

CSIRO Publishing

---

AUSTRALIAN JOURNAL OF  
**CHEMISTRY**  
AN INTERNATIONAL JOURNAL FOR CHEMICAL SCIENCE

---

publishing research papers from all fields of chemical science, including synthesis, structure, new materials, macromolecules, supramolecular chemistry, biological chemistry, nanotechnology, surface chemistry, and analytical techniques.

Volume 55, 2002  
© CSIRO 2002

All enquiries and manuscripts should be directed to:

Dr Alison Green  
*Australian Journal of Chemistry –  
an International Journal for Chemical Science*



CSIRO PUBLISHING  
PO Box 1139 (150 Oxford St)  
Collingwood, Vic. 3066, Australia

Telephone: +61 3 9662 7630  
Fax: +61 3 9662 7611  
E-mail: [publishing.ajc@csiro.au](mailto:publishing.ajc@csiro.au)

Published by CSIRO PUBLISHING  
for CSIRO and the Australian Academy of Science

[www.publish.csiro.au/journals/ajc](http://www.publish.csiro.au/journals/ajc)

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

data\_global

```
_audit_creation_method      Xtal3.6  
_audit_creation_date        01-11-28  
_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
```

```
#-----
```

```
_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_delgn

# 2. EXPERIMENTAL DATA
#-----

_chemical_formula_sum           'C26 H34 O6'
_chemical_formula_moiety       ?
_chemical_formula_weight       442.55
_chemical_melting_point        ?

_symmetry_cell_setting         monoclinic
_symmetry_space_group_name_H-M P_1_21/c_1
_symmetry_space_group_name_Hall -p_2ybc

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

_cell_length_a                 11.108(4)

```

_cell_length_b	31.410(9)
_cell_length_c	14.691(5)
_cell_angle_alpha	90.00000
_cell_angle_beta	108.115(7)
_cell_angle_gamma	90.00000
_cell_volume	4872(3)
_cell_formula_units_Z	8
_exptl_crystal_density_diffn	1.207
_exptl_crystal_density_meas	?
_exptl_crystal_density_method	?
_diffn_radiation_type	'Mo K\alpha'
_diffn_radiation_wavelength	.71073
_cell_measurement_reflns_used	4614
_cell_measurement_theta_min	1.3
_cell_measurement_theta_max	20.5
_cell_measurement_temperature	150
_exptl_absorpt_coefficient_mu	.085
_exptl_crystal_description	bar
_exptl_crystal_size_max	.75
_exptl_crystal_size_mid	.16
_exptl_crystal_size_min	.11
_exptl_crystal_size_rad	?
_exptl_crystal_colour	colourless
_diffn_measurement_device_type	
;	
Bruker SMART CCD diffractometer	
;	
_diffn_measurement_method	'\w scans'
_diffn_detector_area_resol_mean	?
_exptl_absorpt_correction_type	multi-scan
_exptl_absorpt_process_details	
;	
SADABS; Sheldrick, 1996	
;	
_exptl_absorpt_correction_T_min	.58
_exptl_absorpt_correction_T_max	.89
_diffn_reflns_number	46700
_reflns_number_total	8470
_reflns_Friedel_coverage	0
_reflns_number_gt	4807
_reflns_threshold_expression	'F > 4.00 sig(F )'
_diffn_reflns_theta_max	24.88
_diffn_reflns_theta_full	?
_diffn_measured_fraction_theta_max	?
_diffn_measured_fraction_theta_full	?
_diffn_reflns_av_R_equivalents	.072
_diffn_reflns_limit_h_min	-13
_diffn_reflns_limit_h_max	12
_diffn_reflns_limit_k_min	0
_diffn_reflns_limit_k_max	37

```

_diffn_reflms_limit_l_min      0
_diffn_reflms_limit_l_max     17
_diffn_standards_number       ?
_diffn_standards_interval_count ?
_diffn_standards_interval_time ?
_diffn_standards_decay_%      0

_refine_ls_structure_factor_coef F
_refine_ls_R_factor_gt        .064
_refine_ls_wR_factor_ref      .092
_refine_ls_goodness_of_fit_ref 1.198
_refine_ls_number_reflms      4807
_refine_ls_number_parameters   631
_refine_ls_weighting_scheme    calc
_refine_ls_weighting_details   ?
_refine_ls_hydrogen_treatment  noref
_refine_ls_shift/su_max        .075
_refine_diff_density_min       -.263
_refine_diff_density_max       .36

_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 ? 0 208 .002 .002 'Int Tables Vol IV Tables 2.2B and 2.3.1'
  H ? 0 272 0 0 'Int Tables Vol IV Tables 2.2B and 2.3.1'
  O ? 0 48 .008 .006 '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
C11 .2699(4) .58479(13) .6807(3) .038(2) Uani ? ? 1.00000 ?
?
O11 .3296(3) .58741(10) .7666(2) .0565(18) Uani ? ? 1.00000
? ?
C12 .3116(4) .55232(13) .6210(3) .037(2) Uani ? ? 1.00000 ?
?
C121 .4520(4) .55953(17) .6295(3) .057(3) Uani ? ? 1.00000 ?
?
C122 .2969(5) .50777(15) .6599(4) .061(3) Uani ? ? 1.00000 ?
?
C13 .2363(4) .55275(15) .5142(3) .045(2) Uani ? ? 1.00000 ?
?
O13 .2642(3) .52856(11) .4612(2) .071(2) Uani ? ? 1.00000 ?
?
C14 .1269(4) .58363(13) .4728(3) .038(2) Uani ? ? 1.00000 ?
?
C14a .1025(4) .61162(12) .5468(3) .035(2) Uani ? ? 1.00000 ?
?
C141 .1618(6) .61150(17) .3983(4) .069(3) Uani ? ? 1.00000 ?
?
C142 .0076(5) .55721(17) .4226(4) .064(3) Uani ? ? 1.00000 ?
?
C15 -.0892(4) .70586(13) .5023(3) .035(2) Uani ? ? 1.00000 ?
?
C16 -.1066(4) .74283(13) .5469(3) .039(2) Uani ? ? 1.00000 ?
?
O16 -.1873(3) .77294(9) .4976(2) .0490(17) Uani ? ? 1.00000
? ?
C17 -.0433(4) .74891(13) .6457(3) .040(2) Uani ? ? 1.00000 ?
?
C18 .0293(4) .71518(14) .6974(3) .043(2) Uani ? ? 1.00000 ?
?
C18a .0458(4) .67689(13) .6537(3) .035(2) Uani ? ? 1.00000 ?
?
O18 .0871(3) .71774(10) .7932(2) .0572(19) Uani ? ? 1.00000
? ?
C19 .1214(4) .64055(13) .7088(3) .039(2) Uani ? ? 1.00000 ?
?
C19a .1626(4) .61211(12) .6415(3) .033(2) Uani ? ? 1.00000 ?
?
O110 .0048(3) .63917(9) .5053(2) .0379(15) Uani ? ? 1.00000
? ?
C110a -.0114(4) .67452(13) .5560(3) .034(2) Uani ? ? 1.00000
? ?
O11' -.0071(4) .79042(11) .7861(3) .069(2) Uani ? ? 1.00000
? ?
C11' -.0466(4) .78975(15) .6973(4) .048(3) Uani ? ? 1.00000
? ?

