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ENTER ABSTRACT ; _publ_section_exptl_refinement ENTER EXPERIMENTAL SECTION ; _publ_section_comment ENTER TEXT ; _publ_section_references ; Molecular Structure Corporation. (1992-1997). teXsan. Single Crystal Structure Analysis Software. Version 1.7. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA. Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands. Mackay, S., Gilmore, C. J., Edwards, C., Stewart, N. & Shankland, K. (1999). maXus Computer Program for the Solution and Refinement of Crystal Structures. Nonius, The Netherlands, MacScience, Japan & The University of Glasgow. Otwinowski, Z. and Minor, W, (1997). In Methods in Enzymology, 276, edited by C.W. Carter, Jr. & R.M. Sweet pp. 307-326, New York: Academic Press. Coppens, P. (1970). The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis. Crystallographic Computing. F. R. Ahmed, S. R. Hall and C. P. Huber, eds., Munksgaard. Copenhagen. pp 255-270. ; _publ_section_acknowledgements ; ENTER ACKNOWLEDGEMENTS ; _publ_section_table_legends ; ENTER TABLE LEGENDS ; _publ_section_figure_captions Figure 1. Thermal ellipsoid diagram of C50 H32 Au2 F10 P2 with labelling of selected atoms. Ellipsoids show 30 percent probability levels. Hydrogen atoms have been omitted for clarity.

Figure 2. Unit cell diagram of C50.50 H33 Au2 Cl F10 P2 projected down the a axis. Ellipsoids show 30 percent probability levels. Hydrogen atoms have been omitted for clarity. #-----_computing_cell_refinement 'Denzo and Scalepack (Otwinowski & Minor, 1997)' _computing_data_collection 'KappaCCD' _computing_data_reduction 'Denzo and Scalepack (Otwinowski & Minor, 1997)' _computing_structure_solution ; DIRDIF92 PATTY (Beurskens, 1992) ; _computing_structure_refinement 'teXsan (MSC, 1992-1997)' _computing_publication_material 'teXsan (MSC, 1992-1997)' _cell_length_a 11.3818(2) _cell_length_b 13.6538(2) _cell_length_c 14.9228(2) _cell_angle_alpha 87.5070(9) 78.2039(9) _cell_angle_beta _cell_angle_gamma 76.4867(9) _cell_volume 2207.23(6) _cell_formula_units_Z 2 _cell_measurement_temperature 200.0 27641 _cell_measurement_reflns_used _cell_measurement_theta_min 2.910
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C(30) -0.2066(4) 0.4359(3) 0.2774(3) 0.038(1) 1.000 . Uani d ?
C(31) -0.1193(4) 0.4222(3) 0.1972(3) 0.033(1) 1.000 . Uani d ?
C(32) -0.0435(5) 0.2761(4) 0.4501(3) 0.046(1) 1.000. Uani d?
C(33) 0.1966(4) 0.4142(3) 0.0610(3) 0.025(1) 1.000. Uani d ?
C(34) 0.1371(4) 0.5149(3) 0.0809(3) 0.032(1) 1.000 . Uani d ?
C(35) 0.1925(4) 0.5909(3) 0.0413(3) 0.039(1) 1.000 . Uani d ?
C(36) = 0.3059(5) = 0.5675(4) = 0.0172(3) = 0.045(1) = 1.000 Hani d 2
C(37) = 0.3649(4) = 0.4682(4) = 0.0363(3) = 0.044(1) = 1.000 Hani d 2
C(38) = 0.3114(4) = 0.3924(3) = 0.025(3) = 0.033(1) = 0.000 Hani d 2
C(39) = 0.878(4) = 0.2474(3) = 0.0273(3) = 0.026(1) = 1.000 = Hapi = 0.2273(3) = 0.026(1) = 1.000 = Hapi = 0.2273(3) = 0.026(1) = 1.000 = Hapi = 0.2273(3) = 0.026(1) = 1.0000 = 1.0000 = 1.0000 = 1.0000 = 1.0000 = 1.0000 = 1.0000 = 1.0000 = 1.0000 = 1.0000 = 1.0000 = 1.0000 =
C(40) = 0.0076(4) = 0.1844(3) = 0.0573(3) = 0.020(1) = 1.000 = 0.0011 d = 0
C(41) = 0.0299(4) = 0.1334(3) = 0.0038(3) = 0.038(1) = 1.000 = 0.001 = 0.00001 = 0.0001 = 0
C(42) = 0.0225(1) = 0.01351(3) = 0.0050(3) = 0.0050(1) = 1.000 = 0.0011 = 0.0000 = 0.000000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.0000000 = 0.0000000 = 0.0000000 = 0.00000000
C(42) = 0.0111(5) = 0.1115(1) = 0.0571(3) = 0.011(1) = 1.000 = 0.0011(1)
C(44) = 0.1305(4) = 0.2566(3) = 0.0657(3) = 0.032(1) = 0.000 Uani d :
C(44) = 0.1303(4) = 0.2300(3) = 0.0037(3) = 0.032(1) = 1.000 = 0.001 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.000000 = 0.000000 = 0.00000 = 0.00000000
C(45) = 0.5714(5) = 0.1254(5) = 0.1255(2) = 0.025(1) = 1.000 = 0.0011 = 0.000000000000000000
C(47) = 0.4027(4) = 0.1000(3) = 0.1329(3) = 0.020(1) = 1.000 = 0.0001 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.00000 = 0.000000 = 0.000000 = 0.000000 = 0.00000000
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C(48) = 0.6072(4) = 0.0307(3) = 0.0716(3) = 0.031(1) = 1.000 = 0.0411 = 0.0207(3) = 0.0207(3) = 0.0207(1) = 0.027(1) = 0.
C(49) = 0.5205(4) = 0.0228(3) = 0.1008(3) = 0.030(1) = 1.000 = 0.0411 = 0.0228(3) = 0.1008(3) = 0.030(1) = 0.000 = 0.0001 = 0.0
C(50) = 0.4052(4) = 0.0203(3) = 0.1527(3) = 0.020(1) = 1.000 = 0.0011 = 0.000000000000000000
U(51) = 0.533(1) = 0.5330(8) = 0.5171(8) = 0.059(3) = 0.500. Uant d?
H(1) 0.0950 -0.0778 0.4317 0.035 1.000 . 0180 C ?
$H(2) = 0.2103 - 0.0678 = 0.5420 = 0.038 = 1.000 = 0.0180 C^{2}$
H(3) 0.3181 0.0589 0.5334 0.034 1.000 . 0150 C ?
H(4) 0.5649 0.2964 0.3215 0.043 1.000 . 01SO C ?
H(5) 0.7644 0.2287 0.2407 0.051 1.000 . 01s0 C ?
H(6) 0.8307 0.0559 0.2134 0.046 1.000 . 0150 C?
H(7) 0.6991 -0.0503 0.2713 0.042 1.000 . 0180 C ?
H(8) 0.5012 0.0163 0.3532 0.036 1.000 . 0180 C ?
H(9) 0.2059 0.32/3 0.5630 0.040 1.000 . 01so C ?
H(10) 0.21/1 0.3448 0.7154 0.051 1.000 . 0180 C ?
$H(11) = 0.3967 = 0.2661 = 0.7675 = 0.056 = 1.000 = 0.0180 C^{2}$
$H(12) = 0.5623 = 0.1686 = 0.6678 = 0.054 = 1.000 = 0.0180 C^2$
H(13) 0.5501 0.1476 0.5156 0.043 1.000 . 0180 C ?
$H(14) = 0.2385 \ 0.4011 \ 0.4114 \ 0.044 \ 1.000 \ . \ 01so \ C \ ?$
$H(15) = 0.2861 \ 0.4781 \ 0.2784 \ 0.045 \ 1.000 \ . U1SO C ?$
$H(16) = 0.1357 \ 0.4557 \ 0.1424 \ 0.040 \ 1.000 \ . 0150 \ C \ ?$
$H(17) = 0.0592 = 0.5312 = 0.1214 = 0.038 = 1.000 = 0.0180 C^{-2}$
$H(18) = 0.1520 = 0.6594 = 0.0544 = 0.047 = 1.000 = 0.0180 C^{2}$
H(19) 0.3433 0.6198 -0.0444 0.054 1.000 . 0180 C?
H(20) 0.4431 0.4523 - 0.0765 0.053 1.000 . 0180 C?
$H(21) = 0.3533 = 0.3243 - 0.0107 = 0.039 = 1.000 = 0.0180 = C^{2}$
$H(22) = 0.0212 \ 0.1770 \ 0.1210 \ 0.038 \ 1.000 \ . Uiso c ?$
$H(23) = 0.0865 \ 0.0922 \ 0.0174 \ 0.046 \ 1.000 \ . Ulso c ?$
H(24) -0.0102 0.1045 -0.1401 0.053 1.000 . Uiso c ?
H(25) 0.1242 0.2084 -0.1908 0.050 1.000 . Uiso c ?
H(26) U.1846 U.2997 -U.U873 U.U39 1.000 . Uiso c ?
H(27) -0.0120 0.0972 0.2955 0.038 1.000 . Uiso c ?
H(28) 0.0134 -0.0189 0.3065 0.038 1.000 . Uiso c ?
H(29) 0.0967 0.0287 0.2300 0.038 1.000 . Uiso c ?
H(30) 0.0281 0.2918 0.4637 0.056 1.000 . Uiso c ?
H(31) -0.1126 0.3020 0.4972 0.056 1.000 . Uiso c ?
H(32) -0.0317 0.2051 0.4463 0.056 1.000 . Uiso c ?
H(33) 0.4831 0.5825 0.5609 0.070 0.500 . Uiso d ?

