_references
;
Sheldrick, G M. (1996). SADABS. Program for Empirical Absorption Correction
of Area Detector Data. University of Gottingen, Germany.

Siemens (1995). SMART and SAINT. Area-Detector Control and Integration

```

Software. Siemens Analytical X-ray Systems Inc., Madison, Wisconsin, USA.

Hall, S.R., King, G.S.D., and Stewart., J.M. (1995).
The Xtal 3.5 User's Manual. University of Western Australia, Lamb: Perth.

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#####  
  
data_br7071  
  
# 2. EXPERIMENTAL DATA  
#-----  
  
_chemical_formula_sum      'C166 H139 Cu4 Fe8 Ir2 O1 P2'  
_chemical_formula_moiety   ?  
_chemical_formula_weight   3297.29  
_chemical_melting_point    ?  
  
_symmetry_cell_setting     triclinic  
_symmetry_space_group_name_H-M  P_-1  
_symmetry_space_group_name_Hall -p_1  
  
loop_  
_symmetry_equiv_pos_as_xyz  
  +x,+y,+z  -x,-y,-z  
  
_cell_length_a             15.6675(8)  
_cell_length_b             16.4128(8)  
_cell_length_c             26.8380(10)  
_cell_angle_alpha          106.5290(10)  
_cell_angle_beta           92.0770(10)  
_cell_angle_gamma          92.9840(10)  
_cell_volume                6597.8(5)  
_cell_formula_units_Z      2  
  
_exptl_crystal_density_diffn  1.66  
_exptl_crystal_density_meas  ?  
_exptl_crystal_density_method ?  
_diffrn_radiation_type      'Mo K\a'  
_diffrn_radiation_wavelength .71073  
  
_cell_measurement_reflns_used  8192  
_cell_measurement_theta_min    1.6  
_cell_measurement_theta_max    20.4  
_cell_measurement_temperature  150  
  
_exptl_absorpt_coefficient_mu  3.568  
_exptl_crystal_description     bar  
_exptl_crystal_size_max        .35  
_exptl_crystal_size_mid        .15  
_exptl_crystal_size_min        .13
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_exptl_crystal_size_rad          ?
_exptl_crystal_colour           dark_red

_diffrn_measurement_device_type
;
Bruker SMART CCD diffractometer
;
_diffrn_measurement_method       '\w scans'
_diffrn_detector_area_resol_mean ?

_exptl_absorpt_correction_type   multi-scan
_exptl_absorpt_process_details
;
SADABS; Sheldrick, 1996
;
_exptl_absorpt_correction_T_min  .53
_exptl_absorpt_correction_T_max  .75

_diffrn_reflns_number            100092
_reflns_number_total             50442
_reflns_Friedel_coverage         0
_reflns_number_gt                35834
_reflns_threshold_expression      'F > 4.00 sig(F )'

_diffrn_reflns_theta_max         34.17
_diffrn_reflns_theta_full        ?
_diffrn_measured_fraction_theta_max ?
_diffrn_measured_fraction_theta_full ?
_diffrn_reflns_av_R_equivalents  .034
_diffrn_reflns_limit_h_min       -24
_diffrn_reflns_limit_h_max       24
_diffrn_reflns_limit_k_min       -25
_diffrn_reflns_limit_k_max       24
_diffrn_reflns_limit_l_min       0
_diffrn_reflns_limit_l_max       42
_diffrn_standards_number         ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        0

_refine_ls_structure_factor_coef  F
_refine_ls_R_factor_gt           .035
_refine_ls_wR_factor_ref         .038
_refine_ls_goodness_of_fit_ref   1.05
_refine_ls_number_reflns        35834
_refine_ls_number_parameters     1604
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details     ?
_refine_ls_hydrogen_treatment    noref
_refine_ls_shift/su_max          .045
_refine_diff_density_min         -1.942
_refine_diff_density_max         2.821

_refine_ls_extinction_method     ?
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details  ?
_refine_ls_abs_structure_Flack   ?

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3. Information for the "methods" section

#-----

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_computing_data_collection      'Siemens SMART (Siemens, 1995)'  
_computing_cell_refinement      'Siemens SAINT (Siemens, 1995)'  
_computing_data_reduction       xtal  
_computing_structure_solution   xtal  
_computing_structure_refinement 'xtal CRYLSQ'  
_computing_molecular_graphics   xtal  
_computing_publication_material 'xtal BONDLA CIFIO'
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4. Supplementary data for validation and tables

#-----

loop_

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_atom_type_symbol  
_atom_type_description  
_atom_type_oxidation_number  
_atom_type_number_in_cell  
_atom_type_scatter_dispersion_real  
_atom_type_scatter_dispersion_imag  
_atom_type_scatter_source  
C ? 0 332 .002 .002 'Int Tables Vol IV Tables 2.2B and 2.3.1'  
H ? 0 278 0 0 'Int Tables Vol IV Tables 2.2B and 2.3.1'  
Cu ? 0 8 .263 1.266 'Int Tables Vol IV Tables 2.2B and 2.3.1'  
Fe ? 0 16 .301 .845 'Int Tables Vol IV Tables 2.2B and 2.3.1'  
Ir ? 0 4 -2.066 7.99 'Int Tables Vol IV Tables 2.2B and 2.3.1'  
O ? 0 2 .008 .006 'Int Tables Vol IV Tables 2.2B and 2.3.1'  
P ? 0 4 .09 .095 'Int Tables Vol IV Tables 2.2B and 2.3.1'
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loop_

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_atom_site_label  
_atom_site_fract_x  
_atom_site_fract_y  
_atom_site_fract_z  
_atom_site_U_iso_or_equiv  
_atom_site_adp_type  
_atom_site_calc_flag  
_atom_site_calc_attached_atom  
_atom_site_occupancy  
_atom_site_disorder_assembly  
_atom_site_disorder_group  
Ir1 .704471(7) .832210(7) .221593(4) .01323(4) Uani ? ? 1.00000 ? ?  
Ir2 .724659(7) 1.095410(7) .281683(4) .01368(4) Uani ? ? 1.00000 ? ?  
Cu1 .72235(2) .97872(2) .177710(14) .01706(14) Uani ? ? 1.00000 ? ?  
Cu2 .83886(2) .96079(2) .256640(15) .01887(15) Uani ? ? 1.00000 ? ?  
Cu3 .70007(2) .95236(2) .322877(15) .01928(15) Uani ? ? 1.00000 ? ?  
Cu4 .58635(2) .96417(2) .245242(14) .01798(15) Uani ? ? 1.00000 ? ?  
Fe11 .68015(3) .81132(3) -.000072(17) .02023(18) Uani ? ? 1.00000 ?  
?  
Fe21 .69551(3) 1.23705(3) .097130(18) .0232(2) Uani ? ? 1.00000 ? ?  
Fe12 1.05636(3) .75042(3) .29548(2) .0288(2) Uani ? ? 1.00000 ? ?  
Fe22 1.05394(3) 1.01795(3) .165181(18) .02066(18) Uani ? ? 1.00000 ?  
?  
Fe13 .45705(3) .77000(3) .36585(2) .0268(2) Uani ? ? 1.00000 ? ?  
Fe23 .82381(3) .96622(4) .472697(19) .0288(2) Uani ? ? 1.00000 ? ?  
Fe14 .36895(3) .94551(3) .138116(17) .01771(17) Uani ? ? 1.00000 ? ?  
Fe24 .39217(3) 1.12548(3) .381235(18) .0231(2) Uani ? ? 1.00000 ? ?  
P1 .70599(5) .68829(5) .19179(3) .0173(3) Uani ? ? 1.00000 ? ?  
Cl011 .6949(2) .6348(2) .24284(13) .0220(13) Uani ? ? 1.00000 ? ?  
Cl012 .6426(2) .5603(2) .23550(15) .0314(16) Uani ? ? 1.00000 ? ?
```

| | | | | | | | | | | |
|--------|------------|------------|-------------|-----------|------|---|---|---------|---|---|
| C1013 | .6356(3) | .5221(2) | .27523(16) | .041(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C1014 | .6815(3) | .5569(2) | .32219(16) | .042(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C1015 | .7354(3) | .6293(2) | .32940(14) | .0345(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C1016 | .7422(2) | .6684(2) | .28987(13) | .0260(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C1021 | .80465(18) | .64756(18) | .16211(12) | .0188(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C1022 | .8295(2) | .5675(2) | .16332(14) | .0287(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C1023 | .9024(2) | .5350(2) | .13896(16) | .0337(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C1024 | .9510(2) | .5813(2) | .11336(15) | .0316(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C1025 | .9261(2) | .6603(2) | .11146(14) | .0277(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C1026 | .8540(2) | .6934(2) | .13620(12) | .0232(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C1031 | .6216(2) | .6337(2) | .14407(13) | .0232(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C1032 | .6378(2) | .5708(2) | .09824(14) | .0334(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C1033 | .5698(3) | .5249(3) | .06552(15) | .045(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C1034 | .4862(3) | .5424(3) | .07725(18) | .049(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C1035 | .4695(2) | .6055(3) | .12170(18) | .043(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C1036 | .5363(2) | .6506(2) | .15537(16) | .0329(16) | Uani | ? | ? | 1.00000 | ? | ? |
| P2 | .73179(5) | 1.23852(5) | .31780(3) | .0205(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C2011 | .8061(2) | 1.3036(2) | .29151(13) | .0241(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C2012 | .8488(2) | 1.2694(2) | .24593(15) | .0314(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C2013 | .9009(2) | 1.3229(2) | .22607(16) | .0364(18) | Uani | ? | ? | 1.00000 | ? | ? |
| C2014 | .9126(2) | 1.4087(2) | .25176(19) | .044(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2015 | .8683(3) | 1.4422(2) | .2937(2) | .050(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2016 | .8159(3) | 1.3906(2) | .3142(2) | .053(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2021 | .7637(3) | 1.2691(2) | .38684(14) | .0357(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C2022 | .8504(4) | 1.2926(4) | .4033(2) | .072(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C2023 | .8754(5) | 1.3072(5) | .4555(2) | .122(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2024 | .8179(6) | 1.2998(4) | .4909(2) | .120(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C2025 | .7312(5) | 1.2749(3) | .47505(19) | .089(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C2026 | .7047(3) | 1.2576(3) | .42217(16) | .050(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2031 | .6309(2) | 1.2879(2) | .31245(14) | .0277(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C2032 | .5811(2) | 1.2593(2) | .26606(15) | .0317(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C2033 | .5052(2) | 1.2971(2) | .25946(17) | .0371(18) | Uani | ? | ? | 1.00000 | ? | ? |
| C2034 | .4782(3) | 1.3626(3) | .29924(19) | .047(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2035 | .5265(3) | 1.3918(2) | .34587(18) | .048(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2036 | .6030(3) | 1.3551(2) | .35273(16) | .0374(18) | Uani | ? | ? | 1.00000 | ? | ? |
| C111 | .73714(18) | .85352(18) | .15390(11) | .0168(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C112 | .74956(18) | .87368(18) | .11366(12) | .0186(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C1121 | .76870(18) | .8585(2) | .06004(12) | .0195(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C1122 | .7915(2) | .7778(2) | .02765(12) | .0245(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C1123 | .8009(2) | .7841(2) | -.02361(13) | .0297(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C1124 | .7847(2) | .8680(2) | -.02358(13) | .0292(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C1125 | .7644(2) | .9145(2) | .02754(12) | .0236(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C1121' | .5660(2) | .8201(3) | .03423(15) | .0369(18) | Uani | ? | ? | 1.00000 | ? | ? |
| C1122' | .5833(2) | .7338(3) | .01347(17) | .044(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C1123' | .5923(3) | .7179(3) | -.04119(17) | .044(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C1124' | .5799(2) | .7945(3) | -.05417(14) | .0356(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C1125' | .5637(2) | .8579(3) | -.00738(15) | .0339(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C121 | .83030(19) | .83586(18) | .24577(11) | .0187(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C122 | .9068(2) | .84436(19) | .25817(12) | .0205(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C1221 | .99744(18) | .8388(2) | .26763(13) | .0222(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C1222 | 1.0471(2) | .8794(2) | .31508(14) | .0287(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C1223 | 1.1331(2) | .8591(2) | .30686(16) | .0342(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C1224 | 1.1380(2) | .8058(3) | .25567(16) | .0355(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C1225 | 1.0545(2) | .7920(2) | .23109(14) | .0305(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C1221' | .9729(3) | .6478(3) | .2890(2) | .052(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C1222' | .9830(3) | .6970(3) | .3401(2) | .060(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C1223' | 1.0759(4) | .6988(3) | .3547(2) | .074(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C1224' | 1.1122(3) | .6492(3) | .3097(2) | .055(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C1225' | 1.0495(3) | .6192(3) | .2705(2) | .058(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C131 | .65937(18) | .83106(18) | .29170(12) | .0182(12) | Uani | ? | ? | 1.00000 | ? | ? |

| | | | | | | | | | | |
|--------|-------------|-------------|------------|-----------|------|---|---|---------|---|---|
| C132 | .62584(18) | .84072(19) | .33272(12) | .0195(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C1321 | .57499(19) | .8345(2) | .37550(12) | .0215(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C1322 | .5110(2) | .8911(2) | .39798(13) | .0264(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C1323 | .4718(2) | .8606(3) | .43688(13) | .0336(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C1324 | .5105(2) | .7853(3) | .43849(14) | .0343(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C1325 | .5739(2) | .7685(2) | .40115(13) | .0266(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C1321' | .4086(4) | .7495(4) | .2898(2) | .0234(13) | Uiso | ? | ? | .50000 | ? | ? |
| C1322' | .3434(5) | .7697(5) | .3252(3) | .0382(18) | Uiso | ? | ? | .50000 | ? | ? |
| C1323' | .3436(6) | .7030(7) | .3540(4) | .059(3) | Uiso | ? | ? | .50000 | ? | ? |
| C1324' | .4058(6) | .6488(6) | .3348(4) | .048(2) | Uiso | ? | ? | .50000 | ? | ? |
| C1325' | .4488(4) | .6759(5) | .2953(3) | .0299(15) | Uiso | ? | ? | .50000 | ? | ? |
| C1321" | .4317(7) | .7096(7) | .2911(4) | .069(3) | Uiso | ? | ? | .50000 | ? | ? |
| C1322" | .3714(7) | .7654(7) | .3070(4) | .066(3) | Uiso | ? | ? | .50000 | ? | ? |
| C1323" | .3294(5) | .7405(5) | .3464(3) | .0420(19) | Uiso | ? | ? | .50000 | ? | ? |
| C1324" | .3660(5) | .6694(5) | .3519(3) | .0376(17) | Uiso | ? | ? | .50000 | ? | ? |
| C1325" | .4348(6) | .6485(6) | .3197(4) | .054(2) | Uiso | ? | ? | .50000 | ? | ? |
| C141 | .58149(18) | .84397(18) | .19913(11) | .0171(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C142 | .50825(18) | .86145(19) | .18995(12) | .0195(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C1421 | .42158(18) | .85762(19) | .16929(12) | .0184(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C1422 | .34883(19) | .8924(2) | .19721(12) | .0209(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C1423 | .27654(18) | .8738(2) | .16186(13) | .0228(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C1424 | .3026(2) | .8288(2) | .11194(13) | .0236(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C1425 | .3922(2) | .8185(2) | .11627(12) | .0216(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C1421' | .4623(2) | 1.0405(2) | .14572(16) | .0348(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C1422' | .3889(3) | 1.0745(2) | .17092(13) | .0327(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C1423' | .3193(2) | 1.0567(2) | .13355(14) | .0282(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C1424' | .3494(2) | 1.0127(2) | .08534(12) | .0248(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C1425' | .4374(2) | 1.0020(2) | .09205(14) | .0293(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C211 | .70784(18) | 1.10294(18) | .20728(12) | .0174(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C212 | .70566(19) | 1.10323(18) | .16192(12) | .0188(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C2121 | .70597(18) | 1.12138(18) | .11206(11) | .0177(11) | Uani | ? | ? | 1.00000 | ? | ? |
| C2122 | .6339(2) | 1.1190(2) | .07730(12) | .0217(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C2123 | .6634(2) | 1.1388(2) | .03255(12) | .0265(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C2124 | .7537(2) | 1.1537(2) | .03922(13) | .0288(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C2125 | .7805(2) | 1.1442(2) | .08817(13) | .0251(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C2121' | .6938(3) | 1.3334(2) | .16510(16) | .041(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2122' | .6132(3) | 1.3222(3) | .13770(18) | .046(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2123' | .6250(3) | 1.3346(3) | .08920(19) | .048(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2124' | .7121(3) | 1.3538(3) | .08502(18) | .047(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2125' | .7568(3) | 1.3528(2) | .13346(18) | .046(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C221 | .85178(19) | 1.08655(18) | .26851(11) | .0186(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C222 | .92379(19) | 1.06911(19) | .25512(12) | .0202(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C2221 | 1.0092(2) | 1.0771(2) | .23723(12) | .0218(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C2222 | 1.08209(19) | 1.0310(2) | .24255(12) | .0223(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C2223 | 1.1520(2) | 1.0637(2) | .22047(13) | .0258(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C2224 | 1.1236(2) | 1.1301(2) | .20101(14) | .0301(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C2225 | 1.0349(2) | 1.1382(2) | .21075(14) | .0283(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C2221' | .9689(2) | .9177(2) | .12893(15) | .0341(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C2222' | 1.0538(2) | .8913(2) | .12535(13) | .0285(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C2223' | 1.1004(2) | .9401(2) | .09891(13) | .0296(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C2224' | 1.0446(2) | .9975(3) | .08555(14) | .0363(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C2225' | .9631(2) | .9830(3) | .10432(15) | .0391(18) | Uani | ? | ? | 1.00000 | ? | ? |
| C231 | .74331(18) | 1.07301(18) | .35192(12) | .0185(12) | Uani | ? | ? | 1.00000 | ? | ? |