```





O210	.4236(3)	.81929(9)	.5377(2)	.0416(15)	Uani	?	?	1.00000	
? ?									
C210a	.4991(4)	.85602(13)	.5510(3)	.033(2)	Uani	?	?	1.00000	
? ?									
C21'a	.7118(14)	.9716(5)	.5804(12)	.038(7)	Uani	?	?	.50000	?
? ?									
O21'a	.803(2)	.9756(7)	.6549(19)	.045(9)	Uani	?	?	.50000	?
? ?									
C22'a	.6871(12)	1.0056(4)	.5063(9)	.042(6)	Uani	?	?	.50000	?
? ?									
C23'a	.7460(13)	.9987(6)	.4203(9)	.061(8)	Uani	?	?	.50000	?
? ?									
C24'a	.688(2)	1.0308(10)	.3445(17)	.093(15)	Uani	?	?	.50000	
? ?									
C25'a	.8860(9)	1.0056(3)	.4710(9)	.070(7)	Uani	?	?	.50000	?
? ?									
C21'b	.7483(15)	.9575(5)	.5634(10)	.040(8)	Uani	?	?	.50000	?
? ?									
O21'b	.831(2)	.9657(8)	.638(2)	.051(10)	Uani	?	?	.50000	?
C22'b	.7628(9)	.9790(4)	.4732(11)	.061(7)	Uani	?	?	.50000	?
? ?									
C23'b	.6964(16)	1.0175(5)	.4575(14)	.064(10)	Uani	?	?	.50000	
? ?									
C24'b	.687(4)	1.0338(11)	.356(3)	.15(2)	Uani	?	?	.50000	?
C25'b	.7681(9)	1.0492(3)	.5292(8)	.057(6)	Uani	?	?	.50000	?
? ?									
C21"	.5264(4)	.85044(14)	.7853(3)	.041(2)	Uani	?	?	1.00000	?
? ?									
C22"	.5715(4)	.89076(14)	.8424(3)	.040(2)	Uani	?	?	1.00000	?
? ?									
C23"	.6942(5)	.88428(14)	.9211(3)	.051(3)	Uani	?	?	1.00000	?
? ?									
C24"	.4704(5)	.90695(18)	.8840(4)	.068(3)	Uani	?	?	1.00000	?
? ?									
H121A	.48011	.53959	.59248	.09200	Uiso	?	?	1.00000	?
H121B	.50357	.55733	.69465	.09200	Uiso	?	?	1.00000	?
H121C	.46310	.58778	.60762	.09200	Uiso	?	?	1.00000	?
H122A	.32390	.48572	.62628	.10100	Uiso	?	?	1.00000	?
H122B	.21204	.50229	.65793	.10100	Uiso	?	?	1.00000	?
H122C	.34904	.50549	.72684	.10100	Uiso	?	?	1.00000	?
H141A	.09602	.63157	.36821	.11000	Uiso	?	?	1.00000	?
H141B	.17623	.59453	.34817	.11000	Uiso	?	?	1.00000	?
H141C	.23752	.62748	.42737	.11000	Uiso	?	?	1.00000	?
H142A	-.06297	.57507	.39565	.10100	Uiso	?	?	1.00000	?
H142B	-.01203	.53806	.46685	.10100	Uiso	?	?	1.00000	?
H142C	.02190	.54025	.37269	.10100	Uiso	?	?	1.00000	?
H15	-.13037	.70176	.43309	.05000	Uiso	?	?	1.00000	?
H16	-.24642	.76876	.43182	.08000	Uiso	?	?	1.00000	?
H18	.07161	.74566	.82681	.09200	Uiso	?	?	1.00000	?
H19	.19776	.65104	.75589	.05300	Uiso	?	?	1.00000	?
H12'A	-.08078	.85290	.68973	.06900	Uiso	?	?	1.00000	?
H12'B	-.16862	.82842	.60299	.06900	Uiso	?	?	1.00000	?
H13'	.00875	.81894	.54352	.08000	Uiso	?	?	1.00000	?
H14'A	.00914	.89161	.49260	.16900	Uiso	?	?	1.00000	?
H14'B	-.04318	.90594	.57361	.16900	Uiso	?	?	1.00000	?
H14'C	-.12734	.87951	.48869	.16900	Uiso	?	?	1.00000	?
H15'A	.19940	.85506	.61518	.13800	Uiso	?	?	1.00000	?

