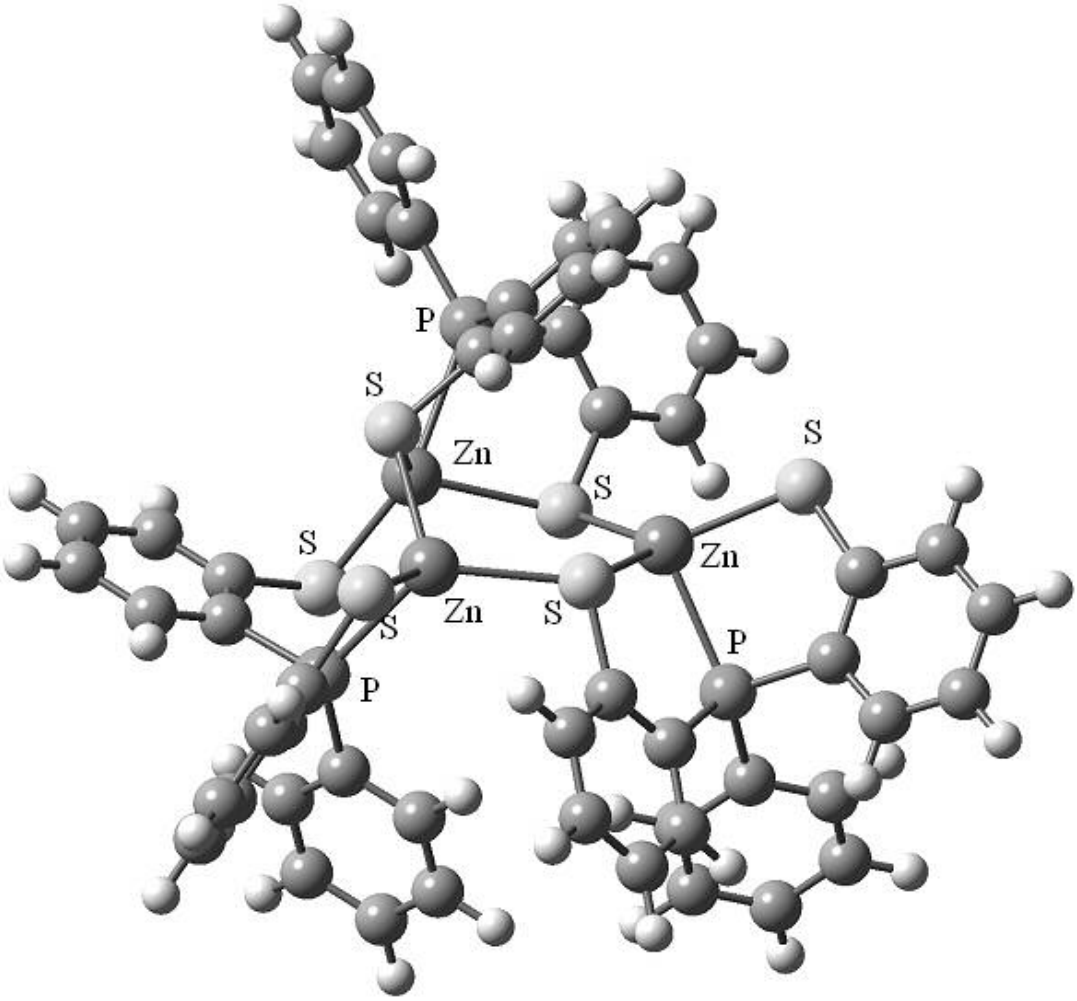
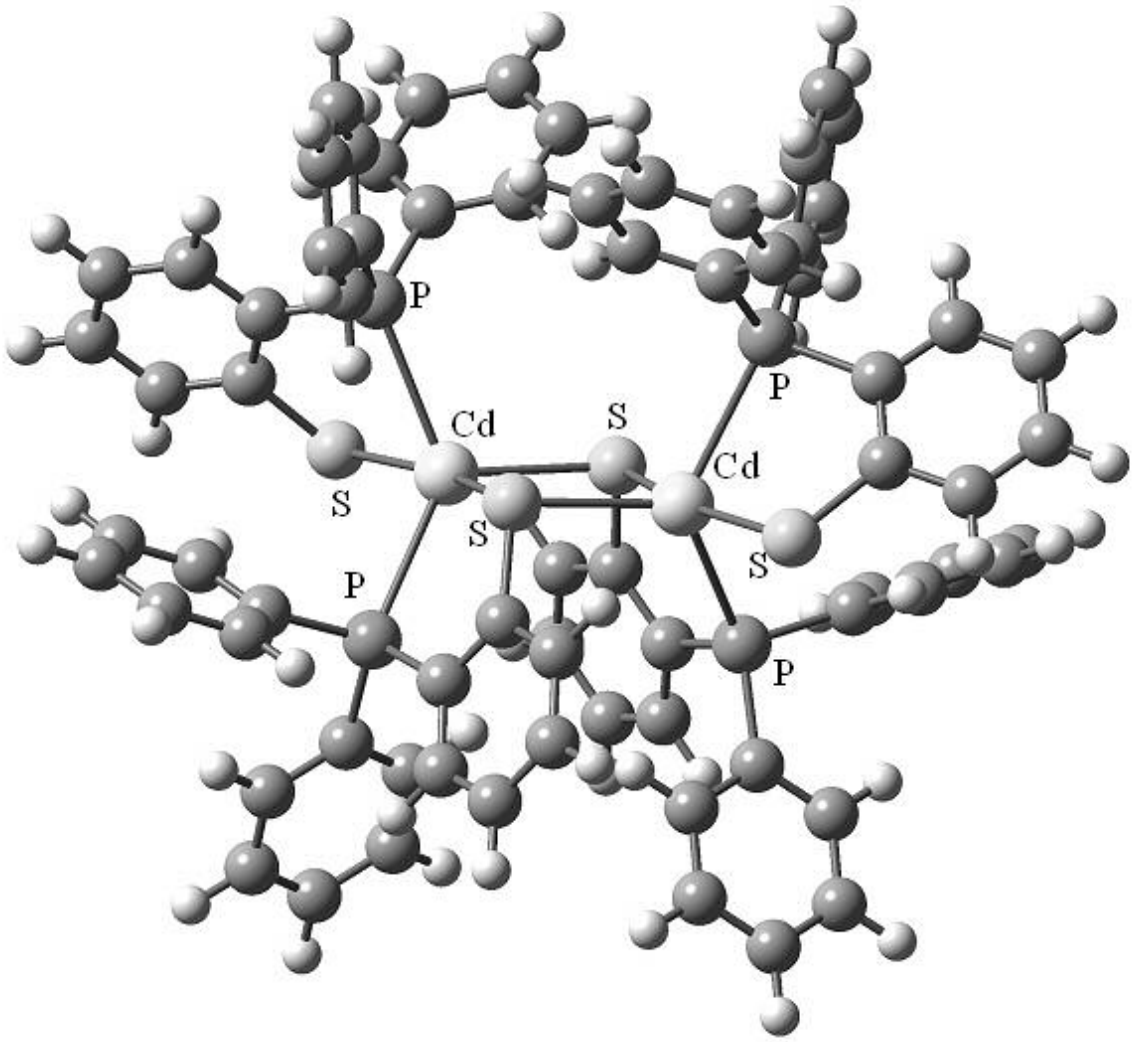
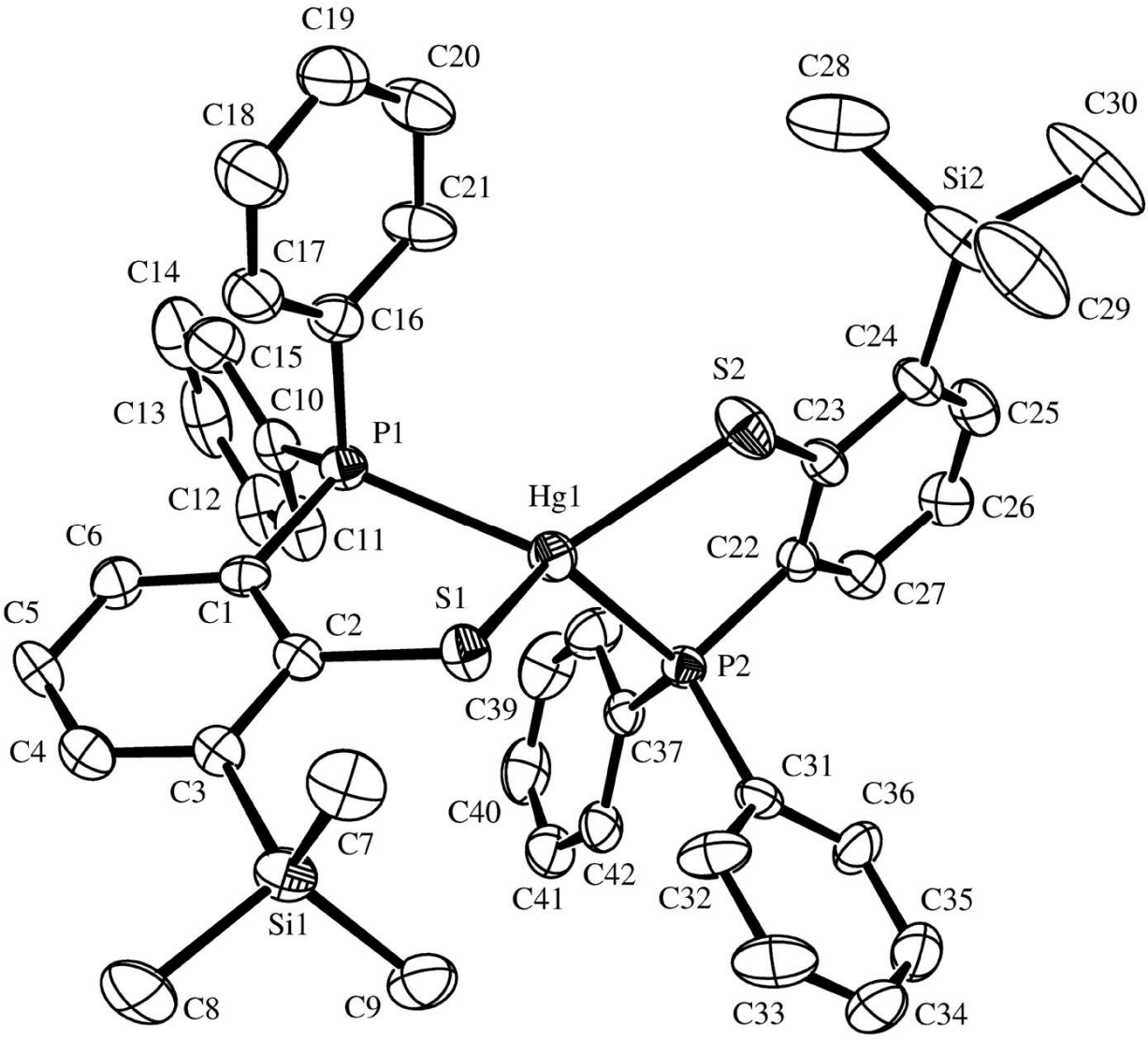