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P(1)	0.021/0(0)	0.01001(0)	0.02020(0)	-0 0055(4)	-0.00561(0)	0.00214(0)
P(2)	0.0231(3) 0.0241(5)	0.0213(5)	0.0210(5)	-0.0027(4)	-0.0036(4)	0.0025(4)
F(1)	0.043(2)	0.036(2)	0.071(2)	0.000(1)	0.012(1)	0.011(1)
F(2)	0.058(2)	0.042(2)	0.072(2)	-0.020(1)	0.001(2)	0.019(1)
F(3)	0.068(2)	0.025(1)	0.073(2)	-0.008(1)	-0.018(2)	0.013(1)
F(4)	0.044(2)	0.037(2)	0.067(2)	0.011(1)	-0.008(1)	0.003(1)
F(5)	0.036(2)	0.043(2)	0.063(2)	-0.011(1)	-0.002(1)	0.010(1)
F(6)	0.034(1)	0.025(1)	0.043(1)	-0.007(1)	-0.003(1)	0.002(1)
F(7)	0.030(1)	0.048(2)	0.054(2)	-0.012(1)	0.001(1)	0.004(1)
F(8)	0.028(1)	0.053(2)	0.052(2)	0.007(1)	0.001(1)	-0.009(1)
F(9)	0.052(2)	0.027(1)	0.048(2)	0.003(1)	-0.010(1)	-0.008(1)
F(10)	0.040(1)	0.028(1)	0.049(2)	-0.011(1)	0.001(1)	-0.002(1)
C(1)	0.022(2)	0.021(2)	0.026(2)	-0.004(2)	-0.004(2)	0.000(2)
C(2)	0.022(2)	0.020(2)	0.020(2)	-0.002(2)	-0.002(2)	0.003(1)
C(3)	0.023(2)	0.026(2)	0.023(2)	-0.004(2)	-0.003(2)	-0.001(2)
C(4)	0.028(2)	0.024(2)	0.035(2)	-0.009(2)	-0.003(2)	0.004(2)
C(5)	0.036(2)	0.030(2)	0.026(2)	-0.00/(2)	-0.002(2)	0.012(2)
C(6)	0.029(2)	0.033(2)	0.024(2)	-0.008(2)	-0.009(2)	0.007(2)
C(7)	0.028(2)	0.029(2)	0.040(2)	-0.009(2)	-0.010(2)	0.002(2)
C(0)	0.024(2)	0.028(2)	0.027(2)	-0.004(2)	-0.007(2)	-0.002(2)
C(9)	0.032(2)	0.052(2)	0.044(3) 0.047(3)	-0.012(2)	-0.003(2)	-0.009(2)
C(10)	0.032(3)	0.052(3)	0.047(3) 0.034(2)	-0,020(2)	-0,007(2)	-0,010(2)
C(12)	0.033(2)	0.037(2)	0.033(2)	0.004(2)	-0.010(2)	-0.005(2)
C(13)	0.031(2)	0.028(2)	0.031(2)	-0.004(2)	-0.011(2)	0.003(2)
C(14)	0.034(2)	0.023(2)	0.025(2)	-0.009(2)	-0.009(2)	0.002(2)
C(15)	0.032(2)	0.032(2)	0.035(2)	-0.007(2)	-0.005(2)	-0.001(2)
C(16)	0.052(3)	0.038(3)	0.036(3)	-0.018(2)	0.004(2)	-0.008(2)
C(17)	0.067(4)	0.049(3)	0.032(3)	-0.026(3)	-0.011(2)	-0.002(2)
C(18)	0.053(3)	0.044(3)	0.044(3)	-0.011(2)	-0.026(2)	0.003(2)
C(19)	0.042(3)	0.033(2)	0.035(2)	-0.007(2)	-0.013(2)	-0.002(2)
C(20)	0.035(2)	0.024(2)	0.028(2)	-0.005(2)	-0.005(2)	-0.001(2)
C(21)	0.036(2)	0.022(2)	0.039(2)	-0.003(2)	-0.004(2)	0.002(2)
C(22)	0.044(3)	0.032(2)	0.036(2)	-0.016(2)	-0.006(2)	0.007(2)
C(23)	0.049(3)	0.019(2)	0.042(3)	-0.005(2)	-0.017(2)	0.004(2)
C(24)	0.036(3)	0.030(2)	0.040(3)	0.002(2)	-0.015(2)	0.001(2)
C(25)	0.031(2)	0.033(2)	0.036(2)	-0.005(2)	-0.011(2)	0.001(2)
C(26)	0.026(2)	0.022(2)	0.027(2)	-0.004(2)	-0.002(2)	-0.001(2)
C(27)	0.024(2)	0.022(2)	0.025(2)	-0.006(2)	-0.001(2)	-0.002(2)
C(20)	0.033(2)	0.027(2)	0.030(2)	-0.006(2)	0.000(2)	-0.003(2)
C(29)	0.031(2)	0.030(3) 0.031(2)	0.033(2)	-0.003(2)	0.000(2)	-0.003(2)
C(30)	0.020(2)	0.031(2)	0.042(3)	0.003(2)	-0 009(2)	0.001(2)
C(32)	0.046(3)	0.054(3)	0.029(2)	-0.003(2)	0.005(2)	0.001(2)
C(33)	0.030(2)	0.023(2)	0.023(2)	-0.006(2)	-0.009(2)	0.006(2)
C(34)	0.035(2)	0.029(2)	0.032(2)	-0.005(2)	-0.009(2)	0.002(2)
C(35)	0.048(3)	0.025(2)	0.049(3)	-0.007(2)	-0.024(2)	0.007(2)

C(36)	0.050(3)	0.044(3)	0.050(3)	-0.026(2)	-0.018(2)	0.018(2)
C(37)	0.037(3)	0.050(3)	0.045(3)	-0.018(2)	-0.001(2)	0.010(2)
C(38)	0.030(2)	0.031(2)	0.037(2)	-0.007(2)	-0.005(2)	0.005(2)
C(39)	0.025(2)	0.022(2)	0.029(2)	-0.004(2)	-0.005(2)	0.000(2)
C(40)	0.029(2)	0.030(2)	0.033(2)	-0.005(2)	-0.003(2)	0.001(2)
C(41)	0.035(3)	0.024(2)	0.057(3)	-0.006(2)	-0.013(2)	-0.006(2)
C(42)	0.046(3)	0.040(3)	0.048(3)	-0.001(2)	-0.022(2)	-0.014(2)
C(43)	0.048(3)	0.045(3)	0.031(2)	-0.006(2)	-0.009(2)	-0.005(2)
C(44)	0.033(2)	0.035(2)	0.026(2)	-0.009(2)	-0.002(2)	0.002(2)
C(45)	0.023(2)	0.021(2)	0.022(2)	-0.001(2)	-0.007(2)	0.002(2)
C(46)	0.029(2)	0.024(2)	0.026(2)	-0.003(2)	-0.010(2)	0.002(2)
C(47)	0.024(2)	0.036(2)	0.032(2)	-0.010(2)	-0.006(2)	0.005(2)
C(48)	0.023(2)	0.038(2)	0.026(2)	0.004(2)	-0.004(2)	-0.005(2)
C(49)	0.034(2)	0.024(2)	0.029(2)	0.001(2)	-0.009(2)	-0.005(2)
C(50)	0.031(2)	0.028(2)	0.025(2)	-0.006(2)	-0.008(2)	0.002(2)
C(51)	0.061(7)	0.049(6)	0.065(7)	-0.031(5)	0.014(6)	-0.019(5)
#						

_refine_special_details

;

 $s^2(Fo)$ is the larger of the value from averaging of equivalent reflections or counting statistics.