H15'B	.17541	.82334	.68821	.13800	Uiso	?	?	1.00000	?	?
H15'C	.14811	.87142	.69520	.13800	Uiso	?	?	1.00000	?	?
H11"A	.03041	.63640	.81206	.07200	Uiso	?	?	1.00000	?	?
H11"B	.10270	.59487	.80593	.07200	Uiso	?	?	1.00000	?	?
H12"	-.11197	.61136	.65128	.09300	Uiso	?	?	1.00000	?	?
H13"A	-.24312	.58069	.74081	.16500	Uiso	?	?	1.00000	?	?
H13"B	-.17863	.62120	.79431	.16500	Uiso	?	?	1.00000	?	?
H13"C	-.12444	.57660	.82980	.16500	Uiso	?	?	1.00000	?	?
H14"A	-.13055	.53702	.64629	.16900	Uiso	?	?	1.00000	?	?
H14"B	-.02004	.53351	.74095	.16900	Uiso	?	?	1.00000	?	?
H14"C	.00549	.54903	.64887	.16900	Uiso	?	?	1.00000	?	?
H221A	.54098	.65032	.76198	.09800	Uiso	?	?	1.00000	?	?
H221B	.50006	.68806	.81341	.09800	Uiso	?	?	1.00000	?	?
H221C	.64223	.67753	.83496	.09800	Uiso	?	?	1.00000	?	?
H222A	.65808	.66568	.63839	.10800	Uiso	?	?	1.00000	?	?
H222B	.75489	.69398	.71213	.10800	Uiso	?	?	1.00000	?	?
H222C	.67975	.71237	.61311	.10800	Uiso	?	?	1.00000	?	?
H241A	.22055	.77446	.49925	.09000	Uiso	?	?	1.00000	?	?
H241B	.24030	.75619	.60054	.09000	Uiso	?	?	1.00000	?	?
H241C	.20870	.72589	.51326	.09000	Uiso	?	?	1.00000	?	?
H242A	.39076	.75981	.41510	.10400	Uiso	?	?	1.00000	?	?
H242B	.37662	.71138	.42943	.10400	Uiso	?	?	1.00000	?	?
H242C	.50850	.73267	.46683	.10400	Uiso	?	?	1.00000	?	?
H25	.40574	.87406	.41309	.05100	Uiso	?	?	1.00000	?	?
H26	.45147	.93797	.34418	.07800	Uiso	?	?	1.00000	?	?
H28	.81528	.93353	.71851	.05900	Uiso	?	?	1.00000	?	?
H29	.69231	.83510	.76162	.05100	Uiso	?	?	1.00000	?	?
H22'aA	.71778	1.03179	.53789	.05200	Uiso	?	?	.50000	?	?
H22'aB	.59615	1.00815	.47838	.05200	Uiso	?	?	.50000	?	?
H23'a	.72359	.97155	.39077	.08400	Uiso	?	?	.50000	?	?
H24'aA	.73808	1.02107	.29226	.10600	Uiso	?	?	.50000	?	?
H24'aB	.71100	1.05583	.35796	.10600	Uiso	?	?	.50000	?	?
H24'aC	.60759	1.02280	.30916	.10600	Uiso	?	?	.50000	?	?
H25'aA	.90023	1.02916	.51323	.10000	Uiso	?	?	.50000	?	?
H25'aB	.93140	1.00871	.42709	.10000	Uiso	?	?	.50000	?	?
H25'aC	.91267	.97979	.50805	.10900	Uiso	?	?	.50000	?	?
H22'bA	.73114	.96067	.41805	.07600	Uiso	?	?	.50000	?	?
H22'bB	.85176	.98372	.48040	.07600	Uiso	?	?	.50000	?	?
H23'b	.61618	1.01091	.46674	.07500	Uiso	?	?	.50000	?	?
H24'bA	.62856	1.06529	.35781	.13800	Uiso	?	?	.50000	?	?
H24'bB	.62770	1.02087	.31175	.13800	Uiso	?	?	.50000	?	?
H24'bC	.75365	1.04559	.35215	.13800	Uiso	?	?	.50000	?	?
H25'bA	.71985	1.07418	.52291	.08600	Uiso	?	?	.50000	?	?
H25'bB	.84563	1.05310	.52270	.08600	Uiso	?	?	.50000	?	?
H25'bC	.77649	1.03715	.59264	.08600	Uiso	?	?	.50000	?	?
H221"A	.52185	.82776	.82884	.06100	Uiso	?	?	1.00000	?	?
H221"B	.43961	.85466	.74399	.06100	Uiso	?	?	1.00000	?	?
H22"	.58821	.91131	.79910	.05700	Uiso	?	?	1.00000	?	?
H23"A	.72411	.90972	.95362	.08200	Uiso	?	?	1.00000	?	?
H23"B	.75921	.87405	.89373	.08200	Uiso	?	?	1.00000	?	?
H23"C	.68544	.86301	.96407	.08200	Uiso	?	?	1.00000	?	?
H24"A	.49663	.93287	.92004	.11100	Uiso	?	?	1.00000	?	?
H24"B	.45239	.88646	.92617	.11100	Uiso	?	?	1.00000	?	?
H24"C	.39205	.91318	.83488	.11100	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