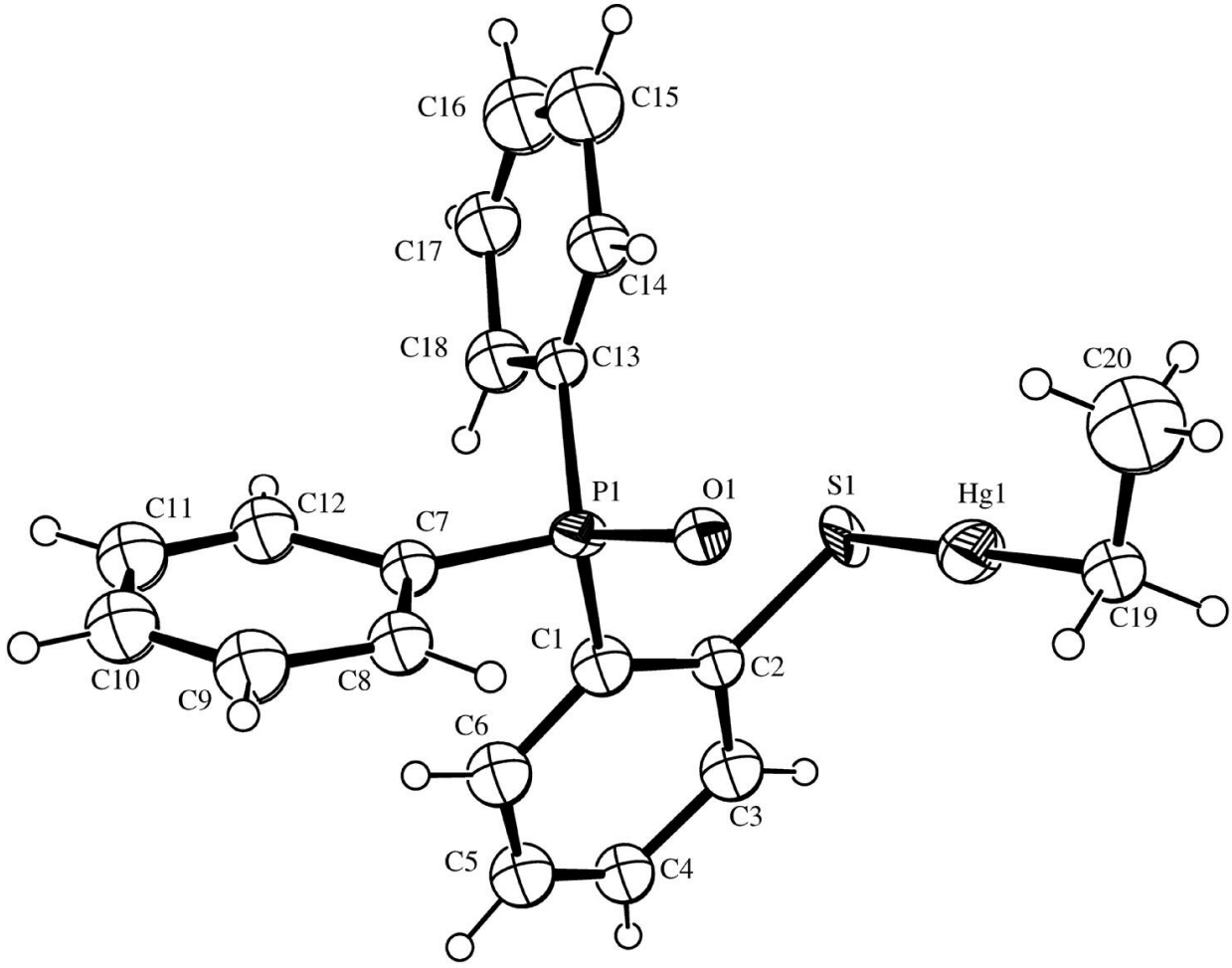
The optimized structure of **1**



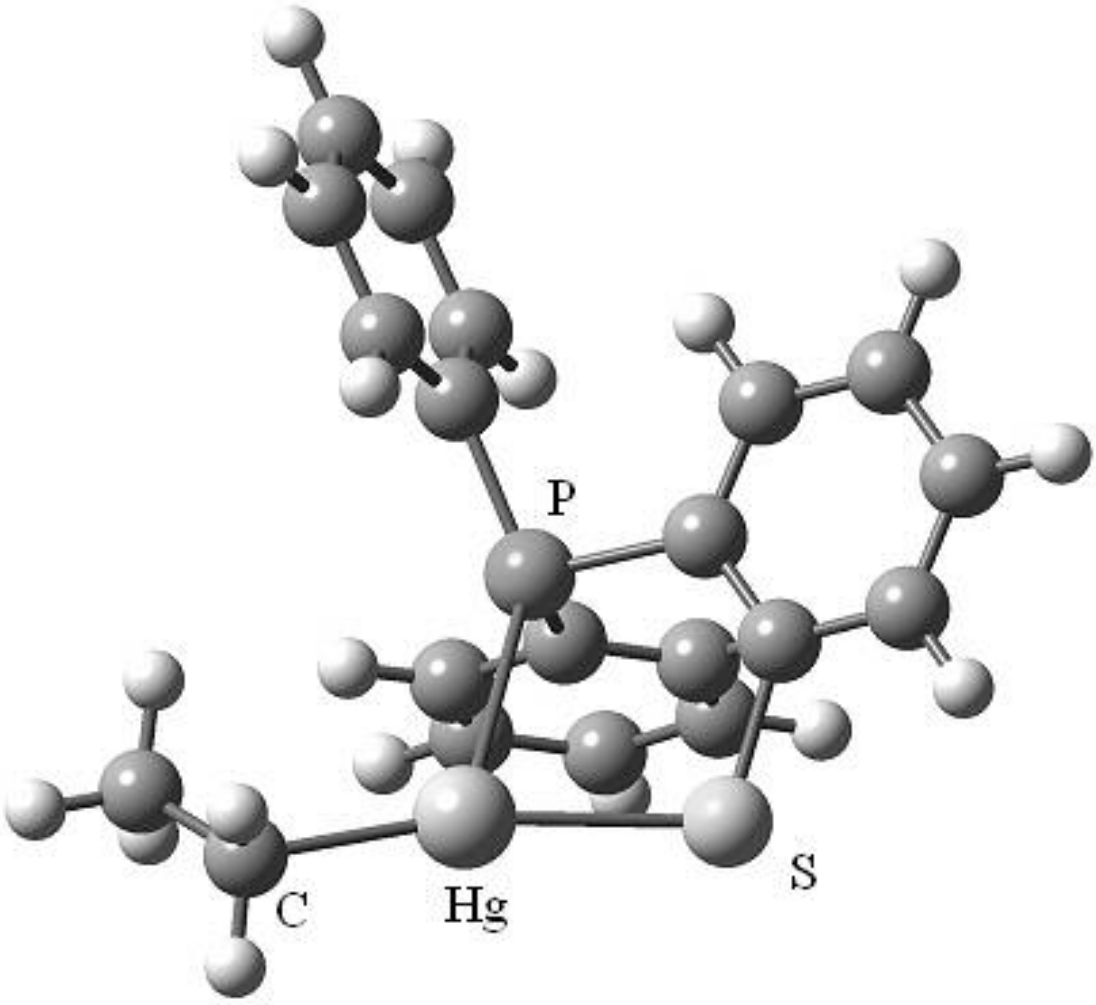
The optimized structure of **2**



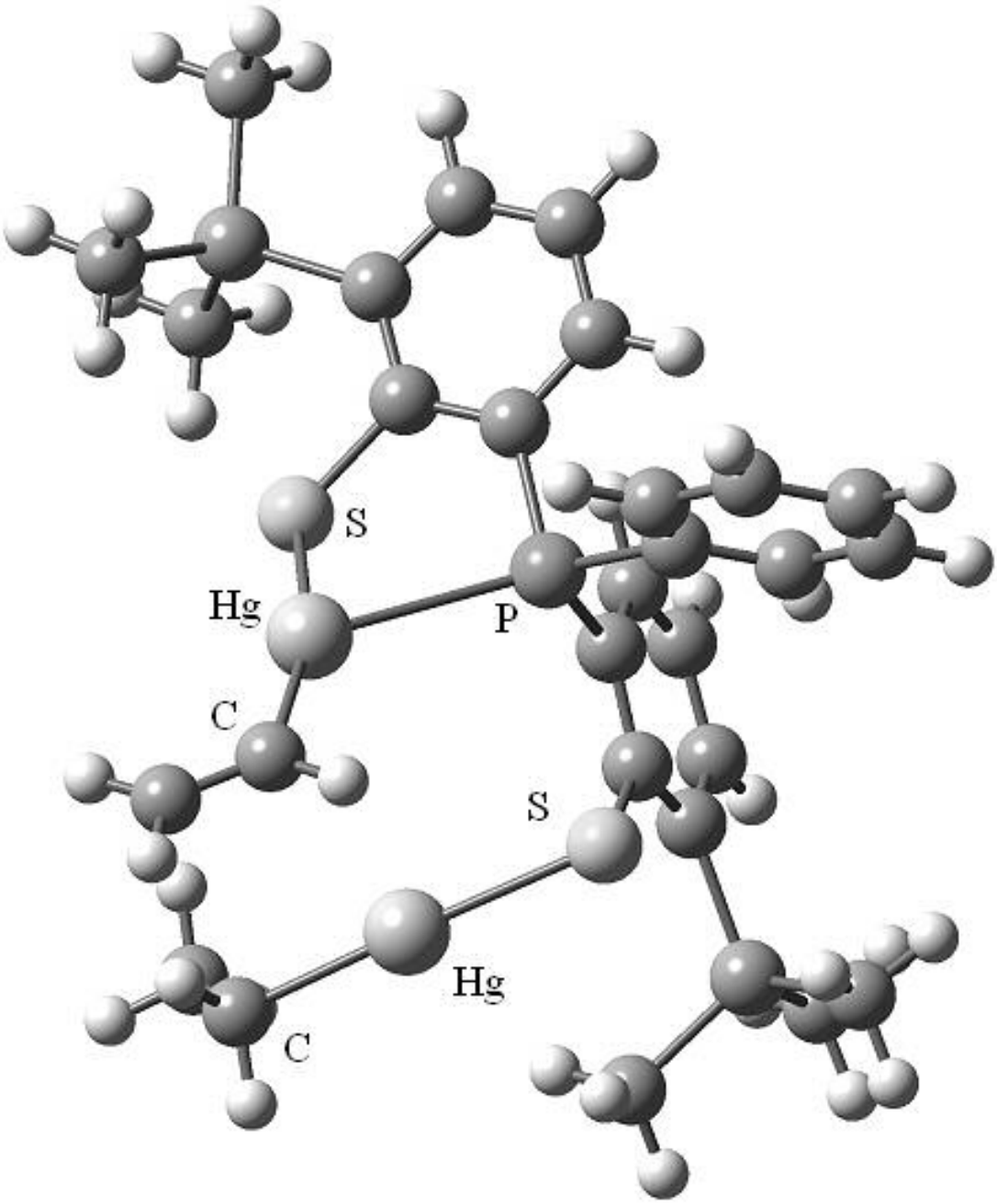
ORTEP diagram of the molecular structure of **6**, with 50% thermal ellipsoid probability



ORTEP diagram of the molecular structure of **7***, with 50% thermal ellipsoid probability



The optimized structure of **7**



The optimized structure of **10**

Compound (1*)

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 'H'  'H'   0.0000   0.0000
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 'O'  'O'   0.0106   0.0060
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 'P'  'P'   0.1023   0.0942
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 'x, y, z'
 '-x, -y, -z'

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_cell_length_c                    20.05(2)
_cell_angle_alpha                 109.455(15)
_cell_angle_beta                  97.335(16)
_cell_angle_gamma                 99.492(16)
_cell_volume                      2938(5)
_cell_formula_units_Z             2
_cell_measurement_temperature     150(2)
_cell_measurement_reflns_used     1016
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_diffrn_radiation_type            MoK\a
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_diffrn_radiation_monochromator   graphite
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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
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 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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S2 S 0.45817(5) 0.17636(5) 0.40625(3) 0.02782(13) Uani 1 1 d . . .
S3 S 0.38265(6) 0.27569(5) 0.24969(3) 0.02865(13) Uani 1 1 d . . .
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S5 S 0.01511(5) 0.18747(4) 0.18670(3) 0.02522(12) Uani 1 1 d . . .
S6 S 0.20827(8) 0.27209(6) 0.06132(4) 0.04731(19) Uani 1 1 d . . .
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P2 P 0.45323(6) 0.06389(5) 0.17967(3) 0.02875(14) Uani 1 1 d . . .
P3 P 0.12387(6) 0.41921(5) 0.20518(3) 0.03123(15) Uani 1 1 d . . .
O1 O 0.19520(13) 0.22966(12) 0.34960(8) 0.0235(3) Uani 1 1 d . . .
C1 C 0.0371(2) 0.25000(18) 0.44429(12) 0.0243(5) Uani 1 1 d . . .
C2 C -0.0649(2) 0.17227(18) 0.40279(12) 0.0244(5) Uani 1 1 d . . .
C3 C -0.1808(2) 0.1826(2) 0.41902(13) 0.0290(5) Uani 1 1 d . . .
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H4 H -0.2735 0.2713 0.4835 0.044 Uiso 1 1 calc R . .
C5 C -0.0951(2) 0.3456(2) 0.51143(15) 0.0414(7) Uani 1 1 d . . .
H5 H -0.1057 0.4051 0.5475 0.050 Uiso 1 1 calc R . .
C6 C 0.0206(2) 0.3373(2) 0.49734(14) 0.0342(6) Uani 1 1 d . . .
H6 H 0.0892 0.3915 0.5239 0.041 Uiso 1 1 calc R . .
C7 C 0.2350(2) 0.14229(17) 0.45346(12) 0.0245(5) Uani 1 1 d . . .
C8 C 0.3445(2) 0.11134(18) 0.43917(12) 0.0248(5) Uani 1 1 d . . .
C9 C 0.3699(2) 0.0288(2) 0.45624(15) 0.0359(6) Uani 1 1 d . . .
H9 H 0.4415 0.0050 0.4452 0.043 Uiso 1 1 calc R . .
C10 C 0.2923(3) -0.0194(2) 0.48906(17) 0.0446(7) Uani 1 1 d . . .
H10 H 0.3114 -0.0756 0.5004 0.054 Uiso 1 1 calc R . .
C11 C 0.1879(3) 0.0134(2) 0.50543(16) 0.0402(6) Uani 1 1 d . . .
H11 H 0.1361 -0.0189 0.5290 0.048 Uiso 1 1 calc R . .
C12 C 0.1590(2) 0.09355(19) 0.48742(13) 0.0300(5) Uani 1 1 d . . .
H12 H 0.0865 0.1158 0.4983 0.036 Uiso 1 1 calc R . .
C13 C 0.2879(2) 0.36249(17) 0.48607(12) 0.0246(5) Uani 1 1 d . . .
C14 C 0.2990(2) 0.44343(18) 0.46171(14) 0.0310(5) Uani 1 1 d . . .
H14 H 0.2605 0.4332 0.4141 0.037 Uiso 1 1 calc R . .
C15 C 0.3662(2) 0.53914(19) 0.50700(15) 0.0363(6) Uani 1 1 d . . .
H15 H 0.3747 0.5946 0.4903 0.044 Uiso 1 1 calc R . .
C16 C 0.4211(2) 0.5540(2) 0.57676(15) 0.0386(6) Uani 1 1 d . . .
H16 H 0.4667 0.6198 0.6079 0.046 Uiso 1 1 calc R . .
C17 C 0.4102(2) 0.4742(2) 0.60108(14) 0.0370(6) Uani 1 1 d . . .
H17 H 0.4481 0.4852 0.6490 0.044 Uiso 1 1 calc R . .
C18 C 0.3436(2) 0.3773(2) 0.55595(13) 0.0314(5) Uani 1 1 d . . .
H18 H 0.3364 0.3219 0.5727 0.038 Uiso 1 1 calc R . .
C19 C 0.5282(2) 0.1725(2) 0.16156(12) 0.0291(5) Uani 1 1 d . . .
C20 C 0.4937(2) 0.2658(2) 0.19248(12) 0.0291(5) Uani 1 1 d . . .
C21 C 0.5471(2) 0.3512(2) 0.18062(15) 0.0378(6) Uani 1 1 d . . .
H21 H 0.5228 0.4137 0.2011 0.045 Uiso 1 1 calc R . .
C22 C 0.6371(3) 0.3463(2) 0.13854(15) 0.0428(7) Uani 1 1 d . . .
H22 H 0.6731 0.4054 0.1300 0.051 Uiso 1 1 calc R . .
C23 C 0.6741(2) 0.2558(2) 0.10930(14) 0.0413(7) Uani 1 1 d . . .
H23 H 0.7367 0.2531 0.0817 0.050 Uiso 1 1 calc R . .
C24 C 0.6198(2) 0.1695(2) 0.12034(13) 0.0357(6) Uani 1 1 d . . .
H24 H 0.6447 0.1072 0.0998 0.043 Uiso 1 1 calc R . .
C25 C 0.3058(2) 0.01944(18) 0.11808(12) 0.0282(5) Uani 1 1 d . . .
C26 C 0.1996(2) -0.01208(17) 0.14097(13) 0.0272(5) Uani 1 1 d . . .
C27 C 0.0898(2) -0.05653(19) 0.09062(15) 0.0351(6) Uani 1 1 d . . .
H27 H 0.0174 -0.0787 0.1058 0.042 Uiso 1 1 calc R . .
C28 C 0.0857(2) -0.0685(2) 0.01903(14) 0.0378(6) Uani 1 1 d . . .
H28 H 0.0116 -0.1023 -0.0151 0.045 Uiso 1 1 calc R . .
C29 C 0.1889(2) -0.0317(2) -0.00334(14) 0.0378(6) Uani 1 1 d . . .
H29 H 0.1845 -0.0363 -0.0520 0.045 Uiso 1 1 calc R . .
C30 C 0.2981(2) 0.0118(2) 0.04577(13) 0.0358(6) Uani 1 1 d . . .
H30 H 0.3690 0.0370 0.0306 0.043 Uiso 1 1 calc R . .
C31 C 0.5375(2) -0.0349(2) 0.14817(13) 0.0327(6) Uani 1 1 d . . .
C32 C 0.6496(3) -0.0254(2) 0.19043(17) 0.0499(8) Uani 1 1 d . . .
H32 H 0.6778 0.0300 0.2352 0.060 Uiso 1 1 calc R . .
C33 C 0.7198(3) -0.0955(3) 0.16798(19) 0.0600(9) Uani 1 1 d . . .
H33 H 0.7973 -0.0872 0.1966 0.072 Uiso 1 1 calc R . .
C34 C 0.6791(3) -0.1772(3) 0.10466(18) 0.0614(10) Uani 1 1 d . . .
H34 H 0.7276 -0.2261 0.0898 0.074 Uiso 1 1 calc R . .
C35 C 0.5685(3) -0.1884(3) 0.06264(17) 0.0672(11) Uani 1 1 d . . .
H35 H 0.5405 -0.2451 0.0185 0.081 Uiso 1 1 calc R . .
C36 C 0.4976(3) -0.1180(3) 0.08408(15) 0.0514(8) Uani 1 1 d . . .
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C37 C -0.0001(2) 0.39186(19) 0.24948(13) 0.0303(5) Uani 1 1 d . . .
C38 C -0.0437(2) 0.29042(18) 0.24160(12) 0.0266(5) Uani 1 1 d . . .
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C39 C -0.1416(2) 0.2664(2) 0.27359(13) 0.0312(5) Uani 1 1 d . . .
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C40 C -0.1936(3) 0.3431(2) 0.31319(14) 0.0385(6) Uani 1 1 d . . .
H40 H -0.2597 0.3263 0.3351 0.046 Uiso 1 1 calc R . .
C41 C -0.1506(3) 0.4433(2) 0.32124(15) 0.0415(7) Uani 1 1 d . . .
H41 H -0.1871 0.4953 0.3483 0.050 Uiso 1 1 calc R . .
C42 C -0.0540(3) 0.4678(2) 0.28964(15) 0.0390(6) Uani 1 1 d . . .
H42 H -0.0241 0.5370 0.2953 0.047 Uiso 1 1 calc R . .
C43 C 0.0479(3) 0.3997(2) 0.11431(14) 0.0381(6) Uani 1 1 d . . .
C44 C 0.0869(3) 0.3362(2) 0.05555(15) 0.0424(7) Uani 1 1 d . . .
C45 C 0.0232(3) 0.3196(3) -0.01400(17) 0.0577(9) Uani 1 1 d . . .
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C46 C -0.0751(4) 0.3624(3) -0.0233(2) 0.0692(11) Uani 1 1 d . . .
H46 H -0.1174 0.3493 -0.0707 0.083 Uiso 1 1 calc R . .
C47 C -0.1135(3) 0.4243(3) 0.0353(2) 0.0633(10) Uani 1 1 d . . .
H47 H -0.1812 0.4540 0.0283 0.076 Uiso 1 1 calc R . .
C48 C -0.0524(3) 0.4423(2) 0.10389(18) 0.0498(8) Uani 1 1 d . . .
H48 H -0.0789 0.4842 0.1444 0.060 Uiso 1 1 calc R . .
C49 C 0.1994(3) 0.5527(2) 0.25049(16) 0.0409(6) Uani 1 1 d . . .
C50 C 0.1898(5) 0.6241(3) 0.2199(3) 0.1003(18) Uani 1 1 d . . .
H50 H 0.1405 0.6057 0.1735 0.120 Uiso 1 1 calc R . .
C51 C 0.2548(6) 0.7264(3) 0.2587(4) 0.132(2) Uani 1 1 d . . .
H51 H 0.2460 0.7774 0.2388 0.158 Uiso 1 1 calc R . .
C52 C 0.3293(5) 0.7526(3) 0.3238(3) 0.0957(16) Uani 1 1 d . . .
H52 H 0.3725 0.8214 0.3491 0.115 Uiso 1 1 calc R . .
C53 C 0.3416(4) 0.6809(3) 0.3524(2) 0.0704(11) Uani 1 1 d . . .
H53 H 0.3942 0.6989 0.3977 0.085 Uiso 1 1 calc R . .
C54 C 0.2782(3) 0.5814(3) 0.31605(18) 0.0586(9) Uani 1 1 d . . .
H54 H 0.2889 0.5312 0.3365 0.070 Uiso 1 1 calc R . .