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|--------|------------|-------------|-------------|-----------|------|---|---|---------|---|---|
| C232 | .7474(2) | 1.0532(2) | .39253(12) | .0221(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C2321 | .7620(2) | 1.0531(2) | .44593(12) | .0253(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C2322 | .7073(2) | 1.0157(2) | .47634(12) | .0269(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C2323 | .7463(2) | 1.0343(3) | .52743(13) | .0345(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C2324 | .8256(3) | 1.0811(3) | .52844(14) | .0391(18) | Uani | ? | ? | 1.00000 | ? | ? |
| C2325 | .8362(2) | 1.0928(2) | .47880(14) | .0335(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C2321' | .8567(3) | .8768(3) | .40762(16) | .047(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2322' | .8039(3) | .8396(3) | .4380(2) | .054(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2323' | .8467(3) | .8533(3) | .4870(2) | .058(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C2324' | .9243(3) | .8993(3) | .48688(18) | .051(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C2325' | .9310(3) | .9151(3) | .43857(18) | .047(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C241 | .59603(19) | 1.08449(18) | .29024(11) | .0183(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C242 | .5210(2) | 1.06934(19) | .29515(11) | .0195(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C2421 | .43173(19) | 1.0736(2) | .30805(12) | .0206(12) | Uani | ? | ? | 1.00000 | ? | ? |
| C2422 | .3803(2) | 1.0121(2) | .32468(12) | .0246(13) | Uani | ? | ? | 1.00000 | ? | ? |
| C2423 | .2979(2) | 1.0448(2) | .33541(14) | .0319(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C2424 | .2982(2) | 1.1250(2) | .32620(14) | .0314(15) | Uani | ? | ? | 1.00000 | ? | ? |
| C2425 | .3803(2) | 1.1437(2) | .30951(13) | .0255(14) | Uani | ? | ? | 1.00000 | ? | ? |
| C2421' | .4999(2) | 1.1476(3) | .42896(14) | .0337(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C2422' | .4354(3) | 1.1039(2) | .44858(14) | .0374(18) | Uani | ? | ? | 1.00000 | ? | ? |
| C2423' | .3645(3) | 1.1540(3) | .45824(14) | .0394(18) | Uani | ? | ? | 1.00000 | ? | ? |
| C2424' | .3835(2) | 1.2296(2) | .44466(14) | .0358(17) | Uani | ? | ? | 1.00000 | ? | ? |
| C2425' | .4683(2) | 1.2256(2) | .42615(14) | .0323(16) | Uani | ? | ? | 1.00000 | ? | ? |
| C101 | 1.0158(2) | .7991(3) | -.04052(16) | .0397(18) | Uani | ? | ? | 1.00000 | ? | ? |
| C102 | .9899(3) | .7739(3) | -.09227(17) | .044(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C103 | .9596(3) | .6910(3) | -.11587(16) | .048(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C104 | .9564(3) | .6331(3) | -.0874(2) | .052(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C105 | .9826(3) | .6580(3) | -.0358(2) | .052(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C106 | 1.0118(3) | .7407(3) | -.01223(17) | .046(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C201 | .2985(3) | 1.4974(3) | .23376(19) | .058(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C202 | .3709(3) | 1.4784(4) | .2071(2) | .066(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C203 | .3796(4) | 1.3965(5) | .1777(2) | .090(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C204 | .3160(5) | 1.3343(4) | .1756(3) | .110(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C205 | .2451(4) | 1.3555(4) | .2022(3) | .096(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C206 | .2349(4) | 1.4371(4) | .2323(2) | .070(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C301 | 1.0972(4) | .3670(4) | .3285(3) | .087(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C302 | 1.1090(4) | .4543(4) | .3503(3) | .089(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C303 | 1.1894(4) | .4915(4) | .3705(3) | .087(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C304 | 1.2587(4) | .4408(4) | .3691(3) | .082(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C305 | 1.2455(4) | .3534(3) | .3468(2) | .072(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C306 | 1.1651(4) | .3167(4) | .3267(3) | .078(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C401 | .2306(4) | .4715(3) | .0430(2) | .071(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C402 | .1951(4) | .5178(5) | .0140(2) | .094(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C403 | .1701(3) | .5974(6) | .0374(4) | .131(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C404 | .1820(4) | .6281(4) | .0909(4) | .121(5) | Uani | ? | ? | 1.00000 | ? | ? |
| C405 | .2164(4) | .5789(4) | .1190(3) | .094(4) | Uani | ? | ? | 1.00000 | ? | ? |
| C406 | .2400(3) | .5030(4) | .0939(2) | .076(3) | Uani | ? | ? | 1.00000 | ? | ? |
| C501 | .9181(10) | .6662(8) | .4784(5) | .139(3) | Uiso | ? | ? | .50000 | ? | ? |
| C502 | .9381(6) | .5938(12) | .4394(5) | .139(3) | Uiso | ? | ? | .50000 | ? | ? |
| C503 | .8903(11) | .5166(8) | .4323(4) | .139(3) | Uiso | ? | ? | .50000 | ? | ? |
| C504 | .8227(10) | .5117(8) | .4642(5) | .139(3) | Uiso | ? | ? | .50000 | ? | ? |
| C505 | .8027(6) | .5842(12) | .5033(5) | .139(3) | Uiso | ? | ? | .50000 | ? | ? |
| C506 | .8506(12) | .6614(8) | .5103(4) | .139(3) | Uiso | ? | ? | .50000 | ? | ? |
| H501 | .9454(16) | .7189(11) | .4783(8) | .15600 | Uiso | ? | ? | .50000 | ? | ? |
| H502 | .9852(8) | .595(2) | .4173(7) | .15600 | Uiso | ? | ? | .50000 | ? | ? |
| H503 | .9103(18) | .4638(11) | .4093(5) | .15600 | Uiso | ? | ? | .50000 | ? | ? |
| H504 | .7960(16) | .4564(11) | .4624(8) | .15600 | Uiso | ? | ? | .50000 | ? | ? |
| H505 | .7562(8) | .580(2) | .5235(7) | .15600 | Uiso | ? | ? | .50000 | ? | ? |
| H506 | .8312(18) | .7117(11) | .5314(5) | .15600 | Uiso | ? | ? | .50000 | ? | ? |
| C501' | .8845(7) | .6435(5) | .4479(3) | .0972(18) | Uiso | ? | ? | .50000 | ? | ? |

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|--------|-----------|-----------|------------|-----------|------|---|---|---------|---|---|
| C502' | .9467(5) | .5837(7) | .4357(3) | .0972(18) | Uiso | ? | ? | .50000 | ? | ? |
| C503' | .9566(5) | .5265(6) | .4651(3) | .0972(18) | Uiso | ? | ? | .50000 | ? | ? |
| C504' | .9043(7) | .5290(5) | .5067(3) | .0972(18) | Uiso | ? | ? | .50000 | ? | ? |
| C505' | .8421(5) | .5887(7) | .5188(3) | .0972(18) | Uiso | ? | ? | .50000 | ? | ? |
| C506' | .8321(5) | .6461(6) | .4894(3) | .0972(18) | Uiso | ? | ? | .50000 | ? | ? |
| H501' | .8755(10) | .6788(7) | .4262(4) | .09400 | Uiso | ? | ? | .50000 | ? | ? |
| H502' | .9813(7) | .5799(10) | .4066(4) | .09400 | Uiso | ? | ? | .50000 | ? | ? |
| H503' | 1.0013(7) | .4872(8) | .4579(5) | .09400 | Uiso | ? | ? | .50000 | ? | ? |
| H504' | .9155(10) | .4934(7) | .5287(4) | .09400 | Uiso | ? | ? | .50000 | ? | ? |
| H505' | .8095(7) | .5921(10) | .5483(4) | .09400 | Uiso | ? | ? | .50000 | ? | ? |
| H506' | .7895(7) | .6850(8) | .4970(5) | .09400 | Uiso | ? | ? | .50000 | ? | ? |
| C601 | .5590(9) | .5488(6) | .4807(4) | .205(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C602 | .4758(9) | .5641(5) | .4841(4) | .192(9) | Uani | ? | ? | 1.00000 | ? | ? |
| C603 | .4188(8) | .5194(5) | .5012(4) | .187(8) | Uani | ? | ? | 1.00000 | ? | ? |
| 00 | .9795(2) | 1.0849(3) | .38450(14) | .078(2) | Uani | ? | ? | 1.00000 | ? | ? |
| C0 | 1.0444(4) | 1.1405(4) | .3782(2) | .079(3) | Uani | ? | ? | 1.00000 | ? | ? |
| H1012 | .61171 | .53472 | .20234 | .04000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1013 | .59778 | .47197 | .27028 | .04900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1014 | .67650 | .53044 | .34961 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1015 | .76799 | .65219 | .36204 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1016 | .77980 | .71914 | .29522 | .03300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1022 | .79538 | .53424 | .18064 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1023 | .91960 | .48008 | .14041 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1024 | 1.00152 | .55851 | .09619 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1025 | .96031 | .69259 | .09382 | .03500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1026 | .83779 | .74875 | .13523 | .02900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1032 | .69612 | .55909 | .08951 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1033 | .58203 | .48104 | .03438 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1034 | .43914 | .50965 | .05472 | .05900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1035 | .41124 | .61808 | .12897 | .05300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1036 | .52388 | .69374 | .18724 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2012 | .84207 | 1.20925 | .22857 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2013 | .92926 | 1.29976 | .19419 | .04500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2014 | .95157 | 1.44455 | .23883 | .05100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2015 | .87223 | 1.50319 | .30977 | .06300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2016 | .78601 | 1.41562 | .34527 | .06500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2022 | .89295 | 1.29548 | .37693 | .09000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2023 | .93740 | 1.32222 | .46765 | .13600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2024 | .83554 | 1.31234 | .52723 | .13700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2025 | .68856 | 1.27102 | .50049 | .11100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2026 | .64540 | 1.23751 | .40964 | .06700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2032 | .59932 | 1.21215 | .23777 | .04000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2033 | .47101 | 1.27732 | .22693 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2034 | .42546 | 1.38787 | .29483 | .05900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2035 | .50679 | 1.43670 | .37358 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2036 | .63732 | 1.37683 | .38501 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1122 | .79931 | .72808 | .03907 | .03100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1123 | .81527 | .73864 | -.05319 | .03700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1124 | .78679 | .88955 | -.05326 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1125 | .74980 | .97313 | .03833 | .02900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1121' | .55880 | .84909 | .07084 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1122' | .58728 | .69188 | .03241 | .05500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1123' | .60499 | .66420 | -.06529 | .05400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1124' | .58249 | .80239 | -.08834 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1125' | .55268 | .91674 | -.00502 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2122 | .57534 | 1.10591 | .08345 | .02700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2123 | .62796 | 1.14238 | .00318 | .03400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2124 | .79113 | 1.16726 | .01436 | .03500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2125 | .83844 | 1.15152 | .10282 | .03200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2121' | .70327 | 1.32888 | .20005 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2122' | .55896 | 1.30777 | .15075 | .06000 | Uiso | ? | ? | 1.00000 | ? | ? |

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|--------|---------|---------|--------|--------|------|---|---|---------|---|---|
| H2123' | .58065 | 1.33081 | .06264 | .06100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2124' | .73858 | 1.36576 | .05593 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2125' | .81807 | 1.36264 | .14155 | .05800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1222 | 1.02558 | .91487 | .34694 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1223 | 1.18071 | .87835 | .33207 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1224 | 1.18901 | .78357 | .24029 | .04400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1225 | 1.03940 | .75798 | .19580 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1221' | .91871 | .63491 | .26924 | .06500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1222' | .93866 | .72422 | .36174 | .07700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1223' | 1.10575 | .72828 | .38819 | .08900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1224' | 1.17160 | .63823 | .30688 | .06600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1225' | 1.05822 | .58477 | .23500 | .07600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2222 | 1.08368 | .98558 | .25850 | .02800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2223 | 1.20916 | 1.04458 | .21920 | .03200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2224 | 1.15808 | 1.16323 | .18402 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2225 | .99826 | 1.17749 | .20140 | .03500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2221' | .92298 | .89444 | .14495 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2222' | 1.07608 | .84771 | .13881 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2223' | 1.15950 | .93522 | .09050 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2224' | 1.06003 | 1.03894 | .06726 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2225' | .91239 | 1.01258 | .10138 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1322 | .49711 | .94168 | .38826 | .03500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1323 | .42643 | .88620 | .45849 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1324 | .49688 | .75138 | .46145 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1325 | .61007 | .72123 | .39408 | .03400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1321' | .42282 | .78074 | .26648 | .03000 | Uiso | ? | ? | .50000 | ? | ? |
| H1322' | .30678 | .81389 | .33057 | .05500 | Uiso | ? | ? | .50000 | ? | ? |
| H1323' | .30769 | .69803 | .38000 | .07300 | Uiso | ? | ? | .50000 | ? | ? |
| H1324' | .42041 | .60075 | .34550 | .05700 | Uiso | ? | ? | .50000 | ? | ? |
| H1325' | .49472 | .65093 | .27611 | .03600 | Uiso | ? | ? | .50000 | ? | ? |
| H1321" | .46726 | .71242 | .26484 | .03000 | Uiso | ? | ? | .50000 | ? | ? |
| H1322" | .35906 | .81196 | .29463 | .05500 | Uiso | ? | ? | .50000 | ? | ? |
| H1323" | .28435 | .76670 | .36531 | .05200 | Uiso | ? | ? | .50000 | ? | ? |
| H1324" | .34897 | .63713 | .37388 | .07300 | Uiso | ? | ? | .50000 | ? | ? |
| H1325" | .47380 | .60710 | .31597 | .05700 | Uiso | ? | ? | .50000 | ? | ? |
| H2322 | .65384 | .98387 | .46437 | .03300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2323 | .72277 | 1.01783 | .55597 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2324 | .86463 | 1.10122 | .55816 | .04900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2325 | .88472 | 1.12284 | .46895 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2321' | .84378 | .87716 | .37149 | .06000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2322' | .74903 | .80845 | .42678 | .06600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2323' | .82650 | .83570 | .51616 | .07200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2324' | .96666 | .91780 | .51607 | .06400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2325' | .97821 | .94590 | .42840 | .06000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1422 | .34919 | .92266 | .23363 | .02600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1423 | .21926 | .88887 | .17041 | .02800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1424 | .26648 | .80893 | .08082 | .02900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1425 | .42665 | .79090 | .08816 | .02700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1421' | .51886 | 1.04296 | .16191 | .04300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1422' | .38658 | 1.10453 | .20723 | .04000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1423' | .26158 | 1.07225 | .14019 | .03600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1424' | .31533 | .99240 | .05272 | .03200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H1425' | .47419 | .97425 | .06515 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2422 | .39791 | .95790 | .32760 | .03200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2423 | .25032 | 1.01670 | .34678 | .03800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2424 | .25155 | 1.16204 | .33081 | .03900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2425 | .39798 | 1.19410 | .30049 | .03200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2421' | .55580 | 1.12741 | .41903 | .04200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2422' | .43930 | 1.04856 | .45424 | .04700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2423' | .31176 | 1.13961 | .47187 | .04800 | Uiso | ? | ? | 1.00000 | ? | ? |
| H2424' | .34613 | 1.27562 | .44760 | .04600 | Uiso | ? | ? | 1.00000 | ? | ? |

| | | | | | | | | | | |
|--------|---------|---------|---------|--------|------|---|---|---------|---|---|
| H2425' | .49865 | 1.26809 | .41388 | .04100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H101 | 1.03637 | .85772 | -.02358 | .05000 | Uiso | ? | ? | 1.00000 | ? | ? |
| H102 | .99431 | .81443 | -.11219 | .05400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H103 | .94033 | .67372 | -.15247 | .06200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H104 | .93493 | .57419 | -.10398 | .06600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H105 | .98101 | .61728 | -.01538 | .06400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H106 | 1.02939 | .75878 | .02459 | .05600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H201 | .29188 | 1.55495 | .25412 | .07500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H202 | .41540 | 1.52439 | .20961 | .08400 | Uiso | ? | ? | 1.00000 | ? | ? |
| H203 | .43069 | 1.38350 | .15713 | .10700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H204 | .32419 | 1.27711 | .15565 | .13200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H205 | .20000 | 1.31169 | .20285 | .11600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H206 | .18291 | 1.45199 | .25097 | .08600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H301 | 1.03981 | .33998 | .31527 | .10200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H302 | 1.05986 | .48960 | .35055 | .10700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H303 | 1.19906 | .55271 | .38717 | .11500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H304 | 1.31524 | .46610 | .38170 | .09700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H305 | 1.29477 | .31803 | .34758 | .08500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H306 | 1.15757 | .25479 | .30974 | .09700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H401 | .24971 | .41493 | .02507 | .09600 | Uiso | ? | ? | 1.00000 | ? | ? |
| H402 | .18061 | .49874 | -.02436 | .12100 | Uiso | ? | ? | 1.00000 | ? | ? |
| H403 | .14643 | .64257 | .02578 | .13900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H404 | .17195 | .68531 | .11538 | .11900 | Uiso | ? | ? | 1.00000 | ? | ? |
| H405 | .22178 | .59474 | .15809 | .11300 | Uiso | ? | ? | 1.00000 | ? | ? |
| H406 | .26657 | .46707 | .11296 | .09500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H601 | .58743 | .58963 | .46244 | .22500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H602 | .44396 | .60662 | .47274 | .21700 | Uiso | ? | ? | 1.00000 | ? | ? |
| H603 | .35401 | .52490 | .50544 | .25200 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0a | 1.02517 | 1.16488 | .35165 | .11500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0b | 1.09220 | 1.10724 | .36538 | .11500 | Uiso | ? | ? | 1.00000 | ? | ? |
| H0c | 1.06273 | 1.18242 | .41008 | .11500 | Uiso | ? | ? | 1.00000 | ? | ? |

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

| | | | | | | |
|-------|------------|------------|------------|-------------|-------------|------------|
| Ir1 | .01143(5) | .01219(5) | .01671(5) | .00121(4) | .00073(4) | .00512(4) |
| Ir2 | .01305(5) | .01227(5) | .01581(5) | .00058(4) | .00202(4) | .00407(4) |
| Cu1 | .01797(17) | .01240(16) | .02070(18) | .00201(13) | .00132(13) | .00437(14) |
| Cu2 | .02003(17) | .01427(17) | .02327(19) | .00072(14) | .00133(14) | .00697(14) |
| Cu3 | .01860(17) | .01649(18) | .02212(18) | -.00133(14) | -.00111(14) | .00519(14) |
| Cu4 | .01864(17) | .01457(17) | .01967(18) | .00145(13) | .00006(14) | .00326(14) |
| Fe11 | .0177(2) | .0239(2) | .0197(2) | .00352(17) | .00052(16) | .00688(18) |
| Fe21 | .0269(2) | .0180(2) | .0267(2) | -.00309(18) | -.00307(19) | .01107(19) |
| Fe12 | .0165(2) | .0283(3) | .0489(3) | .00276(19) | -.0001(2) | .0229(2) |
| Fe22 | .0146(2) | .0221(2) | .0258(2) | .00232(16) | .00247(17) | .00736(18) |
| Fe13 | .0203(2) | .0332(3) | .0270(2) | -.0044(2) | .00185(18) | .0099(2) |
| Fe23 | .0203(2) | .0442(3) | .0238(2) | -.0008(2) | -.00297(18) | .0140(2) |
| Fe14 | .01410(18) | .0197(2) | .0205(2) | .00054(16) | .00009(16) | .00799(17) |
| Fe24 | .0210(2) | .0262(2) | .0210(2) | .00000(18) | .00595(17) | .00451(19) |
| P1 | .0164(3) | .0135(3) | .0228(4) | .0015(3) | .0035(3) | .0059(3) |
| C1011 | .0228(15) | .0177(15) | .0294(16) | .0057(12) | .0087(12) | .0113(13) |
| C1012 | .0357(19) | .0223(17) | .038(2) | -.0016(14) | .0096(16) | .0116(15) |
| C1013 | .059(3) | .025(2) | .045(2) | -.0020(18) | .016(2) | .0179(17) |
| C1014 | .060(3) | .033(2) | .046(2) | .0160(19) | .022(2) | .0272(19) |
| C1015 | .048(2) | .030(2) | .0314(19) | .0135(17) | .0049(16) | .0153(16) |
| C1016 | .0258(16) | .0213(16) | .0343(18) | .0069(13) | .0042(14) | .0123(14) |