A molecule of dichloromethane is disordered across a centre of inversion. The images of the two Cl atoms almost coincide, so the Cl atoms were assigned isotropic displacement factors which were constrained to be equal. Initially restraints were imposed on Cl--C distances and the Cl--C--Cl angle, but these restraints were removed later in the refinement.

Hydrogen atoms were included at geometrically determined positions which were periodically recalculated but were not refined. Methyl hydrogens were oriented

to best-fit peaks in inner-data difference map.

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_refine_ls_structure_factor_coef	F
_refine_ls_matrix_type	full
_refine_ls_weighting_scheme	sigma
_refine_ls_weighting_details	$w = 1/[s^2(Fo)]$
_refine_ls_hydrogen_treatment	noref
_refine_ls_extinction_method	none
_refine_ls_extinction_coef	?
_refine_ls_abs_structure_details	?
_refine_ls_abs_structure_Flack	?
_refine_ls_number_reflns	8125
_refine_ls_number_parameters	593
_refine_ls_number_restraints	0
_refine_ls_number_constraints	1
_refine_ls_R_factor_all	0.0379
_refine_ls_R_factor_gt	0.0272
_refine_ls_wR_factor_all	0.0338
_refine_ls_wR_factor_ref	0.0302
_refine_ls_goodness_of_fit_all	0.858
_refine_ls_goodness_of_fit_ref	0.856
_refine_ls_shift/su_max	0.0360
_refine_ls_shift/su_mean	0.0010
_refine_diff_density_min	-1.25

_refine_diff_density_max

#----loop_ _geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_1 _geom_bond_site_symmetry_2 _geom_bond_publ_flag Au(1) P(1) 2.274(1) . . yes Au(1) C(20) 2.056(4) . . yes Au(2) P(2) 2.374(1) . . yes Au(2) C(2) 2.077(4) . . yes Au(2) C(27) 2.099(4) . . yes Au(2) C(45) 2.098(4) . . yes Cl(1) Cl(2) 0.626(5) . 2_666 no Cl(1) C(51) 1.73(1) . . yes Cl(1) C(51) 1.75(1) . 2_666 no Cl(2) C(51) 1.74(1) . . yes Cl(2) C(51) 1.29(1) . 2_666 no P(1) C(1) 1.809(4) . . yes P(1) C(8) 1.825(4) . . yes P(1) C(14) 1.819(4) . . yes P(2) C(26) 1.795(4) . . yes P(2) C(33) 1.797(4) . . yes P(2) C(39) 1.818(4) . . yes F(1) C(21) 1.366(5) . . yes F(2) C(22) 1.350(5) . . yes F(3) C(23) 1.347(4) . . yes F(4) C(24) 1.357(5) . . yes F(5) C(25) 1.350(5) . . yes F(6) C(46) 1.352(4) . . yes F(7) C(47) 1.352(5) . . yes F(8) C(48) 1.339(4) . . yes F(9) C(49) 1.352(4) . . yes F(10) C(50) 1.347(4) . . yes C(1) C(2) 1.399(5) . . yes C(1) C(6) 1.405(5) . . yes C(2) C(3) 1.405(5) . . yes C(3) C(4) 1.391(5) . . yes C(3) C(7) 1.509(5) . . yes C(4) C(5) 1.387(6) . . yes C(4) H(1) 0.95 . . no C(5) C(6) 1.378(6) . . yes C(5) H(2) 0.95 . . no C(6) H(3) 0.95 . . no C(7) H(27) 0.95 . . no C(7) H(28) 0.95 . . no C(7) H(29) 0.95 . . no C(8) C(9) 1.387(6) . . yes C(8) C(13) 1.385(5) . . yes C(9) C(10) 1.388(6) . . yes C(9) H(4) 0.95 . . no C(10) C(11) 1.380(6) . . yes C(10) H(5) 0.95 . . no C(11) C(12) 1.388(6) . . yes C(11) H(6) 0.95 . . no

C(12)	C(13)	1.378(6)	• •	yes
C(12)	H('/) ().951	10	
C(13)	H(8)	$1.95 \cdot 1$	10	
C(14)	C(19)	1.390(0) 1.390(6)	• •	yes
C(15)	C(16)	1.383(6)	•••	ves
C(15)	H(9) ().95 1	••• 10	YCD
C(16)	C(17)	1.392(7)	•••	yes
C(10)	C(18)	0.95 1.373(7)	110	Veg
C(17)	H(11)	0.95	 no	YCD
C(18)	C(19)	1.394(6)		yes
C(18)	H(12)	0.95	no	
C(19)	H(13)	0.95	no	
C(20)	C(21)	1.379(6)	•••	yes
C(20)	C(25)	1.3/1(6)	• •	yes
C(21)	C(22)	1.369(6)	• •	yes
C(22)	C(23)	1.300(0) 1.371(6)	•••	ves
C(24)	C(25)	1.388(6)		yes
C(26)	C(27)	1.396(5)		yes
C(26)	C(31)	1.389(5)		yes
C(27)	C(28)	1.407(5)	• •	yes
C(28)	C(29)	1.388(6)	• •	yes
C(28)	C(32)	1.495(6)	• •	yes
C(29)	C(30)	1.385(6)	•••	yes
C(29)	C(31)	1 379(6)	110	Veg
C(30)	H(15)	0.95	no .	100
C(31)	H(16)	0.95	no	
C(32)	H(30)	0.95	no	
C(32)	H(31)	0.95	no	
C(32)	H(32)	0.95	no	
C(33)	C(34)	1.399(5)	• •	yes
C(33)	C(38)	1.390(6) 1.397(6)	• •	yes
C(34)	H(17)	0.95	· · no	усь
C(35)	C(36)	1.378(7)		ves
C(35)	H(18)	0.95	no	-
C(36)	C(37)	1.378(7)		yes
C(36)	H(19)	0.95	no	
C(37)	C(38)	1.369(6)	•••	yes
C(37)	H(20)	0.95	no	
C(30)	C(40)	1 393(6)	110	ves
C(39)	C(44)	1.384(5)		ves
C(40)	C(41)	1.361(6)		yes
C(40)	H(22)	0.95	no	
C(41)	C(42)	1.393(7)	• •	yes
C(41)	H(23)	0.95	no	
C(42)	С(43) H(24)	1.3/U(/) 0.95	•••	yes
C(43)	C(44)	1.382(6)		ves
C(43)	H(25)	0.95	no	1 -~
C(44)	H(26)	0.95	no	
C(45)	C(46)	1.384(5)		yes
C(45)	C(50)	1.387(5)		yes

C(46) C(47) 1.375(5) . . yes C(47) C(48) 1.379(6) . . yes C(48) C(49) 1.369(6) . . yes C(49) C(50) 1.379(6) . . yes C(51) C(51) 1.47(2) . 2_666 no C(51) H(33) 0.95 . . no C(51) H(34) 0.95 . . no #------_____ loop_ _geom_angle_atom_site_label_1 _geom_angle_atom_site_label_2 _geom_angle_atom_site_label_3 _geom_angle _geom_angle_site_symmetry_1 _geom_angle_site_symmetry_2 _geom_angle_site_symmetry_3 _geom_angle_publ_flag P(1) Au(1) C(20) 169.1(1) . . . yes P(2) Au(2) C(2) 163.4(1) . . . yes P(2) Au(2) C(27) 68.1(1) . . . yes P(2) Au(2) C(45) 101.5(1) . . . yes C(2) Au(2) C(27) 99.2(1) . . . yes C(2) Au(2) C(45) 91.1(1) . . . yes C(27) Au(2) C(45) 169.6(1) . . . yes Au(1) P(1) C(1) 117.1(1) . . . yes Au(1) P(1) C(8) 111.5(1) . . . yes Au(1) P(1) C(14) 111.0(1) . . . yes C(1) P(1) C(8) 106.5(2) . . . yes C(14) 105.0(2) . . . yes C(1) P(1) C(8) P(1) C(14) 104.8(2) . . . yes Au(2) P(2) C(26) 83.4(1) . . . yes C(33) 125.6(1) . . . yes Au(2) P(2) C(39) 114.6(1) . . . yes Au(2) P(2) C(33) 113.1(2) . . . yes C(26) P(2) C(39) 107.6(2) . . . yes C(26) P(2) C(33) P(2) C(39) 108.8(2) . . . yes P(1) C(1) C(2) 120.0(3) . . . yes P(1) C(1) C(6) 119.5(3) . . . yes C(2) C(1) C(6) 120.5(3) . . . yes Au(2) C(2) C(1) 124.2(3) . . . yes Au(2) C(2) C(3) 117.0(3) . . . yes C(1) C(2) C(3) 118.9(3) . . . yes C(2) C(3) C(4) 119.7(3) . . . yes C(2) C(3) C(7) 121.8(3) . . . yes C(4) C(3) C(7) 118.5(4) . . . yes C(3) C(4) C(5) 121.2(4) . . . yes C(3) C(4) H(1) 119.4 . . . no C(5) C(4) H(1) 119.4 . . . no C(4) C(5) C(6) 119.7(4) . . . yes C(4) C(5) H(2) 120.1 . . . no C(6) C(5) H(2) 120.1 . . . no C(1) C(6) C(5) 120.0(4) . . . yes C(1) C(6) H(3) 120.0 . . . no H(3) 120.0 . . . no C(5) C(6) H(27) 109.5 . . . no C(3) C(7) H(28) 109.5 . . . no C(3) C(7) C(3) C(7) H(29) 109.5 . . . no