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0.00056(12)
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S3 0.0279(3) 0.0310(3) 0.0219(3) 0.0056(2) 0.0069(2) -0.0002(2)
S4 0.0274(3) 0.0233(3) 0.0303(3) 0.0072(2) 0.0104(2) 0.0040(2)
S5 0.0264(3) 0.0274(3) 0.0184(3) 0.0056(2) 0.0039(2) 0.0027(2)
S6 0.0569(5) 0.0565(5) 0.0280(3) 0.0136(3) 0.0190(3) 0.0068(4)
P1 0.0170(3) 0.0236(3) 0.0201(3) 0.0064(2) 0.0030(2) 0.0031(2)
P2 0.0256(3) 0.0347(3) 0.0183(3) 0.0035(3) 0.0033(2) -0.0006(3)
P3 0.0354(4) 0.0290(3) 0.0283(3) 0.0105(3) 0.0072(3) 0.0035(3)
O1 0.0189(8) 0.0278(8) 0.0220(8) 0.0082(7) 0.0039(6) 0.0021(6)
C1 0.0196(11) 0.0307(12) 0.0245(11) 0.0114(10) 0.0050(9) 0.0075(9)
C2 0.0215(11) 0.0314(13) 0.0238(11) 0.0141(10) 0.0048(9) 0.0063(10)
C3 0.0213(12) 0.0387(14) 0.0314(13) 0.0173(11) 0.0077(10) 0.0065(10)
C4 0.0247(13) 0.0516(17) 0.0405(15) 0.0183(13) 0.0129(11) 0.0157(12)
C5 0.0341(15) 0.0444(16) 0.0412(15) 0.0036(13) 0.0123(12) 0.0175(13)
C6 0.0267(13) 0.0383(15) 0.0318(13) 0.0051(11) 0.0059(10) 0.0077(11)
C7 0.0231(12) 0.0248(12) 0.0239(11) 0.0083(10) 0.0033(9) 0.0027(9)
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C10 0.0440(17) 0.0452(17) 0.0620(19) 0.0360(15) 0.0162(14) 0.0173(14)
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0.0091(12)
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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
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 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Compound 2*

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
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 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
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based
 on F^2^ are statistically about twice as large as those based on F,
and R-
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Cd2 Cd 0.26267(2) -0.00721(4) 0.58586(2) 0.05603(17) Uani 1 1 d . . .
O1 O 0.1612(3) 0.1603(5) 0.4270(3) 0.162(3) Uani 1 1 d . . .
S1 S 0.22798(9) 0.06998(14) 0.32273(9) 0.0718(7) Uani 1 1 d . . .
S2 S 0.16319(8) -0.04636(13) 0.51779(8) 0.0537(6) Uani 1 1 d . . .
S3 S 0.31710(7) 0.01782(13) 0.48317(7) 0.0546(5) Uani 1 1 d . . .
S4 S 0.24150(8) -0.01347(15) 0.68710(8) 0.0737(6) Uani 1 1 d . . .
P1 P 0.14247(11) 0.22363(19) 0.38207(10) 0.0716(8) Uani 1 1 d . . .
P2 P 0.13589(9) -0.14451(14) 0.39569(9) 0.0536(6) Uani 1 1 d . . .
P3 P 0.36117(8) -0.12347(14) 0.59189(9) 0.0548(6) Uani 1 1 d . . .
P4 P 0.27833(9) 0.19002(15) 0.62129(9) 0.0623(6) Uani 1 1 d . . .
C1 C 0.1157(4) 0.1714(5) 0.3118(3) 0.049(2) Uani 1 1 d . . .
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C2 C 0.1522(3) 0.1025(5) 0.2884(3) 0.055(2) Uani 1 1 d . . .
C3 C 0.1272(4) 0.0605(5) 0.2364(4) 0.069(2) Uani 1 1 d . . .
H3 H 0.1500 0.0122 0.2205 0.082 Uiso 1 1 calc R . .
C4 C 0.0689(4) 0.0873(7) 0.2067(3) 0.080(3) Uani 1 1 d . . .
H4 H 0.0536 0.0580 0.1713 0.096 Uiso 1 1 calc R . .
C5 C 0.0334(4) 0.1585(6) 0.2302(4) 0.070(3) Uani 1 1 d . . .
H5 H -0.0055 0.1780 0.2109 0.084 Uiso 1 1 calc R . .
C6 C 0.0574(4) 0.1978(5) 0.2816(3) 0.061(2) Uani 1 1 d . . .
H6 H 0.0341 0.2448 0.2978 0.073 Uiso 1 1 calc R . .
C7 C 0.1989(3) 0.3218(5) 0.3784(4) 0.057(2) Uani 1 1 d . . .
C8 C 0.1980(4) 0.3738(6) 0.3277(4) 0.082(3) Uani 1 1 d . . .
H8 H 0.1704 0.3530 0.2952 0.099 Uiso 1 1 calc R . .
C9 C 0.2371(4) 0.4554(7) 0.3246(4) 0.113(4) Uani 1 1 d . . .
H9 H 0.2376 0.4886 0.2902 0.135 Uiso 1 1 calc R . .
C10 C 0.2750(5) 0.4858(8) 0.3733(6) 0.116(4) Uani 1 1 d . . .
H10 H 0.3005 0.5430 0.3725 0.139 Uiso 1 1 calc R . .
C11 C 0.2769(5) 0.4346(9) 0.4236(4) 0.121(4) Uani 1 1 d . . .
H11 H 0.3043 0.4557 0.4562 0.145 Uiso 1 1 calc R . .
C12 C 0.2380(4) 0.3516(7) 0.4259(4) 0.099(3) Uani 1 1 d . . .
H12 H 0.2388 0.3165 0.4600 0.119 Uiso 1 1 calc R . .
C13 C 0.0788(3) 0.2918(8) 0.4037(3) 0.061(2) Uani 1 1 d . . .
C14 C 0.0751(4) 0.3971(8) 0.4056(4) 0.098(3) Uani 1 1 d . . .
H14 H 0.1055 0.4376 0.3947 0.118 Uiso 1 1 calc R . .
C15 C 0.0269(6) 0.4442(9) 0.4235(5) 0.127(4) Uani 1 1 d . . .
H15 H 0.0250 0.5164 0.4255 0.152 Uiso 1 1 calc R . .
C16 C -0.0187(6) 0.3842(11) 0.4385(5) 0.123(5) Uani 1 1 d . . .
H16 H -0.0516 0.4162 0.4503 0.148 Uiso 1 1 calc R . .
C17 C -0.0163(5) 0.2807(10) 0.4362(4) 0.111(4) Uani 1 1 d . . .
H17 H -0.0480 0.2412 0.4454 0.133 Uiso 1 1 calc R . .
C18 C 0.0330(5) 0.2318(7) 0.4202(3) 0.085(3) Uani 1 1 d . . .
H18 H 0.0356 0.1595 0.4204 0.102 Uiso 1 1 calc R . .
C19 C 0.1536(3) -0.2284(6) 0.4566(3) 0.048(2) Uani 1 1 d . . .
C20 C 0.1678(3) -0.1821(5) 0.5096(3) 0.0435(19) Uani 1 1 d . . .
C21 C 0.1830(3) -0.2460(6) 0.5576(3) 0.057(2) Uani 1 1 d . . .
H21 H 0.1896 -0.2168 0.5938 0.069 Uiso 1 1 calc R . .
C22 C 0.1883(3) -0.3523(7) 0.5515(4) 0.074(3) Uani 1 1 d . . .
H22 H 0.2000 -0.3936 0.5837 0.089 Uiso 1 1 calc R . .
C23 C 0.1765(4) -0.3981(6) 0.4991(4) 0.082(3) Uani 1 1 d . . .
H23 H 0.1797 -0.4697 0.4952 0.098 Uiso 1 1 calc R . .
C24 C 0.1597(3) -0.3347(6) 0.4518(3) 0.066(2) Uani 1 1 d . . .
H24 H 0.1523 -0.3647 0.4159 0.079 Uiso 1 1 calc R . .
C25 C 0.1295(4) -0.2256(5) 0.3338(3) 0.054(2) Uani 1 1 d . . .
C26 C 0.0802(4) -0.2884(6) 0.3156(4) 0.094(3) Uani 1 1 d . . .
H26 H 0.0479 -0.2890 0.3351 0.112 Uiso 1 1 calc R . .
C27 C 0.0772(5) -0.3520(8) 0.2679(5) 0.122(4) Uani 1 1 d . . .
H27 H 0.0429 -0.3929 0.2544 0.146 Uiso 1 1 calc R . .
C28 C 0.1271(6) -0.3519(8) 0.2416(5) 0.121(5) Uani 1 1 d . . .
H28 H 0.1268 -0.3960 0.2109 0.146 Uiso 1 1 calc R . .
C29 C 0.1762(5) -0.2900(8) 0.2591(5) 0.120(4) Uani 1 1 d . . .
H29 H 0.2088 -0.2893 0.2400 0.144 Uiso 1 1 calc R . .
C30 C 0.1773(4) -0.2280(6) 0.3057(4) 0.088(3) Uani 1 1 d . . .
H30 H 0.2115 -0.1864 0.3185 0.106 Uiso 1 1 calc R . .
C31 C 0.0574(3) -0.1009(5) 0.3931(4) 0.051(2) Uani 1 1 d . . .
C32 C 0.0318(4) -0.0399(5) 0.3478(3) 0.062(2) Uani 1 1 d . . .
H32 H 0.0541 -0.0244 0.3199 0.074 Uiso 1 1 calc R . .
C33 C -0.0267(4) -0.0015(6) 0.3433(3) 0.076(2) Uani 1 1 d . . .
H33 H -0.0438 0.0383 0.3118 0.092 Uiso 1 1 calc R . .
C34 C -0.0600(3) -0.0205(6) 0.3838(4) 0.078(3) Uani 1 1 d . . .
H34 H -0.0996 0.0059 0.3804 0.094 Uiso 1 1 calc R . .
C35 C -0.0343(4) -0.0792(6) 0.4297(4) 0.085(3) Uani 1 1 d . . .
H35 H -0.0561 -0.0920 0.4584 0.102 Uiso 1 1 calc R . .
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C36 C 0.0239(4) -0.1195(6) 0.4337(4) 0.078(3) Uani 1 1 d . . .
H36 H 0.0407 -0.1604 0.4649 0.094 Uiso 1 1 calc R . .
C37 C 0.3645(3) -0.1728(6) 0.5217(3) 0.049(2) Uani 1 1 d . . .
C38 C 0.3399(3) -0.1107(5) 0.4749(3) 0.049(2) Uani 1 1 d . . .
C39 C 0.3374(3) -0.1540(6) 0.4207(3) 0.062(2) Uani 1 1 d . . .
H39 H 0.3204 -0.1155 0.3886 0.075 Uiso 1 1 calc R . .
C40 C 0.3597(3) -0.2526(7) 0.4142(4) 0.066(3) Uani 1 1 d . . .
H40 H 0.3576 -0.2797 0.3780 0.080 Uiso 1 1 calc R . .
C41 C 0.3850(4) -0.3110(6) 0.4609(4) 0.078(3) Uani 1 1 d . . .
H41 H 0.4004 -0.3771 0.4564 0.094 Uiso 1 1 calc R . .
C42 C 0.3874(3) -0.2708(6) 0.5146(4) 0.065(2) Uani 1 1 d . . .
H42 H 0.4046 -0.3100 0.5463 0.078 Uiso 1 1 calc R . .
C43 C 0.3766(4) -0.2297(5) 0.6405(3) 0.056(2) Uani 1 1 d . . .
C44 C 0.3286(4) -0.2756(6) 0.6611(3) 0.075(3) Uani 1 1 d . . .
H44 H 0.2891 -0.2487 0.6501 0.090 Uiso 1 1 calc R . .
C45 C 0.3378(5) -0.3594(8) 0.6974(4) 0.106(4) Uani 1 1 d . . .
H45 H 0.3048 -0.3885 0.7106 0.127 Uiso 1 1 calc R . .
C46 C 0.3952(6) -0.3994(8) 0.7138(5) 0.131(5) Uani 1 1 d . . .
H46 H 0.4014 -0.4577 0.7373 0.157 Uiso 1 1 calc R . .
C47 C 0.4431(5) -0.3549(9) 0.6963(5) 0.128(4) Uani 1 1 d . . .
H47 H 0.4825 -0.3809 0.7091 0.153 Uiso 1 1 calc R . .
C48 C 0.4345(4) -0.2719(7) 0.6599(4) 0.092(3) Uani 1 1 d . . .
H48 H 0.4683 -0.2431 0.6480 0.110 Uiso 1 1 calc R . .
C49 C 0.4276(3) -0.0407(5) 0.6131(4) 0.055(2) Uani 1 1 d . . .
C50 C 0.4688(4) -0.0205(6) 0.5787(3) 0.079(3) Uani 1 1 d . . .
H50 H 0.4632 -0.0506 0.5428 0.094 Uiso 1 1 calc R . .
C51 C 0.5185(4) 0.0439(7) 0.5969(4) 0.102(3) Uani 1 1 d . . .
H51 H 0.5465 0.0565 0.5735 0.122 Uiso 1 1 calc R . .
C52 C 0.5264(4) 0.0892(6) 0.6494(5) 0.091(3) Uani 1 1 d . . .
H52 H 0.5593 0.1342 0.6611 0.109 Uiso 1 1 calc R . .
C53 C 0.4868(4) 0.0695(6) 0.6846(4) 0.077(3) Uani 1 1 d . . .
H53 H 0.4933 0.0990 0.7207 0.092 Uiso 1 1 calc R . .
C54 C 0.4366(3) 0.0050(6) 0.6665(3) 0.064(2) Uani 1 1 d . . .
H54 H 0.4089 -0.0077 0.6902 0.077 Uiso 1 1 calc R . .
C55 C 0.3113(3) 0.1677(6) 0.6947(3) 0.052(2) Uani 1 1 d . . .
C56 C 0.2953(3) 0.0773(6) 0.7207(3) 0.059(2) Uani 1 1 d . . .
C57 C 0.3232(4) 0.0595(6) 0.7767(4) 0.081(3) Uani 1 1 d . . .
H57 H 0.3134 -0.0005 0.7947 0.097 Uiso 1 1 calc R . .
C58 C 0.3653(4) 0.1287(9) 0.8067(4) 0.105(4) Uani 1 1 d . . .
H58 H 0.3844 0.1136 0.8439 0.125 Uiso 1 1 calc R . .
C59 C 0.3786(4) 0.2182(7) 0.7820(4) 0.096(3) Uani 1 1 d . . .
H59 H 0.4050 0.2666 0.8029 0.115 Uiso 1 1 calc R . .
C60 C 0.3530(3) 0.2373(5) 0.7264(4) 0.070(2) Uani 1 1 d . . .
H60 H 0.3636 0.2977 0.7093 0.084 Uiso 1 1 calc R . .
C61 C 0.3266(4) 0.2888(7) 0.6000(3) 0.069(3) Uani 1 1 d . . .
C62 C 0.3144(4) 0.3935(9) 0.5982(3) 0.099(3) Uani 1 1 d . . .
H62 H 0.2785 0.4174 0.6083 0.118 Uiso 1 1 calc R . .
C63 C 0.3548(5) 0.4650(7) 0.5814(4) 0.120(4) Uani 1 1 d . . .
H63 H 0.3443 0.5351 0.5784 0.144 Uiso 1 1 calc R . .
C64 C 0.4095(5) 0.4330(9) 0.5694(4) 0.106(4) Uani 1 1 d . . .
H64 H 0.4373 0.4813 0.5604 0.127 Uiso 1 1 calc R . .
C65 C 0.4230(4) 0.3301(10) 0.5709(4) 0.100(3) Uani 1 1 d . . .
H65 H 0.4599 0.3074 0.5623 0.121 Uiso 1 1 calc R . .
C66 C 0.3811(5) 0.2572(6) 0.5854(4) 0.083(3) Uani 1 1 d . . .
H66 H 0.3902 0.1866 0.5851 0.099 Uiso 1 1 calc R . .
C67 C 0.2064(4) 0.2505(6) 0.6222(4) 0.062(2) Uani 1 1 d . . .
C68 C 0.1683(5) 0.2771(7) 0.5721(4) 0.101(3) Uani 1 1 d . . .
H68 H 0.1811 0.2638 0.5382 0.121 Uiso 1 1 calc R . .
C69 C 0.1107(6) 0.3235(9) 0.5702(5) 0.132(5) Uani 1 1 d . . .
H69 H 0.0865 0.3442 0.5359 0.158 Uiso 1 1 calc R . .
C70 C 0.0912(5) 0.3373(7) 0.6201(6) 0.111(4) Uani 1 1 d . . .
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H70 H 0.0529 0.3673 0.6195 0.134 Uiso 1 1 calc R . .
C71 C 0.1259(5) 0.3088(7) 0.6699(5) 0.105(4) Uani 1 1 d . . .
H71 H 0.1117 0.3167 0.7036 0.126 Uiso 1 1 calc R . .
C72 C 0.1829(4) 0.2675(6) 0.6697(4) 0.089(3) Uani 1 1 d . . .
H72 H 0.2073 0.2499 0.7046 0.107 Uiso 1 1 calc R . .
N1S N 0.4495(5) 0.4070(9) 0.4159(6) 0.174(5) Uani 1 1 d . . .
C1S C 0.4246(6) 0.3328(10) 0.4148(6) 0.134(5) Uani 1 1 d . . .
C2S C 0.3921(5) 0.2356(7) 0.4153(4) 0.172(5) Uani 1 1 d . . .
H2S1 H 0.3764 0.2304 0.4497 0.258 Uiso 1 1 calc R . .
H2S2 H 0.4197 0.1788 0.4134 0.258 Uiso 1 1 calc R . .
H2S3 H 0.3586 0.2328 0.3832 0.258 Uiso 1 1 calc R . .