| | | | | | | |
|--------|-----------|-----------|-----------|------------|------------|-----------|
| C1021 | .0169(13) | .0139(13) | .0247(15) | .0029(10) | .0024(11) | .0034(11) |
| C1022 | .0271(17) | .0214(16) | .042(2) | .0086(13) | .0123(15) | .0133(15) |
| C1023 | .0318(18) | .0190(16) | .056(2) | .0120(14) | .0165(17) | .0159(16) |
| C1024 | .0269(17) | .0272(18) | .041(2) | .0072(14) | .0153(15) | .0087(16) |
| C1025 | .0276(17) | .0241(17) | .0347(19) | .0050(13) | .0125(14) | .0116(14) |
| C1026 | .0239(15) | .0214(15) | .0262(16) | .0069(12) | .0069(12) | .0082(13) |
| C1031 | .0255(15) | .0153(14) | .0292(17) | -.0014(12) | .0008(13) | .0075(12) |
| C1032 | .046(2) | .0258(18) | .0271(18) | .0035(16) | -.0040(16) | .0055(14) |
| C1033 | .068(3) | .030(2) | .033(2) | -.007(2) | -.018(2) | .0041(17) |
| C1034 | .051(3) | .038(2) | .057(3) | -.018(2) | -.028(2) | .019(2) |
| C1035 | .0286(19) | .034(2) | .066(3) | -.0056(16) | -.0117(19) | .018(2) |
| C1036 | .0243(17) | .0215(17) | .051(2) | -.0018(13) | -.0005(16) | .0087(16) |
| P2 | .0224(4) | .0141(4) | .0240(4) | -.0000(3) | .0068(3) | .0036(3) |
| C2011 | .0222(15) | .0184(15) | .0306(17) | .0002(12) | .0063(13) | .0048(13) |
| C2012 | .0317(18) | .0240(17) | .041(2) | .0016(14) | .0086(15) | .0123(15) |
| C2013 | .0303(19) | .036(2) | .048(2) | .0014(16) | .0112(17) | .0193(18) |
| C2014 | .032(2) | .025(2) | .077(3) | -.0023(16) | .018(2) | .020(2) |
| C2015 | .049(3) | .0196(19) | .082(3) | -.0025(17) | .027(2) | .012(2) |
| C2016 | .052(3) | .0203(19) | .086(4) | -.0004(18) | .040(2) | .008(2) |
| C2021 | .057(2) | .0180(16) | .0269(18) | -.0075(16) | .0020(17) | .0003(14) |
| C2022 | .087(4) | .071(4) | .054(3) | -.045(3) | -.031(3) | .024(3) |
| C2023 | .182(8) | .104(5) | .067(4) | -.085(5) | -.077(5) | .034(4) |
| C2024 | .246(10) | .062(4) | .035(3) | -.041(5) | -.041(4) | .004(3) |
| C2025 | .191(7) | .049(3) | .036(3) | .041(4) | .044(4) | .016(2) |
| C2026 | .083(3) | .038(2) | .036(2) | .023(2) | .024(2) | .0144(19) |
| C2031 | .0302(17) | .0169(15) | .040(2) | .0039(13) | .0156(15) | .0132(14) |
| C2032 | .0270(17) | .0214(17) | .051(2) | .0068(13) | .0121(16) | .0149(16) |
| C2033 | .0260(17) | .033(2) | .063(3) | .0097(15) | .0114(17) | .027(2) |
| C2034 | .039(2) | .040(2) | .078(3) | .0228(18) | .034(2) | .038(2) |
| C2035 | .058(3) | .030(2) | .069(3) | .0257(19) | .044(2) | .026(2) |
| C2036 | .048(2) | .0237(18) | .045(2) | .0106(16) | .0231(18) | .0123(16) |
| C111 | .0157(13) | .0117(13) | .0221(14) | .0025(10) | .0011(11) | .0030(11) |
| C112 | .0176(13) | .0152(14) | .0225(15) | .0037(11) | .0011(11) | .0041(11) |
| C1121 | .0149(13) | .0215(15) | .0239(15) | .0016(11) | .0007(11) | .0092(12) |
| C1122 | .0225(15) | .0311(18) | .0219(15) | .0098(13) | .0017(12) | .0094(13) |
| C1123 | .0249(16) | .043(2) | .0213(16) | .0137(15) | .0046(13) | .0062(15) |
| C1124 | .0213(15) | .044(2) | .0272(17) | .0048(14) | .0060(13) | .0171(16) |
| C1125 | .0220(15) | .0259(16) | .0250(16) | .0016(12) | .0025(12) | .0104(13) |
| C1121' | .0179(16) | .062(3) | .039(2) | .0034(16) | .0067(14) | .027(2) |
| C1122' | .030(2) | .053(3) | .057(3) | -.0138(18) | -.0115(18) | .033(2) |
| C1123' | .043(2) | .035(2) | .048(2) | -.0098(18) | -.0174(19) | .0070(19) |
| C1124' | .0271(18) | .048(2) | .032(2) | -.0005(16) | -.0092(15) | .0149(17) |
| C1125' | .0146(14) | .053(2) | .040(2) | .0065(15) | .0018(14) | .0231(19) |
| C121 | .0215(14) | .0148(13) | .0209(14) | .0008(11) | .0027(11) | .0067(11) |
| C122 | .0221(14) | .0161(14) | .0262(16) | .0034(11) | .0024(12) | .0100(12) |
| C1221 | .0150(13) | .0230(16) | .0321(17) | .0001(11) | .0006(12) | .0139(13) |
| C1222 | .0241(16) | .0256(17) | .037(2) | -.0002(13) | -.0069(14) | .0117(15) |
| C1223 | .0208(16) | .032(2) | .054(2) | -.0030(14) | -.0082(16) | .0213(18) |
| C1224 | .0159(15) | .044(2) | .058(2) | .0070(15) | .0082(15) | .030(2) |
| C1225 | .0235(16) | .034(2) | .038(2) | .0071(14) | .0042(14) | .0167(16) |
| C1221' | .034(2) | .043(3) | .090(4) | -.0034(18) | .004(2) | .038(3) |
| C1222' | .071(3) | .049(3) | .082(4) | .014(2) | .039(3) | .044(3) |
| C1223' | .125(5) | .051(3) | .059(3) | -.024(3) | -.034(3) | .044(3) |
| C1224' | .038(2) | .041(3) | .099(4) | .004(2) | -.012(2) | .040(3) |
| C1225' | .057(3) | .029(2) | .093(4) | -.001(2) | .003(3) | .025(2) |
| C131 | .0174(13) | .0162(14) | .0218(14) | .0013(11) | -.0014(11) | .0071(11) |
| C132 | .0175(13) | .0173(14) | .0247(15) | .0003(11) | -.0014(11) | .0085(12) |
| C1321 | .0190(14) | .0245(16) | .0222(15) | -.0015(12) | .0002(11) | .0093(12) |
| C1322 | .0283(17) | .0279(17) | .0231(16) | .0027(13) | .0045(13) | .0069(13) |
| C1323 | .0320(19) | .043(2) | .0237(17) | -.0008(16) | .0077(14) | .0055(16) |
| C1324 | .035(2) | .046(2) | .0255(17) | -.0066(17) | .0038(15) | .0180(16) |

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|--------|-----------|-----------|-----------|------------|------------|------------|
| C1325 | .0244(16) | .0312(18) | .0291(17) | .0011(13) | .0000(13) | .0167(15) |
| C141 | .0165(13) | .0118(13) | .0223(14) | .0008(10) | .0017(11) | .0037(11) |
| C142 | .0178(13) | .0167(14) | .0237(15) | -.0017(11) | .0000(11) | .0058(12) |
| C1421 | .0151(13) | .0178(14) | .0236(15) | -.0007(10) | -.0001(11) | .0085(12) |
| C1422 | .0173(13) | .0223(15) | .0240(15) | -.0002(11) | .0026(11) | .0082(12) |
| C1423 | .0129(13) | .0276(17) | .0306(17) | -.0003(12) | .0012(12) | .0129(14) |
| C1424 | .0182(14) | .0232(16) | .0285(17) | -.0038(12) | -.0045(12) | .0075(13) |
| C1425 | .0196(14) | .0173(14) | .0264(16) | -.0011(11) | .0000(12) | .0046(12) |
| C1421' | .0259(17) | .034(2) | .051(2) | -.0099(15) | -.0106(16) | .0267(18) |
| C1422' | .057(2) | .0180(16) | .0246(17) | -.0032(15) | .0009(16) | .0089(13) |
| C1423' | .0329(18) | .0236(17) | .0334(18) | .0105(14) | .0107(14) | .0139(14) |
| C1424' | .0298(17) | .0261(17) | .0219(15) | .0050(13) | .0016(13) | .0122(13) |
| C1425' | .0275(17) | .0282(18) | .038(2) | .0035(14) | .0143(15) | .0177(15) |
| C211 | .0149(13) | .0126(13) | .0248(15) | .0035(10) | .0037(11) | .0046(11) |
| C212 | .0191(14) | .0119(13) | .0257(15) | .0025(10) | .0033(11) | .0052(11) |
| C2121 | .0199(14) | .0135(13) | .0204(14) | .0008(10) | .0019(11) | .0061(11) |
| C2122 | .0218(14) | .0194(15) | .0251(16) | -.0027(12) | -.0017(12) | .0093(12) |
| C2123 | .0348(18) | .0248(17) | .0212(15) | -.0035(14) | -.0038(13) | .0103(13) |
| C2124 | .0332(18) | .0327(19) | .0245(16) | .0034(15) | .0059(14) | .0137(14) |
| C2125 | .0213(15) | .0301(18) | .0278(17) | .0022(13) | .0044(13) | .0141(14) |
| C2121' | .053(3) | .0216(18) | .045(2) | .0080(17) | -.003(2) | .0049(17) |
| C2122' | .049(2) | .032(2) | .056(3) | .0173(19) | .004(2) | .008(2) |
| C2123' | .053(3) | .029(2) | .067(3) | .0056(19) | -.012(2) | .022(2) |
| C2124' | .064(3) | .027(2) | .056(3) | -.002(2) | -.001(2) | .025(2) |
| C2125' | .050(3) | .023(2) | .061(3) | -.0113(17) | -.008(2) | .0090(19) |
| C221 | .0206(14) | .0151(13) | .0208(14) | .0006(11) | .0021(11) | .0062(11) |
| C222 | .0195(14) | .0167(14) | .0253(15) | .0012(11) | .0028(12) | .0073(12) |
| C2221 | .0193(14) | .0190(15) | .0265(16) | -.0001(11) | .0043(12) | .0055(12) |
| C2222 | .0177(14) | .0262(16) | .0226(15) | -.0009(12) | .0006(11) | .0069(13) |
| C2223 | .0157(14) | .0291(17) | .0284(17) | -.0022(12) | .0015(12) | .0020(14) |
| C2224 | .0245(16) | .0229(17) | .041(2) | -.0037(13) | .0109(14) | .0049(15) |
| C2225 | .0262(16) | .0223(16) | .041(2) | .0057(13) | .0147(15) | .0140(15) |
| C2221' | .0178(15) | .039(2) | .037(2) | -.0079(14) | -.0007(14) | -.0002(16) |
| C2222' | .0285(17) | .0255(17) | .0291(18) | .0017(14) | -.0003(14) | .0040(14) |
| C2223' | .0227(16) | .033(2) | .0288(18) | .0032(14) | .0027(13) | .0025(15) |
| C2224' | .038(2) | .042(2) | .0281(19) | .0053(17) | -.0022(16) | .0102(17) |
| C2225' | .0245(18) | .049(2) | .037(2) | .0096(16) | -.0082(15) | .0006(18) |
| C231 | .0142(13) | .0157(14) | .0241(15) | -.0016(10) | .0018(11) | .0035(11) |
| C232 | .0212(14) | .0201(15) | .0232(15) | -.0005(12) | -.0013(12) | .0040(12) |
| C2321 | .0252(16) | .0323(18) | .0174(14) | -.0010(13) | -.0009(12) | .0063(13) |
| C2322 | .0213(15) | .039(2) | .0208(15) | -.0010(14) | .0003(12) | .0092(14) |
| C2323 | .0327(19) | .051(2) | .0199(16) | .0000(17) | .0004(14) | .0116(16) |
| C2324 | .039(2) | .052(3) | .0198(17) | -.0050(18) | -.0074(15) | .0025(16) |
| C2325 | .0309(18) | .042(2) | .0247(17) | -.0104(16) | -.0037(14) | .0078(16) |
| C2321' | .048(2) | .051(3) | .039(2) | .019(2) | -.006(2) | .006(2) |
| C2322' | .031(2) | .039(2) | .090(4) | .0050(18) | -.013(2) | .016(2) |
| C2323' | .039(2) | .076(4) | .080(4) | .014(2) | .007(2) | .051(3) |
| C2324' | .032(2) | .072(3) | .050(3) | .011(2) | -.0127(19) | .018(2) |
| C2325' | .029(2) | .059(3) | .052(3) | .005(2) | .0027(18) | .016(2) |
| C241 | .0225(14) | .0135(13) | .0188(14) | .0033(11) | .0013(11) | .0043(11) |
| C242 | .0227(14) | .0177(14) | .0192(14) | .0058(11) | .0046(11) | .0057(11) |
| C2421 | .0189(14) | .0229(15) | .0194(14) | .0008(12) | .0025(11) | .0050(12) |
| C2422 | .0233(15) | .0250(16) | .0239(16) | -.0030(13) | .0004(12) | .0054(13) |
| C2423 | .0228(16) | .042(2) | .0273(17) | -.0049(15) | .0037(13) | .0057(16) |
| C2424 | .0194(15) | .042(2) | .0315(18) | .0094(14) | .0046(13) | .0069(16) |
| C2425 | .0225(15) | .0316(18) | .0248(16) | .0059(13) | .0041(12) | .0108(14) |
| C2421' | .0325(19) | .041(2) | .0237(17) | .0015(16) | -.0018(14) | .0044(15) |
| C2422' | .055(2) | .035(2) | .0208(17) | -.0013(18) | .0027(16) | .0063(15) |
| C2423' | .045(2) | .046(2) | .0234(18) | -.0008(19) | .0153(16) | .0036(16) |
| C2424' | .041(2) | .031(2) | .031(2) | .0067(16) | .0087(16) | .0002(16) |
| C2425' | .0350(19) | .0305(19) | .0271(18) | -.0072(15) | .0019(15) | .0029(15) |

| | | | | | | |
|------|----------|---------|----------|------------|-----------|-----------|
| C101 | .030(2) | .043(2) | .046(2) | -.0004(17) | .0061(17) | .0119(19) |
| C102 | .036(2) | .056(3) | .050(3) | .008(2) | .0152(19) | .027(2) |
| C103 | .035(2) | .065(3) | .037(2) | .008(2) | .0123(18) | .003(2) |
| C104 | .033(2) | .037(2) | .079(3) | .0107(18) | .019(2) | .001(2) |
| C105 | .042(2) | .049(3) | .076(3) | .014(2) | .009(2) | .033(3) |
| C106 | .039(2) | .059(3) | .044(2) | .007(2) | .0005(19) | .023(2) |
| C201 | .060(3) | .054(3) | .050(3) | .004(2) | -.010(2) | -.001(2) |
| C202 | .058(3) | .092(4) | .046(3) | .004(3) | -.007(2) | .017(3) |
| C203 | .078(4) | .132(6) | .050(3) | .060(4) | -.009(3) | .003(3) |
| C204 | .116(6) | .065(4) | .119(6) | .052(4) | -.049(5) | -.025(4) |
| C205 | .088(5) | .049(3) | .145(6) | -.008(3) | -.035(4) | .025(4) |
| C206 | .064(3) | .068(4) | .072(4) | .000(3) | -.002(3) | .009(3) |
| C301 | .064(4) | .088(5) | .123(6) | .012(3) | .010(4) | .051(4) |
| C302 | .075(4) | .090(5) | .116(5) | .029(4) | .027(4) | .046(4) |
| C303 | .112(5) | .057(4) | .093(5) | .024(4) | .016(4) | .019(3) |
| C304 | .084(4) | .064(4) | .100(5) | .000(3) | .010(4) | .030(4) |
| C305 | .070(4) | .057(3) | .094(4) | .017(3) | .012(3) | .028(3) |
| C306 | .069(4) | .058(4) | .107(5) | .007(3) | -.012(3) | .027(3) |
| C401 | .065(3) | .049(3) | .088(4) | -.011(3) | .006(3) | .008(3) |
| C402 | .052(3) | .170(7) | .068(4) | -.012(4) | -.007(3) | .049(4) |
| C403 | .041(3) | .214(9) | .223(9) | .032(4) | .035(4) | .193(8) |
| C404 | .071(4) | .048(3) | .258(10) | .006(3) | .082(5) | .060(5) |
| C405 | .060(4) | .091(5) | .104(5) | -.032(3) | .001(3) | -.009(4) |
| C406 | .056(3) | .086(4) | .096(5) | .001(3) | -.017(3) | .043(4) |
| C601 | .340(17) | .105(7) | .119(8) | -.057(9) | .012(9) | -.036(6) |
| C602 | .338(16) | .059(5) | .142(8) | -.017(7) | -.035(9) | -.019(5) |
| C603 | .295(14) | .074(6) | .143(8) | .006(7) | -.047(9) | -.039(5) |
| O0 | .061(2) | .117(3) | .063(2) | .001(2) | .0006(19) | .039(2) |
| C0 | .088(4) | .104(5) | .041(3) | -.022(4) | -.005(3) | .018(3) |

5. Molecular Geometry

#-----

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_distance

_geom_bond_publ_flag

#<< enter YES for value to be published

| | | | | | |
|-----|------|---|---|-----------|---|
| Ir1 | P1 | . | . | 2.2698(8) | ? |
| Ir1 | C111 | . | . | 2.024(3) | ? |
| Ir1 | C121 | . | . | 2.045(3) | ? |
| Ir1 | C131 | . | . | 2.038(3) | ? |
| Ir1 | C141 | . | . | 2.033(3) | ? |
| Ir2 | P2 | . | . | 2.2668(8) | ? |
| Ir2 | C211 | . | . | 2.044(3) | ? |
| Ir2 | C221 | . | . | 2.041(3) | ? |
| Ir2 | C231 | . | . | 2.034(3) | ? |
| Ir2 | C241 | . | . | 2.041(3) | ? |
| Cu1 | C111 | . | . | 1.999(3) | ? |
| Cu1 | C112 | . | . | 2.134(3) | ? |
| Cu1 | C211 | . | . | 1.995(3) | ? |
| Cu1 | C212 | . | . | 2.228(3) | ? |
| Cu2 | C121 | . | . | 1.984(3) | ? |
| Cu2 | C122 | . | . | 2.245(3) | ? |
| Cu2 | C221 | . | . | 1.995(3) | ? |
| Cu2 | C222 | . | . | 2.175(3) | ? |
| Cu3 | C131 | . | . | 1.988(3) | ? |
| Cu3 | C132 | . | . | 2.203(3) | ? |

| | | | | | |
|------|--------|---|---|-----------|---|
| Cu3 | C231 | . | . | 1.983(3) | ? |
| Cu3 | C232 | . | . | 2.189(3) | ? |
| Cu4 | C141 | . | . | 2.004(3) | ? |
| Cu4 | C142 | . | . | 2.184(3) | ? |
| Cu4 | C241 | . | . | 1.995(3) | ? |
| Cu4 | C242 | . | . | 2.189(3) | ? |
| Fe11 | C1121 | . | . | 2.035(3) | ? |
| Fe11 | C1122 | . | . | 2.035(3) | ? |
| Fe11 | C1123 | . | . | 2.047(3) | ? |
| Fe11 | C1124 | . | . | 2.049(4) | ? |
| Fe11 | C1125 | . | . | 2.035(3) | ? |
| Fe11 | C1121' | . | . | 2.034(4) | ? |
| Fe11 | C1122' | . | . | 2.039(4) | ? |
| Fe11 | C1123' | . | . | 2.042(4) | ? |
| Fe11 | C1124' | . | . | 2.053(4) | ? |
| Fe11 | C1125' | . | . | 2.039(4) | ? |
| Fe21 | C2121 | . | . | 2.062(3) | ? |
| Fe21 | C2122 | . | . | 2.038(3) | ? |
| Fe21 | C2123 | . | . | 2.030(3) | ? |
| Fe21 | C2124 | . | . | 2.035(3) | ? |
| Fe21 | C2125 | . | . | 2.044(3) | ? |
| Fe21 | C2121' | . | . | 2.048(4) | ? |
| Fe21 | C2122' | . | . | 2.055(4) | ? |
| Fe21 | C2123' | . | . | 2.046(5) | ? |
| Fe21 | C2124' | . | . | 2.038(5) | ? |
| Fe21 | C2125' | . | . | 2.042(4) | ? |
| Fe12 | C1221 | . | . | 2.055(4) | ? |
| Fe12 | C1222 | . | . | 2.045(4) | ? |
| Fe12 | C1223 | . | . | 2.039(4) | ? |
| Fe12 | C1224 | . | . | 2.033(4) | ? |
| Fe12 | C1225 | . | . | 2.030(4) | ? |
| Fe12 | C1221' | . | . | 2.041(4) | ? |
| Fe12 | C1222' | . | . | 2.029(6) | ? |
| Fe12 | C1223' | . | . | 2.023(6) | ? |
| Fe12 | C1224' | . | . | 2.040(5) | ? |
| Fe12 | C1225' | . | . | 2.061(4) | ? |
| Fe22 | C2221 | . | . | 2.067(3) | ? |
| Fe22 | C2222 | . | . | 2.055(3) | ? |
| Fe22 | C2223 | . | . | 2.051(3) | ? |
| Fe22 | C2224 | . | . | 2.052(3) | ? |
| Fe22 | C2225 | . | . | 2.048(3) | ? |
| Fe22 | C2221' | . | . | 2.049(3) | ? |
| Fe22 | C2222' | . | . | 2.049(3) | ? |
| Fe22 | C2223' | . | . | 2.055(3) | ? |
| Fe22 | C2224' | . | . | 2.065(4) | ? |
| Fe22 | C2225' | . | . | 2.058(4) | ? |
| Fe13 | C1321 | . | . | 2.051(3) | ? |
| Fe13 | C1322 | . | . | 2.051(3) | ? |
| Fe13 | C1323 | . | . | 2.054(3) | ? |
| Fe13 | C1324 | . | . | 2.037(4) | ? |
| Fe13 | C1325 | . | . | 2.035(3) | ? |
| Fe13 | C1321' | . | . | 2.078(7) | ? |
| Fe13 | C1322' | . | . | 2.053(8) | ? |
| Fe13 | C1323' | . | . | 2.006(10) | ? |
| Fe13 | C1324' | . | . | 2.034(9) | ? |
| Fe13 | C1325' | . | . | 2.071(6) | ? |
| Fe13 | C1321" | . | . | 1.982(11) | ? |
| Fe13 | C1322" | . | . | 2.017(11) | ? |
| Fe13 | C1323" | . | . | 2.045(8) | ? |
| Fe13 | C1324" | . | . | 2.066(8) | ? |
| Fe13 | C1325" | . | . | 2.031(9) | ? |