H(27) C(7)	H(28) 109.5 no
H(27) C(7)	H(29) 109.5 no
H(28) C(7)	H(29) 109.5 no
P(1) C(8)	C(9) 118.7(3) ves
P(1) C(8)	C(13) 121.5(3) ves
C(9) C(8)	C(13) 119 $8(4)$ ves
C(9) C(0)	C(10) 119 $O(1)$
C(0) C(0)	U(4) = 120 0 mo
C(0) C(9)	H(4) 120.0
C(10) C(9)	H(4) 120.0 no
C(9) C(10)	C(11) 120.3(4) yes
C(9) C(10)	H(5) 119.9 no
C(11) C(10)	H(5) 119.9 no
C(10) C(11)	C(12) 119.6(4) yes
C(10) C(11)	H(6) 120.2 no
C(12) C(11)	H(6) 120.2 no
C(11) C(12)	C(13) 120.4(4) yes
C(11) C(12)	H(7) 119.8 no
C(13) C(12)	H(7) 119.8 no
C(8) C(13)	C(12) 120.0(4) ves
C(8) $C(13)$	H(8) 120 0 no
C(12) $C(13)$	H(8) 120 0 no
D(1) C(14)	C(15) 118 $F(3)$
P(1) C(14) D(1) C(14)	C(13) 110.3(3) yes
P(1) C(14)	$C(19) 122.9(3) \dots $ yes
C(15) $C(14)$	C(19) 118.6(4) yes
C(14) $C(15)$	C(16) 120.7(4) yes
C(14) $C(15)$	H(9) 119.7no
C(16) C(15)	H(9) 119.7 no
C(15) C(16)	C(17) 120.0(4) yes
C(15) C(16)	$H(10) 120.0 \dots no$
C(17) C(16)	H(10) 120.0 no
C(16) C(17)	C(18) 119.9(4) yes
C(16) C(17)	H(11) 120.0 no
C(18) C(17)	H(11) 120.0 no
C(17) C(18)	C(19) 120.2(4) yes
C(17) C(18)	H(12) 119.9 no
C(19) C(18)	H(12) 119.9 no
C(14) C(19)	C(18) 120.5(4) yes
C(14) C(19)	H(13) 119.7 no
C(18) C(19)	H(13) 119.7 no
Au(1) C(20)	C(21) 118.9(3) yes
Au(1) C(20)	C(25) 125.4(3) yes
C(21) C(20)	C(25) 115.1(4) yes
F(1) C(21)	C(20) 119.3(4) yes
F(1) C(21)	C(22) 116.5(4) ves
C(20) C(21)	C(22) 124 2(4) ves
F(2) C(22)	C(21) 121 $G(4)$ ves
F(2) C(22)	C(23) 119 $5(4)$ Ves
C(21) C(22)	C(23) 118 9(4) Ves
F(3) C(23)	C(22) 120 3(4) veg
F(3) C(23)	C(24) 120.3(4) yes
(22) - (22)	C(24) 119 $G(4)$ 200
$r(\Delta) c(\Delta 3)$	C(23) 119 1(4) yes
$\mathbf{F}(\mathbf{A}) = \mathbf{C}(\mathbf{A}\mathbf{F})$	C(25) 121 $C(4)$ yes
P(2) = (22) = (24)	C(25) = 110 - 7(A)
U(23) U(24) F(5) C(25)	C(20) = 120 - 7(4) + yes
$\mathbf{r}(5) = \mathbf{C}(25)$ $\mathbf{r}(5) = \mathbf{C}(25)$	C(20) = 120.7(4) yes
r(5) C(25)	$C(24) \pm 0.7(4) \dots \text{ yes}$
C(20) $C(25)$	U(24) 122.5(4) Yes

P(2) C(26)	C(27) 103.3(3) yes
P(2) C(26)	C(31) 132.8(3) yes
C(27) C(26)	C(31) 123.9(4) yes
Au(2) C(27)	C(26) 105.1(3) yes
Au(2) C(27)	C(28) 136.2(3) yes
C(26) C(27)	C(28) 118.7(4) yes
C(27) C(28)	C(29) 116.5(4) yes
C(27) C(28)	C(32) 123.7(4) yes
C(29) C(28)	C(32) 119.8(4) yes
C(28) C(29)	C(30) 124.1(4) yes
C(28) C(29)	H(14) 118.0 no
C(30) C(29)	H(14) 118.0 no
C(29) C(30)	C(31) 119.8(4) yes
C(29) C(30)	H(15) 120.1 no
C(31) C(30)	H(15) 120.1 no
C(26) C(31)	C(30) 117.0(4) yes
C(26) C(31)	H(16) 121.5 no
C(30) C(31)	H(16) 121.5 no
C(28) C(32)	H(30) 109.5 no
C(28) C(32)	H(31) 109.5 no
C(28) C(32)	H(32) 109.5 no
H(30) C(32)	H(31) 109.5 no
H(30) C(32)	H(32) 109.5 no
H(31) C(32)	H(32) 109.5 no
P(2) C(33)	C(34) 120.9(3) yes
P(2) C(33)	C(38) 120.1(3) yes
C(34) C(33)	C(38) 118.9(4) yes
C(33) C(34)	C(35) 119.7(4) yes
C(33) C(34)	H(17) 120.1 no
C(35) C(34)	H(17) 120.1 no
C(34) C(35)	C(36) 120.3(4) yes
C(34) C(35)	H(18) 119.9 no
C(36) C(35)	H(18) 119.9 no
C(35) $C(36)$	C(37) 120.0(4) yes
C(35) C(36)	H(19) 120.0 no
C(37) C(36)	$H(19) 120.0 \dots 100$
C(36) C(37)	U(20) 110 9 no
C(30) C(37)	H(20) 119.0
C(33) $C(37)$	C(37) 120 $T(4)$ vec
C(33) $C(38)$	H(21) 119 6 no
C(33) $C(30)$	H(21) 119.0
P(2) C(39)	C(40) 117 2(3) Ves
P(2) C(39)	C(44) 123 7(3) Ves
C(40) C(39)	C(44) 119 1(4) veg
C(39) C(40)	C(41) 120.7(4)
C(39) C(40)	H(22) 119.7 no
C(41) C(40)	H(22) 119.7 no
C(40) C(41)	C(42) 120.3(4) ves
C(40) C(41)	H(23) 119.9 no
C(42) C(41)	H(23) 119.9 no
C(41) C(42)	C(43) 119.2(4) yes
C(41) C(42)	H(24) 120.4 no
C(43) C(42)	H(24) 120.4 no
C(42) C(43)	C(44) 121.0(4) yes
C(42) C(43)	H(25) 119.5 no
C(44) C(43)	H(25) 119.5 no

```
C(39) C(44)
            C(43) 119.7(4) . . . yes
C(39) C(44)
            H(26) 120.2 . . . no
C(43) C(44)
            H(26) 120.2 . . . no
            C(46) 119.7(3) . . . yes
Au(2) C(45)
            C(50) 125.7(3) . . . yes
Au(2) C(45)
C(46) C(45) C(50) 114.5(3) . . . yes
F(6) C(46) C(45) 120.1(3) . . . yes
F(6) C(46) C(47) 116.3(4) . . . yes
C(45) C(46) C(47) 123.6(4) . . . yes
F(7) C(47) C(46) 121.1(4) . . . yes
F(7) C(47) C(48) 119.1(4) . . . yes
C(46) C(47) C(48) 119.8(4) . . . yes
F(8) C(48) C(47) 120.4(4) . . . yes
F(8) C(48) C(49) 120.9(4) . . . yes
C(47) C(48) C(49) 118.7(4) . . . yes
F(9) C(49) C(48) 119.2(4) . . . yes
F(9) C(49) C(50) 120.6(4) . . . yes
C(48) C(49) C(50) 120.1(4) . . . yes
F(10) C(50) C(45) 120.5(3) . . . yes
F(10) C(50) C(49) 116.3(3) . . . yes
C(45) C(50) C(49) 123.2(4) . . . yes
Cl(1) C(51) Cl(2) 111.0(5) . . . yes
 Cl(1) C(51) H(33) 109.1 . . . no
Cl(1) C(51) H(34) 109.1 . . . no
 Cl(2) C(51) H(33) 109.1 . . . no
Cl(2) C(51) H(34) 109.1 . . . no
H(33) C(51) H(34) 109.5 . . . no
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
        C(18)
                  3.298(6)
                              . . no
Cl(1)
         C(19)
                   3.401(6)
Cl(1)
                              . . no
                              . 2_666 no
Cl(1)
         C(21)
                  3.445(6)
                              . . no
Cl(1)
         C(17)
                  3.475(6)
                              . 2_666 no
Cl(1)
         F(1)
                  3.508(5)
                              . . no
Cl(2)
         F(1)
                  3.212(5)
Cl(2)
         C(21)
                  3.301(6)
                             . . no
Cl(2)
         C(20)
                  3.572(6)
                             . . no
F(1)
         C(37)
                  3.250(5)
                             . 2_665 no
F(2)
         C(37)
                  3.346(6)
                             . 2_665 no
F(2)
         F(9)
                  3.392(4)
                             . 1_565 no
         C(17)
                  3.442(6)
                             . 2_666 no
F(2)
                  2.895(4)
                             . 1_565 no
F(3)
         F(10)
                   3.112(5)
                            . 1_565 no
F(3)
         C(7)
         C(42)
                   3.232(5)
                            . 2_565 no
F(3)
                             . 1_565 no
                   3.541(4)
F(3)
         C(3)
F(3)
          C(4)
                   3.596(5)
                             . 1_565 no
                             . 2_566 no
F(4)
         C(15)
                   3.250(5)
                             . 2_565 no
F(4)
          C(43)
                   3.398(5)
                             . 2_566 no
          C(32)
                   3.404(5)
F(4)
                             . 2_566 no
F(4)
          C(16)
                   3.423(6)
```