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Cd2 0.0502(3) 0.0607(4) 0.0569(4) -0.0084(3) 0.0098(3) -0.0035(3)
O1 0.159(7) 0.157(7) 0.176(9) -0.023(6) 0.048(6) -0.024(5)
S1 0.0604(15) 0.0945(16) 0.0653(17) 0.0191(12) 0.0235(13) 0.0058(12)
S2 0.0502(13) 0.0657(14) 0.0471(14) -0.0068(10) 0.0141(10) 0.0000(10)
S3 0.0515(12) 0.0586(13) 0.0543(13) 0.0025(11) 0.0117(10) -0.0042(11)
S4 0.0827(15) 0.0768(15) 0.0692(15) -0.0088(13) 0.0337(12) -0.0193(13)
P1 0.0693(18) 0.094(2) 0.0499(19) 0.0105(14) 0.0085(15) -0.0190(15)
P2 0.0536(14) 0.0624(14) 0.0471(15) -0.0018(11) 0.0153(12) -0.0035(11)
P3 0.0456(14) 0.0636(14) 0.0546(16) 0.0022(12) 0.0082(12) -0.0035(11)
P4 0.0553(15) 0.0779(16) 0.0533(16) 0.0123(12) 0.0097(13) -0.0039(12)
C1 0.057(6) 0.059(5) 0.030(5) 0.001(4) 0.011(5) -0.015(4)
C2 0.063(6) 0.063(6) 0.043(6) 0.002(4) 0.019(5) -0.004(5)
C3 0.088(7) 0.077(6) 0.047(7) -0.012(5) 0.026(5) -0.009(5)
C4 0.088(8) 0.114(8) 0.037(6) 0.005(5) 0.010(6) -0.031(6)
C5 0.069(7) 0.087(7) 0.049(7) 0.006(5) 0.001(6) -0.005(5)
C6 0.064(6) 0.063(5) 0.051(6) 0.005(5) -0.001(5) 0.000(4)
C7 0.041(5) 0.077(6) 0.057(7) -0.007(5) 0.017(5) -0.022(4)
C8 0.072(7) 0.091(7) 0.086(9) 0.014(6) 0.020(6) -0.020(5)
C9 0.113(9) 0.115(9) 0.119(10) 0.001(7) 0.047(7) -0.055(6)
C10 0.107(9) 0.107(8) 0.150(12) -0.044(9) 0.064(9) -0.062(7)
C11 0.097(8) 0.181(12) 0.086(10) -0.059(8) 0.024(8) -0.064(8)
C12 0.079(7) 0.143(9) 0.078(9) -0.041(6) 0.025(6) -0.058(6)
C13 0.037(6) 0.098(7) 0.055(6) -0.015(5) 0.023(4) -0.004(5)
C14 0.090(9) 0.096(9) 0.112(9) -0.018(7) 0.030(7) 0.002(7)
C15 0.092(10) 0.134(11) 0.151(12) -0.033(8) 0.015(8) 0.014(8)
C16 0.073(9) 0.214(16) 0.076(9) -0.032(10) 0.000(7) 0.023(12)
C17 0.045(8) 0.236(14) 0.053(7) -0.002(9) 0.016(6) -0.026(10)
C18 0.056(7) 0.145(8) 0.055(7) -0.003(6) 0.012(5) -0.018(7)
C19 0.045(5) 0.050(5) 0.048(6) -0.008(4) 0.012(4) -0.001(4)
C20 0.030(4) 0.060(5) 0.043(6) 0.008(5) 0.011(4) -0.003(4)
C21 0.050(5) 0.086(6) 0.036(6) 0.005(5) 0.010(4) -0.003(5)
C22 0.070(6) 0.070(7) 0.078(8) 0.025(6) 0.003(6) 0.000(5)
C23 0.104(7) 0.043(6) 0.097(9) -0.013(6) 0.018(7) -0.005(5)
C24 0.073(6) 0.073(7) 0.054(6) 0.008(5) 0.018(5) -0.008(5)
C25 0.056(6) 0.060(5) 0.047(6) -0.009(4) 0.012(5) 0.000(5)
C26 0.099(8) 0.110(8) 0.071(8) -0.042(6) 0.016(6) -0.023(6)
C27 0.109(10) 0.148(10) 0.096(11) -0.049(8) -0.010(8) -0.010(8)
C28 0.156(13) 0.102(9) 0.098(10) -0.052(7) 0.006(10) 0.026(9)
C29 0.146(11) 0.118(9) 0.110(11) -0.045(7) 0.057(9) -0.011(8)
C30 0.093(8) 0.092(7) 0.085(8) -0.036(6) 0.030(7) 0.001(6)
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C31 0.061(6) 0.043(5) 0.048(6) 0.000(4) 0.007(5) -0.002(4)
C32 0.057(6) 0.064(6) 0.070(7) 0.000(5) 0.027(5) -0.004(4)
C33 0.074(7) 0.083(6) 0.073(7) 0.005(6) 0.015(5) 0.006(6)
C34 0.040(5) 0.103(7) 0.083(7) -0.009(6) -0.006(5) 0.005(5)
C35 0.047(6) 0.141(8) 0.076(8) 0.014(6) 0.032(5) 0.017(5)
C36 0.060(7) 0.103(7) 0.073(8) 0.033(5) 0.014(6) 0.002(6)
C37 0.038(5) 0.049(5) 0.060(6) -0.007(5) 0.014(4) -0.001(4)
C38 0.034(5) 0.067(6) 0.045(6) -0.010(5) 0.009(4) -0.014(4)
C39 0.052(5) 0.075(6) 0.059(7) -0.005(5) 0.009(5) -0.022(5)
C40 0.069(7) 0.071(7) 0.068(7) -0.029(6) 0.035(5) -0.022(5)
C41 0.092(7) 0.039(6) 0.105(9) -0.010(6) 0.024(7) -0.009(5)
C42 0.066(6) 0.061(6) 0.067(7) -0.006(5) 0.008(5) 0.002(5)
C43 0.041(5) 0.066(6) 0.061(6) 0.012(4) 0.007(5) 0.004(5)
C44 0.060(7) 0.093(7) 0.072(7) 0.023(5) 0.017(5) 0.002(5)
C45 0.135(11) 0.108(9) 0.074(8) 0.033(6) 0.018(7) -0.041(7)
C46 0.161(14) 0.113(9) 0.104(10) 0.055(7) -0.012(10) 0.013(10)
C47 0.099(10) 0.131(11) 0.141(12) 0.050(8) -0.004(8) 0.020(8)
C48 0.074(8) 0.094(7) 0.101(9) 0.025(6) -0.002(6) 0.010(6)
C49 0.042(5) 0.069(6) 0.055(6) 0.006(5) 0.010(5) 0.006(4)
C50 0.061(6) 0.104(7) 0.072(7) -0.034(5) 0.015(5) -0.034(5)
C51 0.091(8) 0.145(9) 0.074(8) -0.036(6) 0.031(6) -0.053(6)
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C53 0.070(7) 0.084(7) 0.074(8) -0.018(5) 0.009(6) -0.013(5)
C54 0.056(5) 0.079(6) 0.058(6) 0.002(5) 0.012(4) 0.002(5)
C55 0.042(5) 0.059(5) 0.054(6) -0.003(5) 0.010(4) -0.003(4)
C56 0.059(6) 0.086(6) 0.032(6) 0.003(5) 0.009(5) 0.012(5)
C57 0.072(7) 0.104(7) 0.069(8) 0.031(6) 0.019(6) 0.001(5)
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C61 0.077(7) 0.068(7) 0.058(6) 0.008(5) 0.005(5) 0.005(6)
C62 0.109(9) 0.090(8) 0.106(9) 0.014(6) 0.044(6) 0.007(7)
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C65 0.065(7) 0.140(10) 0.097(8) 0.026(8) 0.018(6) -0.017(8)
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C69 0.089(11) 0.171(11) 0.115(12) 0.058(10) -0.029(9) 0.008(8)
C70 0.078(9) 0.101(8) 0.154(14) 0.033(9) 0.018(10) 0.023(6)
C71 0.090(9) 0.112(8) 0.116(11) 0.020(7) 0.031(8) 0.040(6)
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 All esds (except the esd in the dihedral angle between two l.s.
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 are estimated using the full covariance matrix.  The cell esds are
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angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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C26 C27 1.397(10) . ?
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based
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of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
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based
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and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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C2 C -0.1123(3) 0.42182(17) 0.17098(15) 0.0356(8) Uani 1 1 d . . .
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H3 H -0.2755 0.3823 0.1782 0.060 Uiso 1 1 calc R . .
C4 C -0.2702(4) 0.3692(2) 0.0937(2) 0.0609(12) Uani 1 1 d . . .
H4 H -0.3472 0.3487 0.0819 0.073 Uiso 1 1 calc R . .
C5 C -0.1999(4) 0.3788(2) 0.05290(19) 0.0580(11) Uani 1 1 d . . .
H5 H -0.2279 0.3635 0.0141 0.070 Uiso 1 1 calc R . .
C6 C -0.0876(3) 0.41144(19) 0.07087(16) 0.0450(9) Uani 1 1 d . . .
H6 H -0.0404 0.4187 0.0436 0.054 Uiso 1 1 calc R . .
C7 C 0.2014(3) 0.42939(17) 0.11114(14) 0.0312(7) Uani 1 1 d . . .
C8 C 0.2425(3) 0.36099(18) 0.13203(14) 0.0352(8) Uani 1 1 d . . .
C9 C 0.3226(3) 0.3246(2) 0.10473(16) 0.0492(10) Uani 1 1 d . . .
H9 H 0.3511 0.2793 0.1181 0.059 Uiso 1 1 calc R . .
C10 C 0.3599(3) 0.3554(2) 0.05793(17) 0.0536(11) Uani 1 1 d . . .
H10 H 0.4149 0.3312 0.0408 0.064 Uiso 1 1 calc R . .
C11 C 0.3166(3) 0.4216(2) 0.03644(17) 0.0517(10) Uani 1 1 d . . .
H11 H 0.3404 0.4413 0.0042 0.062 Uiso 1 1 calc R . .
C12 C 0.2376(3) 0.4584(2) 0.06303(15) 0.0420(9) Uani 1 1 d . . .
H12 H 0.2083 0.5031 0.0486 0.050 Uiso 1 1 calc R . .
C13 C 0.0839(3) 0.56622(17) 0.11688(14) 0.0329(7) Uani 1 1 d . . .
C14 C -0.0241(3) 0.59016(19) 0.08106(16) 0.0428(9) Uani 1 1 d . . .
H14 H -0.0891 0.5585 0.0694 0.051 Uiso 1 1 calc R . .
C15 C -0.0366(4) 0.6612(2) 0.06226(18) 0.0568(11) Uani 1 1 d . . .
H15 H -0.1097 0.6767 0.0379 0.068 Uiso 1 1 calc R . .
C16 C 0.0578(4) 0.7084(2) 0.07936(18) 0.0561(11) Uani 1 1 d . . .
H16 H 0.0486 0.7560 0.0672 0.067 Uiso 1 1 calc R . .
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C17 C 0.1661(4) 0.6853(2) 0.11440(18) 0.0550(10) Uani 1 1 d . . .
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C18 C 0.1798(3) 0.61516(19) 0.13312(17) 0.0465(9) Uani 1 1 d . . .
H18 H 0.2538 0.6001 0.1569 0.056 Uiso 1 1 calc R . .
C19 C 0.0188(3) 0.6283(2) 0.24350(18) 0.0508(10) Uani 1 1 d . . .
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H20 H -0.0590 0.7247 0.2223 0.071 Uiso 1 1 calc R . .
C21 C 0.1156(4) 0.7411(2) 0.26266(19) 0.0642(12) Uani 1 1 d . . .
H21 H 0.1145 0.7909 0.2600 0.077 Uiso 1 1 calc R . .
C22 C 0.2202(4) 0.7051(2) 0.28963(19) 0.0628(12) Uani 1 1 d . . .
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C23 C 0.2188(3) 0.6319(2) 0.29214(17) 0.0484(10) Uani 1 1 d . . .
H23 H 0.2897 0.6081 0.3111 0.058 Uiso 1 1 calc R . .
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C25 C 0.6121(3) 0.34710(17) 0.33766(17) 0.0412(9) Uani 1 1 d . . .
C26 C 0.7285(3) 0.3781(2) 0.3576(2) 0.0570(11) Uani 1 1 d . . .
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C27 C 0.7743(4) 0.3942(2) 0.4155(2) 0.0715(14) Uani 1 1 d . . .
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C28 C 0.7090(4) 0.3799(2) 0.4572(2) 0.0695(13) Uani 1 1 d . . .
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H29 H 0.5497 0.3386 0.4669 0.064 Uiso 1 1 calc R . .
C30 C 0.3007(3) 0.33822(17) 0.39876(14) 0.0331(7) Uani 1 1 d . . .
C31 C 0.2577(3) 0.40680(18) 0.37898(15) 0.0369(8) Uani 1 1 d . . .
C32 C 0.1807(3) 0.4420(2) 0.40824(17) 0.0505(10) Uani 1 1 d . . .
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C33 C 0.1488(4) 0.4113(2) 0.45640(18) 0.0586(11) Uani 1 1 d . . .
H33 H 0.0965 0.4355 0.4752 0.070 Uiso 1 1 calc R . .
C34 C 0.1939(4) 0.3448(2) 0.47688(17) 0.0540(10) Uani 1 1 d . . .
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C35 C 0.2688(3) 0.3081(2) 0.44764(16) 0.0445(9) Uani 1 1 d . . .
H35 H 0.2980 0.2629 0.4608 0.053 Uiso 1 1 calc R . .
C36 C 0.4113(3) 0.19935(17) 0.38523(14) 0.0322(7) Uani 1 1 d . . .
C37 C 0.3136(3) 0.15344(19) 0.36485(16) 0.0453(9) Uani 1 1 d . . .
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C38 C 0.3236(3) 0.08040(19) 0.37445(17) 0.0483(9) Uani 1 1 d . . .
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C39 C 0.4319(4) 0.05230(19) 0.40497(17) 0.0476(9) Uani 1 1 d . . .
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C41 C 0.5187(3) 0.1699(2) 0.41747(16) 0.0452(9) Uani 1 1 d . . .
H41 H 0.5852 0.1994 0.4327 0.054 Uiso 1 1 calc R . .
C42 C 0.2867(3) 0.1407(2) 0.20649(17) 0.0492(10) Uani 1 1 d . . .
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C44 C 0.3949(4) 0.0319(2) 0.2267(2) 0.0667(12) Uani 1 1 d . . .
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C45 C 0.4936(4) 0.0703(2) 0.25437(19) 0.0593(11) Uani 1 1 d . . .
H45 H 0.5668 0.0473 0.2709 0.071 Uiso 1 1 calc R . .
C46 C 0.4846(3) 0.14337(19) 0.25782(17) 0.0466(9) Uani 1 1 d . . .
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C1S C 0.9853(5) 0.3565(4) 0.5849(2) 0.0821(16) Uani 1 1 d . . .
C2S C 0.9415(6) 0.2842(3) 0.5830(3) 0.121(2) Uani 1 1 d . . .
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H2S2 H 0.9900 0.2575 0.6153 0.181 Uiso 1 1 calc R . .
H2S3 H 0.9472 0.2623 0.5464 0.181 Uiso 1 1 calc R . .
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C3S C 0.4911(6) 0.3770(4) 0.5823(2) 0.096(2) Uani 1 1 d . . .
C4S C 0.4470(7) 0.4478(4) 0.5697(3) 0.135(3) Uani 1 1 d . . .
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H4S2 H 0.5039 0.4812 0.5925 0.202 Uiso 1 1 calc R . .
H4S3 H 0.3695 0.4526 0.5797 0.202 Uiso 1 1 calc R . .

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N2 0.0414(17) 0.0298(15) 0.0448(17) -0.0017(13) 0.0108(14) 0.0038(13)
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C3 0.030(2) 0.042(2) 0.078(3) 0.013(2) 0.015(2) -0.0005(16)
C4 0.035(2) 0.055(3) 0.083(3) 0.013(2) -0.006(2) -0.0092(19)
C5 0.049(3) 0.058(3) 0.057(3) 0.002(2) -0.007(2) -0.008(2)
C6 0.039(2) 0.045(2) 0.045(2) 0.0065(17) -0.0005(17) -0.0016(17)
C7 0.0272(17) 0.0333(18) 0.0325(18) -0.0028(14) 0.0056(14) -0.0031(14)
C8 0.0274(18) 0.038(2) 0.0390(19) -0.0038(15) 0.0046(15) 0.0013(14)
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C12 0.039(2) 0.044(2) 0.042(2) 0.0027(17) 0.0098(17) -0.0046(16)
C13 0.0316(18) 0.0307(18) 0.0371(19) 0.0036(15) 0.0092(15) 0.0021(14)
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C27 0.039(3) 0.059(3) 0.106(4) 0.009(3) -0.005(3) -0.012(2)
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0.0011(14)
C31 0.0325(19) 0.0360(19) 0.040(2) -0.0017(15) 0.0040(16) 0.0022(15)
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C34 0.054(3) 0.063(3) 0.050(2) 0.000(2) 0.022(2) -0.005(2)
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C38 0.047(2) 0.037(2) 0.060(3) 0.0031(18) 0.010(2) -0.0094(17)
C39 0.060(3) 0.0281(19) 0.058(2) 0.0070(17) 0.020(2) 0.0036(18)
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C44 0.076(3) 0.035(2) 0.086(3) -0.009(2) 0.012(3) 0.004(2)
C45 0.056(3) 0.043(2) 0.071(3) -0.007(2) -0.002(2) 0.015(2)
C46 0.043(2) 0.039(2) 0.057(2) -0.0052(18) 0.0100(19) 0.0025(17)
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C2S 0.154(6) 0.096(5) 0.100(5) 0.015(4) 0.007(4) -0.006(4)
N2S 0.135(5) 0.132(6) 0.127(5) 0.025(4) -0.023(4) -0.017(5)
C3S 0.104(5) 0.116(6) 0.053(3) 0.006(4) -0.009(3) -0.034(5)
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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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C9 C8 C7 118.6(3) . . ?
C9 C8 S2 122.6(3) . . ?
C7 C8 S2 118.8(2) . . ?
C10 C9 C8 120.5(4) . . ?
C11 C10 C9 120.7(4) . . ?
C10 C11 C12 119.6(4) . . ?
C11 C12 C7 120.7(4) . . ?
C14 C13 C18 118.1(3) . . ?
C14 C13 P1 123.9(3) . . ?
C18 C13 P1 117.7(3) . . ?
C13 C14 C15 120.6(3) . . ?
C16 C15 C14 120.3(4) . . ?
C15 C16 C17 119.8(4) . . ?
C16 C17 C18 120.4(4) . . ?
C17 C18 C13 120.8(3) . . ?
N1 C19 C20 122.9(4) . . ?
C21 C20 C19 119.6(4) . . ?
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```
C20 C21 C22 118.2(4) . . ?
C23 C22 C21 119.3(4) . . ?
N1 C23 C22 122.9(4) . . ?
C29 C24 C25 120.0(3) . . ?
C29 C24 P2 120.2(3) . . ?
C25 C24 P2 119.8(3) . . ?
C24 C25 C26 117.3(4) . . ?
C24 C25 S3 125.5(3) . . ?
C26 C25 S3 117.1(3) . . ?
C27 C26 C25 121.7(4) . . ?
C26 C27 C28 121.0(4) . . ?
C27 C28 C29 118.7(4) . . ?
C24 C29 C28 121.2(4) . . ?
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C35 C30 P2 122.4(3) . . ?
C31 C30 P2 117.6(2) . . ?
C32 C31 C30 118.4(3) . . ?
C32 C31 S4 122.6(3) . . ?
C30 C31 S4 118.9(3) . . ?
C33 C32 C31 121.0(4) . . ?
C34 C33 C32 120.5(4) . . ?
C33 C34 C35 119.4(4) . . ?
C34 C35 C30 120.6(4) . . ?
C41 C36 C37 117.9(3) . . ?
C41 C36 P2 124.4(3) . . ?
C37 C36 P2 117.1(2) . . ?
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C39 C40 C41 121.2(4) . . ?
C40 C41 C36 120.1(3) . . ?
N2 C42 C43 123.3(4) . . ?
C44 C43 C42 118.3(4) . . ?
C45 C44 C43 119.3(4) . . ?
C44 C45 C46 119.3(4) . . ?
N2 C46 C45 122.9(4) . . ?
N1S C1S C2S 179.2(8) . . ?
N2S C3S C4S 179.6(9) . . ?