| | | | | | |
|-------|--------|---|---|----------|---|
| Fe23 | C2321 | . | . | 2.041(4) | ? |
| Fe23 | C2322 | . | . | 2.030(3) | ? |
| Fe23 | C2323 | . | . | 2.053(4) | ? |
| Fe23 | C2324 | . | . | 2.045(4) | ? |
| Fe23 | C2325 | . | . | 2.036(4) | ? |
| Fe23 | C2321' | . | . | 2.038(4) | ? |
| Fe23 | C2322' | . | . | 2.023(4) | ? |
| Fe23 | C2323' | . | . | 2.043(6) | ? |
| Fe23 | C2324' | . | . | 2.051(5) | ? |
| Fe23 | C2325' | . | . | 2.046(4) | ? |
| Fe14 | C1421 | . | . | 2.055(3) | ? |
| Fe14 | C1422 | . | . | 2.042(4) | ? |
| Fe14 | C1423 | . | . | 2.050(3) | ? |
| Fe14 | C1424 | . | . | 2.053(3) | ? |
| Fe14 | C1425 | . | . | 2.054(3) | ? |
| Fe14 | C1421' | . | . | 2.042(4) | ? |
| Fe14 | C1422' | . | . | 2.051(3) | ? |
| Fe14 | C1423' | . | . | 2.053(4) | ? |
| Fe14 | C1424' | . | . | 2.052(4) | ? |
| Fe14 | C1425' | . | . | 2.045(4) | ? |
| Fe24 | C2421 | . | . | 2.039(3) | ? |
| Fe24 | C2422 | . | . | 2.035(3) | ? |
| Fe24 | C2423 | . | . | 2.046(3) | ? |
| Fe24 | C2424 | . | . | 2.045(4) | ? |
| Fe24 | C2425 | . | . | 2.034(4) | ? |
| Fe24 | C2421' | . | . | 2.033(4) | ? |
| Fe24 | C2422' | . | . | 2.038(4) | ? |
| Fe24 | C2423' | . | . | 2.053(4) | ? |
| Fe24 | C2424' | . | . | 2.055(3) | ? |
| Fe24 | C2425' | . | . | 2.035(3) | ? |
| P1 | C1011 | . | . | 1.835(4) | ? |
| P1 | C1021 | . | . | 1.834(3) | ? |
| P1 | C1031 | . | . | 1.814(3) | ? |
| C1011 | C1012 | . | . | 1.397(5) | ? |
| C1011 | C1016 | . | . | 1.393(4) | ? |
| C1012 | C1013 | . | . | 1.387(6) | ? |
| C1012 | H1012 | . | . | .968 | ? |
| C1013 | C1014 | . | . | 1.383(6) | ? |
| C1013 | H1013 | . | . | .962 | ? |
| C1014 | C1015 | . | . | 1.384(6) | ? |
| C1014 | H1014 | . | . | .959 | ? |
| C1015 | C1016 | . | . | 1.392(6) | ? |
| C1015 | H1015 | . | . | .964 | ? |
| C1016 | H1016 | . | . | .967 | ? |
| C1021 | C1022 | . | . | 1.399(5) | ? |
| C1021 | C1026 | . | . | 1.387(5) | ? |
| C1022 | C1023 | . | . | 1.391(5) | ? |
| C1022 | H1022 | . | . | .965 | ? |
| C1023 | C1024 | . | . | 1.379(6) | ? |
| C1023 | H1023 | . | . | .966 | ? |
| C1024 | C1025 | . | . | 1.389(5) | ? |
| C1024 | H1024 | . | . | .968 | ? |
| C1025 | C1026 | . | . | 1.387(5) | ? |
| C1025 | H1025 | . | . | .961 | ? |
| C1026 | H1026 | . | . | .964 | ? |
| C1031 | C1032 | . | . | 1.404(4) | ? |
| C1031 | C1036 | . | . | 1.406(5) | ? |
| C1032 | C1033 | . | . | 1.394(5) | ? |
| C1032 | H1032 | . | . | .967 | ? |
| C1033 | C1034 | . | . | 1.384(6) | ? |
| C1033 | H1033 | . | . | .968 | ? |

| | | | | | |
|--------|--------|---|---|-----------|---|
| C1034 | C1035 | . | . | 1.383(6) | ? |
| C1034 | H1034 | . | . | .970 | ? |
| C1035 | C1036 | . | . | 1.389(5) | ? |
| C1035 | H1035 | . | . | .961 | ? |
| C1036 | H1036 | . | . | .976 | ? |
| P2 | C2011 | . | . | 1.831(4) | ? |
| P2 | C2021 | . | . | 1.820(4) | ? |
| P2 | C2031 | . | . | 1.834(4) | ? |
| C2011 | C2012 | . | . | 1.402(5) | ? |
| C2011 | C2016 | . | . | 1.383(5) | ? |
| C2012 | C2013 | . | . | 1.395(6) | ? |
| C2012 | H2012 | . | . | .962 | ? |
| C2013 | C2014 | . | . | 1.380(5) | ? |
| C2013 | H2013 | . | . | .966 | ? |
| C2014 | C2015 | . | . | 1.340(6) | ? |
| C2014 | H2014 | . | . | .966 | ? |
| C2015 | C2016 | . | . | 1.384(7) | ? |
| C2015 | H2015 | . | . | .969 | ? |
| C2016 | H2016 | . | . | .968 | ? |
| C2021 | C2022 | . | . | 1.412(7) | ? |
| C2021 | C2026 | . | . | 1.392(6) | ? |
| C2022 | C2023 | . | . | 1.389(8) | ? |
| C2022 | H2022 | . | . | .999 | ? |
| C2023 | C2024 | . | . | 1.359(11) | ? |
| C2023 | H2023 | . | . | 1.008 | ? |
| C2024 | C2025 | . | . | 1.411(12) | ? |
| C2024 | H2024 | . | . | .966 | ? |
| C2025 | C2026 | . | . | 1.408(7) | ? |
| C2025 | H2025 | . | . | .985 | ? |
| C2026 | H2026 | . | . | .983 | ? |
| C2031 | C2032 | . | . | 1.392(5) | ? |
| C2031 | C2036 | . | . | 1.407(5) | ? |
| C2032 | C2033 | . | . | 1.398(5) | ? |
| C2032 | H2032 | . | . | .981 | ? |
| C2033 | C2034 | . | . | 1.379(5) | ? |
| C2033 | H2033 | . | . | .970 | ? |
| C2034 | C2035 | . | . | 1.386(6) | ? |
| C2034 | H2034 | . | . | .961 | ? |
| C2035 | C2036 | . | . | 1.399(6) | ? |
| C2035 | H2035 | . | . | .959 | ? |
| C2036 | H2036 | . | . | .968 | ? |
| C111 | C112 | . | . | 1.235(5) | ? |
| C112 | C1121 | . | . | 1.434(4) | ? |
| C1121 | C1122 | . | . | 1.433(4) | ? |
| C1121 | C1125 | . | . | 1.439(5) | ? |
| C1122 | C1123 | . | . | 1.421(5) | ? |
| C1122 | H1122 | . | . | .962 | ? |
| C1123 | C1124 | . | . | 1.414(6) | ? |
| C1123 | H1123 | . | . | .965 | ? |
| C1124 | C1125 | . | . | 1.424(4) | ? |
| C1124 | H1124 | . | . | .960 | ? |
| C1125 | H1125 | . | . | .965 | ? |
| C1121' | C1122' | . | . | 1.411(6) | ? |
| C1121' | C1125' | . | . | 1.424(7) | ? |
| C1121' | H1121' | . | . | .976 | ? |
| C1122' | C1123' | . | . | 1.429(6) | ? |
| C1122' | H1122' | . | . | .968 | ? |
| C1123' | C1124' | . | . | 1.418(7) | ? |
| C1123' | H1123' | . | . | .968 | ? |
| C1124' | C1125' | . | . | 1.426(5) | ? |
| C1124' | H1124' | . | . | .964 | ? |

C1125' H1125' . . .974 ?
C121 C122 . . 1.222(4) ?
C122 C1221 . . 1.446(4) ?
C1221 C1222 . . 1.436(4) ?
C1221 C1225 . . 1.434(5) ?
C1222 C1223 . . 1.414(5) ?
C1222 H1222 . . .971 ?
C1223 C1224 . . 1.411(5) ?
C1223 H1223 . . .965 ?
C1224 C1225 . . 1.422(5) ?
C1224 H1224 . . .954 ?
C1225 H1225 . . .966 ?
C1221' C1222' . . 1.378(7) ?
C1221' C1225' . . 1.371(7) ?
C1221' H1221' . . .965 ?
C1222' C1223' . . 1.491(8) ?
C1222' H1222' . . .966 ?
C1223' C1224' . . 1.407(7) ?
C1223' H1223' . . .980 ?
C1224' C1225' . . 1.378(7) ?
C1224' H1224' . . .958 ?
C1225' H1225' . . .977 ?
C131 C132 . . 1.210(4) ?
C132 C1321 . . 1.445(5) ?
C1321 C1322 . . 1.433(5) ?
C1321 C1325 . . 1.439(5) ?
C1322 C1323 . . 1.425(6) ?
C1322 H1322 . . .971 ?
C1323 C1324 . . 1.416(6) ?
C1323 H1323 . . .970 ?
C1324 C1325 . . 1.417(5) ?
C1324 H1324 . . .963 ?
C1325 H1325 . . .964 ?
C1321' C1322' . . 1.409(10) ?
C1321' C1325' . . 1.432(11) ?
C1321' H1321' . . .941 ?
C1322' C1323' . . 1.508(15) ?
C1322' H1322' . . .930 ?
C1323' C1324' . . 1.369(14) ?
C1323' H1323' . . .931 ?
C1324' C1325' . . 1.436(13) ?
C1324' H1324' . . .949 ?
C1325' H1325' . . .943 ?
C1321" C1322" . . 1.346(16) ?
C1321" C1325" . . 1.427(18) ?
C1321" H1321" . . .925 ?
C1322" C1323" . . 1.410(16) ?
C1322" H1322" . . .941 ?
C1323" C1324" . . 1.368(13) ?
C1323" H1323" . . .935 ?
C1324" C1325" . . 1.402(13) ?
C1324" H1324" . . .934 ?
C1325" H1325" . . .924 ?
C141 C142 . . 1.230(4) ?
C142 C1421 . . 1.439(4) ?
C1421 C1422 . . 1.440(4) ?
C1421 C1425 . . 1.432(4) ?
C1422 C1423 . . 1.413(4) ?
C1422 H1422 . . .962 ?
C1423 C1424 . . 1.420(4) ?
C1423 H1423 . . .962 ?

| | | | | | |
|--------|--------|---|---|----------|---|
| C1424 | C1425 | . | . | 1.426(4) | ? |
| C1424 | H1424 | . | . | .957 | ? |
| C1425 | H1425 | . | . | .963 | ? |
| C1421' | C1422' | . | . | 1.414(5) | ? |
| C1421' | C1425' | . | . | 1.429(5) | ? |
| C1421' | H1421' | . | . | .967 | ? |
| C1422' | C1423' | . | . | 1.414(5) | ? |
| C1422' | H1422' | . | . | .962 | ? |
| C1423' | C1424' | . | . | 1.402(5) | ? |
| C1423' | H1423' | . | . | .962 | ? |
| C1424' | C1425' | . | . | 1.410(5) | ? |
| C1424' | H1424' | . | . | .972 | ? |
| C1425' | H1425' | . | . | .965 | ? |
| C211 | C212 | . | . | 1.218(5) | ? |
| C212 | C2121 | . | . | 1.451(5) | ? |
| C2121 | C2122 | . | . | 1.430(4) | ? |
| C2121 | C2125 | . | . | 1.435(5) | ? |
| C2122 | C2123 | . | . | 1.417(5) | ? |
| C2122 | H2122 | . | . | .962 | ? |
| C2123 | C2124 | . | . | 1.419(5) | ? |
| C2123 | H2123 | . | . | .965 | ? |
| C2124 | C2125 | . | . | 1.418(5) | ? |
| C2124 | H2124 | . | . | .968 | ? |
| C2125 | H2125 | . | . | .964 | ? |
| C2121' | C2122' | . | . | 1.413(6) | ? |
| C2121' | C2125' | . | . | 1.407(7) | ? |
| C2121' | H2121' | . | . | .969 | ? |
| C2122' | C2123' | . | . | 1.391(7) | ? |
| C2122' | H2122' | . | . | .974 | ? |
| C2123' | C2124' | . | . | 1.400(6) | ? |
| C2123' | H2123' | . | . | .964 | ? |
| C2124' | C2125' | . | . | 1.459(7) | ? |
| C2124' | H2124' | . | . | .960 | ? |
| C2125' | H2125' | . | . | .971 | ? |
| C221 | C222 | . | . | 1.220(4) | ? |
| C222 | C2221 | . | . | 1.450(4) | ? |
| C2221 | C2222 | . | . | 1.426(5) | ? |
| C2221 | C2225 | . | . | 1.434(5) | ? |
| C2222 | C2223 | . | . | 1.416(5) | ? |
| C2222 | H2222 | . | . | .961 | ? |
| C2223 | C2224 | . | . | 1.419(6) | ? |
| C2223 | H2223 | . | . | .963 | ? |
| C2224 | C2225 | . | . | 1.431(5) | ? |
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| C2225 | H2225 | . | . | .963 | ? |
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| C2221' | H2221' | . | . | .966 | ? |
| C2222' | C2223' | . | . | 1.407(6) | ? |
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| C2223' | C2224' | . | . | 1.427(6) | ? |
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| C2225' | H2225' | . | . | .965 | ? |
| C231 | C232 | . | . | 1.224(5) | ? |
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| C2325 | H2325 | . | . | .969 | ? |
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| C242 | C2421 | . | . | 1.453(4) | ? |
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| C1122 | Fe11 | C1123' | . . . | 119.09(16) | ? |
| C1122 | Fe11 | C1124' | . . . | 153.08(13) | ? |
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| C1123 | Fe11 | C1124' | . . . | 120.15(14) | ? |
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| C2121 | Fe21 | C2124 | . . . | 68.52(14) | ? |
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| C2121 | Fe21 | C2121' | . . . | 110.76(15) | ? |
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| C2221 | Fe22 | C2225 | . . . | 40.80(15) | ? |
| C2221 | Fe22 | C2221' | . . . | 107.79(13) | ? |
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| C2222 | Fe22 | C2224 | . . . | 68.07(15) | ? |
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| C2222 | Fe22 | C2223' | . . . | 131.32(14) | ? |
| C2222 | Fe22 | C2224' | . . . | 170.94(14) | ? |
| C2222 | Fe22 | C2225' | . . . | 146.88(14) | ? |
| C2223 | Fe22 | C2224 | . . . | 40.48(15) | ? |
| C2223 | Fe22 | C2225 | . . . | 68.42(13) | ? |
| C2223 | Fe22 | C2221' | . . . | 146.77(16) | ? |
| C2223 | Fe22 | C2222' | . . . | 115.66(14) | ? |
| C2223 | Fe22 | C2223' | . . . | 109.79(13) | ? |
| C2223 | Fe22 | C2224' | . . . | 133.01(15) | ? |
| C2223 | Fe22 | C2225' | . . . | 172.07(17) | ? |
| C2224 | Fe22 | C2225 | . . . | 40.84(13) | ? |
| C2224 | Fe22 | C2221' | . . . | 171.06(15) | ? |
| C2224 | Fe22 | C2222' | . . . | 148.03(14) | ? |
| C2224 | Fe22 | C2223' | . . . | 117.35(14) | ? |
| C2224 | Fe22 | C2224' | . . . | 110.68(16) | ? |
| C2224 | Fe22 | C2225' | . . . | 133.08(17) | ? |
| C2225 | Fe22 | C2221' | . . . | 131.13(14) | ? |
| C2225 | Fe22 | C2222' | . . . | 169.71(15) | ? |
| C2225 | Fe22 | C2223' | . . . | 149.25(16) | ? |
| C2225 | Fe22 | C2224' | . . . | 117.02(17) | ? |
| C2225 | Fe22 | C2225' | . . . | 109.48(15) | ? |
| C2221' | Fe22 | C2222' | . . . | 40.50(14) | ? |
| C2221' | Fe22 | C2223' | . . . | 67.83(14) | ? |
| C2221' | Fe22 | C2224' | . . . | 67.97(16) | ? |
| C2221' | Fe22 | C2225' | . . . | 40.31(18) | ? |
| C2222' | Fe22 | C2223' | . . . | 40.10(15) | ? |
| C2222' | Fe22 | C2224' | . . . | 67.87(16) | ? |
| C2222' | Fe22 | C2225' | . . . | 67.80(16) | ? |
| C2223' | Fe22 | C2224' | . . . | 40.52(16) | ? |
| C2223' | Fe22 | C2225' | . . . | 67.82(14) | ? |
| C2224' | Fe22 | C2225' | . . . | 40.37(16) | ? |
| C1321 | Fe13 | C1322 | . . . | 40.90(13) | ? |
| C1321 | Fe13 | C1323 | . . . | 68.76(13) | ? |
| C1321 | Fe13 | C1324 | . . . | 68.88(15) | ? |
| C1321 | Fe13 | C1325 | . . . | 41.24(15) | ? |
| C1321 | Fe13 | C1321' | . . . | 109.6(2) | ? |
| C1321 | Fe13 | C1322' | . . . | 136.6(3) | ? |
| C1321 | Fe13 | C1323' | . . . | 177.6(3) | ? |
| C1321 | Fe13 | C1324' | . . . | 138.1(3) | ? |
| C1321 | Fe13 | C1325' | . . . | 109.2(2) | ? |
| C1321 | Fe13 | C1321" | . . . | 109.7(4) | ? |
| C1321 | Fe13 | C1322" | . . . | 123.6(4) | ? |
| C1321 | Fe13 | C1323" | . . . | 159.9(3) | ? |
| C1321 | Fe13 | C1324" | . . . | 159.6(2) | ? |
| C1321 | Fe13 | C1325" | . . . | 122.8(3) | ? |