C11	.039(3)	.033(3)	.033(3)	-.002(2)	-.000(2)	.002(2)
O11	.062(2)	.052(2)	.036(2)	.0165(17)	-.0131(16)	-.0063(16)
C12	.032(2)	.030(2)	.039(3)	.001(2)	-.002(2)	.002(2)
C121	.043(3)	.076(4)	.047(3)	-.009(3)	.006(2)	.002(3)
C122	.075(4)	.041(3)	.069(4)	-.005(3)	.024(3)	.004(3)
C13	.046(3)	.038(3)	.044(3)	.003(2)	.003(2)	-.011(2)
O13	.073(2)	.069(2)	.053(2)	.035(2)	-.0086(18)	-.022(2)
C14	.041(3)	.032(2)	.030(2)	.007(2)	-.003(2)	.001(2)
C14a	.031(2)	.028(2)	.039(3)	-.003(2)	-.001(2)	.001(2)
C141	.087(4)	.067(4)	.060(3)	.025(3)	.034(3)	.008(3)
C142	.050(3)	.060(3)	.065(4)	.007(3)	-.007(3)	-.027(3)
C15	.035(2)	.033(2)	.029(2)	-.001(2)	-.002(2)	.002(2)
C16	.034(2)	.032(3)	.045(3)	.000(2)	.005(2)	-.000(2)
O16	.049(2)	.0374(18)	.047(2)	.0118(15)	-.0047(15)	-.0032(15)
C17	.040(2)	.031(3)	.041(3)	-.001(2)	.003(2)	-.005(2)
C18	.045(3)	.038(3)	.037(3)	.001(2)	.000(2)	-.005(2)
C18a	.032(2)	.035(3)	.032(3)	-.001(2)	.003(2)	-.003(2)
O18	.078(2)	.048(2)	.0319(19)	.0105(17)	-.0017(17)	-.0093(15)
C19	.044(3)	.033(2)	.029(2)	.001(2)	-.002(2)	-.004(2)
C19a	.034(2)	.027(2)	.033(3)	-.002(2)	.001(2)	.002(2)
O110	.0361(16)	.0323(17)	.0351(17)	.0069(14)	-.0036(13)	-.0024(14)
C110a	.030(2)	.031(2)	.037(3)	-.003(2)	.004(2)	-.004(2)
O11'	.096(3)	.053(2)	.049(2)	.012(2)	.006(2)	-.0143(19)
C11'	.048(3)	.045(3)	.046(3)	.004(2)	.007(2)	-.010(3)
C12'	.054(3)	.040(3)	.057(3)	.004(2)	.014(3)	-.017(2)
C13'	.069(4)	.042(3)	.052(3)	-.012(3)	.013(3)	-.005(3)
C14'	.133(7)	.079(5)	.126(6)	.011(4)	.045(5)	.039(5)
C15'	.074(4)	.097(5)	.074(4)	-.027(4)	.020(3)	-.026(4)
C11"	.063(3)	.049(3)	.038(3)	.008(3)	.018(3)	.007(2)
C12"	.071(4)	.064(4)	.055(3)	-.008(3)	.024(3)	.010(3)
C13"	.088(5)	.101(5)	.117(6)	.011(4)	.045(4)	.018(4)
C14"	.094(5)	.083(5)	.117(6)	-.020(4)	.043(4)	-.021(4)
C21	.036(2)	.040(3)	.042(3)	-.006(2)	.003(2)	.007(2)
O21	.061(2)	.044(2)	.045(2)	-.0083(17)	-.0106(17)	.0072(16)
C22	.043(3)	.034(3)	.039(3)	-.003(2)	.008(2)	.000(2)
C221	.076(4)	.043(3)	.052(3)	-.013(3)	.009(3)	.007(3)
C222	.053(3)	.063(4)	.080(4)	-.005(3)	.019(3)	-.014(3)
C23	.045(3)	.036(3)	.053(3)	-.012(2)	.013(2)	-.001(2)
O23	.072(2)	.040(2)	.076(3)	-.023(2)	-.006(2)	.0033(18)
C24	.046(3)	.034(3)	.038(3)	-.014(2)	.007(2)	-.005(2)
C24a	.036(2)	.034(3)	.032(3)	-.004(2)	.007(2)	.004(2)
C241	.042(3)	.049(3)	.069(3)	-.014(2)	.006(2)	.003(3)
C242	.087(4)	.046(3)	.048(3)	-.018(3)	.018(3)	-.012(3)
C25	.033(2)	.040(3)	.032(3)	-.010(2)	.003(2)	-.007(2)
C26	.038(2)	.043(3)	.028(2)	-.009(2)	.007(2)	.003(2)
O26	.050(2)	.059(2)	.0316(17)	-.0254(16)	-.0038(14)	.0088(16)
C27	.035(2)	.046(3)	.032(3)	-.018(2)	.006(2)	-.000(2)
C28	.031(2)	.035(2)	.028(2)	-.005(2)	.006(2)	-.003(2)
O28	.0340(16)	.0403(17)	.0316(16)	-.0107(14)	.0010(13)	-.0033(14)

```

C28a .028(2) .030(2) .031(2) -.003(2) .0072(19) -.002(2)
C29 .035(2) .031(2) .030(2) -.007(2) .002(2) -.001(2)
C29a .034(2) .032(2) .034(3) -.009(2) .005(2) -.001(2)
O210 .0414(17) .0375(18) .0364(17) -.0137(15) -.0017(14)
.0007(15)
C210a .030(2) .032(2) .036(3) -.006(2) .008(2) -.004(2)
C21'a .043(8) .039(8) .038(8) -.004(6) .023(6) -.022(6)
O21'a .051(11) .048(9) .031(8) -.030(7) .008(6) -.009(6)
C22'a .050(7) .026(7) .033(7) -.012(5) -.011(6) .006(6)
C23'a .052(8) .080(11) .044(9) -.020(7) .005(7) .040(9)
C24'a .052(11) .15(2) .068(14) -.011(12) -.001(10) .087(14)
C25'a .041(6) .064(7) .109(9) -.011(5) .030(6) -.012(7)
C21'b .051(9) .049(10) .020(7) -.021(7) .011(6) -.002(6)
O21'b .043(9) .068(12) .034(10) -.016(7) .000(6) .001(7)
C22'b .026(6) .079(9) .073(9) -.019(6) .011(6) -.000(8)
C23'b .068(10) .057(11) .049(12) -.017(8) -.011(9) .005(9)
C24'b .18(3) .08(2) .14(3) -.063(19) -.03(2) .010(17)
C25'b .040(6) .047(6) .081(7) -.005(5) .012(5) -.015(6)
C21" .050(3) .041(3) .030(2) -.009(2) .010(2) -.000(2)
C22" .044(3) .044(3) .035(3) -.002(2) .014(2) .002(2)
C23" .059(3) .044(3) .044(3) -.001(2) .009(3) -.001(2)
C24" .073(4) .082(4) .059(3) .004(3) .034(3) -.004(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