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Compound (5)

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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'P'  'P'   0.1023   0.0942
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'S'  'S'   0.1246   0.1234
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Hg'  'Hg'  -2.3894   9.2266
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'C 2/c'

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 '-x, y, -z+1/2'
 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

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_cell_length_b                    9.2713(16)
_cell_length_c                    20.907(4)
_cell_angle_alpha                 90.00
_cell_angle_beta                  98.067(3)
_cell_angle_gamma                 90.00
_cell_volume                      3132.3(9)
_cell_formula_units_Z             4
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_diffrn_radiation_monochromator   graphite
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_diffrn_standards_decay_%         ?
_diffrn_reflns_number             4242
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_diffrn_reflns_av_sigmaI/netI     0.0276
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_diffrn_reflns_limit_k_max        11
_diffrn_reflns_limit_l_min        -26
_diffrn_reflns_limit_l_max        16
_diffrn_reflns_theta_min          1.97
_diffrn_reflns_theta_max          26.37
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_reflns_number_gt                 2964
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        'BRUKER Smart'
_computing_data_reduction         ?
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_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
```

```
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0184P)^2^+3.6007P] where
P=(Fo^2^+2Fc^2^)/3'
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 _atom_site_fract_z
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 _atom_site_symmetry_multiplicity
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 _atom_site_refinement_flags
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 _atom_site_disorder_group
Hg1 Hg 0.0000 0.116245(18) 0.7500 0.03693(6) Uani 1 2 d S . .
S1 S 0.06533(5) -0.00722(8) 0.66370(3) 0.03932(17) Uani 1 1 d . . .
P1 P -0.09069(4) 0.23109(7) 0.65707(3) 0.02823(14) Uani 1 1 d . . .
C1 C -0.02944(17) 0.2092(3) 0.59204(12) 0.0307(6) Uani 1 1 d . . .
C2 C 0.03616(17) 0.1091(3) 0.59775(13) 0.0303(5) Uani 1 1 d . . .
C3 C 0.0819(2) 0.0987(3) 0.54569(14) 0.0403(7) Uani 1 1 d . . .
H3 H 0.1258 0.0339 0.5484 0.048 Uiso 1 1 calc R . .
C4 C 0.0636(2) 0.1814(4) 0.49096(15) 0.0470(8) Uani 1 1 d . . .
H4 H 0.0945 0.1712 0.4571 0.056 Uiso 1 1 calc R . .
C5 C -0.0005(2) 0.2797(4) 0.48622(15) 0.0504(8) Uani 1 1 d . . .
H5 H -0.0124 0.3363 0.4494 0.061 Uiso 1 1 calc R . .
C6 C -0.0465(2) 0.2936(3) 0.53591(14) 0.0427(7) Uani 1 1 d . . .
```

```
H6 H -0.0897 0.3599 0.5324 0.051 Uiso 1 1 calc R . .
C7 C -0.18615(17) 0.1311(3) 0.63577(13) 0.0318(6) Uani 1 1 d . . .
C8 C -0.2106(2) 0.0763(3) 0.57414(15) 0.0415(7) Uani 1 1 d . . .
H8 H -0.1789 0.0944 0.5413 0.050 Uiso 1 1 calc R . .
C9 C -0.2827(2) -0.0059(4) 0.56154(17) 0.0513(8) Uani 1 1 d . . .
H9 H -0.2982 -0.0449 0.5206 0.062 Uiso 1 1 calc R . .
C10 C -0.3305(2) -0.0294(4) 0.60907(18) 0.0548(9) Uani 1 1 d . . .
H10 H -0.3791 -0.0826 0.6002 0.066 Uiso 1 1 calc R . .
C11 C -0.3073(2) 0.0251(4) 0.66987(18) 0.0581(9) Uani 1 1 d . . .
H11 H -0.3402 0.0087 0.7021 0.070 Uiso 1 1 calc R . .
C12 C -0.2352(2) 0.1044(4) 0.68346(17) 0.0476(8) Uani 1 1 d . . .
H12 H -0.2195 0.1400 0.7249 0.057 Uiso 1 1 calc R . .
C13 C -0.11886(18) 0.4209(3) 0.65674(13) 0.0307(6) Uani 1 1 d . . .
C14 C -0.19954(19) 0.4710(3) 0.64591(15) 0.0415(7) Uani 1 1 d . . .
H14 H -0.2431 0.4063 0.6362 0.050 Uiso 1 1 calc R . .
C15 C -0.2156(2) 0.6177(3) 0.64951(18) 0.0535(9) Uani 1 1 d . . .
H15 H -0.2699 0.6511 0.6422 0.064 Uiso 1 1 calc R . .
C16 C -0.1513(2) 0.7137(3) 0.66395(17) 0.0529(9) Uani 1 1 d . . .
H16 H -0.1623 0.8117 0.6667 0.064 Uiso 1 1 calc R . .
C17 C -0.0714(2) 0.6651(4) 0.67428(17) 0.0533(9) Uani 1 1 d . . .
H17 H -0.0282 0.7308 0.6833 0.064 Uiso 1 1 calc R . .
C18 C -0.0541(2) 0.5189(3) 0.67150(15) 0.0433(7) Uani 1 1 d . . .
H18 H 0.0003 0.4865 0.6794 0.052 Uiso 1 1 calc R . .

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S1 0.0453(4) 0.0358(4) 0.0390(4) 0.0004(3) 0.0136(3) 0.0098(3)
P1 0.0256(3) 0.0317(3) 0.0282(3) 0.0002(3) 0.0065(3) 0.0016(3)
C1 0.0294(14) 0.0348(14) 0.0286(13) -0.0013(11) 0.0068(11) -0.0007(11)
C2 0.0286(14) 0.0314(13) 0.0314(13) -0.0073(11) 0.0062(10) -0.0067(11)
C3 0.0379(17) 0.0441(17) 0.0413(16) -0.0091(13) 0.0144(13) -0.0011(13)
C4 0.051(2) 0.058(2) 0.0365(16) -0.0045(14) 0.0211(14) -0.0029(16)
C5 0.062(2) 0.058(2) 0.0343(16) 0.0104(14) 0.0146(15) 0.0015(17)
C6 0.0473(18) 0.0472(18) 0.0345(15) 0.0058(13) 0.0092(13) 0.0056(14)
C7 0.0302(14) 0.0288(14) 0.0367(14) 0.0001(11) 0.0057(11) 0.0037(11)
C8 0.0411(18) 0.0452(17) 0.0384(16) -0.0030(13) 0.0063(13) 0.0010(13)
C9 0.046(2) 0.053(2) 0.0505(19) -0.0119(15) -0.0079(15) -0.0043(15)
C10 0.0333(18) 0.052(2) 0.076(2) -0.0028(18) -0.0025(16) -0.0098(15)
C11 0.0406(19) 0.072(2) 0.064(2) -0.0010(19) 0.0184(16) -0.0171(18)
C12 0.0387(18) 0.060(2) 0.0461(18) -0.0031(15) 0.0119(14) -0.0089(15)
C13 0.0345(15) 0.0310(14) 0.0279(13) 0.0016(10) 0.0094(11) 0.0025(11)
C14 0.0332(16) 0.0377(16) 0.0523(18) -0.0029(13) 0.0021(13) 0.0019(13)
C15 0.050(2) 0.0449(18) 0.064(2) 0.0011(16) 0.0048(17) 0.0140(16)
C16 0.074(3) 0.0303(16) 0.057(2) 0.0050(14) 0.0161(18) 0.0074(16)
C17 0.063(2) 0.0384(17) 0.060(2) 0.0013(15) 0.0152(17) -0.0142(16)
C18 0.0338(16) 0.0432(17) 0.0536(18) 0.0020(14) 0.0091(13) -0.0018(13)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
```

```
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Hg1 S1 2.4986(7) . ?
Hg1 P1 2.5085(7) 2_556 ?
Hg1 P1 2.5085(7) . ?
S1 C2 1.762(3) . ?
P1 C1 1.808(3) . ?
P1 C7 1.814(3) . ?
P1 C13 1.819(3) . ?
C1 C6 1.406(4) . ?
C1 C2 1.409(4) . ?
C2 C3 1.407(4) . ?
C3 C4 1.375(5) . ?
C4 C5 1.380(5) . ?
C5 C6 1.371(4) . ?
C7 C12 1.385(4) . ?
C7 C8 1.391(4) . ?
C8 C9 1.396(5) . ?
C9 C10 1.364(5) . ?
C10 C11 1.371(5) . ?
C11 C12 1.384(5) . ?
C13 C14 1.385(4) . ?
C13 C18 1.395(4) . ?
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S1 Hg1 P1 84.28(3) 2_556 2_556 ?
S1 Hg1 P1 119.24(3) . 2_556 ?
S1 Hg1 P1 119.24(3) 2_556 . ?
S1 Hg1 P1 84.28(3) . . ?
P1 Hg1 P1 129.77(3) 2_556 . ?
C2 S1 Hg1 100.89(9) . . ?
C1 P1 C7 107.73(13) . . ?
C1 P1 C13 105.78(12) . . ?
C7 P1 C13 106.59(13) . . ?
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C1 P1 Hg1 101.90(9) . . ?
C7 P1 Hg1 111.49(9) . . ?
C13 P1 Hg1 122.34(9) . . ?
C6 C1 C2 119.8(2) . . ?
C6 C1 P1 119.9(2) . . ?
C2 C1 P1 120.3(2) . . ?
C3 C2 C1 117.3(3) . . ?
C3 C2 S1 116.7(2) . . ?
C1 C2 S1 126.0(2) . . ?
C4 C3 C2 121.9(3) . . ?
C3 C4 C5 120.1(3) . . ?
C6 C5 C4 119.9(3) . . ?
C5 C6 C1 121.0(3) . . ?
C12 C7 C8 118.8(3) . . ?
C12 C7 P1 118.5(2) . . ?
C8 C7 P1 122.6(2) . . ?
C7 C8 C9 120.0(3) . . ?
C10 C9 C8 120.2(3) . . ?
C9 C10 C11 120.4(3) . . ?
C10 C11 C12 120.1(3) . . ?
C11 C12 C7 120.6(3) . . ?
C14 C13 C18 119.4(3) . . ?
C14 C13 P1 124.0(2) . . ?
C18 C13 P1 116.5(2) . . ?
C13 C14 C15 120.2(3) . . ?
C16 C15 C14 120.0(3) . . ?
C17 C16 C15 120.2(3) . . ?
C16 C17 C18 120.6(3) . . ?
C17 C18 C13 119.6(3) . . ?

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Compound (6)

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;
_chemical_name_common             ?
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_chemical_formula_moiety          ?
_chemical_formula_sum
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_chemical_formula_weight          3981.19

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Si'  'Si'   0.0817   0.0704
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'P'  'P'   0.1023   0.0942
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'S'  'S'   0.1246   0.1234
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Hg'  'Hg'  -2.3894   9.2266
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cl'  'Cl'   0.1484   0.1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'C 2/c'

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 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

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_cell_length_b                    11.8702(8)
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_cell_angle_beta                  114.6160(10)
_cell_angle_gamma                 90.00
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_cell_formula_units_Z             4
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_exptl_absorpt_coefficient_mu     3.656
_exptl_absorpt_correction_type    'multi-scan'
_exptl_absorpt_correction_T_min   0.2900
_exptl_absorpt_correction_T_max   0.8383
_exptl_absorpt_process_details    ?

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature       293(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Smart-CCD-1000 BRUKER'
_diffrn_measurement_method        'omega scans'
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_number          ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             83214
_diffrn_reflns_av_R_equivalents   0.0863
_diffrn_reflns_av_sigmaI/netI     0.0597
_diffrn_reflns_limit_h_min        -57
_diffrn_reflns_limit_h_max        52
_diffrn_reflns_limit_k_min        0
_diffrn_reflns_limit_k_max        13
_diffrn_reflns_limit_l_min        0
_diffrn_reflns_limit_l_max        37
_diffrn_reflns_theta_min          0.87
_diffrn_reflns_theta_max          23.31
_reflns_number_total              13353
_reflns_number_gt                 8349
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'BRUKER Smart'
_computing_cell_refinement        'BRUKER Smart'
_computing_data_reduction         ?
_computing_structure_solution     ?
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
```

```
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0497P)^2^+181.3905P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     'constr'
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          13353
_refine_ls_number_parameters      955
_refine_ls_number_restraints      4
_refine_ls_R_factor_all           0.1018
_refine_ls_R_factor_gt            0.0442
_refine_ls_wR_factor_ref          0.1341
_refine_ls_wR_factor_gt           0.1021
_refine_ls_goodness_of_fit_ref    1.036
_refine_ls_restrained_S_all       1.036
_refine_ls_shift/su_max           0.002
_refine_ls_shift/su_mean          0.000