F(5)

C(15)

3.556(5)

. 2_566 no

F(7)	C(41)	3.337(5)	. 1_655 no
F(7)	C(36)	3.457(5)	. 2_665 no
F(8)	F(10)	3.273(4)	. 2_655 no
F(8)	C(50)	3.296(5)	. 2_655 no
F(8)	C(44)	3.421(5)	. 2_655 no
F(8)	C(39)	3.425(4)	. 2_655 no
F(8)	C(43)	3.425(5)	. 2_655 no
F(8)	C(40)	3.442(5)	. 2_655 no
F(8)	C(42)	3.459(5)	. 2_655 no
F(8)	C(41)	3.478(5)	. 2_655 no
F(9)	C(47)	3.308(5)	. 2_655 no
F(9)	C(48)	3.372(5)	. 2_655 no
F(9)	C(17)	3.536(5)	. 2_656 no
F(9)	C(46)	3.546(4)	. 2_655 no
C(4)	C(4)	3.398(8)	. 2_556 no
C(7)	C(11)	3.516(6)	. 1_455 no
C(14)	C(51)	3.56(1)	. 2_666 no
C(16)	C(30)	3.507(6)	. 2_566 no
C(41)	C(41)	3.547(8)	. 2 no
C(48)	C(49)	3.301(5)	. 2_655 no
C(48)	C(50)	3.507(5)	. 2_655 no
C(49)	C(49)	3.327(8)	. 2_655 no
Au(1)	Au(2)	3.1948(2)	no
#			
TOOD	atom atom	aita labal 1	
_geom_tor	sion_atom	_site_label_l	
_geom_tor	sion_atom	_SILE_IADEL_2	
_geom_tor	sion_atom	_site_label_3	
_geom_tor	sion_atom	_SILE_IADEL_4	
_geom_tor	sion site	_Symmetry_1	
_geom_tor	sion site	_symmetry_2	
_geom_tor	sion site	_symmetry 4	
_geom_tor	sion_bicc		
_geom_tor	sion nubl	flag	
$A_{11}(1) P($	1) $C(1)$ $C(1)$	(2) 3	32 6(3) no
$A_{11}(1) P($	1) C(1) C(1) C(1) C(1) C(1) C(1) C(1) C((6) -	-1464(3) no
Au(1) P(1) C(8) C(1) C(1) C(1) C(1) C(1) C(1) C(1) C(1	(9)	36.7(4) no
Au(1) P(1) C(8) C(8) C(8) C(8) C(8) C(8) C(8) C(8	(13)	-142.7(3) no
Au(1) P(1) $C(14)$	C(15)	46.3(4) no
Au(1) P(1) $C(14)$	C(19)	-134.5(3) no
Au(1) C(20) C(21)	F(1)	7.8(5) no
Au(1) C(20) C(21)	C(22)	169.4(4) no
Au(1) C(20) C(25)	F(5)	-9.3(6) no
Au(1) C(20) C(25)	C(24)	. 168.7(3) no
Au(2) P(2) C(26)	C(27)	2.6(2) no
Au(2) P(2) C(26)	C(31)	-174.7(4) no
Au(2) P(2) C(33)	C(34)	-104.4(3) no
Au(2) P(2) C(33)	C(38)	72.3(4) no
Au(2) P(2) C(39)	С(40)	49.5(3) no
Au(2) P(2) C(39)	С(44)	-130.7(3) no
Au(2) C(2) C(1) P	(1) 2	2.3(4) no
Au(2) C(2) C(1) C	(6)	178.7(3) no
Au(2) C(2) C(3) C	(4) 1	.77.2(3) no
Au(2) C(2) C(3) C	(7)	6.2(5) no
Au(2) C(27) C(26)	P(2)	-3.0(3) no
-	-		