```

C11 O11 . . 1.232(5) ?
C11 C12 . . 1.509(6) ?
C11 C19a . . 1.436(6) ?
C12 C121 . . 1.541(7) ?
C12 C122 . . 1.540(6) ?
C12 C13 . . 1.531(6) ?
C121 H121A . . .945 ?
C121 H121B . . .952 ?
C121 H121C . . .965 ?
C122 H122A . . .952 ?
C122 H122B . . .949 ?
C122 H122C . . .977 ?
C13 O13 . . 1.196(6) ?
C13 C14 . . 1.526(6) ?
C14 C14a . . 1.488(6) ?
C14 C141 . . 1.542(8) ?
C14 C142 . . 1.543(6) ?
C14a C19a . . 1.342(6) ?
C14a O110 . . 1.374(5) ?
C141 H141A . . .962 ?
C141 H141B . . .962 ?
C141 H141C . . .958 ?

```

C142	H142A	. .	.945	?
C142	H142B	. .	.959	?
C142	H142C	. .	.959	?
C15	C16	. .	1.376(6)	?
C15	C110a	. .	1.384(5)	?
C15	H15	. .	.985	?
C16	O16	. .	1.349(5)	?
C16	C17	. .	1.415(6)	?
O16	H16	. .	.994	?
C17	C18	. .	1.403(6)	?
C17	C11'	. .	1.496(7)	?
C18	C18a	. .	1.402(6)	?
C18	O18	. .	1.356(5)	?
C18a	C19	. .	1.497(5)	?
C18a	C110a	. .	1.378(6)	?
O18	H18	. .	1.047	?
C19	C19a	. .	1.505(6)	?
C19	C11"	. .	1.557(7)	?
C19	H19	. .	.970	?
O110	C110a	. .	1.380(5)	?
O11'	C11'	. .	1.240(6)	?
C11'	C12'	. .	1.478(7)	?
C12'	C13'	. .	1.511(8)	?
C12'	H12'A	. .	.961	?
C12'	H12'B	. .	.980	?
C13'	C14'	. .	1.528(8)	?
C13'	C15'	. .	1.529(7)	?
C13'	H13'	. .	.984	?
C14'	H14'A	. .	.953	?
C14'	H14'B	. .	.948	?
C14'	H14'C	. .	.994	?
C15'	H15'A	. .	.958	?
C15'	H15'B	. .	.934	?
C15'	H15'C	. .	.980	?
C11"	C12"	. .	1.527(7)	?
C11"	H11"A	. .	.966	?
C11"	H11"B	. .	.975	?
C12"	C13"	. .	1.540(11)	?
C12"	C14"	. .	1.463(9)	?
C12"	H12"	. .	.993	?
C13"	H13"A	. .	.930	?
C13"	H13"B	. .	.989	?
C13"	H13"C	. .	.960	?
C14"	H14"A	. .	.943	?
C14"	H14"B	. .	.989	?
C14"	H14"C	. .	.955	?
C21	O21	. .	1.222(5)	?
C21	C22	. .	1.531(6)	?
C21	C29a	. .	1.441(6)	?
C22	C221	. .	1.517(7)	?
C22	C222	. .	1.545(8)	?
C22	C23	. .	1.518(5)	?
C221	H221A	. .	.979	?
C221	H221B	. .	.942	?
C221	H221C	. .	.972	?
C222	H222A	. .	.975	?
C222	H222B	. .	.947	?

C222 H222C . . .954 ?  
C23 O23 . . 1.200(6) ?  
C23 C24 . . 1.541(6) ?  
C24 C24a . . 1.519(6) ?  
C24 C241 . . 1.543(7) ?  
C24 C242 . . 1.529(7) ?  
C24a C29a . . 1.335(5) ?  
C24a O210 . . 1.373(5) ?  
C241 H241A . . .967 ?  
C241 H241B . . .965 ?  
C241 H241C . . .953 ?  
C242 H242A . . .958 ?  
C242 H242B . . .950 ?  
C242 H242C . . .970 ?  
C25 C26 . . 1.384(6) ?  
C25 C210a . . 1.373(6) ?  
C25 H25 . . .983 ?  
C26 O26 . . 1.342(5) ?  
C26 C27 . . 1.414(5) ?  
O26 H26 . . .977 ?  
C27 C28 . . 1.421(6) ?  
C27 C21'a . . 1.541(15) ?  
C27 C21'b . . 1.462(17) ?  
C28 O28 . . 1.350(4) ?  
C28 C28a . . 1.393(6) ?  
O28 H28 . . 1.055 ?  
C28a C29 . . 1.505(6) ?  
C28a C210a . . 1.377(5) ?  
C29 C29a . . 1.526(5) ?  
C29 C21" . . 1.531(7) ?  
C29 H29 . . .986 ?  
O210 C210a . . 1.404(5) ?  
C21'a O21'a . . 1.25(3) ?  
C21'a C22'a . . 1.49(2) ?  
C22'a C23'a . . 1.61(2) ?  
C22'a H22'aA . . .955 ?  
C22'a H22'aB . . .968 ?  
C23'a C24'a . . 1.49(3) ?  
C23'a C25'a . . 1.516(16) ?  
C23'a H23'a . . .955 ?  
C24'a H24'aA . . 1.12 ?  
C24'a H24'aB . . .83 ?  
C24'a H24'aC . . .92 ?  
C25'a H25'aA . . .947 ?  
C25'a H25'aB . . .939 ?  
C25'a H25'aC . . .970 ?  
C21'b O21'b . . 1.22(3) ?  
C21'b C22'b . . 1.54(2) ?  
C22'b C23'b . . 1.40(2) ?  
C22'b H22'bA . . .968 ?  
C22'b H22'bB . . .971 ?  
C23'b C24'b . . 1.55(5) ?  
C23'b C25'b . . 1.487(19) ?  
C23'b H23'b . . .96 ?  
C24'b H24'bA . . 1.19 ?  
C24'b H24'bB . . .86 ?  
C24'b H24'bC . . .85 ?

C25'b H25'bA . . .938 ?  
 C25'b H25'bB . . .903 ?  
 C25'b H25'bC . . .984 ?  
 C21" C22" . . 1.516(6) ?  
 C21" H221"A . . .969 ?  
 C21" H221"B . . .976 ?  
 C22" C23" . . 1.502(6) ?  
 C22" C24" . . 1.523(8) ?  
 C22" H22" . . .964 ?  
 C23" H23"A . . .938 ?  
 C23" H23"B . . .983 ?  
 C23" H23"C . . .945 ?  
 C24" H24"A . . .966 ?  
 C24" H24"B . . .957 ?  
 C24" H24"C . . .962 ?

loop\_

\_geom\_angle\_atom\_site\_label\_1  
 \_geom\_angle\_atom\_site\_label\_2  
 \_geom\_angle\_atom\_site\_label\_3  
 \_geom\_angle\_site\_symmetry\_1  
 \_geom\_angle\_site\_symmetry\_2  
 \_geom\_angle\_site\_symmetry\_3  
 \_geom\_angle

\_geom\_angle\_publ\_flag  
 published

#<< enter YES for value to be

O11 C11 C12 . . . 118.4(4) ?  