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| C1322 | Fe13 | C1323 | . . . | 40.61(16) | ? |
| C1322 | Fe13 | C1324 | . . . | 68.34(16) | ? |
| C1322 | Fe13 | C1325 | . . . | 68.78(14) | ? |
| C1322 | Fe13 | C1321' | . . . | 112.8(2) | ? |
| C1322 | Fe13 | C1322' | . . . | 111.8(3) | ? |
| C1322 | Fe13 | C1323' | . . . | 141.4(3) | ? |
| C1322 | Fe13 | C1324' | . . . | 178.6(3) | ? |
| C1322 | Fe13 | C1325' | . . . | 139.3(2) | ? |
| C1322 | Fe13 | C1321" | . . . | 127.9(4) | ? |
| C1322 | Fe13 | C1322" | . . . | 111.3(3) | ? |
| C1322 | Fe13 | C1323" | . . . | 124.6(3) | ? |
| C1322 | Fe13 | C1324" | . . . | 157.6(2) | ? |
| C1322 | Fe13 | C1325" | . . . | 162.2(3) | ? |
| C1323 | Fe13 | C1324 | . . . | 40.50(16) | ? |
| C1323 | Fe13 | C1325 | . . . | 68.54(14) | ? |
| C1323 | Fe13 | C1321' | . . . | 142.5(2) | ? |
| C1323 | Fe13 | C1322' | . . . | 114.7(2) | ? |
| C1323 | Fe13 | C1323' | . . . | 113.5(3) | ? |
| C1323 | Fe13 | C1324' | . . . | 139.0(3) | ? |
| C1323 | Fe13 | C1325' | . . . | 176.7(2) | ? |
| C1323 | Fe13 | C1321" | . . . | 164.1(4) | ? |
| C1323 | Fe13 | C1322" | . . . | 127.3(3) | ? |
| C1323 | Fe13 | C1323" | . . . | 109.3(2) | ? |
| C1323 | Fe13 | C1324" | . . . | 121.4(2) | ? |
| C1323 | Fe13 | C1325" | . . . | 153.0(3) | ? |
| C1324 | Fe13 | C1325 | . . . | 40.74(14) | ? |
| C1324 | Fe13 | C1321' | . . . | 176.4(2) | ? |
| C1324 | Fe13 | C1322' | . . . | 143.4(3) | ? |
| C1324 | Fe13 | C1323' | . . . | 112.2(3) | ? |
| C1324 | Fe13 | C1324' | . . . | 110.6(3) | ? |
| C1324 | Fe13 | C1325' | . . . | 136.5(3) | ? |
| C1324 | Fe13 | C1321" | . . . | 155.0(4) | ? |
| C1324 | Fe13 | C1322" | . . . | 161.9(3) | ? |
| C1324 | Fe13 | C1323" | . . . | 123.6(3) | ? |
| C1324 | Fe13 | C1324" | . . . | 106.5(3) | ? |
| C1324 | Fe13 | C1325" | . . . | 116.7(3) | ? |
| C1325 | Fe13 | C1321' | . . . | 136.0(2) | ? |
| C1325 | Fe13 | C1322' | . . . | 175.9(2) | ? |
| C1325 | Fe13 | C1323' | . . . | 138.3(4) | ? |
| C1325 | Fe13 | C1324' | . . . | 109.9(3) | ? |
| C1325 | Fe13 | C1325' | . . . | 108.2(2) | ? |
| C1325 | Fe13 | C1321" | . . . | 121.5(3) | ? |
| C1325 | Fe13 | C1322" | . . . | 157.2(3) | ? |
| C1325 | Fe13 | C1323" | . . . | 158.3(3) | ? |
| C1325 | Fe13 | C1324" | . . . | 122.4(3) | ? |
| C1325 | Fe13 | C1325" | . . . | 103.3(3) | ? |
| C1321' | Fe13 | C1322' | . . . | 39.9(3) | ? |
| C1321' | Fe13 | C1323' | . . . | 69.2(4) | ? |
| C1321' | Fe13 | C1324' | . . . | 68.2(3) | ? |
| C1321' | Fe13 | C1325' | . . . | 40.4(3) | ? |
| C1322' | Fe13 | C1323' | . . . | 43.6(4) | ? |
| C1322' | Fe13 | C1324' | . . . | 69.5(4) | ? |
| C1322' | Fe13 | C1325' | . . . | 68.6(3) | ? |
| C1323' | Fe13 | C1324' | . . . | 39.6(4) | ? |
| C1323' | Fe13 | C1325' | . . . | 68.5(3) | ? |
| C1324' | Fe13 | C1325' | . . . | 41.0(4) | ? |
| C1321" | Fe13 | C1322" | . . . | 39.3(5) | ? |
| C1321" | Fe13 | C1323" | . . . | 66.3(4) | ? |
| C1321" | Fe13 | C1324" | . . . | 65.7(4) | ? |
| C1321" | Fe13 | C1325" | . . . | 41.6(5) | ? |
| C1322" | Fe13 | C1323" | . . . | 40.6(4) | ? |

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| C1322" | Fe13 | C1324" | . . . | 66.6(4) | ? |
| C1322" | Fe13 | C1325" | . . . | 69.6(4) | ? |
| C1323" | Fe13 | C1324" | . . . | 38.9(4) | ? |
| C1323" | Fe13 | C1325" | . . . | 68.4(4) | ? |
| C1324" | Fe13 | C1325" | . . . | 40.0(4) | ? |
| C2321 | Fe23 | C2322 | . . . | 41.27(15) | ? |
| C2321 | Fe23 | C2323 | . . . | 68.84(15) | ? |
| C2321 | Fe23 | C2324 | . . . | 68.75(15) | ? |
| C2321 | Fe23 | C2325 | . . . | 41.38(13) | ? |
| C2321 | Fe23 | C2321' | . . . | 105.16(17) | ? |
| C2321 | Fe23 | C2322' | . . . | 121.55(17) | ? |
| C2321 | Fe23 | C2323' | . . . | 159.23(15) | ? |
| C2321 | Fe23 | C2324' | . . . | 157.35(18) | ? |
| C2321 | Fe23 | C2325' | . . . | 120.52(18) | ? |
| C2322 | Fe23 | C2323 | . . . | 40.81(14) | ? |
| C2322 | Fe23 | C2324 | . . . | 68.74(14) | ? |
| C2322 | Fe23 | C2325 | . . . | 69.42(14) | ? |
| C2322 | Fe23 | C2321' | . . . | 121.10(15) | ? |
| C2322 | Fe23 | C2322' | . . . | 106.69(15) | ? |
| C2322 | Fe23 | C2323' | . . . | 124.12(17) | ? |
| C2322 | Fe23 | C2324' | . . . | 161.02(18) | ? |
| C2322 | Fe23 | C2325' | . . . | 156.84(17) | ? |
| C2323 | Fe23 | C2324 | . . . | 40.59(15) | ? |
| C2323 | Fe23 | C2325 | . . . | 68.63(16) | ? |
| C2323 | Fe23 | C2321' | . . . | 158.32(15) | ? |
| C2323 | Fe23 | C2322' | . . . | 123.35(18) | ? |
| C2323 | Fe23 | C2323' | . . . | 109.9(2) | ? |
| C2323 | Fe23 | C2324' | . . . | 125.91(17) | ? |
| C2323 | Fe23 | C2325' | . . . | 160.53(15) | ? |
| C2324 | Fe23 | C2325 | . . . | 40.53(16) | ? |
| C2324 | Fe23 | C2321' | . . . | 158.51(18) | ? |
| C2324 | Fe23 | C2322' | . . . | 159.9(2) | ? |
| C2324 | Fe23 | C2323' | . . . | 124.7(2) | ? |
| C2324 | Fe23 | C2324' | . . . | 109.99(16) | ? |
| C2324 | Fe23 | C2325' | . . . | 123.53(16) | ? |
| C2325 | Fe23 | C2321' | . . . | 121.45(18) | ? |
| C2325 | Fe23 | C2322' | . . . | 158.1(2) | ? |
| C2325 | Fe23 | C2323' | . . . | 159.01(16) | ? |
| C2325 | Fe23 | C2324' | . . . | 122.78(17) | ? |
| C2325 | Fe23 | C2325' | . . . | 106.21(18) | ? |
| C2321' | Fe23 | C2322' | . . . | 40.8(2) | ? |
| C2321' | Fe23 | C2323' | . . . | 67.9(2) | ? |
| C2321' | Fe23 | C2324' | . . . | 67.29(18) | ? |
| C2321' | Fe23 | C2325' | . . . | 40.48(16) | ? |
| C2322' | Fe23 | C2323' | . . . | 40.5(2) | ? |
| C2322' | Fe23 | C2324' | . . . | 67.62(18) | ? |
| C2322' | Fe23 | C2325' | . . . | 68.43(18) | ? |
| C2323' | Fe23 | C2324' | . . . | 39.91(19) | ? |
| C2323' | Fe23 | C2325' | . . . | 67.8(2) | ? |
| C2324' | Fe23 | C2325' | . . . | 40.0(2) | ? |
| C1421 | Fe14 | C1422 | . . . | 41.15(12) | ? |
| C1421 | Fe14 | C1423 | . . . | 68.48(13) | ? |
| C1421 | Fe14 | C1424 | . . . | 68.56(12) | ? |
| C1421 | Fe14 | C1425 | . . . | 40.80(12) | ? |
| C1421 | Fe14 | C1421' | . . . | 106.16(14) | ? |
| C1421 | Fe14 | C1422' | . . . | 123.18(13) | ? |
| C1421 | Fe14 | C1423' | . . . | 160.21(12) | ? |
| C1421 | Fe14 | C1424' | . . . | 157.39(13) | ? |
| C1421 | Fe14 | C1425' | . . . | 121.11(13) | ? |
| C1422 | Fe14 | C1423 | . . . | 40.41(12) | ? |
| C1422 | Fe14 | C1424 | . . . | 68.37(13) | ? |

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| C1422 | Fe14 | C1425 | . . . | 68.72(13) | ? |
| C1422 | Fe14 | C1421' | . . . | 120.86(14) | ? |
| C1422 | Fe14 | C1422' | . . . | 107.27(13) | ? |
| C1422 | Fe14 | C1423' | . . . | 124.17(13) | ? |
| C1422 | Fe14 | C1424' | . . . | 160.74(13) | ? |
| C1422 | Fe14 | C1425' | . . . | 157.02(13) | ? |
| C1423 | Fe14 | C1424 | . . . | 40.48(12) | ? |
| C1423 | Fe14 | C1425 | . . . | 68.25(13) | ? |
| C1423 | Fe14 | C1421' | . . . | 156.93(14) | ? |
| C1423 | Fe14 | C1422' | . . . | 122.41(14) | ? |
| C1423 | Fe14 | C1423' | . . . | 108.98(14) | ? |
| C1423 | Fe14 | C1424' | . . . | 125.36(13) | ? |
| C1423 | Fe14 | C1425' | . . . | 161.11(13) | ? |
| C1424 | Fe14 | C1425 | . . . | 40.64(12) | ? |
| C1424 | Fe14 | C1421' | . . . | 160.43(14) | ? |
| C1424 | Fe14 | C1422' | . . . | 158.14(15) | ? |
| C1424 | Fe14 | C1423' | . . . | 123.14(13) | ? |
| C1424 | Fe14 | C1424' | . . . | 109.16(13) | ? |
| C1424 | Fe14 | C1425' | . . . | 124.38(13) | ? |
| C1425 | Fe14 | C1421' | . . . | 123.23(13) | ? |
| C1425 | Fe14 | C1422' | . . . | 159.73(14) | ? |
| C1425 | Fe14 | C1423' | . . . | 158.19(13) | ? |
| C1425 | Fe14 | C1424' | . . . | 122.72(13) | ? |
| C1425 | Fe14 | C1425' | . . . | 107.44(14) | ? |
| C1421' | Fe14 | C1422' | . . . | 40.44(15) | ? |
| C1421' | Fe14 | C1423' | . . . | 68.06(15) | ? |
| C1421' | Fe14 | C1424' | . . . | 68.06(15) | ? |
| C1421' | Fe14 | C1425' | . . . | 40.93(15) | ? |
| C1422' | Fe14 | C1423' | . . . | 40.31(14) | ? |
| C1422' | Fe14 | C1424' | . . . | 67.48(14) | ? |
| C1422' | Fe14 | C1425' | . . . | 68.05(14) | ? |
| C1423' | Fe14 | C1424' | . . . | 39.94(13) | ? |
| C1423' | Fe14 | C1425' | . . . | 67.77(15) | ? |
| C1424' | Fe14 | C1425' | . . . | 40.26(14) | ? |
| C2421 | Fe24 | C2422 | . . . | 41.34(14) | ? |
| C2421 | Fe24 | C2423 | . . . | 69.09(13) | ? |
| C2421 | Fe24 | C2424 | . . . | 68.97(13) | ? |
| C2421 | Fe24 | C2425 | . . . | 41.11(14) | ? |
| C2421 | Fe24 | C2421' | . . . | 105.55(13) | ? |
| C2421 | Fe24 | C2422' | . . . | 127.68(15) | ? |
| C2421 | Fe24 | C2423' | . . . | 166.84(16) | ? |
| C2421 | Fe24 | C2424' | . . . | 149.87(15) | ? |
| C2421 | Fe24 | C2425' | . . . | 115.09(14) | ? |
| C2422 | Fe24 | C2423 | . . . | 41.09(13) | ? |
| C2422 | Fe24 | C2424 | . . . | 68.73(14) | ? |
| C2422 | Fe24 | C2425 | . . . | 69.17(14) | ? |
| C2422 | Fe24 | C2421' | . . . | 116.25(14) | ? |
| C2422 | Fe24 | C2422' | . . . | 108.17(15) | ? |
| C2422 | Fe24 | C2423' | . . . | 129.88(16) | ? |
| C2422 | Fe24 | C2424' | . . . | 168.24(15) | ? |
| C2422 | Fe24 | C2425' | . . . | 149.24(14) | ? |
| C2423 | Fe24 | C2424 | . . . | 40.23(17) | ? |
| C2423 | Fe24 | C2425 | . . . | 68.50(15) | ? |
| C2423 | Fe24 | C2421' | . . . | 151.36(17) | ? |
| C2423 | Fe24 | C2422' | . . . | 119.47(17) | ? |
| C2423 | Fe24 | C2423' | . . . | 110.64(15) | ? |
| C2423 | Fe24 | C2424' | . . . | 130.13(15) | ? |
| C2423 | Fe24 | C2425' | . . . | 167.50(16) | ? |
| C2424 | Fe24 | C2425 | . . . | 40.85(14) | ? |
| C2424 | Fe24 | C2421' | . . . | 166.02(17) | ? |
| C2424 | Fe24 | C2422' | . . . | 152.71(16) | ? |

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| C2424 | Fe24 | C2423' | . | . | . | 119.91(15) | ? |
| C2424 | Fe24 | C2424' | . | . | . | 109.33(15) | ? |
| C2424 | Fe24 | C2425' | . | . | . | 128.65(16) | ? |
| C2425 | Fe24 | C2421' | . | . | . | 126.80(15) | ? |
| C2425 | Fe24 | C2422' | . | . | . | 165.55(15) | ? |
| C2425 | Fe24 | C2423' | . | . | . | 151.89(16) | ? |
| C2425 | Fe24 | C2424' | . | . | . | 117.51(16) | ? |
| C2425 | Fe24 | C2425' | . | . | . | 106.35(15) | ? |
| C2421' | Fe24 | C2422' | . | . | . | 40.54(17) | ? |
| C2421' | Fe24 | C2423' | . | . | . | 68.03(15) | ? |
| C2421' | Fe24 | C2424' | . | . | . | 68.54(15) | ? |
| C2421' | Fe24 | C2425' | . | . | . | 40.78(16) | ? |
| C2422' | Fe24 | C2423' | . | . | . | 40.17(17) | ? |
| C2422' | Fe24 | C2424' | . | . | . | 67.88(16) | ? |
| C2422' | Fe24 | C2425' | . | . | . | 68.25(16) | ? |
| C2423' | Fe24 | C2424' | . | . | . | 40.15(17) | ? |
| C2423' | Fe24 | C2425' | . | . | . | 68.16(16) | ? |
| C2424' | Fe24 | C2425' | . | . | . | 41.01(15) | ? |
| Ir1 | P1 | C1011 | . | . | . | 113.64(9) | ? |
| Ir1 | P1 | C1021 | . | . | . | 115.65(10) | ? |
| Ir1 | P1 | C1031 | . | . | . | 116.64(11) | ? |
| C1011 | P1 | C1021 | . | . | . | 102.49(15) | ? |
| C1011 | P1 | C1031 | . | . | . | 102.49(15) | ? |
| C1021 | P1 | C1031 | . | . | . | 104.10(13) | ? |
| P1 | C1011 | C1012 | . | . | . | 122.2(3) | ? |
| P1 | C1011 | C1016 | . | . | . | 118.7(2) | ? |
| C1012 | C1011 | C1016 | . | . | . | 119.1(3) | ? |
| C1011 | C1012 | C1013 | . | . | . | 120.4(3) | ? |
| C1011 | C1012 | H1012 | . | . | . | 119.8 | ? |
| C1013 | C1012 | H1012 | . | . | . | 119.8 | ? |
| C1012 | C1013 | C1014 | . | . | . | 120.1(4) | ? |
| C1012 | C1013 | H1013 | . | . | . | 119.8 | ? |
| C1014 | C1013 | H1013 | . | . | . | 120.1 | ? |
| C1013 | C1014 | C1015 | . | . | . | 120.1(4) | ? |
| C1013 | C1014 | H1014 | . | . | . | 120.0 | ? |
| C1015 | C1014 | H1014 | . | . | . | 120.0 | ? |
| C1014 | C1015 | C1016 | . | . | . | 120.1(3) | ? |
| C1014 | C1015 | H1015 | . | . | . | 119.2 | ? |
| C1016 | C1015 | H1015 | . | . | . | 120.6 | ? |
| C1011 | C1016 | C1015 | . | . | . | 120.2(3) | ? |
| C1011 | C1016 | H1016 | . | . | . | 120.1 | ? |
| C1015 | C1016 | H1016 | . | . | . | 119.7 | ? |
| P1 | C1021 | C1022 | . | . | . | 120.2(3) | ? |
| P1 | C1021 | C1026 | . | . | . | 121.1(2) | ? |
| C1022 | C1021 | C1026 | . | . | . | 118.6(3) | ? |
| C1021 | C1022 | C1023 | . | . | . | 120.2(3) | ? |
| C1021 | C1022 | H1022 | . | . | . | 119.8 | ? |
| C1023 | C1022 | H1022 | . | . | . | 119.9 | ? |
| C1022 | C1023 | C1024 | . | . | . | 120.6(3) | ? |
| C1022 | C1023 | H1023 | . | . | . | 119.7 | ? |
| C1024 | C1023 | H1023 | . | . | . | 119.7 | ? |
| C1023 | C1024 | C1025 | . | . | . | 119.5(3) | ? |
| C1023 | C1024 | H1024 | . | . | . | 120.5 | ? |
| C1025 | C1024 | H1024 | . | . | . | 119.9 | ? |
| C1024 | C1025 | C1026 | . | . | . | 120.1(4) | ? |
| C1024 | C1025 | H1025 | . | . | . | 119.3 | ? |
| C1026 | C1025 | H1025 | . | . | . | 120.5 | ? |
| C1021 | C1026 | C1025 | . | . | . | 120.9(3) | ? |
| C1021 | C1026 | H1026 | . | . | . | 119.5 | ? |
| C1025 | C1026 | H1026 | . | . | . | 119.6 | ? |
| P1 | C1031 | C1032 | . | . | . | 122.6(3) | ? |