Au(2)	C(27)	C(28)	C(29)		174.5(3) no
Au(2)	C(27)	C(28)	C(32)		6.5(7) no
Au(2)	C(45)	C(46)	F(6)		3.3(5) no
Au(2)	C(45)	C(46)	C(47)		177.1(3) no
Au(2)	C(45)	C(50)	F(10)		1.5(5) no
Au(2)	C(45)	C(50)	C(49)		178.6(3) no
Cl(1)	Cl(2)	C(51)	Cl(2)		2 666 43(1) no
Cl(1)	C1(2)	C(51)	C(51)		2 666 . 2 666 43(1) no
Cl(1)	Cl(2)	C(51)	C1(2)		26662666 - 145(1) no
Cl(1)	C1(2)	C(51)	C(51)		2 666 2 666145(1) no
Cl(1)	C(51)	Cl(1)	C1(2)		2666 - 27.5(9) no
Cl(1)	C(51)	Cl(1)	C(51)		. 2 666 2 666 0.0000(1) no
Cl(1)	C(51)	Cl(2)	C(51)		2 666 12.7(4) no
Cl(1)	C(51)	Cl(2)	C(51)		26662666-43(1) no
Cl(1)	C(51)	C(51)	Cl(1)		. 2 666 2 666 180.0000 no
Cl(1)	C(51)	C(51)	Cl(2)		. 2 666167.0(4) no
Cl(1)	C(51)	C(51)	C1(2)		. 2 666 2 666 13.0(4) no
Cl(1)	C(51)	Cl(1)	Cl(2)		2 666 2 666 . 132(2) no
Cl(1)	C(51)	Cl(1)	C(51)		2 666 2 666 . 0.0000 no
Cl(1)	C(51)	Cl(2)	C(51)		2 66618.4(6) no
Cl(1)	C(51)	Cl(2)	C(51)		2 666 2 666 . 145(1) no
Cl(1)	C(51)	C(51)	Cl(1)		2 666 . 2 666 -180.0000 no
Cl(1)	C(51)	C(51)	C1(2)		2_666 167.0(4) no
Cl(1)	C(51)	C(51)	Cl(2)		2_666 . 2_666 -13.0(4) no
Cl(2)	Cl(1)	C(51)	C(51)		2_666 . 2_666 -27.5(9) no
Cl(2)	Cl(1)	C(51)	C(51)		2_666 2_666 . 132(2) no
Cl(2)	C(51)	Cl(1)	C(51)		2_666 -10.1(3) no
Cl(2)	C(51)	Cl(1)	C(51)		. 2_666 2_666 27.5(9) no
Cl(2)	C(51)	Cl(2)	C(51)		. 2_666 2_666 0.0000 no
Cl(2)	C(51)	C(51)	Cl(2)		. 2_666 2_666 180.0000 no
Cl(2)	C(51)	Cl(1)	C(51)	•	2_666 20.0(6) no
Cl(2)	C(51)	Cl(1)	C(51)	•	2_666 2_666132(2) no
Cl(2)	C(51)	Cl(2)	C(51)	•	2_666 2_666 . 0.0000 no
Cl(2)	C(51)	C(51)	Cl(2)	•	2_666 . 2_666 -180.0000 no
P(1) i	Au(1) (2(20)	C(21)	• •	47.7(8) no
P(1) 7	Au(1) (2(20)	C(25)	•••	122.7(6) no
P(1) (C(1) C(1)	2) C(3)	•	-178.8(3) no
P(I) (C(1) C(1)	6) C(5)	•	-179.5(3) no
P(I) (2(8) C((9) C(10) .	• •	-179.5(3) no
P(1) (C(8) C(3)	(15) C	(± 2) .	•	177 [(3)] no
P(1) ((14) ((14) ((15)	C(10)	• •	179, 2/2 no
P(1) ((14) (14) (14)	2(19) 7(2) C	C(18)	• •	142 E(2) no
P(Z) I	$\operatorname{Au}(Z)$ ((2)	·(⊥) • 1(2)	• •	-143.5(5) IIO
P(Z) I	$\operatorname{Au}(Z)$ (-(ム) し コ(ロワ)	C(2)	• •	24(2) no
P(Z) I	$\operatorname{Au}(Z)$ (- (ユノ) マ(クワ)	C(20)	• •	180 0(4) no
P(2)	$\Delta_{11}(2)$ (-(27) 	C(20)	•••	62 6(3) no
P(2)	$\Delta_{11}(2)$ (r(45)	C(50)	•••	-115 1(3) no
P(2)	(26)	1(27)	C(28)	•••	178.9(3) no
P(2) (C(26)	2(31)	C(30)		. 177.8(3) no
P(2) (2)	2(33)	2(34)	C(35)		177.7(3) no
P(2)	C(33)	2(38)	C(37)		177.8(3) no
P(2) (2(39) (C(40)	C(41)		179.0(3) no
P(2) (C(39) C	C(44)	C(43)		179.6(3) no
F(1) (C(21) C	2(20)	C(25)	• •	179.2(4) no
F(1) (C(21) C	2(22)	F(2) .		2.2(6) no
F(1) (C(21) (2(22)	C(23)		178.3(4) no

F(2)	C(22) C(21) C(20)	179.5(4) no
F(2)	C(22) C(23) F(3)	1.3(6) no
F(2)	C(22) C(23) C(24)	179.5(4) no
F(3)	C(23) C(22) C(21)	179.2(4) no
F(3)	C(23) C(24) F(4)	0.1(6) no
F(3)	C(23) C(24) C(25)	179.2(4) no
F(4)	C(24) C(23) C(22)	179.1(4) no
F(4)	C(24) C(25) F(5)	0.1(6) no
F(4)	C(24) C(25) C(20)	178.0(4) no
F(5)	C(25) C(20) C(21)	180.0(4) no
F(5)	C(25) C(24) C(23)	179.2(4) no
F(6)	C(46) C(45) C(50)	178.8(3) no
F(6)	C(46) C(47) F(7)	1.2(6) no
F(6)	C(46) C(47) C(48)	178.4(3) no
F(7)	C(47) C(46) C(45)	179.1(4) no
F(7)	C(47) C(48) F(8)	0.8(6) no
F(7)	C(47) C(48) C(49)	179.7(4) no
F(8)	C(48) C(47) C(46)	178.8(4) no
F(8)	C(48) C(49) F(9)	1.0(6) no
F(8)	C(48) C(49) C(50)	179.6(4) no
F(9)	C(49) C(48) C(47)	179.8(3) no
F(9)	C(49) C(50) F(10)	0.6(5) no
F(9)	C(49) C(50) C(45)	179.3(3) no
F(10)) C(50) C(45) C(46)	179.2(3) no
F(10)) C(50) C(49) C(48)	178.0(4) no
C(1)	P(1) Au(1) C(20)	173.3(6) no
C(1)	$P(1) C(8) C(9) \dots$. 165.5(3) no
C(1)	P(1) C(8) C(13)	13.9(4) no
C(1)	P(1) C(14) C(15)	81.1(3) no
C(1)	P(1) C(14) C(19)	98.0(4) no
C(1)	C(2) Au(2) C(27)	-104.4(3) no
C(1)	C(2) Au(2) C(45)	1.0(5) no
C(1)	$C(2) C(3) C(4) \dots$	-1.8(5) no
C(1)	$C(2) C(3) C(7) \dots$	174.9(3) no
C(1)	$C(6) C(5) C(4) \dots$	-1.7(6) no
C(2)	Au(2) P(2) C(20)	154 1(4) = 20
C(2)	Au(2) P(2) C(33)	-66 0(4) no
C(2)	Au(2) P(2) C(33)	-166 4(3) no
C(2)	Au(2) C(27) C(20).	11 2(4) no
C(2)	Au(2) C(27) C(20)	-128 4(3) no
C(2)	$A_{11}(2) C(45) C(50)$	53 9(3) no
C(2)	C(1) P(1) C(8)	-92.9(3) no
C(2)	$C(1) P(1) C(14) \dots$	156.2(3) no
C(2)	C(1) $C(6)$ $C(5)$	1.6(6) no
C(2)	$C(3) C(4) C(5) \dots$	1.8(6) no
C(3)	C(2) Au(2) C(27)	76.7(3) no
C(3)	C(2) Au(2) C(45)	101.8(3) no
C(3)	C(2) C(1) C(6)	0.2(5) no
C(3)	C(4) C(5) C(6)	0.0(6) no
C(5)	C(4) C(3) C(7)	175.0(4) no
C(6)	C(1) P(1) C(8)	. 88.1(3) no
C(6)	C(1) P(1) C(14)	22.8(4) no
C(8)	P(1) Au(1) C(20)	63.8(6) no
C(8)	P(1) C(14) C(15)	166.8(3) no
C(8)	P(1) C(14) C(19)	14.0(4) no
C(8)	C(9) C(10) C(11)	0.8(7) no

C(8)	C(13) C(12) C(11)	. 0.0(6) no
C(9) (C(8) P(1) C(14)	-83.5(4) no
C(9)	C(8) C(13) C(12)	0.4(6) no
C(9) (C(10) C(11) C(12)	1.1(7) no
C(10)	C(9) C(8) C(13)	. 0.0(6) no
C(10)	C(11) C(12) C(13)	0.7(7) no
C(13)	C(8) P(1) C(14)	. 97.1(3) no
C(14)	P(1) Au(1) C(20)	. 52.7(6) no
C(14)	C(15) C(16) C(17)	1.4(7) no
C(14)	C(19) C(18) C(17)	0.1(7) no
C(15)	C(14) C(19) C(18)	0.9(6) no
C(15)	C(16) C(17) C(18)	0.4(7) no
C(16)	C(15) C(14) C(19)	1.6(6) no
C(16)	C(17) C(18) C(19)	0.4(7) no
C(20)	C(21) C(22) C(23)	1.0(7) no
C(20)	C(25) C(24) C(23)	1.1(7) no
C(21)	C(20) C(25) C(24)	2.0(6) no
C(21)	C(22) C(23) C(24)	0.0(7) no
C(22)	C(21) C(20) C(25)	2.0(7) no
C(22)	C(23) C(24) C(25)	0.0(7) no
C(26)	P(2) Au(2) C(27)	1.8(2) no
C(26)	P(2) Au(2) C(45)	. 178.7(2) no
C(26)	P(2) C(33) C(34)	5.6(4) no
C(26)	P(2) C(33) C(38)	. 171.1(3) no
C(26)	P(2) C(39) C(40)	41.3(4) no
C(26)	P(2) C(39) C(44)	. 138.6(3) no
C(26)	C(27) Au(2) C(45)	5.0(9) no
C(26)	C(27) C(28) C(29)	2.9(6) no
C(26)	C(27) C(28) C(32)	176.1(4) no
C(26)	C(31) C(30) C(29)	2.0(6) no
C(27)	Au(2) P(2) C(33)	. 112.0(2) no
C(27)	Au(2) P(2) C(39)	108.1(2) no
C(27)	Au(2) C(45) C(46)	60.1(9) no
C(27)	Au(2) C(45) C(50)	117.6(7) no
C(27)	C(26) P(2) C(33)	123.5(3) no
C(27)	C(26) P(2) C(39)	. 116.4(3) no
C(27)	C(26) C(31) C(30)	1.0(6) no
C(27)	C(28) C(29) C(30).	-0.1(7) no
C(28)	C(27) Au(2) $C(45)$.	177.4(6) no
C(28)	C(27) C(26) C(31)	-3.5(6) no
C(28)	C(29) C(30) C(31)	-2.5(7) no
C(30)	C(29) C(28) C(32).	1/9.0(4) no
C(31)	$C(26) P(2) C(33) \dots$. 59.2(5) no
C(31)	$C(26) P(2) C(39) \dots$	-60.9(4) no
C(33)	P(2) Au(2) C(45)	-6/.5(2) no
C(33)	$P(2) C(39) C(40) \dots$	-164.1(3) no
C(33)	$P(2) C(39) C(44) \dots$	15.7(4) no
C(33)	C(34) C(35) C(36)	-0.3(6) no
C(33)	C(30) C(37) C(30)	112 0(2) mc
C(34)	$C(33) P(2) C(39) \dots$	-1 1(6) po
C(34)	C(35) C(36) C(37).	-0.2(7) no
C(24)	C(34) C(33) C(37)	1.0(6) no
C(35)	$C(34) C(33) C(30) \cdot \cdot$	0 1(7) 20
C(33)	C(33) P(2) C(39)	-69 4(4) no
C(20)	$P(2) = \Delta_{11}(2) = C(35) + \cdots + C(35)$	72 4(2) no
C(39)	C(40) C(41) C(42)	1.9(7) no
- ()		