 O11 C11 C19a . . . 119.1(4) ?  
 C12 C11 C19a . . . 122.5(4) ?  
 C11 C12 C121 . . . 109.8(3) ?  
 C11 C12 C122 . . . 108.1(4) ?  
 C11 C12 C13 . . . 114.9(3) ?  
 C121 C12 C122 . . . 109.0(4) ?  
 C121 C12 C13 . . . 107.4(4) ?  
 C122 C12 C13 . . . 107.5(3) ?  
 C12 C121 H121A . . . 111.3 ?  
 C12 C121 H121B . . . 110.4 ?  
 C12 C121 H121C . . . 109.8 ?  
 H121A C121 H121B . . . 109.1 ?  
 H121A C121 H121C . . . 108.5 ?  
 H121B C121 H121C . . . 107.6 ?  
 C12 C122 H122A . . . 112.4 ?  
 C12 C122 H122B . . . 111.9 ?  
 C12 C122 H122C . . . 110.0 ?  
 H122A C122 H122B . . . 108.8 ?  
 H122A C122 H122C . . . 106.6 ?  
 H122B C122 H122C . . . 106.8 ?  
 C12 C13 O13 . . . 119.5(4) ?  
 C12 C13 C14 . . . 121.9(4) ?  
 O13 C13 C14 . . . 118.6(4) ?  
 C13 C14 C14a . . . 112.8(3) ?  
 C13 C14 C141 . . . 107.4(4) ?  
 C13 C14 C142 . . . 107.9(4) ?  
 C14a C14 C141 . . . 109.1(4) ?  
 C14a C14 C142 . . . 110.0(4) ?  
 C141 C14 C142 . . . 109.6(4) ?  
 C14 C14a C19a . . . 128.3(4) ?

C14	C14a	O110	.	.	.	110.2(3)	?
C19a	C14a	O110	.	.	.	121.5(4)	?
C14	C141	H141A	.	.	.	112.0	?
C14	C141	H141B	.	.	.	111.5	?
C14	C141	H141C	.	.	.	111.1	?
H141A	C141	H141B	.	.	.	107.2	?
H141A	C141	H141C	.	.	.	107.3	?
H141B	C141	H141C	.	.	.	107.5	?
C14	C142	H142A	.	.	.	111.0	?
C14	C142	H142B	.	.	.	110.9	?
C14	C142	H142C	.	.	.	110.0	?
H142A	C142	H142B	.	.	.	108.9	?
H142A	C142	H142C	.	.	.	108.8	?
H142B	C142	H142C	.	.	.	107.2	?
C16	C15	C110a	.	.	.	119.0(4)	?
C16	C15	H15	.	.	.	120.8	?
C110a	C15	H15	.	.	.	120.2	?
C15	C16	O16	.	.	.	120.3(4)	?
C15	C16	C17	.	.	.	120.2(4)	?
O16	C16	C17	.	.	.	119.5(4)	?
C16	O16	H16	.	.	.	123.9	?
C16	C17	C18	.	.	.	118.1(4)	?
C16	C17	C11'	.	.	.	123.5(4)	?
C18	C17	C11'	.	.	.	118.3(4)	?
C17	C18	C18a	.	.	.	122.3(4)	?
C17	C18	O18	.	.	.	121.6(4)	?
C18a	C18	O18	.	.	.	116.1(4)	?
C18	C18a	C19	.	.	.	122.5(4)	?
C18	C18a	C110a	.	.	.	116.1(4)	?
C19	C18a	C110a	.	.	.	121.4(4)	?
C18	O18	H18	.	.	.	116.4	?
C18a	C19	C19a	.	.	.	109.3(3)	?
C18a	C19	C11"	.	.	.	111.3(4)	?
C18a	C19	H19	.	.	.	110.2	?
C19a	C19	C11"	.	.	.	113.3(4)	?
C19a	C19	H19	.	.	.	107.1	?
C11"	C19	H19	.	.	.	105.4	?
C11	C19a	C14a	.	.	.	119.5(4)	?
C11	C19a	C19	.	.	.	118.3(3)	?
C14a	C19a	C19	.	.	.	122.2(4)	?
C14a	O110	C110a	.	.	.	119.0(3)	?
C15	C110a	C18a	.	.	.	124.0(4)	?
C15	C110a	O110	.	.	.	115.3(3)	?
C18a	C110a	O110	.	.	.	120.7(3)	?
C17	C11'	O11'	.	.	.	119.4(4)	?
C17	C11'	C12'	.	.	.	121.5(4)	?
O11'	C11'	C12'	.	.	.	118.7(4)	?
C11'	C12'	C13'	.	.	.	112.7(4)	?
C11'	C12'	H12'A	.	.	.	109.6	?
C11'	C12'	H12'B	.	.	.	108.5	?
C13'	C12'	H12'A	.	.	.	109.6	?
C13'	C12'	H12'B	.	.	.	110.6	?
H12'A	C12'	H12'B	.	.	.	105.7	?
C12'	C13'	C14'	.	.	.	109.3(5)	?
C12'	C13'	C15'	.	.	.	112.8(4)	?
C12'	C13'	H13'	.	.	.	110.2	?
C14'	C13'	C15'	.	.	.	109.6(5)	?



C14'	C13'	H13'	. . .	109.5 ?
C15'	C13'	H13'	. . .	105.4 ?
C13'	C14'	H14'A	. . .	114.1 ?
C13'	C14'	H14'B	. . .	111.9 ?
C13'	C14'	H14'C	. . .	110.8 ?
H14'A	C14'	H14'B	. . .	108.7 ?
H14'A	C14'	H14'C	. . .	105.2 ?
H14'B	C14'	H14'C	. . .	105.6 ?
C13'	C15'	H15'A	. . .	112.4 ?
C13'	C15'	H15'B	. . .	112.2 ?
C13'	C15'	H15'C	. . .	108.5 ?
H15'A	C15'	H15'B	. . .	109.6 ?
H15'A	C15'	H15'C	. . .	105.7 ?
H15'B	C15'	H15'C	. . .	108.1 ?
C19	C11"	C12"	. . .	117.0(4) ?
C19	C11"	H11"A	. . .	108.2 ?
C19	C11"	H11"B	. . .	108.3 ?
C12"	C11"	H11"A	. . .	109.9 ?
C12"	C11"	H11"B	. . .	107.0 ?
H11"A	C11"	H11"B	. . .	105.9 ?
C11"	C12"	C13"	. . .	108.7(5) ?
C11"	C12"	C14"	. . .	113.3(5) ?
C11"	C12"	H12"	. . .	106.6 ?
C13"	C12"	C14"	. . .	108.1(5) ?
C13"	C12"	H12"	. . .	111.9 ?
C14"	C12"	H12"	. . .	108.4 ?
C12"	C13"	H13"A	. . .	113.5 ?
C12"	C13"	H13"B	. . .	110.8 ?
C12"	C13"	H13"C	. . .	109.6 ?
H13"A	C13"	H13"B	. . .	107.6 ?
H13"A	C13"	H13"C	. . .	109.8 ?
H13"B	C13"	H13"C	. . .	105.3 ?
C12"	C14"	H14"A	. . .	113.7 ?
C12"	C14"	H14"B	. . .	108.8 ?
C12"	C14"	H14"C	. . .	113.1 ?
H14"A	C14"	H14"B	. . .	106.3 ?
H14"A	C14"	H14"C	. . .	109.1 ?
H14"B	C14"	H14"C	. . .	105.2 ?
O21	C21	C22	. . .	119.5(4) ?
O21	C21	C29a	. . .	120.1(4) ?
C22	C21	C29a	. . .	120.3(3) ?
C21	C22	C221	. . .	110.2(4) ?
C21	C22	C222	. . .	105.9(4) ?
C21	C22	C23	. . .	113.8(3) ?