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|-------|-------|-------|---|---|---|------------|---|
| P1 | C1031 | C1036 | . | . | . | 118.5(2) | ? |
| C1032 | C1031 | C1036 | . | . | . | 118.7(3) | ? |
| C1031 | C1032 | C1033 | . | . | . | 120.1(4) | ? |
| C1031 | C1032 | H1032 | . | . | . | 119.8 | ? |
| C1033 | C1032 | H1032 | . | . | . | 120.1 | ? |
| C1032 | C1033 | C1034 | . | . | . | 120.4(3) | ? |
| C1032 | C1033 | H1033 | . | . | . | 119.1 | ? |
| C1034 | C1033 | H1033 | . | . | . | 120.5 | ? |
| C1033 | C1034 | C1035 | . | . | . | 120.1(4) | ? |
| C1033 | C1034 | H1034 | . | . | . | 120.1 | ? |
| C1035 | C1034 | H1034 | . | . | . | 119.8 | ? |
| C1034 | C1035 | C1036 | . | . | . | 120.3(4) | ? |
| C1034 | C1035 | H1035 | . | . | . | 119.3 | ? |
| C1036 | C1035 | H1035 | . | . | . | 120.3 | ? |
| C1031 | C1036 | C1035 | . | . | . | 120.3(3) | ? |
| C1031 | C1036 | H1036 | . | . | . | 119.9 | ? |
| C1035 | C1036 | H1036 | . | . | . | 119.8 | ? |
| Ir2 | P2 | C2011 | . | . | . | 117.93(10) | ? |
| Ir2 | P2 | C2021 | . | . | . | 112.30(12) | ? |
| Ir2 | P2 | C2031 | . | . | . | 114.24(10) | ? |
| C2011 | P2 | C2021 | . | . | . | 103.43(16) | ? |
| C2011 | P2 | C2031 | . | . | . | 101.40(17) | ? |
| C2021 | P2 | C2031 | . | . | . | 106.13(17) | ? |
| P2 | C2011 | C2012 | . | . | . | 122.2(2) | ? |
| P2 | C2011 | C2016 | . | . | . | 119.8(3) | ? |
| C2012 | C2011 | C2016 | . | . | . | 117.8(4) | ? |
| C2011 | C2012 | C2013 | . | . | . | 119.7(3) | ? |
| C2011 | C2012 | H2012 | . | . | . | 119.9 | ? |
| C2013 | C2012 | H2012 | . | . | . | 120.4 | ? |
| C2012 | C2013 | C2014 | . | . | . | 120.5(4) | ? |
| C2012 | C2013 | H2013 | . | . | . | 119.8 | ? |
| C2014 | C2013 | H2013 | . | . | . | 119.7 | ? |
| C2013 | C2014 | C2015 | . | . | . | 119.8(4) | ? |
| C2013 | C2014 | H2014 | . | . | . | 119.7 | ? |
| C2015 | C2014 | H2014 | . | . | . | 120.5 | ? |
| C2014 | C2015 | C2016 | . | . | . | 120.8(4) | ? |
| C2014 | C2015 | H2015 | . | . | . | 119.9 | ? |
| C2016 | C2015 | H2015 | . | . | . | 119.3 | ? |
| C2011 | C2016 | C2015 | . | . | . | 121.3(4) | ? |
| C2011 | C2016 | H2016 | . | . | . | 119.0 | ? |
| C2015 | C2016 | H2016 | . | . | . | 119.7 | ? |
| P2 | C2021 | C2022 | . | . | . | 119.9(3) | ? |
| P2 | C2021 | C2026 | . | . | . | 119.3(3) | ? |
| C2022 | C2021 | C2026 | . | . | . | 120.3(4) | ? |
| C2021 | C2022 | C2023 | . | . | . | 119.3(6) | ? |
| C2021 | C2022 | H2022 | . | . | . | 119.3 | ? |
| C2023 | C2022 | H2022 | . | . | . | 121.3 | ? |
| C2022 | C2023 | C2024 | . | . | . | 121.1(7) | ? |
| C2022 | C2023 | H2023 | . | . | . | 120.3 | ? |
| C2024 | C2023 | H2023 | . | . | . | 118.6 | ? |
| C2023 | C2024 | C2025 | . | . | . | 120.5(6) | ? |
| C2023 | C2024 | H2024 | . | . | . | 120.4 | ? |
| C2025 | C2024 | H2024 | . | . | . | 119.1 | ? |
| C2024 | C2025 | C2026 | . | . | . | 119.5(6) | ? |
| C2024 | C2025 | H2025 | . | . | . | 121.2 | ? |
| C2026 | C2025 | H2025 | . | . | . | 119.3 | ? |
| C2021 | C2026 | C2025 | . | . | . | 119.3(5) | ? |
| C2021 | C2026 | H2026 | . | . | . | 119.3 | ? |
| C2025 | C2026 | H2026 | . | . | . | 121.5 | ? |
| P2 | C2031 | C2032 | . | . | . | 118.5(2) | ? |
| P2 | C2031 | C2036 | . | . | . | 122.7(3) | ? |

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|--------|--------|--------|---|---|---|-----------|---|
| C2032 | C2031 | C2036 | . | . | . | 118.8(3) | ? |
| C2031 | C2032 | C2033 | . | . | . | 120.6(3) | ? |
| C2031 | C2032 | H2032 | . | . | . | 119.8 | ? |
| C2033 | C2032 | H2032 | . | . | . | 119.6 | ? |
| C2032 | C2033 | C2034 | . | . | . | 120.2(4) | ? |
| C2032 | C2033 | H2033 | . | . | . | 120.3 | ? |
| C2034 | C2033 | H2033 | . | . | . | 119.5 | ? |
| C2033 | C2034 | C2035 | . | . | . | 120.1(4) | ? |
| C2033 | C2034 | H2034 | . | . | . | 120.1 | ? |
| C2035 | C2034 | H2034 | . | . | . | 119.8 | ? |
| C2034 | C2035 | C2036 | . | . | . | 120.2(4) | ? |
| C2034 | C2035 | H2035 | . | . | . | 119.7 | ? |
| C2036 | C2035 | H2035 | . | . | . | 120.1 | ? |
| C2031 | C2036 | C2035 | . | . | . | 120.1(3) | ? |
| C2031 | C2036 | H2036 | . | . | . | 120.1 | ? |
| C2035 | C2036 | H2036 | . | . | . | 119.8 | ? |
| Ir1 | C111 | Cu1 | . | . | . | 95.11(11) | ? |
| Ir1 | C111 | C112 | . | . | . | 172.2(3) | ? |
| Cu1 | C111 | C112 | . | . | . | 78.7(2) | ? |
| Cu1 | C112 | C111 | . | . | . | 66.75(17) | ? |
| Cu1 | C112 | C1121 | . | . | . | 138.1(2) | ? |
| C111 | C112 | C1121 | . | . | . | 155.2(3) | ? |
| Fe11 | C1121 | C112 | . | . | . | 123.4(2) | ? |
| Fe11 | C1121 | C1122 | . | . | . | 69.37(17) | ? |
| Fe11 | C1121 | C1125 | . | . | . | 69.30(17) | ? |
| C112 | C1121 | C1122 | . | . | . | 123.6(3) | ? |
| C112 | C1121 | C1125 | . | . | . | 129.4(3) | ? |
| C1122 | C1121 | C1125 | . | . | . | 106.9(3) | ? |
| Fe11 | C1122 | C1121 | . | . | . | 69.40(18) | ? |
| Fe11 | C1122 | C1123 | . | . | . | 70.1(2) | ? |
| Fe11 | C1122 | H1122 | . | . | . | 126.5 | ? |
| C1121 | C1122 | C1123 | . | . | . | 108.6(3) | ? |
| C1121 | C1122 | H1122 | . | . | . | 125.2 | ? |
| C1123 | C1122 | H1122 | . | . | . | 126.2 | ? |
| Fe11 | C1123 | C1122 | . | . | . | 69.2(2) | ? |
| Fe11 | C1123 | C1124 | . | . | . | 69.9(2) | ? |
| Fe11 | C1123 | H1123 | . | . | . | 126.2 | ? |
| C1122 | C1123 | C1124 | . | . | . | 108.0(3) | ? |
| C1122 | C1123 | H1123 | . | . | . | 125.7 | ? |
| C1124 | C1123 | H1123 | . | . | . | 126.3 | ? |
| Fe11 | C1124 | C1123 | . | . | . | 69.7(2) | ? |
| Fe11 | C1124 | C1125 | . | . | . | 69.1(2) | ? |
| Fe11 | C1124 | H1124 | . | . | . | 126.7 | ? |
| C1123 | C1124 | C1125 | . | . | . | 108.6(3) | ? |
| C1123 | C1124 | H1124 | . | . | . | 125.3 | ? |
| C1125 | C1124 | H1124 | . | . | . | 126.1 | ? |
| Fe11 | C1125 | C1121 | . | . | . | 69.29(17) | ? |
| Fe11 | C1125 | C1124 | . | . | . | 70.11(19) | ? |
| Fe11 | C1125 | H1125 | . | . | . | 125.7 | ? |
| C1121 | C1125 | C1124 | . | . | . | 108.0(3) | ? |
| C1121 | C1125 | H1125 | . | . | . | 126.1 | ? |
| C1124 | C1125 | H1125 | . | . | . | 125.9 | ? |
| Fe11 | C1121' | C1122' | . | . | . | 69.9(2) | ? |
| Fe11 | C1121' | C1125' | . | . | . | 69.7(2) | ? |
| Fe11 | C1121' | H1121' | . | . | . | 124.5 | ? |
| C1122' | C1121' | C1125' | . | . | . | 108.0(3) | ? |
| C1122' | C1121' | H1121' | . | . | . | 125.9 | ? |
| C1125' | C1121' | H1121' | . | . | . | 126.1 | ? |
| Fe11 | C1122' | C1121' | . | . | . | 69.5(2) | ? |
| Fe11 | C1122' | C1123' | . | . | . | 69.6(2) | ? |
| Fe11 | C1122' | H1122' | . | . | . | 127.3 | ? |

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|--------|--------|--------|-------|-----------|---|
| C1121' | C1122' | C1123' | . . . | 108.0(4) | ? |
| C1121' | C1122' | H1122' | . . . | 126.6 | ? |
| C1123' | C1122' | H1122' | . . . | 125.3 | ? |
| Fe11 | C1123' | C1122' | . . . | 69.4(2) | ? |
| Fe11 | C1123' | C1124' | . . . | 70.2(2) | ? |
| Fe11 | C1123' | H1123' | . . . | 126.0 | ? |
| C1122' | C1123' | C1124' | . . . | 108.2(3) | ? |
| C1122' | C1123' | H1123' | . . . | 126.1 | ? |
| C1124' | C1123' | H1123' | . . . | 125.7 | ? |
| Fe11 | C1124' | C1123' | . . . | 69.3(2) | ? |
| Fe11 | C1124' | C1125' | . . . | 69.1(2) | ? |
| Fe11 | C1124' | H1124' | . . . | 126.4 | ? |
| C1123' | C1124' | C1125' | . . . | 107.5(4) | ? |
| C1123' | C1124' | H1124' | . . . | 126.3 | ? |
| C1125' | C1124' | H1124' | . . . | 126.2 | ? |
| Fe11 | C1125' | C1121' | . . . | 69.3(2) | ? |
| Fe11 | C1125' | C1124' | . . . | 70.1(2) | ? |
| Fe11 | C1125' | H1125' | . . . | 126.5 | ? |
| C1121' | C1125' | C1124' | . . . | 108.2(4) | ? |
| C1121' | C1125' | H1125' | . . . | 126.8 | ? |
| C1124' | C1125' | H1125' | . . . | 125.0 | ? |
| Ir1 | C121 | Cu2 | . . . | 89.41(13) | ? |
| Ir1 | C121 | C122 | . . . | 173.8(3) | ? |
| Cu2 | C121 | C122 | . . . | 85.4(2) | ? |
| Cu2 | C122 | C121 | . . . | 61.7(2) | ? |
| Cu2 | C122 | C1221 | . . . | 127.4(2) | ? |
| C121 | C122 | C1221 | . . . | 169.9(3) | ? |
| Fe12 | C1221 | C122 | . . . | 127.8(3) | ? |
| Fe12 | C1221 | C1222 | . . . | 69.1(2) | ? |
| Fe12 | C1221 | C1225 | . . . | 68.5(2) | ? |
| C122 | C1221 | C1222 | . . . | 126.5(3) | ? |
| C122 | C1221 | C1225 | . . . | 126.2(3) | ? |
| C1222 | C1221 | C1225 | . . . | 107.4(3) | ? |
| Fe12 | C1222 | C1221 | . . . | 69.87(19) | ? |
| Fe12 | C1222 | C1223 | . . . | 69.5(2) | ? |
| Fe12 | C1222 | H1222 | . . . | 126.6 | ? |
| C1221 | C1222 | C1223 | . . . | 107.7(3) | ? |
| C1221 | C1222 | H1222 | . . . | 126.1 | ? |
| C1223 | C1222 | H1222 | . . . | 126.2 | ? |
| Fe12 | C1223 | C1222 | . . . | 69.9(2) | ? |
| Fe12 | C1223 | C1224 | . . . | 69.5(2) | ? |
| Fe12 | C1223 | H1223 | . . . | 126.4 | ? |
| C1222 | C1223 | C1224 | . . . | 108.8(3) | ? |
| C1222 | C1223 | H1223 | . . . | 125.8 | ? |
| C1224 | C1223 | H1223 | . . . | 125.4 | ? |
| Fe12 | C1224 | C1223 | . . . | 70.0(2) | ? |
| Fe12 | C1224 | C1225 | . . . | 69.4(2) | ? |
| Fe12 | C1224 | H1224 | . . . | 126.9 | ? |
| C1223 | C1224 | C1225 | . . . | 108.2(3) | ? |
| C1223 | C1224 | H1224 | . . . | 125.5 | ? |
| C1225 | C1224 | H1224 | . . . | 126.3 | ? |
| Fe12 | C1225 | C1221 | . . . | 70.4(2) | ? |
| Fe12 | C1225 | C1224 | . . . | 69.6(2) | ? |
| Fe12 | C1225 | H1225 | . . . | 126.4 | ? |
| C1221 | C1225 | C1224 | . . . | 107.8(3) | ? |
| C1221 | C1225 | H1225 | . . . | 126.4 | ? |
| C1224 | C1225 | H1225 | . . . | 125.7 | ? |
| Fe12 | C1221' | C1222' | . . . | 69.7(3) | ? |
| Fe12 | C1221' | C1225' | . . . | 71.3(3) | ? |
| Fe12 | C1221' | H1221' | . . . | 126.6 | ? |
| C1222' | C1221' | C1225' | . . . | 111.0(4) | ? |

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|--------|--------|--------|-------|-------------|
| C1222' | C1221' | H1221' | . . . | 124.1 ? |
| C1225' | C1221' | H1221' | . . . | 124.9 ? |
| Fe12 | C1222' | C1221' | . . . | 70.7(3) ? |
| Fe12 | C1222' | C1223' | . . . | 68.2(3) ? |
| Fe12 | C1222' | H1222' | . . . | 125.7 ? |
| C1221' | C1222' | C1223' | . . . | 105.6(4) ? |
| C1221' | C1222' | H1222' | . . . | 126.7 ? |
| C1223' | C1222' | H1222' | . . . | 127.6 ? |
| Fe12 | C1223' | C1222' | . . . | 68.6(3) ? |
| Fe12 | C1223' | C1224' | . . . | 70.4(3) ? |
| Fe12 | C1223' | H1223' | . . . | 125.0 ? |
| C1222' | C1223' | C1224' | . . . | 105.2(4) ? |
| C1222' | C1223' | H1223' | . . . | 127.7 ? |
| C1224' | C1223' | H1223' | . . . | 127.1 ? |
| Fe12 | C1224' | C1223' | . . . | 69.1(3) ? |
| Fe12 | C1224' | C1225' | . . . | 71.2(3) ? |
| Fe12 | C1224' | H1224' | . . . | 125.9 ? |
| C1223' | C1224' | C1225' | . . . | 109.7(4) ? |
| C1223' | C1224' | H1224' | . . . | 125.1 ? |
| C1225' | C1224' | H1224' | . . . | 125.2 ? |
| Fe12 | C1225' | C1221' | . . . | 69.7(3) ? |
| Fe12 | C1225' | C1224' | . . . | 69.5(3) ? |
| Fe12 | C1225' | H1225' | . . . | 125.2 ? |
| C1221' | C1225' | C1224' | . . . | 108.5(4) ? |
| C1221' | C1225' | H1225' | . . . | 125.5 ? |
| C1224' | C1225' | H1225' | . . . | 126.0 ? |
| Ir1 | C131 | Cu3 | . . . | 91.09(13) ? |
| Ir1 | C131 | C132 | . . . | 170.1(3) ? |
| Cu3 | C131 | C132 | . . . | 83.3(2) ? |
| Cu3 | C132 | C131 | . . . | 63.6(2) ? |
| Cu3 | C132 | C1321 | . . . | 128.9(2) ? |
| C131 | C132 | C1321 | . . . | 167.0(3) ? |
| Fe13 | C1321 | C132 | . . . | 123.5(2) ? |
| Fe13 | C1321 | C1322 | . . . | 69.55(18) ? |
| Fe13 | C1321 | C1325 | . . . | 68.79(18) ? |
| C132 | C1321 | C1322 | . . . | 125.5(3) ? |
| C132 | C1321 | C1325 | . . . | 127.5(3) ? |
| C1322 | C1321 | C1325 | . . . | 106.9(3) ? |
| Fe13 | C1322 | C1321 | . . . | 69.55(18) ? |
| Fe13 | C1322 | C1323 | . . . | 69.8(2) ? |
| Fe13 | C1322 | H1322 | . . . | 126.5 ? |
| C1321 | C1322 | C1323 | . . . | 108.4(3) ? |
| C1321 | C1322 | H1322 | . . . | 125.5 ? |
| C1323 | C1322 | H1322 | . . . | 126.1 ? |
| Fe13 | C1323 | C1322 | . . . | 69.58(18) ? |
| Fe13 | C1323 | C1324 | . . . | 69.1(2) ? |
| Fe13 | C1323 | H1323 | . . . | 126.6 ? |
| C1322 | C1323 | C1324 | . . . | 107.9(3) ? |
| C1322 | C1323 | H1323 | . . . | 126.7 ? |
| C1324 | C1323 | H1323 | . . . | 125.5 ? |
| Fe13 | C1324 | C1323 | . . . | 70.4(2) ? |
| Fe13 | C1324 | C1325 | . . . | 69.6(2) ? |
| Fe13 | C1324 | H1324 | . . . | 126.6 ? |
| C1323 | C1324 | C1325 | . . . | 108.7(4) ? |
| C1323 | C1324 | H1324 | . . . | 125.9 ? |
| C1325 | C1324 | H1324 | . . . | 125.4 ? |
| Fe13 | C1325 | C1321 | . . . | 69.97(19) ? |
| Fe13 | C1325 | C1324 | . . . | 69.7(2) ? |
| Fe13 | C1325 | H1325 | . . . | 126.0 ? |
| C1321 | C1325 | C1324 | . . . | 108.1(3) ? |
| C1321 | C1325 | H1325 | . . . | 125.7 ? |