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Hg1 Hg 0.606826(8) 0.31875(3) 0.173785(13) 0.05491(13) Uani 1 1 d . .
.
S1 S 0.65533(5) 0.3159(2) 0.24017(8) 0.0547(6) Uani 1 1 d . . .
S2 S 0.57199(6) 0.4432(3) 0.18779(9) 0.0763(9) Uani 1 1 d . . .
P1 P 0.61037(5) 0.1155(2) 0.18878(8) 0.0484(6) Uani 1 1 d . . .
P2 P 0.59562(5) 0.4423(2) 0.10911(8) 0.0457(6) Uani 1 1 d . . .
Si1 Si 0.72357(6) 0.2743(3) 0.28630(9) 0.0604(8) Uani 1 1 d . . .
Si2 Si 0.51139(8) 0.5563(5) 0.17165(13) 0.1103(16) Uani 1 1 d . . .
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```
C1 C 0.64830(18) 0.0895(8) 0.2144(3) 0.044(2) Uani 1 1 d . . .
C2 C 0.66713(18) 0.1788(8) 0.2362(3) 0.045(2) Uani 1 1 d . . .
C3 C 0.69697(19) 0.1596(8) 0.2565(3) 0.048(2) Uani 1 1 d . . .
C4 C 0.7064(2) 0.0519(9) 0.2543(3) 0.056(3) Uani 1 1 d . . .
H4 H 0.7260 0.0377 0.2672 0.067 Uiso 1 1 calc R . .
C5 C 0.6881(2) -0.0346(9) 0.2340(3) 0.060(3) Uani 1 1 d . . .
H5 H 0.6954 -0.1062 0.2340 0.072 Uiso 1 1 calc R . .
C6 C 0.6591(2) -0.0171(8) 0.2137(3) 0.058(3) Uani 1 1 d . . .
H6 H 0.6468 -0.0762 0.1997 0.069 Uiso 1 1 calc R . .
C7 C 0.7193(2) 0.3215(10) 0.3363(3) 0.086(4) Uani 1 1 d . . .
H7A H 0.7008 0.3544 0.3278 0.129 Uiso 1 1 calc R . .
H7B H 0.7338 0.3763 0.3517 0.129 Uiso 1 1 calc R . .
H7C H 0.7213 0.2580 0.3552 0.129 Uiso 1 1 calc R . .
C8 C 0.7599(2) 0.2112(11) 0.3047(4) 0.089(4) Uani 1 1 d . . .
H8A H 0.7614 0.1468 0.3230 0.133 Uiso 1 1 calc R . .
H8B H 0.7740 0.2660 0.3212 0.133 Uiso 1 1 calc R . .
H8C H 0.7629 0.1884 0.2793 0.133 Uiso 1 1 calc R . .
C9 C 0.7222(2) 0.3980(10) 0.2515(4) 0.081(3) Uani 1 1 d . . .
H9A H 0.7037 0.4329 0.2415 0.122 Uiso 1 1 calc R . .
H9B H 0.7255 0.3740 0.2265 0.122 Uiso 1 1 calc R . .
H9C H 0.7366 0.4512 0.2685 0.122 Uiso 1 1 calc R . .
C10 C 0.59471(19) 0.0175(8) 0.1437(3) 0.056(3) Uani 1 1 d . . .
C11 C 0.5957(2) 0.0424(10) 0.1038(4) 0.077(3) Uani 1 1 d . . .
H11 H 0.6058 0.1055 0.1018 0.093 Uiso 1 1 calc R . .
C12 C 0.5821(3) -0.0237(13) 0.0673(4) 0.096(4) Uani 1 1 d . . .
H12 H 0.5831 -0.0057 0.0407 0.115 Uiso 1 1 calc R . .
C13 C 0.5674(3) -0.1149(14) 0.0701(6) 0.113(6) Uani 1 1 d . . .
H13 H 0.5582 -0.1595 0.0452 0.136 Uiso 1 1 calc R . .
C14 C 0.5658(3) -0.1432(12) 0.1082(6) 0.109(5) Uani 1 1 d . . .
H14 H 0.5555 -0.2065 0.1095 0.131 Uiso 1 1 calc R . .
C15 C 0.5797(2) -0.0766(10) 0.1460(4) 0.080(3) Uani 1 1 d . . .
H15 H 0.5788 -0.0959 0.1724 0.096 Uiso 1 1 calc R . .
C16 C 0.5970(2) 0.0821(8) 0.2295(3) 0.058(3) Uani 1 1 d . . .
C17 C 0.6140(3) 0.0352(11) 0.2697(4) 0.091(4) Uani 1 1 d . . .
H17 H 0.6329 0.0171 0.2761 0.109 Uiso 1 1 calc R . .
C18 C 0.6033(3) 0.0148(14) 0.3004(5) 0.133(7) Uani 1 1 d . . .
H18 H 0.6152 -0.0167 0.3275 0.160 Uiso 1 1 calc R . .
C19 C 0.5756(3) 0.0396(13) 0.2923(5) 0.109(5) Uani 1 1 d . . .
H19 H 0.5683 0.0220 0.3127 0.131 Uiso 1 1 calc R . .
C20 C 0.5590(3) 0.0915(13) 0.2530(5) 0.097(4) Uani 1 1 d . . .
H20 H 0.5403 0.1113 0.2471 0.117 Uiso 1 1 calc R . .
C21 C 0.5698(2) 0.1145(11) 0.2223(4) 0.082(4) Uani 1 1 d . . .
H21 H 0.5585 0.1524 0.1964 0.098 Uiso 1 1 calc R . .
C22 C 0.56139(18) 0.5003(7) 0.1008(3) 0.046(2) Uani 1 1 d . . .
C23 C 0.55235(18) 0.5010(8) 0.1351(3) 0.050(2) Uani 1 1 d . . .
C24 C 0.5256(2) 0.5515(9) 0.1277(4) 0.062(3) Uani 1 1 d . . .
C25 C 0.5097(2) 0.5963(9) 0.0861(4) 0.072(3) Uani 1 1 d . . .
H25 H 0.4922 0.6294 0.0810 0.086 Uiso 1 1 calc R . .
C26 C 0.5180(2) 0.5949(9) 0.0524(4) 0.072(3) Uani 1 1 d . . .
H26 H 0.5064 0.6253 0.0250 0.086 Uiso 1 1 calc R . .
C27 C 0.5442(2) 0.5472(8) 0.0598(3) 0.060(3) Uani 1 1 d . . .
H27 H 0.5504 0.5463 0.0372 0.072 Uiso 1 1 calc R . .
C28 C 0.5033(4) 0.4134(17) 0.1866(6) 0.168(8) Uani 1 1 d . . .
H28A H 0.5206 0.3706 0.1996 0.253 Uiso 1 1 calc R . .
H28B H 0.4902 0.3758 0.1604 0.253 Uiso 1 1 calc R . .
H28C H 0.4948 0.4203 0.2073 0.253 Uiso 1 1 calc R . .
C29 C 0.5350(3) 0.6310(17) 0.2218(5) 0.172(9) Uani 1 1 d . . .
H29A H 0.5532 0.5936 0.2346 0.258 Uiso 1 1 calc R . .
H29B H 0.5265 0.6314 0.2426 0.258 Uiso 1 1 calc R . .
H29C H 0.5376 0.7071 0.2144 0.258 Uiso 1 1 calc R . .
C30 C 0.4769(3) 0.6366(19) 0.1483(6) 0.198(11) Uani 1 1 d . . .
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H30A H 0.4803 0.7112 0.1405 0.297 Uiso 1 1 calc R . .
H30B H 0.4692 0.6410 0.1700 0.297 Uiso 1 1 calc R . .
H30C H 0.4635 0.5986 0.1225 0.297 Uiso 1 1 calc R . .
C31 C 0.62015(18) 0.5590(8) 0.1205(3) 0.050(2) Uani 1 1 d . . .
C32 C 0.6465(2) 0.5524(11) 0.1553(4) 0.079(4) Uani 1 1 d . . .
H32 H 0.6516 0.4876 0.1726 0.095 Uiso 1 1 calc R . .
C33 C 0.6654(3) 0.6419(14) 0.1649(5) 0.105(5) Uani 1 1 d . . .
H33 H 0.6832 0.6366 0.1887 0.126 Uiso 1 1 calc R . .
C34 C 0.6584(3) 0.7352(12) 0.1406(6) 0.099(5) Uani 1 1 d . . .
H34 H 0.6710 0.7959 0.1483 0.118 Uiso 1 1 calc R . .
C35 C 0.6331(3) 0.7426(11) 0.1046(6) 0.110(5) Uani 1 1 d . . .
H35 H 0.6286 0.8058 0.0864 0.132 Uiso 1 1 calc R . .
C36 C 0.6138(2) 0.6536(9) 0.0953(4) 0.084(4) Uani 1 1 d . . .
H36 H 0.5962 0.6591 0.0712 0.100 Uiso 1 1 calc R . .
C37 C 0.5917(2) 0.3838(8) 0.0569(3) 0.049(2) Uani 1 1 d . . .
C38 C 0.5690(3) 0.3140(9) 0.0335(4) 0.079(3) Uani 1 1 d . . .
H38 H 0.5552 0.3003 0.0440 0.095 Uiso 1 1 calc R . .
C39 C 0.5666(3) 0.2645(11) -0.0050(4) 0.097(4) Uani 1 1 d . . .
H39 H 0.5506 0.2204 -0.0211 0.116 Uiso 1 1 calc R . .
C40 C 0.5866(4) 0.2789(11) -0.0197(4) 0.092(4) Uani 1 1 d . . .
H40 H 0.5850 0.2434 -0.0456 0.111 Uiso 1 1 calc R . .
C41 C 0.6093(3) 0.3443(10) 0.0026(4) 0.081(4) Uani 1 1 d . . .
H41 H 0.6233 0.3534 -0.0080 0.097 Uiso 1 1 calc R . .
C42 C 0.6123(2) 0.3987(8) 0.0410(3) 0.060(3) Uani 1 1 d . . .
H42 H 0.6280 0.4448 0.0560 0.072 Uiso 1 1 calc R . .
Hg2 Hg 0.630624(9) 0.98162(4) -0.035109(16) 0.06836(15) Uani 1 1 d . .
.
S3 S 0.65447(6) 1.0827(3) 0.03652(9) 0.0700(8) Uani 1 1 d . . .
S4 S 0.57648(5) 0.9689(2) -0.06940(11) 0.0746(9) Uani 1 1 d . . .
P3 P 0.65769(5) 1.1158(2) -0.06093(8) 0.0497(6) Uani 1 1 d . . .
P4 P 0.62637(5) 0.7761(2) -0.04578(9) 0.0527(7) Uani 1 1 d . . .
Si3 Si 0.70562(7) 1.1721(3) 0.12643(10) 0.0737(9) Uani 1 1 d . . .
Si4 Si 0.51111(6) 0.8959(3) -0.08639(12) 0.0745(9) Uani 1 1 d . . .
C43 C 0.6841(2) 1.1763(8) -0.0102(3) 0.049(2) Uani 1 1 d . . .
C44 C 0.68219(18) 1.1574(7) 0.0306(3) 0.047(2) Uani 1 1 d . . .
C45 C 0.7043(2) 1.1988(8) 0.0701(3) 0.054(2) Uani 1 1 d . . .
C46 C 0.7257(2) 1.2638(9) 0.0659(3) 0.062(3) Uani 1 1 d . . .
H46 H 0.7399 1.2949 0.0913 0.075 Uiso 1 1 calc R . .
C47 C 0.7268(2) 1.2836(8) 0.0260(4) 0.062(3) Uani 1 1 d . . .
H47 H 0.7412 1.3277 0.0243 0.074 Uiso 1 1 calc R . .
C48 C 0.7062(2) 1.2372(8) -0.0111(3) 0.056(3) Uani 1 1 d . . .
H48 H 0.7074 1.2477 -0.0380 0.067 Uiso 1 1 calc R . .
C49 C 0.7406(3) 1.2295(16) 0.1680(4) 0.135(6) Uani 1 1 d . . .
H49A H 0.7420 1.2173 0.1973 0.202 Uiso 1 1 calc R . .
H49B H 0.7417 1.3088 0.1631 0.202 Uiso 1 1 calc R . .
H49C H 0.7561 1.1917 0.1647 0.202 Uiso 1 1 calc R . .
C50 C 0.7063(4) 1.0172(12) 0.1373(5) 0.128(6) Uani 1 1 d . . .
H50A H 0.7067 1.0049 0.1661 0.191 Uiso 1 1 calc R . .
H50B H 0.7230 0.9844 0.1360 0.191 Uiso 1 1 calc R . .
H50C H 0.6895 0.9827 0.1155 0.191 Uiso 1 1 calc R . .
C51 C 0.6757(3) 1.2454(12) 0.1327(4) 0.097(4) Uani 1 1 d . . .
H51A H 0.6765 1.2305 0.1616 0.145 Uiso 1 1 calc R . .
H51B H 0.6579 1.2186 0.1107 0.145 Uiso 1 1 calc R . .
H51C H 0.6772 1.3250 0.1292 0.145 Uiso 1 1 calc R . .
C52 C 0.6790(2) 1.0708(8) -0.0896(3) 0.052(2) Uani 1 1 d . . .
C53 C 0.6759(2) 1.1113(10) -0.1300(3) 0.074(3) Uani 1 1 d . . .
H53 H 0.6621 1.1654 -0.1441 0.089 Uiso 1 1 calc R . .
C54 C 0.6927(3) 1.0741(13) -0.1497(4) 0.099(4) Uani 1 1 d . . .
H54 H 0.6904 1.1038 -0.1769 0.119 Uiso 1 1 calc R . .
C55 C 0.7127(3) 0.9945(12) -0.1302(5) 0.090(4) Uani 1 1 d . . .
H55 H 0.7237 0.9674 -0.1443 0.108 Uiso 1 1 calc R . .
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C56 C 0.7168(3) 0.9540(11) -0.0899(5) 0.094(4) Uani 1 1 d . . .
H56 H 0.7312 0.9018 -0.0758 0.113 Uiso 1 1 calc R . .
C57 C 0.6996(3) 0.9899(10) -0.0700(4) 0.081(4) Uani 1 1 d . . .
H57 H 0.7019 0.9592 -0.0431 0.098 Uiso 1 1 calc R . .
C58 C 0.6347(2) 1.2269(8) -0.0946(3) 0.053(2) Uani 1 1 d . . .
C59 C 0.6069(2) 1.1969(9) -0.1212(3) 0.065(3) Uani 1 1 d . . .
H59 H 0.6004 1.1245 -0.1200 0.077 Uiso 1 1 calc R . .
C60 C 0.5891(3) 1.2755(13) -0.1497(5) 0.101(4) Uani 1 1 d . . .
H60 H 0.5704 1.2551 -0.1677 0.121 Uiso 1 1 calc R . .
C61 C 0.5979(3) 1.3812(13) -0.1522(5) 0.108(5) Uani 1 1 d . . .
H61 H 0.5856 1.4326 -0.1723 0.130 Uiso 1 1 calc R . .
C62 C 0.6253(3) 1.4115(11) -0.1245(5) 0.105(5) Uani 1 1 d . . .
H62 H 0.6315 1.4851 -0.1248 0.126 Uiso 1 1 calc R . .
C63 C 0.6440(3) 1.3332(9) -0.0960(4) 0.076(3) Uani 1 1 d . . .
H63 H 0.6627 1.3533 -0.0780 0.091 Uiso 1 1 calc R . .
C64 C 0.59219(19) 0.7458(8) -0.0454(3) 0.047(2) Uani 1 1 d . . .
C65 C 0.57067(19) 0.8283(8) -0.0584(3) 0.050(2) Uani 1 1 d . . .
C66 C 0.54281(19) 0.7972(8) -0.0639(3) 0.051(2) Uani 1 1 d . . .
C67 C 0.5381(2) 0.6857(9) -0.0550(3) 0.068(3) Uani 1 1 d . . .
H67 H 0.5198 0.6647 -0.0585 0.082 Uiso 1 1 calc R . .
C68 C 0.5597(2) 0.6049(9) -0.0411(3) 0.065(3) Uani 1 1 d . . .
H68 H 0.5561 0.5315 -0.0350 0.078 Uiso 1 1 calc R . .
C69 C 0.5865(2) 0.6360(8) -0.0365(3) 0.056(3) Uani 1 1 d . . .
H69 H 0.6011 0.5829 -0.0273 0.067 Uiso 1 1 calc R . .
C70 C 0.5053(3) 0.9429(13) -0.1426(4) 0.123(6) Uani 1 1 d . . .
H70A H 0.5032 0.8783 -0.1610 0.185 Uiso 1 1 calc R . .
H70B H 0.5215 0.9865 -0.1409 0.185 Uiso 1 1 calc R . .
H70C H 0.4884 0.9882 -0.1548 0.185 Uiso 1 1 calc R . .
C71 C 0.5150(3) 1.0178(12) -0.0499(5) 0.125(6) Uani 1 1 d . . .
H71A H 0.4985 1.0651 -0.0627 0.187 Uiso 1 1 calc R . .
H71B H 0.5317 1.0600 -0.0466 0.187 Uiso 1 1 calc R . .
H71C H 0.5170 0.9917 -0.0215 0.187 Uiso 1 1 calc R . .
C72 C 0.4792(2) 0.8159(11) -0.0898(5) 0.107(5) Uani 1 1 d . . .
H72A H 0.4762 0.7523 -0.1090 0.160 Uiso 1 1 calc R . .
H72B H 0.4627 0.8640 -0.1012 0.160 Uiso 1 1 calc R . .
H72C H 0.4822 0.7901 -0.0608 0.160 Uiso 1 1 calc R . .
C73 C 0.6220(2) 0.7360(8) -0.1008(3) 0.055(3) Uani 1 1 d . . .
C74 C 0.5961(3) 0.7039(10) -0.1334(4) 0.075(3) Uani 1 1 d . . .
H74 H 0.5801 0.6994 -0.1270 0.090 Uiso 1 1 calc R . .
C75 C 0.5934(3) 0.6780(11) -0.1758(4) 0.093(4) Uani 1 1 d . . .
H75 H 0.5759 0.6557 -0.1975 0.112 Uiso 1 1 calc R . .
C76 C 0.6166(4) 0.6857(13) -0.1850(5) 0.107(5) Uani 1 1 d . . .
H76 H 0.6146 0.6692 -0.2134 0.128 Uiso 1 1 calc R . .
C77 C 0.6422(4) 0.7161(13) -0.1546(5) 0.104(5) Uani 1 1 d . . .
H77 H 0.6578 0.7200 -0.1617 0.124 Uiso 1 1 calc R . .
C78 C 0.6453(3) 0.7424(11) -0.1114(4) 0.087(4) Uani 1 1 d . . .
H78 H 0.6630 0.7641 -0.0901 0.104 Uiso 1 1 calc R . .
C79 C 0.65294(19) 0.6856(9) -0.0063(3) 0.055(2) Uani 1 1 d . . .
C80 C 0.6573(2) 0.5744(10) -0.0142(4) 0.082(3) Uani 1 1 d . . .
H80 H 0.6463 0.5436 -0.0418 0.098 Uiso 1 1 calc R . .
C81 C 0.6772(3) 0.5081(12) 0.0173(5) 0.103(5) Uani 1 1 d . . .
H81 H 0.6792 0.4329 0.0113 0.124 Uiso 1 1 calc R . .
C82 C 0.6938(3) 0.5512(14) 0.0566(5) 0.107(5) Uani 1 1 d . . .
H82 H 0.7077 0.5072 0.0779 0.128 Uiso 1 1 calc R . .
C83 C 0.6901(4) 0.6579(16) 0.0650(5) 0.137(7) Uani 1 1 d . . .
H83 H 0.7014 0.6875 0.0928 0.165 Uiso 1 1 calc R . .
C84 C 0.6701(3) 0.7263(12) 0.0339(4) 0.101(4) Uani 1 1 d . . .
H84 H 0.6685 0.8012 0.0407 0.121 Uiso 1 1 calc R . .
Cl1S Cl 0.62243(18) 1.2618(7) -0.2445(3) 0.262(4) Uani 1 1 d . . .
Cl2S Cl 0.6723(2) 1.3774(7) -0.2060(3) 0.304(5) Uani 1 1 d . . .
C1S C 0.6384(5) 1.3892(15) -0.2355(8) 0.196(10) Uani 1 1 d . . .
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H1S1 H 0.6351 1.4240 -0.2636 0.235 Uiso 1 1 calc R . .
H1S2 H 0.6301 1.4373 -0.2204 0.235 Uiso 1 1 calc R . .
Cl3A Cl 0.7166(6) 0.449(3) 0.4484(13) 0.262(18) Uani 0.30 1 d PD A 1
Cl4A Cl 0.7662(5) 0.3622(16) 0.4579(5) 0.178(9) Uani 0.30 1 d PD A 1
C2SA C 0.7483(5) 0.4863(18) 0.4484(9) 0.141(17) Uani 0.30 1 d PD A 1
H2S1 H 0.7583 0.5404 0.4716 0.169 Uiso 0.30 1 calc PR A 1
H2S2 H 0.7458 0.5180 0.4202 0.169 Uiso 0.30 1 calc PR A 1
Cl3B Cl 0.7367(9) 0.367(3) 0.4646(10) 0.24(2) Uani 0.20 1 d PD B 2
Cl4B Cl 0.7175(7) 0.543(2) 0.4126(8) 0.177(13) Uani 0.20 1 d PD B 2
C2SB C 0.7483(5) 0.4863(18) 0.4484(9) 0.141(17) Uani 0.20 1 d PD B 2
H2S3 H 0.7582 0.5361 0.4732 0.169 Uiso 0.20 1 calc PR B 2
H2S4 H 0.7609 0.4684 0.4342 0.169 Uiso 0.20 1 calc PR B 2