C221	C22	C222	. . .	110.6(4) ?
C221	C22	C23	. . .	110.6(4) ?
C222	C22	C23	. . .	105.6(4) ?
C22	C221	H221A	. . .	111.5 ?
C22	C221	H221B	. . .	113.2 ?
C22	C221	H221C	. . .	111.5 ?
H221A	C221	H221B	. . .	107.3 ?
H221A	C221	H221C	. . .	105.0 ?
H221B	C221	H221C	. . .	107.8 ?
C22	C222	H222A	. . .	110.2 ?
C22	C222	H222B	. . .	111.8 ?
C22	C222	H222C	. . .	111.5 ?
H222A	C222	H222B	. . .	107.3 ?

H222A	C222	H222C	.	.	.	106.9	?
H222B	C222	H222C	.	.	.	108.9	?
C22	C23	O23	.	.	.	120.0(4)	?
C22	C23	C24	.	.	.	121.7(4)	?
O23	C23	C24	.	.	.	118.2(4)	?
C23	C24	C24a	.	.	.	110.9(3)	?
C23	C24	C241	.	.	.	108.3(4)	?
C23	C24	C242	.	.	.	108.5(4)	?
C24a	C24	C241	.	.	.	109.6(4)	?
C24a	C24	C242	.	.	.	110.1(4)	?
C241	C24	C242	.	.	.	109.6(4)	?
C24	C24a	C29a	.	.	.	128.3(4)	?
C24	C24a	O210	.	.	.	109.3(3)	?
C29a	C24a	O210	.	.	.	122.4(4)	?
C24	C241	H241A	.	.	.	111.5	?
C24	C241	H241B	.	.	.	111.2	?
C24	C241	H241C	.	.	.	112.2	?
H241A	C241	H241B	.	.	.	106.3	?
H241A	C241	H241C	.	.	.	107.7	?
H241B	C241	H241C	.	.	.	107.6	?
C24	C242	H242A	.	.	.	111.4	?
C24	C242	H242B	.	.	.	111.9	?
C24	C242	H242C	.	.	.	110.4	?
H242A	C242	H242B	.	.	.	108.6	?
H242A	C242	H242C	.	.	.	106.8	?
H242B	C242	H242C	.	.	.	107.4	?
C26	C25	C210a	.	.	.	118.3(3)	?
C26	C25	H25	.	.	.	121.9	?
C210a	C25	H25	.	.	.	119.8	?
C25	C26	O26	.	.	.	119.7(3)	?
C25	C26	C27	.	.	.	120.9(4)	?
O26	C26	C27	.	.	.	119.4(4)	?
C26	O26	H26	.	.	.	119.2	?
C26	C27	C28	.	.	.	117.2(4)	?
C26	C27	C21'a	.	.	.	123.4(6)	?
C26	C27	C21'b	.	.	.	123.2(6)	?
C28	C27	C21'a	.	.	.	117.5(7)	?
C28	C27	C21'b	.	.	.	117.6(6)	?
C27	C28	O28	.	.	.	120.4(4)	?
C27	C28	C28a	.	.	.	122.7(3)	?
O28	C28	C28a	.	.	.	116.9(3)	?
C28	O28	H28	.	.	.	112.7	?
C28	C28a	C29	.	.	.	124.1(3)	?
C28	C28a	C210a	.	.	.	115.8(4)	?
C29	C28a	C210a	.	.	.	120.1(4)	?
C28a	C29	C29a	.	.	.	108.4(3)	?
C28a	C29	C21"	.	.	.	112.7(3)	?
C28a	C29	H29	.	.	.	107.7	?
C29a	C29	C21"	.	.	.	109.6(4)	?
C29a	C29	H29	.	.	.	112.6	?
C21"	C29	H29	.	.	.	105.9	?
C21	C29a	C24a	.	.	.	120.3(4)	?
C21	C29a	C29	.	.	.	119.1(3)	?
C24a	C29a	C29	.	.	.	120.4(3)	?
C24a	O210	C210a	.	.	.	117.5(3)	?
C25	C210a	C28a	.	.	.	125.1(4)	?
C25	C210a	O210	.	.	.	114.2(3)	?

C28a	C210a	O210	.	.	.	120.7(4)	?
C27	C21'a	O21'a	.	.	.	117.4(15)	?
C27	C21'a	C22'a	.	.	.	122.5(11)	?
O21'a	C21'a	C22'a	.	.	.	119.0(16)	?
C21'a	C22'a	C23'a	.	.	.	116.8(12)	?
C21'a	C22'a	H22'aA	.	.	.	107.8	?
C21'a	C22'a	H22'aB	.	.	.	107.5	?
C23'a	C22'a	H22'aA	.	.	.	109.0(13)	?
C23'a	C22'a	H22'aB	.	.	.	107.7(10)	?
H22'aA	C22'a	H22'aB	.	.	.	107.6(12)	?
C22'a	C23'a	C24'a	.	.	.	108.1(16)	?
C22'a	C23'a	C25'a	.	.	.	101.6(10)	?
C22'a	C23'a	H23'a	.	.	.	111.4(15)	?
C24'a	C23'a	C25'a	.	.	.	114.2(16)	?
C24'a	C23'a	H23'a	.	.	.	105.9(14)	?
C25'a	C23'a	H23'a	.	.	.	115.7(15)	?
C23'a	C24'a	H24'aA	.	.	.	98(2)	?
C23'a	C24'a	H24'aB	.	.	.	116(2)	?
C23'a	C24'a	H24'aC	.	.	.	111(3)	?
H24'aA	C24'a	H24'aB	.	.	.	104(3)	?
H24'aA	C24'a	H24'aC	.	.	.	98(2)	?
H24'aB	C24'a	H24'aC	.	.	.	124(3)	?
C23'a	C25'a	H25'aA	.	.	.	111.7	?
C23'a	C25'a	H25'aB	.	.	.	111.4	?
C23'a	C25'a	H25'aC	.	.	.	104.1	?
H25'aA	C25'a	H25'aB	.	.	.	110.7	?
H25'aA	C25'a	H25'aC	.	.	.	109.0	?
H25'aB	C25'a	H25'aC	.	.	.	109.7	?
C27	C21'b	O21'b	.	.	.	120.8(18)	?
C27	C21'b	C22'b	.	.	.	123.5(10)	?
O21'b	C21'b	C22'b	.	.	.	115.7(18)	?
C21'b	C22'b	C23'b	.	.	.	109.4(14)	?
C21'b	C22'b	H22'bA	.	.	.	110.5	?
C21'b	C22'b	H22'bB	.	.	.	110.4	?
C23'b	C22'b	H22'bA	.	.	.	110.0	?
C23'b	C22'b	H22'bB	.	.	.	110.7	?
H22'bA	C22'b	H22'bB	.	.	.	105.9	?
C22'b	C23'b	C24'b	.	.	.	109(2)	?
C22'b	C23'b	C25'b	.	.	.	108.8(12)	?
C22'b	C23'b	H23'b	.	.	.	104.7	?
C24'b	C23'b	C25'b	.	.	.	108.8(17)	?
C24'b	C23'b	H23'b	.	.	.	115	?
C25'b	C23'b	H23'b	.	.	.	111.1	?
C23'b	C24'b	H24'bA	.	.	.	97	?
C23'b	C24'b	H24'bB	.	.	.	112	?
C23'b	C24'b	H24'bC	.	.	.	114	?
H24'bA	C24'b	H24'bB	.	.	.	97	?
H24'bA	C24'b	H24'bC	.	.	.	98	?
H24'bB	C24'b	H24'bC	.	.	.	129	?
C23'b	C25'b	H25'bA	.	.	.	109.0	?
C23'b	C25'b	H25'bB	.	.	.	109.5	?
C23'b	C25'b	H25'bC	.	.	.	106.5	?
H25'bA	C25'b	H25'bB	.	.	.	114.3	?
H25'bA	C25'b	H25'bC	.	.	.	107.3	?
H25'bB	C25'b	H25'bC	.	.	.	109.8	?
C29	C21"	C22"	.	.	.	117.2(4)	?
C29	C21"	H221"A	.	.	.	108.8	?