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|--------|--------|--------|---|---|---|-----------|---|
| C1324 | C1325 | H1325 | . | . | . | 126.2 | ? |
| Fe13 | C1321' | C1322' | . | . | . | 69.1(4) | ? |
| Fe13 | C1321' | C1325' | . | . | . | 69.5(4) | ? |
| Fe13 | C1321' | H1321' | . | . | . | 127.8 | ? |
| C1322' | C1321' | C1325' | . | . | . | 109.8(7) | ? |
| C1322' | C1321' | H1321' | . | . | . | 123.9 | ? |
| C1325' | C1321' | H1321' | . | . | . | 126.3 | ? |
| Fe13 | C1322' | C1321' | . | . | . | 71.0(4) | ? |
| Fe13 | C1322' | C1323' | . | . | . | 66.5(5) | ? |
| Fe13 | C1322' | H1322' | . | . | . | 126.7 | ? |
| C1321' | C1322' | C1323' | . | . | . | 105.3(7) | ? |
| C1321' | C1322' | H1322' | . | . | . | 129.1 | ? |
| C1323' | C1322' | H1322' | . | . | . | 125.6 | ? |
| Fe13 | C1323' | C1322' | . | . | . | 69.9(5) | ? |
| Fe13 | C1323' | C1324' | . | . | . | 71.3(6) | ? |
| Fe13 | C1323' | H1323' | . | . | . | 125.3 | ? |
| C1322' | C1323' | C1324' | . | . | . | 108.1(9) | ? |
| C1322' | C1323' | H1323' | . | . | . | 127.0 | ? |
| C1324' | C1323' | H1323' | . | . | . | 124.9 | ? |
| Fe13 | C1324' | C1323' | . | . | . | 69.1(5) | ? |
| Fe13 | C1324' | C1325' | . | . | . | 70.9(5) | ? |
| Fe13 | C1324' | H1324' | . | . | . | 125.8 | ? |
| C1323' | C1324' | C1325' | . | . | . | 109.7(9) | ? |
| C1323' | C1324' | H1324' | . | . | . | 126.8 | ? |
| C1325' | C1324' | H1324' | . | . | . | 123.5 | ? |
| Fe13 | C1325' | C1321' | . | . | . | 70.1(4) | ? |
| Fe13 | C1325' | C1324' | . | . | . | 68.1(4) | ? |
| Fe13 | C1325' | H1325' | . | . | . | 126.8 | ? |
| C1321' | C1325' | C1324' | . | . | . | 107.1(6) | ? |
| C1321' | C1325' | H1325' | . | . | . | 125.2 | ? |
| C1324' | C1325' | H1325' | . | . | . | 127.7 | ? |
| Fe13 | C1321" | C1322" | . | . | . | 71.7(6) | ? |
| Fe13 | C1321" | C1325" | . | . | . | 71.0(6) | ? |
| Fe13 | C1321" | H1321" | . | . | . | 124.4 | ? |
| C1322" | C1321" | C1325" | . | . | . | 112.8(11) | ? |
| C1322" | C1321" | H1321" | . | . | . | 122.2 | ? |
| C1325" | C1321" | H1321" | . | . | . | 125.0 | ? |
| Fe13 | C1322" | C1321" | . | . | . | 68.9(7) | ? |
| Fe13 | C1322" | C1323" | . | . | . | 70.8(6) | ? |
| Fe13 | C1322" | H1322" | . | . | . | 125.0 | ? |
| C1321" | C1322" | C1323" | . | . | . | 106.2(11) | ? |
| C1321" | C1322" | H1322" | . | . | . | 127.7(12) | ? |
| C1323" | C1322" | H1322" | . | . | . | 126.2 | ? |
| Fe13 | C1323" | C1322" | . | . | . | 68.6(6) | ? |
| Fe13 | C1323" | C1324" | . | . | . | 71.4(5) | ? |
| Fe13 | C1323" | H1323" | . | . | . | 126.0 | ? |
| C1322" | C1323" | C1324" | . | . | . | 107.5(8) | ? |
| C1322" | C1323" | H1323" | . | . | . | 127.0 | ? |
| C1324" | C1323" | H1323" | . | . | . | 125.5 | ? |
| Fe13 | C1324" | C1323" | . | . | . | 69.8(5) | ? |
| Fe13 | C1324" | C1325" | . | . | . | 68.6(5) | ? |
| Fe13 | C1324" | H1324" | . | . | . | 129.2 | ? |
| C1323" | C1324" | C1325" | . | . | . | 111.6(9) | ? |
| C1323" | C1324" | H1324" | . | . | . | 126.5 | ? |
| C1325" | C1324" | H1324" | . | . | . | 122.0 | ? |
| Fe13 | C1325" | C1321" | . | . | . | 67.4(6) | ? |
| Fe13 | C1325" | C1324" | . | . | . | 71.3(5) | ? |
| Fe13 | C1325" | H1325" | . | . | . | 123.9 | ? |
| C1321" | C1325" | C1324" | . | . | . | 101.8(9) | ? |
| C1321" | C1325" | H1325" | . | . | . | 125.8 | ? |
| C1324" | C1325" | H1325" | . | . | . | 132.4 | ? |

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|--------|--------|--------|---|---|---|-----------|---|
| Ir1 | C141 | Cu4 | . | . | . | 90.61(10) | ? |
| Ir1 | C141 | C142 | . | . | . | 171.8(2) | ? |
| Cu4 | C141 | C142 | . | . | . | 81.14(19) | ? |
| Cu4 | C142 | C141 | . | . | . | 65.04(16) | ? |
| Cu4 | C142 | C1421 | . | . | . | 131.3(2) | ? |
| C141 | C142 | C1421 | . | . | . | 163.6(3) | ? |
| Fe14 | C1421 | C142 | . | . | . | 126.2(2) | ? |
| Fe14 | C1421 | C1422 | . | . | . | 68.9(2) | ? |
| Fe14 | C1421 | C1425 | . | . | . | 69.58(19) | ? |
| C142 | C1421 | C1422 | . | . | . | 127.1(3) | ? |
| C142 | C1421 | C1425 | . | . | . | 125.7(3) | ? |
| C1422 | C1421 | C1425 | . | . | . | 107.2(2) | ? |
| Fe14 | C1422 | C1421 | . | . | . | 69.9(2) | ? |
| Fe14 | C1422 | C1423 | . | . | . | 70.1(2) | ? |
| Fe14 | C1422 | H1422 | . | . | . | 126.0 | ? |
| C1421 | C1422 | C1423 | . | . | . | 108.1(3) | ? |
| C1421 | C1422 | H1422 | . | . | . | 126.0 | ? |
| C1423 | C1422 | H1422 | . | . | . | 125.9 | ? |
| Fe14 | C1423 | C1422 | . | . | . | 69.47(19) | ? |
| Fe14 | C1423 | C1424 | . | . | . | 69.85(19) | ? |
| Fe14 | C1423 | H1423 | . | . | . | 126.9 | ? |
| C1422 | C1423 | C1424 | . | . | . | 108.6(3) | ? |
| C1422 | C1423 | H1423 | . | . | . | 125.5 | ? |
| C1424 | C1423 | H1423 | . | . | . | 125.9 | ? |
| Fe14 | C1424 | C1423 | . | . | . | 69.67(17) | ? |
| Fe14 | C1424 | C1425 | . | . | . | 69.72(17) | ? |
| Fe14 | C1424 | H1424 | . | . | . | 126.2 | ? |
| C1423 | C1424 | C1425 | . | . | . | 108.0(3) | ? |
| C1423 | C1424 | H1424 | . | . | . | 126.0 | ? |
| C1425 | C1424 | H1424 | . | . | . | 126.0 | ? |
| Fe14 | C1425 | C1421 | . | . | . | 69.63(17) | ? |
| Fe14 | C1425 | C1424 | . | . | . | 69.64(18) | ? |
| Fe14 | C1425 | H1425 | . | . | . | 125.5 | ? |
| C1421 | C1425 | C1424 | . | . | . | 108.1(3) | ? |
| C1421 | C1425 | H1425 | . | . | . | 126.3 | ? |
| C1424 | C1425 | H1425 | . | . | . | 125.6 | ? |
| Fe14 | C1421' | C1422' | . | . | . | 70.1(2) | ? |
| Fe14 | C1421' | C1425' | . | . | . | 69.7(2) | ? |
| Fe14 | C1421' | H1421' | . | . | . | 125.6 | ? |
| C1422' | C1421' | C1425' | . | . | . | 107.4(3) | ? |
| C1422' | C1421' | H1421' | . | . | . | 126.2 | ? |
| C1425' | C1421' | H1421' | . | . | . | 126.4 | ? |
| Fe14 | C1422' | C1421' | . | . | . | 69.4(2) | ? |
| Fe14 | C1422' | C1423' | . | . | . | 69.95(19) | ? |
| Fe14 | C1422' | H1422' | . | . | . | 126.3 | ? |
| C1421' | C1422' | C1423' | . | . | . | 108.2(3) | ? |
| C1421' | C1422' | H1422' | . | . | . | 125.9 | ? |
| C1423' | C1422' | H1422' | . | . | . | 125.8 | ? |
| Fe14 | C1423' | C1422' | . | . | . | 69.7(2) | ? |
| Fe14 | C1423' | C1424' | . | . | . | 70.0(2) | ? |
| Fe14 | C1423' | H1423' | . | . | . | 126.0 | ? |
| C1422' | C1423' | C1424' | . | . | . | 108.0(3) | ? |
| C1422' | C1423' | H1423' | . | . | . | 125.8 | ? |
| C1424' | C1423' | H1423' | . | . | . | 126.2 | ? |
| Fe14 | C1424' | C1423' | . | . | . | 70.1(2) | ? |
| Fe14 | C1424' | C1425' | . | . | . | 69.6(2) | ? |
| Fe14 | C1424' | H1424' | . | . | . | 125.7 | ? |
| C1423' | C1424' | C1425' | . | . | . | 108.7(3) | ? |
| C1423' | C1424' | H1424' | . | . | . | 125.8 | ? |
| C1425' | C1424' | H1424' | . | . | . | 125.5 | ? |
| Fe14 | C1425' | C1421' | . | . | . | 69.4(2) | ? |

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|--------|--------|--------|-------|--------------|
| Fe14 | C1425' | C1424' | . . . | 70.1(2) ? |
| Fe14 | C1425' | H1425' | . . . | 126.4 ? |
| C1421' | C1425' | C1424' | . . . | 107.6(3) ? |
| C1421' | C1425' | H1425' | . . . | 126.2 ? |
| C1424' | C1425' | H1425' | . . . | 126.1 ? |
| Ir2 | C211 | Cu1 | . . . | 91.71(14) ? |
| Ir2 | C211 | C212 | . . . | 173.2(3) ? |
| Cu1 | C211 | C212 | . . . | 84.1(2) ? |
| Cu1 | C212 | C211 | . . . | 62.9(2) ? |
| Cu1 | C212 | C2121 | . . . | 127.74(19) ? |
| C211 | C212 | C2121 | . . . | 168.8(3) ? |
| Fe21 | C2121 | C212 | . . . | 128.22(19) ? |
| Fe21 | C2121 | C2122 | . . . | 68.67(18) ? |
| Fe21 | C2121 | C2125 | . . . | 68.9(2) ? |
| C212 | C2121 | C2122 | . . . | 127.3(3) ? |
| C212 | C2121 | C2125 | . . . | 125.5(3) ? |
| C2122 | C2121 | C2125 | . . . | 107.2(3) ? |
| Fe21 | C2122 | C2121 | . . . | 70.50(17) ? |
| Fe21 | C2122 | C2123 | . . . | 69.31(18) ? |
| Fe21 | C2122 | H2122 | . . . | 126.2 ? |
| C2121 | C2122 | C2123 | . . . | 108.5(3) ? |
| C2121 | C2122 | H2122 | . . . | 125.4 ? |
| C2123 | C2122 | H2122 | . . . | 126.1 ? |
| Fe21 | C2123 | C2122 | . . . | 69.91(16) ? |
| Fe21 | C2123 | C2124 | . . . | 69.74(17) ? |
| Fe21 | C2123 | H2123 | . . . | 125.0 ? |
| C2122 | C2123 | C2124 | . . . | 107.8(3) ? |
| C2122 | C2123 | H2123 | . . . | 125.7 ? |
| C2124 | C2123 | H2123 | . . . | 126.4 ? |
| Fe21 | C2124 | C2123 | . . . | 69.38(18) ? |
| Fe21 | C2124 | C2125 | . . . | 70.03(18) ? |
| Fe21 | C2124 | H2124 | . . . | 127.3 ? |
| C2123 | C2124 | C2125 | . . . | 108.6(3) ? |
| C2123 | C2124 | H2124 | . . . | 125.9 ? |
| C2125 | C2124 | H2124 | . . . | 125.5 ? |
| Fe21 | C2125 | C2121 | . . . | 70.22(18) ? |
| Fe21 | C2125 | C2124 | . . . | 69.3(2) ? |
| Fe21 | C2125 | H2125 | . . . | 126.1 ? |
| C2121 | C2125 | C2124 | . . . | 107.9(3) ? |
| C2121 | C2125 | H2125 | . . . | 126.0 ? |
| C2124 | C2125 | H2125 | . . . | 126.1 ? |
| Fe21 | C2121' | C2122' | . . . | 70.1(2) ? |
| Fe21 | C2121' | C2125' | . . . | 69.6(2) ? |
| Fe21 | C2121' | H2121' | . . . | 126.7 ? |
| C2122' | C2121' | C2125' | . . . | 108.8(4) ? |
| C2122' | C2121' | H2121' | . . . | 125.1 ? |
| C2125' | C2121' | H2121' | . . . | 126.1 ? |
| Fe21 | C2122' | C2121' | . . . | 69.6(2) ? |
| Fe21 | C2122' | C2123' | . . . | 69.8(3) ? |
| Fe21 | C2122' | H2122' | . . . | 126.0 ? |
| C2121' | C2122' | C2123' | . . . | 108.4(4) ? |
| C2121' | C2122' | H2122' | . . . | 125.4 ? |
| C2123' | C2122' | H2122' | . . . | 126.2 ? |
| Fe21 | C2123' | C2122' | . . . | 70.5(3) ? |
| Fe21 | C2123' | C2124' | . . . | 69.6(3) ? |
| Fe21 | C2123' | H2123' | . . . | 126.1 ? |
| C2122' | C2123' | C2124' | . . . | 109.0(4) ? |
| C2122' | C2123' | H2123' | . . . | 125.8 ? |
| C2124' | C2123' | H2123' | . . . | 125.2 ? |
| Fe21 | C2124' | C2123' | . . . | 70.3(3) ? |
| Fe21 | C2124' | C2125' | . . . | 69.2(3) ? |

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| Fe21 | C2124' | H2124' | . . . | 126.0 ? |
| C2123' | C2124' | C2125' | . . . | 107.6(4) ? |
| C2123' | C2124' | H2124' | . . . | 127.1 ? |
| C2125' | C2124' | H2124' | . . . | 125.3 ? |
| Fe21 | C2125' | C2121' | . . . | 70.1(2) ? |
| Fe21 | C2125' | C2124' | . . . | 68.9(2) ? |
| Fe21 | C2125' | H2125' | . . . | 124.9 ? |
| C2121' | C2125' | C2124' | . . . | 106.2(4) ? |
| C2121' | C2125' | H2125' | . . . | 127.5 ? |
| C2124' | C2125' | H2125' | . . . | 126.2 ? |
| Ir2 | C221 | Cu2 | . . . | 90.30(12) ? |
| Ir2 | C221 | C222 | . . . | 169.8(2) ? |
| Cu2 | C221 | C222 | . . . | 81.3(2) ? |
| Cu2 | C222 | C221 | . . . | 65.0(2) ? |
| Cu2 | C222 | C2221 | . . . | 133.4(2) ? |
| C221 | C222 | C2221 | . . . | 160.6(3) ? |
| Fe22 | C2221 | C222 | . . . | 128.1(2) ? |
| Fe22 | C2221 | C2222 | . . . | 69.30(17) ? |
| Fe22 | C2221 | C2225 | . . . | 68.88(18) ? |
| C222 | C2221 | C2222 | . . . | 129.3(3) ? |
| C222 | C2221 | C2225 | . . . | 123.3(3) ? |
| C2222 | C2221 | C2225 | . . . | 107.4(3) ? |
| Fe22 | C2222 | C2221 | . . . | 70.22(19) ? |
| Fe22 | C2222 | C2223 | . . . | 69.7(2) ? |
| Fe22 | C2222 | H2222 | . . . | 126.1 ? |
| C2221 | C2222 | C2223 | . . . | 108.5(3) ? |
| C2221 | C2222 | H2222 | . . . | 125.9 ? |
| C2223 | C2222 | H2222 | . . . | 125.6 ? |
| Fe22 | C2223 | C2222 | . . . | 69.98(17) ? |
| Fe22 | C2223 | C2224 | . . . | 69.82(18) ? |
| Fe22 | C2223 | H2223 | . . . | 126.4 ? |
| C2222 | C2223 | C2224 | . . . | 108.3 ? |
| C2222 | C2223 | H2223 | . . . | 125.9 ? |
| C2224 | C2223 | H2223 | . . . | 125.8 ? |
| Fe22 | C2224 | C2223 | . . . | 69.71(18) ? |
| Fe22 | C2224 | C2225 | . . . | 69.41(18) ? |
| Fe22 | C2224 | H2224 | . . . | 126.0 ? |
| C2223 | C2224 | C2225 | . . . | 107.9(3) ? |
| C2223 | C2224 | H2224 | . . . | 125.8 ? |
| C2225 | C2224 | H2224 | . . . | 126.3(4) ? |
| Fe22 | C2225 | C2221 | . . . | 70.32(18) ? |
| Fe22 | C2225 | C2224 | . . . | 69.75(18) ? |
| Fe22 | C2225 | H2225 | . . . | 125.5 ? |
| C2221 | C2225 | C2224 | . . . | 107.8(3) ? |
| C2221 | C2225 | H2225 | . . . | 125.5 ? |
| C2224 | C2225 | H2225 | . . . | 126.6 ? |
| Fe22 | C2221' | C2222' | . . . | 69.74(18) ? |
| Fe22 | C2221' | C2225' | . . . | 70.2(2) ? |
| Fe22 | C2221' | H2221' | . . . | 126.2 ? |
| C2222' | C2221' | C2225' | . . . | 107.9(3) ? |
| C2222' | C2221' | H2221' | . . . | 125.9 ? |
| C2225' | C2221' | H2221' | . . . | 126.2 ? |
| Fe22 | C2222' | C2221' | . . . | 69.8(2) ? |
| Fe22 | C2222' | C2223' | . . . | 70.2(2) ? |
| Fe22 | C2222' | H2222' | . . . | 125.5 ? |
| C2221' | C2222' | C2223' | . . . | 108.3(4) ? |
| C2221' | C2222' | H2222' | . . . | 126.1 ? |
| C2223' | C2222' | H2222' | . . . | 125.6 ? |
| Fe22 | C2223' | C2222' | . . . | 69.7(2) ? |
| Fe22 | C2223' | C2224' | . . . | 70.1(2) ? |
| Fe22 | C2223' | H2223' | . . . | 126.8 ? |