C(39) C(44) C	(43) C(42)	0.9(7)	no	
C(40) C(39) C	(44) C(43)	0.5(6)	no	
C(40) C(41) C	(42) C(43)	1.5(7)	no	
C(41) C(40) C	(39) C(44)	0.9(6)	no	
C(41) C(42) C	(43) C(44)	0.1(7)	no	
C(45) C(46) C	(47) C(48)	1.3(6)	no	
C(45) C(50) C	(49) C(48)	-2.0(6)	no	
C(46) C(45) C	(50) C(49)	0.8(5)	no	
C(46) C(47) C	(48) C(49)	0 1(6)	no	
C(47) C(46) C(46) C(46) C(47) C(46) C(47) C(46) C(46	(45) C(50)	0 8(6)	no	
C(47) C(48) C(48	(49) C(50)	1 5(6)	no	
#		1.3(0)		
"geom special	details			
;				
,	Table	of Least-S	quares Plan	es
		Plane numb	er 1	
		i i and i i and		
	Atoma Definina	Dlane	Digtanco	697
		(1)		
	Au(2)		0.0000	0.0001
	P(Z)	(<u> </u>	-0.0001	0.0010
	C(27)	(<u> </u>	0.008/	0.0036
	C(45)	(1)	0.0085	0.0037
	Additional Ator	ns	Distance	
	C(2)	(1)	-0.3970	
	Mean deviation	from plane	is 0.0043	angstroms
	Chi-squared:	11.5		
		Plane numb	er 2	
		_		
	Atoms Defining	Plane	Distance	esd
	Au(2)	(1)	0.0000	
	P(2)	(1)	0.0000	
	C(27)	(1)	0.0000	
	Additional Ator	ns	Distance	
	C(26)	(1)	0.0556	
	Mean deviation	from plane	is 0.0000	angstroms
	Chi-squared:	0.0		-
	-			
	Dihedral angles	s between 1	east-square	s planes
	n	lane plane	angle	T00
	P	2 1	179.74	
		-		
		Plane numb	er 3	
	Atoma Definina	Dlane	Digtanco	ard
		(1)		esu
	P(Z)		0.0000	
	C(26)	(<u> </u>	0.0000	
	C(27)	(1)	0.0000	
	Additional Ator	ns	Distance	
	Au(2)	(1)	0.1054	

Mean deviation from plane is 0.0000 angstroms Chi-squared: 0.0 Dihedral angles between least-squares planes plane plane angle 3 1 176.87 2 3 3.29 ----- Plane number 4 ------Distance Atoms Defining Plane esd Au(2) (1) 0.0000 0.0001 P(1) (1) -0.0004 0.0010 (1) 0.0140 0.0036 C(1) C(2) (1) -0.0126 0.0035 Mean deviation from plane is 0.0067 angstroms Chi-squared: 27.5 Dihedral angles between least-squares planes plane plane angle 4 1 101.00 79.25 2 3 4 4 76.77 ----- Plane number 5 -----esd 0.0036 0.0035 0.0037 Atoms Defining Plane Distance C(1)(1)0.0038C(2)(1)0.0064C(3)(1)-0.0116C(4)(1)0.0069C(5)(1)0.0063C(6)(1)-0.01260.0040 0.0041 0.0040 Additional Atoms Distance $\begin{array}{ccc} \text{Au}(2) & (& 1) & 0.0684 \end{array}$ -0.0065 P(1) (1) C(7) (1) -0.1251 Mean deviation from plane is 0.0079 angstroms Chi-squared: 29.3 Dihedral angles between least-squares planes plane plane angle 5 1 101.24 -.24 79.01 5 2 5 3 76.59 5 4 1.46 ----- Plane number 6 -----esd 0.0037 Atoms Defining Plane Distance
 C(8)
 (
 1)
 -0.0023