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S2 0.0715(19) 0.110(2) 0.0504(16) 0.0019(16) 0.0283(14) 0.0294(17)
P1 0.0390(14) 0.0505(15) 0.0502(15) -0.0050(12) 0.0131(12) -0.0061(12)
P2 0.0404(14) 0.0494(14) 0.0458(14) 0.0004(12) 0.0165(11) -0.0003(11)
Si1 0.0422(16) 0.076(2) 0.0524(17) -0.0071(15) 0.0094(13) -0.0080(14)
Si2 0.068(2) 0.188(5) 0.083(3) -0.024(3) 0.039(2) 0.028(3)
C1 0.044(5) 0.057(6) 0.035(5) 0.003(4) 0.019(4) -0.005(5)
C2 0.043(5) 0.058(6) 0.034(5) -0.001(5) 0.017(4) 0.002(5)
C3 0.045(6) 0.058(6) 0.036(5) 0.001(4) 0.013(4) 0.003(5)
C4 0.043(6) 0.073(7) 0.044(6) -0.003(5) 0.011(5) 0.003(5)
C5 0.047(6) 0.070(7) 0.061(7) -0.005(6) 0.021(5) 0.017(5)
C6 0.055(7) 0.051(6) 0.061(6) -0.010(5) 0.018(5) -0.009(5)
C7 0.070(8) 0.109(10) 0.062(7) -0.017(7) 0.012(6) -0.014(7)
C8 0.034(6) 0.118(10) 0.090(9) -0.014(8) 0.002(6) -0.008(6)
C9 0.065(7) 0.086(9) 0.086(8) 0.008(7) 0.024(6) -0.018(6)
C10 0.036(5) 0.056(6) 0.058(7) -0.016(5) 0.002(5) -0.001(5)
C11 0.070(8) 0.078(8) 0.059(8) -0.014(7) 0.002(6) 0.012(6)
C12 0.092(10) 0.102(11) 0.060(8) -0.016(8) -0.001(7) 0.022(9)
C13 0.069(10) 0.091(12) 0.124(14) -0.048(11) -0.016(10) 0.022(9)
C14 0.068(9) 0.070(9) 0.154(15) -0.043(11) 0.013(11) -0.014(7)
C15 0.075(8) 0.073(8) 0.093(9) -0.023(7) 0.034(7) -0.017(7)
C16 0.048(6) 0.063(7) 0.059(7) -0.007(5) 0.020(5) -0.009(5)
C17 0.088(9) 0.108(10) 0.095(9) 0.050(8) 0.058(8) 0.033(8)
C18 0.119(13) 0.171(16) 0.136(14) 0.089(12) 0.078(11) 0.066(12)
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C22 0.039(5) 0.045(6) 0.049(6) 0.000(4) 0.012(5) 0.002(4)
C23 0.039(5) 0.059(6) 0.048(6) -0.011(5) 0.014(4) 0.002(4)
C24 0.049(6) 0.070(7) 0.074(8) -0.011(6) 0.032(6) 0.004(5)
C25 0.040(6) 0.081(8) 0.079(8) -0.010(7) 0.009(6) 0.010(6)
C26 0.061(7) 0.083(8) 0.059(7) 0.010(6) 0.013(6) 0.008(6)
C27 0.053(6) 0.066(7) 0.056(7) -0.007(5) 0.019(5) -0.002(5)
C28 0.159(17) 0.24(2) 0.157(17) 0.005(16) 0.117(14) -0.028(16)
C29 0.140(15) 0.26(2) 0.129(14) -0.095(15) 0.063(12) 0.024(15)
C30 0.109(13) 0.34(3) 0.155(16) -0.021(18) 0.068(12) 0.105(16)
C31 0.035(5) 0.057(6) 0.060(6) -0.011(5) 0.021(5) -0.004(4)
C32 0.056(7) 0.109(10) 0.061(7) 0.018(7) 0.013(6) -0.026(7)
C33 0.055(8) 0.146(14) 0.097(10) -0.011(10) 0.014(7) -0.045(9)
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C34 0.093(11) 0.066(9) 0.151(14) -0.026(9) 0.065(11) -0.032(8)
C35 0.066(9) 0.059(8) 0.194(16) 0.016(9) 0.043(10) 0.004(7)
C36 0.052(7) 0.048(7) 0.133(11) 0.010(7) 0.021(7) -0.008(5)
C37 0.053(6) 0.047(6) 0.045(6) 0.008(5) 0.018(5) 0.009(5)
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C40 0.141(14) 0.068(9) 0.073(9) -0.012(7) 0.049(10) 0.012(9)
C41 0.109(10) 0.074(8) 0.087(9) 0.007(7) 0.067(8) 0.015(8)
C42 0.075(7) 0.051(6) 0.062(7) -0.009(5) 0.035(6) 0.005(5)
Hg2 0.0584(3) 0.0616(3) 0.0871(3) -0.0072(2) 0.0324(2) -0.0139(2)
S3 0.0713(19) 0.088(2) 0.0637(18) -0.0085(15) 0.0407(15) -0.0223(16)
S4 0.0441(15) 0.0521(16) 0.119(3) 0.0134(16) 0.0248(16) -0.0009(13)
P3 0.0484(15) 0.0533(15) 0.0494(15) -0.0023(12) 0.0223(12) -0.0050(12)
P4 0.0461(15) 0.0495(15) 0.0641(17) 0.0019(13) 0.0244(13) 0.0013(12)
Si3 0.074(2) 0.098(3) 0.0491(17) 0.0069(17) 0.0262(16) 0.0135(19)
Si4 0.0399(16) 0.073(2) 0.097(2) 0.0031(19) 0.0151(16) -0.0033(15)
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C46 0.053(6) 0.079(7) 0.050(6) -0.008(6) 0.015(5) 0.003(6)
C47 0.048(6) 0.062(7) 0.079(8) -0.005(6) 0.031(6) -0.014(5)
C48 0.049(6) 0.057(6) 0.060(6) -0.004(5) 0.021(5) -0.012(5)
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C52 0.056(6) 0.054(6) 0.044(6) -0.004(5) 0.018(5) 0.000(5)
C53 0.074(8) 0.093(9) 0.055(7) 0.013(6) 0.026(6) 0.015(7)
C54 0.110(11) 0.138(13) 0.079(9) -0.002(9) 0.068(9) 0.012(10)
C55 0.088(9) 0.115(11) 0.083(10) -0.025(8) 0.052(8) 0.010(8)
C56 0.103(10) 0.095(10) 0.096(10) 0.004(8) 0.053(9) 0.043(8)
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C59 0.041(6) 0.071(7) 0.072(7) -0.005(6) 0.014(5) 0.012(6)
C60 0.065(8) 0.102(11) 0.119(12) -0.007(10) 0.021(8) 0.017(8)
C61 0.096(11) 0.093(11) 0.092(10) 0.001(9) -0.003(9) 0.030(9)
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C65 0.047(6) 0.048(6) 0.052(6) 0.001(5) 0.018(5) 0.002(5)
C66 0.042(5) 0.060(6) 0.046(6) 0.005(5) 0.015(4) -0.007(5)
C67 0.060(7) 0.076(8) 0.071(7) -0.001(6) 0.029(6) -0.020(6)
C68 0.067(7) 0.056(7) 0.071(7) 0.013(6) 0.027(6) -0.007(6)
C69 0.050(6) 0.056(6) 0.063(7) 0.009(5) 0.025(5) 0.005(5)
C70 0.072(9) 0.141(13) 0.112(11) 0.054(10) -0.005(8) -0.008(9)
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C73 0.064(7) 0.049(6) 0.065(7) 0.021(5) 0.040(6) 0.007(5)
C74 0.073(8) 0.089(9) 0.058(7) 0.006(6) 0.022(6) 0.007(7)
C75 0.121(12) 0.102(10) 0.058(8) 0.011(7) 0.039(8) 0.009(9)
C76 0.154(15) 0.110(12) 0.076(10) 0.018(9) 0.067(11) 0.016(12)
C77 0.126(13) 0.125(13) 0.100(11) 0.002(10) 0.085(11) -0.003(10)
C78 0.090(9) 0.095(9) 0.090(9) -0.003(8) 0.052(8) -0.005(7)
C79 0.036(5) 0.066(7) 0.061(7) 0.000(6) 0.019(5) 0.004(5)
C80 0.077(8) 0.077(8) 0.077(8) -0.011(7) 0.018(7) 0.013(7)
C81 0.090(10) 0.091(10) 0.112(12) 0.010(9) 0.026(9) 0.047(8)
C82 0.093(11) 0.125(13) 0.081(10) 0.006(10) 0.014(9) 0.044(10)
C83 0.146(15) 0.148(16) 0.070(10) -0.013(10) -0.002(9) 0.057(13)
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Cl1S 0.248(8) 0.179(7) 0.317(10) -0.022(7) 0.077(7) 0.017(6)
Cl2S 0.237(9) 0.223(8) 0.386(13) 0.141(9) 0.064(9) -0.023(7)
C1S 0.23(3) 0.085(13) 0.26(3) 0.058(15) 0.09(2) 0.058(15)

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C13A 0.20(2) 0.26(3) 0.43(5) -0.19(3) 0.23(3) -0.07(2)
C14A 0.198(19) 0.168(16) 0.093(10) -0.061(10) -0.015(11) 0.044(14)
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C14B 0.27(4) 0.12(2) 0.23(3) -0.08(2) 0.18(3) -0.02(2)
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;
 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
;

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S2 C23 1.759(9) . ?
P1 C10 1.801(9) . ?
P1 C1 1.801(9) . ?
P1 C16 1.802(10) . ?
P2 C22 1.801(9) . ?
P2 C37 1.805(9) . ?
P2 C31 1.805(9) . ?
Si1 C7 1.852(11) . ?
Si1 C9 1.854(11) . ?
Si1 C8 1.864(10) . ?
Si1 C3 1.891(9) . ?
Si2 C29 1.833(15) . ?
Si2 C28 1.862(19) . ?
Si2 C30 1.874(15) . ?
Si2 C24 1.888(10) . ?
C1 C6 1.386(12) . ?
C1 C2 1.416(12) . ?
C2 C3 1.414(12) . ?
C3 C4 1.380(12) . ?
C4 C5 1.366(13) . ?
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C13 C14 1.35(2) . ?
C14 C15 1.402(17) . ?
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C23 C24 1.426(12) . ?
C24 C25 1.388(14) . ?
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C31 C32 1.369(13) . ?
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C37 C42 1.377(13) . ?
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C39 C40 1.324(18) . ?
C40 C41 1.339(17) . ?
C41 C42 1.384(14) . ?
Hg2 P4 2.462(3) . ?
Hg2 S3 2.489(3) . ?
Hg2 P3 2.492(2) . ?
Hg2 S4 2.537(3) . ?
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S4 C65 1.761(9) . ?
P3 C52 1.807(10) . ?
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Si4 C66 1.891(10) . ?
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C81 C82 1.331(17) . ?
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Cl1S C1S 1.69(2) . ?
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P2 Hg1 S1 123.53(8) . . ?
S2 Hg1 S1 111.27(9) . . ?
C2 S1 Hg1 101.0(3) . . ?
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P4 Hg2 P3 127.76(9) . . ?
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Compound (7*)

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 'x, -y-1/2, z-1/2'

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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
```

```
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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S1 S 0.9103(10) 0.6124(15) 0.5307(4) 0.036(4) Uani 1 1 d . . .
P1 P 0.7132(9) 0.6440(13) 0.4575(4) 0.018(3) Uani 1 1 d U . .
O1 O 0.799(2) 0.726(4) 0.4388(9) 0.030(8) Uiso 1 1 d . . .
C1 C 0.706(4) 0.715(6) 0.5051(14) 0.033(13) Uiso 1 1 d . . .
C2 C 0.782(3) 0.707(5) 0.5355(12) 0.017(11) Uiso 1 1 d . . .
C3 C 0.776(4) 0.776(6) 0.5721(15) 0.039(14) Uiso 1 1 d . . .
H3 H 0.8337 0.7785 0.5912 0.046 Uiso 1 1 calc R . .
C4 C 0.675(4) 0.843(6) 0.5772(16) 0.040(14) Uiso 1 1 d . . .
H4 H 0.6648 0.8834 0.6014 0.048 Uiso 1 1 calc R . .
C5 C 0.596(4) 0.851(6) 0.5501(15) 0.044(15) Uiso 1 1 d . . .
H5 H 0.5318 0.8984 0.5542 0.053 Uiso 1 1 calc R . .
C6 C 0.612(5) 0.784(6) 0.5136(16) 0.049(16) Uiso 1 1 d . . .
H6 H 0.5558 0.7865 0.4941 0.059 Uiso 1 1 calc R . .
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C7 C 0.589(4) 0.669(5) 0.4305(13) 0.026(12) Uiso 1 1 d . . .
C8 C 0.575(4) 0.800(6) 0.4035(14) 0.032(13) Uiso 1 1 d . . .
H8 H 0.6294 0.8719 0.4018 0.039 Uiso 1 1 calc R . .
C9 C 0.481(4) 0.811(6) 0.3811(15) 0.041(14) Uiso 1 1 d . . .
H9 H 0.4759 0.8889 0.3623 0.049 Uiso 1 1 calc R . .
C10 C 0.395(5) 0.722(7) 0.3834(16) 0.050(16) Uiso 1 1 d . . .
H10 H 0.3318 0.7388 0.3680 0.060 Uiso 1 1 calc R . .
C11 C 0.407(5) 0.602(7) 0.4100(17) 0.056(17) Uiso 1 1 d . . .
H11 H 0.3482 0.5417 0.4139 0.067 Uiso 1 1 calc R . .
C12 C 0.502(4) 0.570(6) 0.4309(15) 0.044(15) Uiso 1 1 d . . .
H12 H 0.5089 0.4800 0.4458 0.053 Uiso 1 1 calc R . .
C13 C 0.740(4) 0.434(6) 0.4613(14) 0.032(13) Uiso 1 1 d . . .
C14 C 0.787(4) 0.368(6) 0.4347(15) 0.033(13) Uiso 1 1 d . . .
H14 H 0.8079 0.4297 0.4149 0.040 Uiso 1 1 calc R . .
C15 C 0.809(6) 0.202(9) 0.434(2) 0.09(2) Uiso 1 1 d . . .
H15 H 0.8531 0.1556 0.4176 0.105 Uiso 1 1 calc R . .
C16 C 0.756(5) 0.124(8) 0.4609(18) 0.064(19) Uiso 1 1 d . . .
H16 H 0.7584 0.0159 0.4595 0.076 Uiso 1 1 calc R . .
C17 C 0.703(5) 0.179(8) 0.4875(19) 0.064(19) Uiso 1 1 d . . .
H17 H 0.6766 0.1143 0.5057 0.077 Uiso 1 1 calc R . .
C18 C 0.685(4) 0.349(6) 0.4882(15) 0.039(14) Uiso 1 1 d . . .
H18 H 0.6423 0.3964 0.5050 0.047 Uiso 1 1 calc R . .
C19 C 1.066(4) 0.895(6) 0.4421(14) 0.035(13) Uiso 1 1 d . . .
H19A H 1.0181 0.9774 0.4319 0.042 Uiso 1 1 calc R . .
H19B H 1.1279 0.9442 0.4557 0.042 Uiso 1 1 calc R . .
C20 C 1.098(7) 0.809(11) 0.411(2) 0.12(3) Uiso 1 1 d . . .
H20A H 1.1315 0.8767 0.3938 0.182 Uiso 1 1 calc R . .
H20B H 1.0367 0.7616 0.3968 0.182 Uiso 1 1 calc R . .
H20C H 1.1470 0.7296 0.4204 0.182 Uiso 1 1 calc R . .
Hg2 Hg 0.51031(17) 0.5313(2) 0.30338(7) 0.0407(7) Uani 1 1 d . . .
S2 S 0.4355(11) 0.7128(15) 0.2563(4) 0.043(4) Uani 1 1 d . . .
P2 P 0.2229(10) 0.5307(14) 0.2828(4) 0.029(3) Uani 1 1 d . . .
O2 O 0.311(3) 0.441(4) 0.3057(9) 0.038(9) Uiso 1 1 d . . .
C21 C 0.240(3) 0.741(5) 0.2885(12) 0.019(11) Uiso 1 1 d . . .
C22 C 0.332(4) 0.805(6) 0.2788(15) 0.041(14) Uiso 1 1 d . . .
C23 C 0.351(5) 0.971(8) 0.2870(17) 0.064(18) Uiso 1 1 d . . .
H23 H 0.4135 1.0197 0.2821 0.077 Uiso 1 1 calc R . .
C24 C 0.266(5) 1.056(8) 0.3033(17) 0.057(17) Uiso 1 1 d . . .
H24 H 0.2755 1.1616 0.3083 0.069 Uiso 1 1 calc R . .
C25 C 0.177(5) 0.989(7) 0.3112(17) 0.060(18) Uiso 1 1 d . . .
H25 H 0.1234 1.0475 0.3206 0.071 Uiso 1 1 calc R . .
C26 C 0.163(4) 0.822(6) 0.3049(15) 0.039(14) Uiso 1 1 d . . .
H26 H 0.1033 0.7709 0.3120 0.046 Uiso 1 1 calc R . .
C27 C 0.095(4) 0.494(6) 0.3016(14) 0.033(13) Uiso 1 1 d . . .
C28 C 0.102(4) 0.452(6) 0.3398(14) 0.034(13) Uiso 1 1 d . . .
H28 H 0.1683 0.4342 0.3535 0.040 Uiso 1 1 calc R . .
C29 C 0.006(5) 0.438(7) 0.3583(19) 0.059(17) Uiso 1 1 d . . .
H29 H 0.0081 0.4179 0.3846 0.070 Uiso 1 1 calc R . .
C30 C -0.085(5) 0.454(8) 0.3359(18) 0.066(19) Uiso 1 1 d . . .
H30 H -0.1476 0.4435 0.3473 0.079 Uiso 1 1 calc R . .
C31 C -0.092(5) 0.486(7) 0.2949(17) 0.056(17) Uiso 1 1 d . . .
H31 H -0.1582 0.4925 0.2804 0.067 Uiso 1 1 calc R . .
C32 C -0.001(4) 0.506(6) 0.2777(16) 0.045(15) Uiso 1 1 d . . .
H32 H -0.0022 0.5271 0.2514 0.054 Uiso 1 1 calc R . .
C33 C 0.212(4) 0.486(5) 0.2330(13) 0.028(12) Uiso 1 1 d . . .
C34 C 0.148(5) 0.573(8) 0.2074(19) 0.067(19) Uiso 1 1 d . . .
H34 H 0.1121 0.6573 0.2165 0.081 Uiso 1 1 calc R . .
C35 C 0.135(5) 0.538(8) 0.1665(19) 0.067(19) Uiso 1 1 d . . .
H35 H 0.0945 0.6010 0.1490 0.081 Uiso 1 1 calc R . .
C36 C 0.189(4) 0.400(6) 0.1539(16) 0.042(15) Uiso 1 1 d . . .
H36 H 0.1814 0.3702 0.1280 0.050 Uiso 1 1 calc R . .
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C37 C 0.251(4) 0.314(6) 0.1809(15) 0.040(14) Uiso 1 1 d . . .
H37 H 0.2888 0.2294 0.1729 0.048 Uiso 1 1 calc R . .
C38 C 0.259(4) 0.351(6) 0.2191(16) 0.045(15) Uiso 1 1 d . . .
H38 H 0.2964 0.2851 0.2368 0.054 Uiso 1 1 calc R . .
C39 C 0.596(4) 0.401(6) 0.3408(15) 0.036(14) Uiso 1 1 d . . .
H39A H 0.6619 0.3765 0.3300 0.043 Uiso 1 1 calc R . .
H39B H 0.6149 0.4626 0.3639 0.043 Uiso 1 1 calc R . .
C40 C 0.549(5) 0.248(8) 0.3534(19) 0.08(2) Uiso 1 1 d . . .
H40A H 0.5990 0.1966 0.3716 0.113 Uiso 1 1 calc R . .
H40B H 0.5318 0.1831 0.3312 0.113 Uiso 1 1 calc R . .
H40C H 0.4849 0.2695 0.3653 0.113 Uiso 1 1 calc R . .