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|--------|--------|--------|-------|-------------|
| C2222' | C2223' | C2224' | . . . | 108.3(3) ? |
| C2222' | C2223' | H2223' | . . . | 126.3 ? |
| C2224' | C2223' | H2223' | . . . | 125.4 ? |
| Fe22 | C2224' | C2223' | . . . | 69.3(2) ? |
| Fe22 | C2224' | C2225' | . . . | 69.5(2) ? |
| Fe22 | C2224' | H2224' | . . . | 126.0 ? |
| C2223' | C2224' | C2225' | . . . | 107.2(4) ? |
| C2223' | C2224' | H2224' | . . . | 125.9 ? |
| C2225' | C2224' | H2224' | . . . | 126.8 ? |
| Fe22 | C2225' | C2221' | . . . | 69.5(2) ? |
| Fe22 | C2225' | C2224' | . . . | 70.1(2) ? |
| Fe22 | C2225' | H2225' | . . . | 125.6 ? |
| C2221' | C2225' | C2224' | . . . | 108.3(3) ? |
| C2221' | C2225' | H2225' | . . . | 125.2 ? |
| C2224' | C2225' | H2225' | . . . | 126.5 ? |
| Ir2 | C231 | Cu3 | . . . | 91.61(11) ? |
| Ir2 | C231 | C232 | . . . | 173.2(2) ? |
| Cu3 | C231 | C232 | . . . | 82.5(2) ? |
| Cu3 | C232 | C231 | . . . | 63.89(17) ? |
| Cu3 | C232 | C2321 | . . . | 131.6(2) ? |
| C231 | C232 | C2321 | . . . | 164.4(3) ? |
| Fe23 | C2321 | C232 | . . . | 127.5(2) ? |
| Fe23 | C2321 | C2322 | . . . | 69.0(2) ? |
| Fe23 | C2321 | C2325 | . . . | 69.1(2) ? |
| C232 | C2321 | C2322 | . . . | 127.8(3) ? |
| C232 | C2321 | C2325 | . . . | 124.9(3) ? |
| C2322 | C2321 | C2325 | . . . | 107.3(3) ? |
| Fe23 | C2322 | C2321 | . . . | 69.8(2) ? |
| Fe23 | C2322 | C2323 | . . . | 70.5(2) ? |
| Fe23 | C2322 | H2322 | . . . | 125.5 ? |
| C2321 | C2322 | C2323 | . . . | 108.1(3) ? |
| C2321 | C2322 | H2322 | . . . | 125.9 ? |
| C2323 | C2322 | H2322 | . . . | 126.0 ? |
| Fe23 | C2323 | C2322 | . . . | 68.73(19) ? |
| Fe23 | C2323 | C2324 | . . . | 69.4(2) ? |
| Fe23 | C2323 | H2323 | . . . | 127.4 ? |
| C2322 | C2323 | C2324 | . . . | 107.9(3) ? |
| C2322 | C2323 | H2323 | . . . | 125.6 ? |
| C2324 | C2323 | H2323 | . . . | 126.5 ? |
| Fe23 | C2324 | C2323 | . . . | 70.0(2) ? |
| Fe23 | C2324 | C2325 | . . . | 69.4(2) ? |
| Fe23 | C2324 | H2324 | . . . | 126.8 ? |
| C2323 | C2324 | C2325 | . . . | 108.8(3) ? |
| C2323 | C2324 | H2324 | . . . | 124.8 ? |
| C2325 | C2324 | H2324 | . . . | 126.3 ? |
| Fe23 | C2325 | C2321 | . . . | 69.5(2) ? |
| Fe23 | C2325 | C2324 | . . . | 70.1(2) ? |
| Fe23 | C2325 | H2325 | . . . | 126.4 ? |
| C2321 | C2325 | C2324 | . . . | 107.9(3) ? |
| C2321 | C2325 | H2325 | . . . | 126.4 ? |
| C2324 | C2325 | H2325 | . . . | 125.8 ? |
| Fe23 | C2321' | C2322' | . . . | 69.0(2) ? |
| Fe23 | C2321' | C2325' | . . . | 70.0(2) ? |
| Fe23 | C2321' | H2321' | . . . | 125.6 ? |
| C2322' | C2321' | C2325' | . . . | 108.0(4) ? |
| C2322' | C2321' | H2321' | . . . | 126.3 ? |
| C2325' | C2321' | H2321' | . . . | 125.7 ? |
| Fe23 | C2322' | C2321' | . . . | 70.2(2) ? |
| Fe23 | C2322' | C2323' | . . . | 70.5(3) ? |
| Fe23 | C2322' | H2322' | . . . | 126.5 ? |
| C2321' | C2322' | C2323' | . . . | 107.7(4) ? |

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|--------|--------|--------|-------|-------------|
| C2321' | C2322' | H2322' | . . . | 126.4 ? |
| C2323' | C2322' | H2322' | . . . | 125.9 ? |
| Fe23 | C2323' | C2322' | . . . | 69.0(3) ? |
| Fe23 | C2323' | C2324' | . . . | 70.3(3) ? |
| Fe23 | C2323' | H2323' | . . . | 125.1 ? |
| C2322' | C2323' | C2324' | . . . | 107.8(5) ? |
| C2322' | C2323' | H2323' | . . . | 127.0 ? |
| C2324' | C2323' | H2323' | . . . | 125.2 ? |
| Fe23 | C2324' | C2323' | . . . | 69.8(3) ? |
| Fe23 | C2324' | C2325' | . . . | 69.8(3) ? |
| Fe23 | C2324' | H2324' | . . . | 126.1 ? |
| C2323' | C2324' | C2325' | . . . | 109.2(4) ? |
| C2323' | C2324' | H2324' | . . . | 125.2 ? |
| C2325' | C2324' | H2324' | . . . | 125.6 ? |
| Fe23 | C2325' | C2321' | . . . | 69.5(2) ? |
| Fe23 | C2325' | C2324' | . . . | 70.2(3) ? |
| Fe23 | C2325' | H2325' | . . . | 126.1 ? |
| C2321' | C2325' | C2324' | . . . | 107.3(4) ? |
| C2321' | C2325' | H2325' | . . . | 126.7 ? |
| C2324' | C2325' | H2325' | . . . | 126.0 ? |
| Ir2 | C241 | Cu4 | . . . | 92.17(12) ? |
| Ir2 | C241 | C242 | . . . | 173.2(3) ? |
| Cu4 | C241 | C242 | . . . | 82.25(19) ? |
| Cu4 | C242 | C241 | . . . | 64.58(18) ? |
| Cu4 | C242 | C2421 | . . . | 129.7(2) ? |
| C241 | C242 | C2421 | . . . | 165.7(3) ? |
| Fe24 | C2421 | C242 | . . . | 124.0(2) ? |
| Fe24 | C2421 | C2422 | . . . | 69.16(17) ? |
| Fe24 | C2421 | C2425 | . . . | 69.24(18) ? |
| C242 | C2421 | C2422 | . . . | 127.2(3) ? |
| C242 | C2421 | C2425 | . . . | 125.5(3) ? |
| C2422 | C2421 | C2425 | . . . | 107.3(3) ? |
| Fe24 | C2422 | C2421 | . . . | 69.49(17) ? |
| Fe24 | C2422 | C2423 | . . . | 69.87(18) ? |
| Fe24 | C2422 | H2422 | . . . | 126.7 ? |
| C2421 | C2422 | C2423 | . . . | 107.6(3) ? |
| C2421 | C2422 | H2422 | . . . | 126.2 ? |
| C2423 | C2422 | H2422 | . . . | 126.2 ? |
| Fe24 | C2423 | C2422 | . . . | 69.03(17) ? |
| Fe24 | C2423 | C2424 | . . . | 69.9(2) ? |
| Fe24 | C2423 | H2423 | . . . | 127.1 ? |
| C2422 | C2423 | C2424 | . . . | 108.4(3) ? |
| C2422 | C2423 | H2423 | . . . | 125.8 ? |
| C2424 | C2423 | H2423 | . . . | 125.8 ? |
| Fe24 | C2424 | C2423 | . . . | 69.9(2) ? |
| Fe24 | C2424 | C2425 | . . . | 69.1(2) ? |
| Fe24 | C2424 | H2424 | . . . | 126.0 ? |
| C2423 | C2424 | C2425 | . . . | 108.4(3) ? |
| C2423 | C2424 | H2424 | . . . | 126.4 ? |
| C2425 | C2424 | H2424 | . . . | 125.2 ? |
| Fe24 | C2425 | C2421 | . . . | 69.7(2) ? |
| Fe24 | C2425 | C2424 | . . . | 70.0(2) ? |
| Fe24 | C2425 | H2425 | . . . | 126.5 ? |
| C2421 | C2425 | C2424 | . . . | 108.3(3) ? |
| C2421 | C2425 | H2425 | . . . | 125.8 ? |
| C2424 | C2425 | H2425 | . . . | 126.0 ? |
| Fe24 | C2421' | C2422' | . . . | 69.9(2) ? |
| Fe24 | C2421' | C2425' | . . . | 69.7(2) ? |
| Fe24 | C2421' | H2421' | . . . | 125.7 ? |
| C2422' | C2421' | C2425' | . . . | 107.8(3) ? |
| C2422' | C2421' | H2421' | . . . | 125.9 ? |

| | | | | |
|--------|--------|--------|-------|------------|
| C2425' | C2421' | H2421' | . . . | 126.4 ? |
| Fe24 | C2422' | C2421' | . . . | 69.6(2) ? |
| Fe24 | C2422' | C2423' | . . . | 70.5(2) ? |
| Fe24 | C2422' | H2422' | . . . | 125.5 ? |
| C2421' | C2422' | C2423' | . . . | 108.6(4) ? |
| C2421' | C2422' | H2422' | . . . | 125.7 ? |
| C2423' | C2422' | H2422' | . . . | 125.7 ? |
| Fe24 | C2423' | C2422' | . . . | 69.3(2) ? |
| Fe24 | C2423' | C2424' | . . . | 70.0(2) ? |
| Fe24 | C2423' | H2423' | . . . | 126.6 ? |
| C2422' | C2423' | C2424' | . . . | 108.5(4) ? |
| C2422' | C2423' | H2423' | . . . | 126.1 ? |
| C2424' | C2423' | H2423' | . . . | 125.4 ? |
| Fe24 | C2424' | C2423' | . . . | 69.9(2) ? |
| Fe24 | C2424' | C2425' | . . . | 68.7(2) ? |
| Fe24 | C2424' | H2424' | . . . | 126.9 ? |
| C2423' | C2424' | C2425' | . . . | 107.4(4) ? |
| C2423' | C2424' | H2424' | . . . | 126.0 ? |
| C2425' | C2424' | H2424' | . . . | 126.6 ? |
| Fe24 | C2425' | C2421' | . . . | 69.6(2) ? |
| Fe24 | C2425' | C2424' | . . . | 70.2(2) ? |
| Fe24 | C2425' | H2425' | . . . | 125.6 ? |
| C2421' | C2425' | C2424' | . . . | 107.7(4) ? |
| C2421' | C2425' | H2425' | . . . | 125.8 ? |
| C2424' | C2425' | H2425' | . . . | 126.5 ? |
| C102 | C101 | C106 | . . . | 119.6(4) ? |
| C102 | C101 | H101 | . . . | 120.5 ? |
| C106 | C101 | H101 | . . . | 119.9 ? |
| C101 | C102 | C103 | . . . | 120.2(5) ? |
| C101 | C102 | H102 | . . . | 119.4 ? |
| C103 | C102 | H102 | . . . | 120.4 ? |
| C102 | C103 | C104 | . . . | 119.8(4) ? |
| C102 | C103 | H103 | . . . | 119.9 ? |
| C104 | C103 | H103 | . . . | 120.3 ? |
| C103 | C104 | C105 | . . . | 120.1(4) ? |
| C103 | C104 | H104 | . . . | 120.1 ? |
| C105 | C104 | H104 | . . . | 119.8 ? |
| C104 | C105 | C106 | . . . | 120.0(5) ? |
| C104 | C105 | H105 | . . . | 120.7 ? |
| C106 | C105 | H105 | . . . | 119.3 ? |
| C101 | C106 | C105 | . . . | 120.3(4) ? |
| C101 | C106 | H106 | . . . | 119.5 ? |
| C105 | C106 | H106 | . . . | 120.2 ? |
| C202 | C201 | C206 | . . . | 121.9(5) ? |
| C202 | C201 | H201 | . . . | 119.4 ? |
| C206 | C201 | H201 | . . . | 118.6 ? |
| C201 | C202 | C203 | . . . | 119.2(5) ? |
| C201 | C202 | H202 | . . . | 118.8 ? |
| C203 | C202 | H202 | . . . | 122.0 ? |
| C202 | C203 | C204 | . . . | 119.9(6) ? |
| C202 | C203 | H203 | . . . | 119.1 ? |
| C204 | C203 | H203 | . . . | 121.0 ? |
| C203 | C204 | C205 | . . . | 119.2(6) ? |
| C203 | C204 | H204 | . . . | 118.5 ? |
| C205 | C204 | H204 | . . . | 122.2 ? |
| C204 | C205 | C206 | . . . | 122.0(6) ? |
| C204 | C205 | H205 | . . . | 120.9 ? |
| C206 | C205 | H205 | . . . | 116.9 ? |
| C201 | C206 | C205 | . . . | 117.6(5) ? |
| C201 | C206 | H206 | . . . | 120.9 ? |
| C205 | C206 | H206 | . . . | 121.4 ? |

| | | | | | | | |
|-------|-------|-------|---|---|---|-----------|---|
| C302 | C301 | C306 | . | . | . | 119.9(5) | ? |
| C302 | C301 | H301 | . | . | . | 120.8 | ? |
| C306 | C301 | H301 | . | . | . | 119.3 | ? |
| C301 | C302 | C303 | . | . | . | 120.4(6) | ? |
| C301 | C302 | H302 | . | . | . | 118.9 | ? |
| C303 | C302 | H302 | . | . | . | 120.8 | ? |
| C302 | C303 | C304 | . | . | . | 120.2(5) | ? |
| C302 | C303 | H303 | . | . | . | 122.0 | ? |
| C304 | C303 | H303 | . | . | . | 117.8 | ? |
| C303 | C304 | C305 | . | . | . | 118.6(5) | ? |
| C303 | C304 | H304 | . | . | . | 120.9 | ? |
| C305 | C304 | H304 | . | . | . | 120.4 | ? |
| C304 | C305 | C306 | . | . | . | 121.0(6) | ? |
| C304 | C305 | H305 | . | . | . | 117.6 | ? |
| C306 | C305 | H305 | . | . | . | 121.3 | ? |
| C301 | C306 | C305 | . | . | . | 120.0(5) | ? |
| C301 | C306 | H306 | . | . | . | 120.2 | ? |
| C305 | C306 | H306 | . | . | . | 119.8 | ? |
| C402 | C401 | C406 | . | . | . | 120.0(6) | ? |
| C402 | C401 | H401 | . | . | . | 118.5 | ? |
| C406 | C401 | H401 | . | . | . | 121.5 | ? |
| C401 | C402 | C403 | . | . | . | 120.1(6) | ? |
| C401 | C402 | H402 | . | . | . | 126.9 | ? |
| C403 | C402 | H402 | . | . | . | 112.9 | ? |
| C402 | C403 | C404 | . | . | . | 117.7(8) | ? |
| C402 | C403 | H403 | . | . | . | 135.8 | ? |
| C404 | C403 | H403 | . | . | . | 106.4 | ? |
| C403 | C404 | C405 | . | . | . | 120.4(6) | ? |
| C403 | C404 | H404 | . | . | . | 130.7 | ? |
| C405 | C404 | H404 | . | . | . | 108.8 | ? |
| C404 | C405 | C406 | . | . | . | 118.7(7) | ? |
| C404 | C405 | H405 | . | . | . | 124.7 | ? |
| C406 | C405 | H405 | . | . | . | 116.5 | ? |
| C401 | C406 | C405 | . | . | . | 123.0(7) | ? |
| C401 | C406 | H406 | . | . | . | 116.6 | ? |
| C405 | C406 | H406 | . | . | . | 120.4 | ? |
| C502 | C501 | C506 | . | . | . | 120.1(12) | ? |
| C502 | C501 | H501 | . | . | . | 117 | ? |
| C506 | C501 | H501 | . | . | . | 121.8 | ? |
| C501 | C502 | C503 | . | . | . | 119.9(12) | ? |
| C501 | C502 | H502 | . | . | . | 122 | ? |
| C503 | C502 | H502 | . | . | . | 118 | ? |
| C502 | C503 | C504 | . | . | . | 120.0(10) | ? |
| C502 | C503 | H503 | . | . | . | 120 | ? |
| C504 | C503 | H503 | . | . | . | 119 | ? |
| C503 | C504 | C505 | . | . | . | 120.1(12) | ? |
| C503 | C504 | H504 | . | . | . | 118.8 | ? |
| C505 | C504 | H504 | . | . | . | 120 | ? |
| C504 | C505 | C506 | . | . | . | 119.8(12) | ? |
| C504 | C505 | H505 | . | . | . | 119 | ? |
| C506 | C505 | H505 | . | . | . | 121 | ? |
| C501 | C506 | C505 | . | . | . | 120.0(10) | ? |
| C501 | C506 | H506 | . | . | . | 119 | ? |
| C505 | C506 | H506 | . | . | . | 120 | ? |
| C502' | C501' | C506' | . | . | . | 120.0(9) | ? |
| C502' | C501' | H501' | . | . | . | 119.2 | ? |
| C506' | C501' | H501' | . | . | . | 120.6 | ? |
| C501' | C502' | C503' | . | . | . | 120.0(8) | ? |
| C501' | C502' | H502' | . | . | . | 120.8 | ? |
| C503' | C502' | H502' | . | . | . | 119.1 | ? |
| C502' | C503' | C504' | . | . | . | 120.0(8) | ? |

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C502' C503' H503' . . . 120.0 ?
C504' C503' H503' . . . 119.9 ?
C503' C504' C505' . . . 120.1(9) ?
C503' C504' H504' . . . 119.1 ?
C505' C504' H504' . . . 120.5 ?
C504' C505' C506' . . . 120.0(8) ?
C504' C505' H505' . . . 119.2 ?
C506' C505' H505' . . . 120.7 ?
C501' C506' C505' . . . 119.9(8) ?
C501' C506' H506' . . . 120.1 ?
C505' C506' H506' . . . 120.0 ?
C602 C601 H601 . . . 107.8 ?
C602 C601 C603 . . '2 666' 113.8(11) ?
H601 C601 C603 . . '2 666' 138.1 ?
C601 C602 C603 . . . 124.6(11) ?
C601 C602 H602 . . . 129.6 ?
C603 C602 H602 . . . 105.7 ?
C602 C603 H603 . . . 131.5 ?
C602 C603 C601 . . '2 666' 121.5(12) ?
H603 C603 C601 . . '2 666' 107.0 ?
O0 C0 H0a . . . 107.7 ?
O0 C0 H0b . . . 107.3 ?
O0 C0 H0c . . . 112.5 ?
H0a C0 H0b . . . 107.6 ?
H0a C0 H0c . . . 113.0 ?
H0b C0 H0c . . . 108.5 ?

```

```

loop_
  _geom_torsion_atom_site_label_1
  _geom_torsion_atom_site_label_2
  _geom_torsion_atom_site_label_3
  _geom_torsion_atom_site_label_4
  _geom_torsion_site_symmetry_1
  _geom_torsion_site_symmetry_2
  _geom_torsion_site_symmetry_3
  _geom_torsion_site_symmetry_4
  _geom_torsion
  _geom_torsion_publ_flag #<< enter YES for value to be published
  ? ? ? ? ? ? ? ? ? ?

```

```

loop_
  _geom_hbond_atom_site_label_D
  _geom_hbond_atom_site_label_H
  _geom_hbond_atom_site_label_A
  _geom_hbond_site_symmetry_D
  _geom_hbond_site_symmetry_H
  _geom_hbond_site_symmetry_A
  _geom_hbond_distance_DH
  _geom_hbond_distance_HA
  _geom_hbond_distance_DA
  _geom_hbond_angle_DHA
  _geom_hbond_publ_flag #<< enter YES for value to be published
  ? ? ? ? ? ? ? ? ? ?

```

```

#-----
#       Special items requested by author for inclusion in paper
#-----

```

```

loop_
  _publ_manuscript_incl_extra_item

```

```

_publ_manuscript_incl_extra_defn
      ? ?

#-----
#       Items which are non-mandatory for Acta C submissions
#-----

_atom_sites_solution_primary          ?
_atom_sites_solution_secondary        ?
_atom_sites_solution_hydrogens       ?

_geom_special_details                 ?

_cell_special_details
;           ?
;

_exptl_special_details
;           ?
;

_diffrn_special_details
;           ?
;

_chemical_compound_source              ?
_chemical_name_systematic              ?
_chemical_name_common                  ?
_chemical_formula_analytical           ?
_chemical_formula_structural           ?

_exptl_crystal_F_000                  3302

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
  ? ? ?
loop_
_diffrn_attenuator_code
_diffrn_attenuator_scale
  ? ?

_reflns_limit_h_min                   0
_reflns_limit_h_max                   24
_reflns_limit_k_min                   -25
_reflns_limit_k_max                   25
_reflns_limit_l_min                   -42
_reflns_limit_l_max                   42
_reflns_number_observed               ?
_reflns_d_resolution_high              .633
_reflns_d_resolution_low              12.813

_diffrn_reflns_av_sigmaI/netI         .095
_diffrn_reflns_theta_min              1.59
_diffrn_reflns_reduction_process      ?

_diffrn_ambient_temperature           150
_diffrn_radiation_source              'sealed tube'

```