 C(9)
 (
 1)
 -0.0010

 C(10)
 (
 1)
 0.0058
 0.0045 0.0049

C(11)	(1)	-0.0044	0.0042
C(12)	(1)	0.0008	0.0041
C(13)	(1)	0.0023	0.0039
Additional Ato	ma		Distance	
Additional Ato	(1 \		
P(1)	(1) 1	-0.0203	
Mean deviation Chi-squared:	from	plane 3.3	is 0.0028	angstroms
Dihedral angle	s betu	ween le	east-square	es planes
р	lane	plane	angle	
	6	1	61.35	
	6	2	118.60	
	6	3	116.41	
	6	4	94.71	
	б	5	96.09	
	Plane	e numbe	er 7	
Atoms Defining	Plane	2	Distance	esd
C(14)	(1)	-0.0059	0.0039
C(15)	(1)	0.0086	0.0043
C(16)	(1)	-0 0045	0 0045
C(17)	(1)	-0 0022	0 0048
C(18)	(1)	0 0045	0 0049
C(10)	í	1)	0 0012	0 0045
0(1))	(± /	0.0012	0.0013
Additional Ato	ms		Distance	
Additional Ato P(1)	ms (1)	Distance -0.0562	
Additional Ato P(1) Mean deviation Chi-squared:	ms (from	1) plane 8.4	Distance -0.0562 is 0.0045	angstroms
Additional Ato P(1) Mean deviation Chi-squared:	ms (from	1) plane 8.4	Distance -0.0562 is 0.0045	angstroms
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle	ms (from s betw	1) plane 8.4 ween le	Distance -0.0562 is 0.0045 east-square	angstroms es planes
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle P	ms (from s betw lane	1) plane 8.4 ween le plane	Distance -0.0562 is 0.0045 east-square angle	angstroms es planes
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle P	ms (from s betw lane 7	1) plane 8.4 ween le plane 1 2	Distance -0.0562 is 0.0045 east-square angle 30.87	angstroms es planes
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p	ms (from s betw lane 7 7	1) plane 8.4 ween le plane 1 2 2	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22	angstroms es planes
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle P	ms (from s betw lane 7 7 7 7	1) plane 8.4 ween le plane 1 2 3	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70	angstroms es planes
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle P	ms (from s betw lane 7 7 7 7 7	1) plane 8.4 ween le plane 1 2 3 4	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45	angstroms es planes
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p	ms (from s betw lane 7 7 7 7 7 7 7	1) plane 8.4 ween le plane 1 2 3 4 5 6	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61	angstroms es planes
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p	ms (from s betw lane 7 7 7 7 7 7 7 7 7 7 7	1) plane 8.4 ween lo plane 1 2 3 4 5 6	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8	angstroms es planes
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p	ms (from s betw lane 7 7 7 7 7 7 7 9 Lane	1) plane 8.4 ween le plane 1 2 3 4 5 6 e numbe	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8	angstroms es planes
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p Atoms Defining	ms (from s betw lane 7 7 7 7 7 7 7 7 7 9 Lane	1) plane 8.4 ween lo plane 1 2 3 4 5 6 e numbe	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8	angstroms es planes esd
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p Atoms Defining C(20)	ms (from s betw lane 7 7 7 7 7 7 7 7 7 9 Lane (1) plane 8.4 ween lo plane 1 2 3 4 5 6 e numbe e 1) 1)	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073	angstroms es planes esd 0.0039 0.0043
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p Atoms Defining C(20) C(21) C(22)	ms (from s betw lane 7 7 7 7 7 7 7 7 7 7 7 9 1 ane ((1) plane 8.4 ween la plane 1 2 3 4 5 6 e numbe e 1) 1)	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073 -0.0005	angstroms es planes esd 0.0039 0.0043 0.0043
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p Atoms Defining C(20) C(21) C(22)	ms (from s betw lane 7 7 7 7 7 7 7 7 7 7 9 Lane (((1) plane 8.4 ween lo plane 1 2 3 4 5 6 e numbe e 1) 1) 1)	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073 -0.0005 0.0028	angstroms es planes esd 0.0039 0.0043 0.0044 0.0044
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle P Atoms Defining C(20) C(21) C(22) C(23)	ms (from s betw lane 7 7 7 7 7 7 7 7 7 9 Lane ((((1) plane 8.4 ween la plane 1 2 3 4 5 6 e numbe e 1) 1) 1)	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073 -0.0005 0.0038	angstroms es planes esd 0.0039 0.0043 0.0044 0.0043
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle P Atoms Defining C(20) C(21) C(22) C(23) C(24) C(25)	ms (from s betw lane 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	1) plane 8.4 ween lo plane 1 2 3 4 5 6 e numbe e 1) 1) 1) 1) 1)	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073 -0.0005 0.0038 0.0007 -0.0076	angstroms es planes esd 0.0039 0.0043 0.0044 0.0043 0.0042 0.0042 0.0041
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p Atoms Defining C(20) C(21) C(22) C(23) C(24) C(25)	ms (from s betw lane 7 7 7 7 7 7 7 9 Plane ((((((1) plane 8.4 ween le plane 1 2 3 4 5 6 e numbe e 1) 1) 1) 1) 1)	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073 -0.0005 0.0038 0.0007 -0.0076	angstroms es planes esd 0.0039 0.0043 0.0044 0.0043 0.0042 0.0041
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p Atoms Defining C(20) C(21) C(22) C(23) C(24) C(25) Additional Ato	ms (from s betw lane 7 7 7 7 7 7 9 Plane (((((((((((((((((((1) plane 8.4 ween le plane 1 2 3 4 5 6 e numbe e 1) 1) 1) 1) 1)	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073 -0.0005 0.0038 0.0007 -0.0076 Distance	angstroms es planes esd 0.0039 0.0043 0.0044 0.0043 0.0042 0.0041
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p Atoms Defining C(20) C(21) C(22) C(23) C(24) C(25) Additional Ato Au(1)	ms (from s betw lane 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	1) plane 8.4 ween le plane 1 2 3 4 5 6 e numbe e 1) 1) 1) 1) 1)	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073 -0.0005 0.0038 0.0007 -0.0076 Distance 0.3289	angstroms es planes esd 0.0039 0.0043 0.0044 0.0043 0.0042 0.0041
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle p Atoms Defining C(20) C(21) C(22) C(23) C(24) C(25) Additional Ato Au(1) F(1)	ms (from s betw lane 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	1) plane 8.4 ween lo plane 1 2 3 4 5 6 e numbe e 1) 1) 1) 1) 1) 1) 1) 1)	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073 -0.0005 0.0038 0.0007 -0.0076 Distance 0.3289 0.0254	angstroms es planes esd 0.0039 0.0043 0.0043 0.0044 0.0043 0.0042 0.0041
Additional Ato P(1) Mean deviation Chi-squared: Dihedral angle P Atoms Defining C(20) C(21) C(22) C(23) C(24) C(25) Additional Ato Au(1) F(1) F(2)	ms (from s betw lane 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	<pre>1) plane 8.4 ween le plane 1 2 3 4 5 6 e numbe 1) 1) 1) 1) 1) 1) 1) 1) 1) 1) </pre>	Distance -0.0562 is 0.0045 east-square angle 30.87 149.22 150.70 93.45 92.93 91.61 er 8 Distance 0.0098 -0.0073 -0.0005 0.0038 0.0007 -0.0076 Distance 0.3289 0.0254 -0.0083	angstroms es planes esd 0.0039 0.0043 0.0044 0.0043 0.0042 0.0041

	F(3)	(1)	0.0275	
	F(4)	(1)	0.0237	
	F(5)	(1)	0.0063	
Mean dev:	iation	from	plane	is 0.0050	angstroms
Chi-squa	ared:		13.0		
Dihedral	angles	s betw	ween le	east-square	s planes
	p	lane	plane	angle	
		8	1	46.81	
		8	2	133.09	
		8	3	131.38	
		8	4	105.08	
		o g	5	17 04	
		8	7	77 68	
		0	,	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	
		Plane	e numbe	er 9	
Atoms Det	fining	Plane	e	Distance	esd
	C(26)	(1)	0.0138	0.0038
	C(27)	(1)	-0.0185	0.0036
	C(28)	(1)	0.0113	0.0040
	C(29)	(1)	0.0089	0.0045
	C(30)	(1) 1)	-0.0194	0.0045
	C(31)	(L)	0.0042	0.0043
Additiona	al Ator	ns		Distance	
	Au(2)	(1)	-0.1727	
	P(2)	(1)	-0.0080	
	C(32)	(1)	0.0659	
Mean dev:	iation	from	plane	is 0.0127	angstroms
Chi-squa	ared:		68.9		
Dihedral	angles	z hetz	ween le	agt-gauare	a nlanea
Diffecturat	p.	lane	plane	angle	5 prailes
	-	9	1	4.80	
		9	2	175.05	
		9	3	178.32	
		9	4	104.32	
		9	5	104.46	
		9	6	64.89	
		9	.7	28.43	
		9	8	49.72	
		Plane	e numbe	er 10	
Atoms Dei	fining	Plane	5	Distance	esd
_	C(33)	(1)	-0.0047	0.0037
	C(34)	(1)	0.0035	0.0041
	C(35)	(1)	0.0007	0.0043
	C(36)	(1)	-0.0030	0.0046
	C(37)	(1)	0.0000	0.0049
	C(38)	(工)	0.0047	0.0043
Additiona	al Ator	ns		Distance	

P(2) (1) 0.0600

Mean deviation from plane is 0.0028 angstroms Chi-squared: 3.9 Dihedral angles between least-squares planes plane plane angle 10 53.48 1 10 2 126.50 10 3 124.08 10 4 91.66 10 5 92.95 10 б 9.15 10 7 83.18 10 8 14.34 10 9 57.32 ----- Plane number 11 ------Atoms Defining Plane Distance esd C(39) (1) 0.0004 0.0038 1) 0.0041 C(40) (0.0073 -0.0101 C(41) (1) 0.0043 C(42) (1) 0.0044 0.0046 1) 0.0052 0.0048 C(43) (C(44) (1) -0.0064 0.0043 Additional Atoms Distance P(2) (1) -0.0034 Mean deviation from plane is 0.0056 angstroms Chi-squared: 12.7 Dihedral angles between least-squares planes plane plane angle 11 1 96.10 11 2 84.09 11 3 80.82 11 34.09 4 11 5 35.54 11 б 63.47 11 7 106.52 8 11 77.36 9 100.80 11 10 11 63.02 ----- Plane number 12 ------Atoms Defining Plane Distance esd 0.0035 C(45) (1) -0.0013 C(46) (1) 0.0080 0.0037 -0.0061 0.0040 C(47) (1) -0.0041 0.0039 C(48) (1) (0.0110 0.0039 C(49) 1) C(50) (1) -0.0081 0.0038 Additional Atoms Distance

Au(2)	(1)	-0.0699
F(6)	(1)	0.0394
F(7)	(1)	-0.0142
F(8)	(1)	0.0068
F(9)	(1)	0.0175
F(10)	(1)	-0.0329

Mean deviation from plane is 0.0064 angstroms Chi-squared: 20.9

Dihedral angles between least-squares planes plane angle

Prane	prane	angre
12	1	63.27
12	2	116.69
12	3	114.50
12	4	94.45
12	5	95.85
12	6	1.92
12	7	93.53
12	8	18.71
12	9	66.80
12	10	10.89
12	11	62.77

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