```

C29 C21" H221"B . . . 106.9 ?
C22" C21" H221"A . . . 108.9 ?
C22" C21" H221"B . . . 108.8 ?
H221"A C21" H221"B . . . 105.4 ?
C21" C22" C23" . . . 112.2(4) ?
C21" C22" C24" . . . 110.1(4) ?
C21" C22" H22" . . . 107.0 ?
C23" C22" C24" . . . 110.0(4) ?
C23" C22" H22" . . . 106.4 ?
C24" C22" H22" . . . 111.0 ?
C22" C23" H23"A . . . 111.7 ?
C22" C23" H23"B . . . 109.7 ?
C22" C23" H23"C . . . 110.7 ?
H23"A C23" H23"B . . . 107.3 ?
H23"A C23" H23"C . . . 110.8 ?
H23"B C23" H23"C . . . 106.5 ?
C22" C24" H24"A . . . 111.5 ?
C22" C24" H24"B . . . 111.3 ?
C22" C24" H24"C . . . 112.0 ?
H24"A C24" H24"B . . . 107.5 ?
H24"A C24" H24"C . . . 106.8 ?
H24"B C24" H24"C . . . 107.5 ?

```

```

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                  1904

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                    13
_reflns_limit_k_min                    0
_reflns_limit_k_max                    37
_reflns_limit_l_min                    -17

```