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S1 0.016(7) 0.036(8) 0.060(10) 0.010(7) 0.024(7) -0.001(6)
P1 0.013(6) 0.010(6) 0.032(7) 0.002(5) 0.012(5) -0.006(5)
Hg2 0.0346(13) 0.0265(12) 0.0623(16) -0.0009(12) 0.0111(11) -
0.0009(10)
S2 0.036(8) 0.027(8) 0.071(11) 0.015(7) 0.031(8) 0.000(6)
P2 0.032(8) 0.006(6) 0.050(9) -0.002(7) 0.010(7) 0.005(6)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Hg1 S1 2.378(13) . ?
Hg1 O1 2.71(3) . ?
S1 C2 1.84(4) . ?
P1 O1 1.50(3) . ?
P1 C7 1.76(5) . ?
P1 C1 1.78(5) . ?
P1 C13 1.84(5) . ?
C1 C2 1.35(6) . ?
C1 C6 1.39(7) . ?
C2 C3 1.41(6) . ?
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C4 C5 1.30(7) . ?
C5 C6 1.43(7) . ?
C7 C12 1.39(7) . ?
C7 C8 1.46(7) . ?
C8 C9 1.35(7) . ?
C9 C10 1.34(7) . ?
C10 C11 1.38(8) . ?
C11 C12 1.36(7) . ?
C13 C14 1.28(7) . ?
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Hg2 S2 2.386(14) . ?
Hg2 O2 2.65(3) . ?
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P2 O2 1.51(3) . ?
P2 C33 1.76(5) . ?
P2 C27 1.83(5) . ?
P2 C21 1.83(5) . ?
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C22 C23 1.48(8) . ?
C23 C24 1.46(8) . ?
C24 C25 1.32(8) . ?
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C27 C28 1.37(6) . ?
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S1 Hg1 O1 86.5(7) . . ?
C2 S1 Hg1 104.6(14) . . ?
O1 P1 C7 111(2) . . ?
O1 P1 C1 110(2) . . ?
C7 P1 C1 109(2) . . ?
O1 P1 C13 111(2) . . ?
C7 P1 C13 108(2) . . ?
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C1 P1 C13 107(2) . . ?
P1 O1 Hg1 115.9(16) . . ?
C2 C1 C6 114(5) . . ?
C2 C1 P1 128(4) . . ?
C6 C1 P1 118(4) . . ?
C1 C2 C3 126(4) . . ?
C1 C2 S1 121(4) . . ?
C3 C2 S1 113(3) . . ?
C2 C3 C4 114(5) . . ?
C5 C4 C3 124(5) . . ?
C4 C5 C6 117(5) . . ?
C1 C6 C5 125(5) . . ?
C12 C7 C8 116(4) . . ?
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C10 C9 C8 126(6) . . ?
C9 C10 C11 116(6) . . ?
C12 C11 C10 122(6) . . ?
C11 C12 C7 121(5) . . ?
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C14 C13 P1 119(4) . . ?
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C13 C18 C17 114(5) . . ?
C20 C19 Hg1 114(5) . . ?
C39 Hg2 S2 169.6(15) . . ?
C39 Hg2 O2 105.9(16) . . ?
S2 Hg2 O2 84.5(8) . . ?
C22 S2 Hg2 104.2(18) . . ?
O2 P2 C33 112(2) . . ?
O2 P2 C27 111(2) . . ?
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O2 P2 C21 112(2) . . ?
C33 P2 C21 109(2) . . ?
C27 P2 C21 103(2) . . ?
P2 O2 Hg2 119.0(18) . . ?
C22 C21 C26 124(5) . . ?
C22 C21 P2 118(4) . . ?
C26 C21 P2 118(4) . . ?
C21 C22 C23 118(5) . . ?
C21 C22 S2 128(4) . . ?
C23 C22 S2 114(4) . . ?
C24 C23 C22 117(6) . . ?
C25 C24 C23 122(6) . . ?
C24 C25 C26 119(6) . . ?
C21 C26 C25 119(5) . . ?
C28 C27 C32 124(5) . . ?
C28 C27 P2 115(4) . . ?
C32 C27 P2 121(4) . . ?
C27 C28 C29 119(5) . . ?
C30 C29 C28 117(6) . . ?
C29 C30 C31 124(6) . . ?
C32 C31 C30 119(6) . . ?
C31 C32 C27 117(5) . . ?
C34 C33 C38 118(5) . . ?
C34 C33 P2 120(4) . . ?
C38 C33 P2 122(4) . . ?
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C34 C35 C36 117(6) . . ?
C37 C36 C35 119(5) . . ?
C38 C37 C36 121(5) . . ?
C37 C38 C33 122(5) . . ?
C40 C39 Hg2 118(4) . . ?

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Compound (8)

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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
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 'Si'  'Si'   0.0817   0.0704
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 'P'  'P'   0.1023   0.0942
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 '-x, -y, -z'

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_cell_angle_beta                  101.184(3)
_cell_angle_gamma                 91.568(3)
_cell_volume                      1303.3(4)
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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
```

```
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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S1 S 0.37951(11) 0.92296(10) 0.87784(8) 0.0527(2) Uani 1 1 d . . .
P1 P 0.39688(10) 1.13069(9) 0.71847(9) 0.0449(2) Uani 1 1 d . . .
Si1 Si 0.19368(12) 0.66914(11) 0.77512(10) 0.0538(3) Uani 1 1 d . . .
O1 O 0.5432(3) 1.1179(3) 0.7639(3) 0.0585(7) Uani 1 1 d . . .
C1 C 0.2864(4) 0.9021(3) 0.7331(3) 0.0415(8) Uani 1 1 d . . .
C2 C 0.2941(4) 0.9900(3) 0.6635(3) 0.0441(8) Uani 1 1 d . . .
C3 C 0.2164(5) 0.9697(4) 0.5519(4) 0.0561(10) Uani 1 1 d . . .
H3 H 0.2220 1.0266 0.5049 0.067 Uiso 1 1 calc R . .
C4 C 0.1318(5) 0.8674(4) 0.5100(4) 0.0673(13) Uani 1 1 d . . .
H4 H 0.0796 0.8559 0.4355 0.081 Uiso 1 1 calc R . .
C5 C 0.1241(5) 0.7824(4) 0.5776(4) 0.0576(11) Uani 1 1 d . . .
H5 H 0.0665 0.7132 0.5476 0.069 Uiso 1 1 calc R . .
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C6 C 0.2008(4) 0.7957(3) 0.6916(3) 0.0458(8) Uani 1 1 d . . .
C7 C 0.1478(6) 0.7180(5) 0.9189(5) 0.0900(17) Uani 1 1 d . . .
H7A H 0.1457 0.6495 0.9568 0.135 Uiso 1 1 calc R . .
H7B H 0.0598 0.7508 0.9085 0.135 Uiso 1 1 calc R . .
H7C H 0.2144 0.7788 0.9653 0.135 Uiso 1 1 calc R . .
C8 C 0.0584(6) 0.5526(5) 0.6892(5) 0.0829(16) Uani 1 1 d . . .
H8A H 0.0785 0.5251 0.6143 0.124 Uiso 1 1 calc R . .
H8B H -0.0284 0.5877 0.6807 0.124 Uiso 1 1 calc R . .
H8C H 0.0558 0.4852 0.7284 0.124 Uiso 1 1 calc R . .
C9 C 0.3600(5) 0.5981(4) 0.7883(4) 0.0676(12) Uani 1 1 d . . .
H9A H 0.3805 0.5748 0.7130 0.101 Uiso 1 1 calc R . .
H9B H 0.3551 0.5278 0.8232 0.101 Uiso 1 1 calc R . .
H9C H 0.4301 0.6552 0.8355 0.101 Uiso 1 1 calc R . .
C10 C 0.3109(4) 1.2172(3) 0.8214(3) 0.0462(9) Uani 1 1 d . . .
C11 C 0.3872(5) 1.2978(4) 0.9135(4) 0.0570(10) Uani 1 1 d . . .
H11 H 0.4818 1.3029 0.9250 0.068 Uiso 1 1 calc R . .
C12 C 0.3216(6) 1.3706(4) 0.9884(4) 0.0684(12) Uani 1 1 d . . .
H12 H 0.3721 1.4256 1.0500 0.082 Uiso 1 1 calc R . .
C13 C 0.1826(6) 1.3620(5) 0.9722(4) 0.0689(13) Uani 1 1 d . . .
H13 H 0.1394 1.4122 1.0222 0.083 Uiso 1 1 calc R . .
C14 C 0.1066(5) 1.2805(5) 0.8834(4) 0.0683(12) Uani 1 1 d . . .
H14 H 0.0123 1.2739 0.8741 0.082 Uiso 1 1 calc R . .
C15 C 0.1703(5) 1.2084(4) 0.8082(4) 0.0604(11) Uani 1 1 d . . .
H15 H 0.1186 1.1529 0.7476 0.073 Uiso 1 1 calc R . .
C16 C 0.3822(4) 1.2114(3) 0.5986(3) 0.0482(9) Uani 1 1 d . . .
C17 C 0.2927(5) 1.2989(4) 0.5793(4) 0.0630(11) Uani 1 1 d . . .
H17 H 0.2294 1.3159 0.6263 0.076 Uiso 1 1 calc R . .
C18 C 0.2954(6) 1.3627(5) 0.4905(5) 0.0787(15) Uani 1 1 d . . .
H18 H 0.2343 1.4223 0.4784 0.094 Uiso 1 1 calc R . .
C19 C 0.3874(6) 1.3381(5) 0.4207(4) 0.0777(15) Uani 1 1 d . . .
H19 H 0.3894 1.3812 0.3614 0.093 Uiso 1 1 calc R . .
C20 C 0.4765(6) 1.2499(5) 0.4382(4) 0.0769(14) Uani 1 1 d . . .
H20 H 0.5388 1.2328 0.3903 0.092 Uiso 1 1 calc R . .
C21 C 0.4747(5) 1.1864(4) 0.5261(4) 0.0621(11) Uani 1 1 d . . .
H21 H 0.5355 1.1265 0.5372 0.075 Uiso 1 1 calc R . .
C22 C 0.8181(6) 0.9132(8) 0.8611(6) 0.110(2) Uani 1 1 d . . .
H22A H 0.8700 0.9551 0.9350 0.132 Uiso 1 1 calc R . .
H22B H 0.8385 0.8286 0.8541 0.132 Uiso 1 1 calc R . .
C23 C 0.8660(9) 0.9610(9) 0.7722(9) 0.146(4) Uani 1 1 d . . .
H23A H 0.9620 0.9514 0.7797 0.219 Uiso 1 1 calc R . .
H23B H 0.8494 1.0455 0.7789 0.219 Uiso 1 1 calc R . .
H23C H 0.8189 0.9183 0.6981 0.219 Uiso 1 1 calc R . .
O1S O 0.7568(7) 1.2884(9) 0.7798(8) 0.230(5) Uani 1 1 d . . .
H1S H 0.7112 1.2282 0.7414 0.346 Uiso 1 1 calc R . .
C1S C 0.7246(10) 1.3792(7) 0.7345(9) 0.139(3) Uani 1 1 d . . .
H1S1 H 0.6408 1.4068 0.7538 0.208 Uiso 1 1 calc R . .
H1S2 H 0.7133 1.3572 0.6522 0.208 Uiso 1 1 calc R . .
H1S3 H 0.7952 1.4427 0.7630 0.208 Uiso 1 1 calc R . .

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0.01360(8)
S1 0.0543(6) 0.0649(6) 0.0373(5) 0.0109(4) 0.0048(4) -0.0016(5)
P1 0.0413(5) 0.0456(5) 0.0489(5) 0.0125(4) 0.0089(4) 0.0019(4)
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Si1 0.0484(7) 0.0566(7) 0.0610(7) 0.0208(5) 0.0138(5) -0.0005(5)
O1 0.0450(16) 0.0586(17) 0.0737(19) 0.0230(14) 0.0069(14) 0.0029(13)
C1 0.038(2) 0.049(2) 0.0380(18) 0.0072(15) 0.0072(15) 0.0046(16)
C2 0.042(2) 0.049(2) 0.0435(19) 0.0101(16) 0.0110(16) 0.0072(16)
C3 0.063(3) 0.056(2) 0.050(2) 0.0185(18) 0.0051(19) 0.000(2)
C4 0.075(3) 0.069(3) 0.048(2) 0.011(2) -0.012(2) -0.007(2)
C5 0.055(3) 0.057(2) 0.054(2) 0.0103(19) -0.0033(19) -0.011(2)
C6 0.038(2) 0.051(2) 0.048(2) 0.0101(16) 0.0086(16) 0.0032(17)
C7 0.100(5) 0.102(4) 0.089(4) 0.039(3) 0.050(3) 0.011(3)
C8 0.069(3) 0.070(3) 0.109(4) 0.035(3) 0.003(3) -0.018(3)
C9 0.063(3) 0.057(3) 0.083(3) 0.022(2) 0.008(2) 0.007(2)
C10 0.049(2) 0.048(2) 0.045(2) 0.0166(16) 0.0089(17) 0.0008(17)
C11 0.051(3) 0.058(2) 0.057(2) 0.0076(19) 0.0039(19) -0.001(2)
C12 0.079(4) 0.064(3) 0.055(3) 0.000(2) 0.009(2) 0.003(2)
C13 0.078(4) 0.076(3) 0.058(3) 0.012(2) 0.026(2) 0.019(3)
C14 0.055(3) 0.089(3) 0.066(3) 0.017(3) 0.024(2) 0.006(3)
C15 0.049(3) 0.071(3) 0.060(3) 0.009(2) 0.012(2) -0.005(2)
C16 0.047(2) 0.047(2) 0.054(2) 0.0131(17) 0.0138(18) -0.0006(18)
C17 0.067(3) 0.070(3) 0.063(3) 0.028(2) 0.025(2) 0.017(2)
C18 0.094(4) 0.080(3) 0.076(3) 0.040(3) 0.025(3) 0.032(3)
C19 0.100(4) 0.083(3) 0.062(3) 0.032(3) 0.029(3) 0.009(3)
C20 0.087(4) 0.087(4) 0.069(3) 0.021(3) 0.041(3) 0.009(3)
C21 0.068(3) 0.060(3) 0.069(3) 0.020(2) 0.029(2) 0.015(2)
C22 0.063(4) 0.175(7) 0.108(5) 0.054(5) 0.023(3) 0.050(4)
C23 0.099(6) 0.171(8) 0.210(10) 0.091(7) 0.078(6) 0.027(5)
O1S 0.126(5) 0.295(10) 0.267(9) 0.202(8) -0.085(5) -0.111(6)
C1S 0.149(8) 0.102(5) 0.153(7) 0.014(5) 0.014(6) -0.051(5)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Hg1 S1 2.3739(12) . ?
S1 C1 1.779(4) . ?
P1 O1 1.483(3) . ?
P1 C10 1.805(4) . ?
P1 C2 1.810(4) . ?
P1 C16 1.813(4) . ?
Si1 C9 1.859(5) . ?
Si1 C7 1.867(5) . ?
Si1 C8 1.874(5) . ?
Si1 C6 1.883(4) . ?
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C1 C2 1.409(5) . ?
C2 C3 1.390(5) . ?
C3 C4 1.368(6) . ?
C4 C5 1.365(7) . ?
C5 C6 1.415(5) . ?
C10 C11 1.384(5) . ?
C10 C15 1.388(6) . ?
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C12 C13 1.367(7) . ?
C13 C14 1.365(7) . ?
C14 C15 1.370(6) . ?
C16 C17 1.368(6) . ?
C16 C21 1.393(6) . ?
C17 C18 1.387(6) . ?
C18 C19 1.365(7) . ?
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C20 C21 1.374(7) . ?
C22 C23 1.429(10) . ?
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C1 S1 Hg1 105.74(13) . . ?
O1 P1 C10 114.13(18) . . ?
O1 P1 C2 115.56(17) . . ?
C10 P1 C2 105.74(18) . . ?
O1 P1 C16 108.72(18) . . ?
C10 P1 C16 105.99(18) . . ?
C2 P1 C16 106.00(18) . . ?
C9 Si1 C7 111.8(3) . . ?
C9 Si1 C8 108.1(2) . . ?
C7 Si1 C8 107.0(3) . . ?
C9 Si1 C6 108.2(2) . . ?
C7 Si1 C6 113.6(2) . . ?
C8 Si1 C6 108.0(2) . . ?
C6 C1 C2 121.0(3) . . ?
C6 C1 S1 117.4(3) . . ?
C2 C1 S1 121.5(3) . . ?
C3 C2 C1 118.8(4) . . ?
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C1 C2 P1 121.4(3) . . ?
C4 C3 C2 121.2(4) . . ?
C5 C4 C3 119.9(4) . . ?
C4 C5 C6 122.4(4) . . ?
C1 C6 C5 116.7(3) . . ?
C1 C6 Si1 123.6(3) . . ?
C5 C6 Si1 119.6(3) . . ?
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C11 C10 P1 119.0(3) . . ?
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C13 C12 C11 120.2(4) . . ?
C14 C13 C12 120.8(4) . . ?
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C23 C22 Hg1 117.2(5) . . ?

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Compound (9)

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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'P'  'P'   0.1023   0.0942
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'S'  'S'   0.1246   0.1234
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 'x, y, z'
 '-x, -y, -z'

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_cell_length_c                    12.764(3)
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_cell_angle_gamma                 100.074(3)
_cell_volume                      1141.6(4)
_cell_formula_units_Z             2
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
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```
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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Hg2 Hg 1.44051(5) 0.01122(3) 0.66388(3) 0.06200(14) Uani 1 1 d . . .
S1 S 0.9207(3) 0.0963(3) 0.7048(2) 0.0657(7) Uani 1 1 d . . .
S2 S 1.3541(3) 0.1286(2) 0.55737(19) 0.0536(6) Uani 1 1 d . . .
P1 P 1.2299(2) 0.33950(19) 0.74201(18) 0.0404(5) Uani 1 1 d . . .
C1 C 1.2342(9) 0.2380(7) 0.8234(6) 0.0418(19) Uani 1 1 d . . .
C2 C 1.1012(9) 0.1372(7) 0.8040(7) 0.0427(19) Uani 1 1 d . . .
C3 C 1.1100(11) 0.0625(8) 0.8689(8) 0.058(2) Uani 1 1 d . . .
H3 H 1.0234 -0.0050 0.8560 0.070 Uiso 1 1 calc R . .
C4 C 1.2435(11) 0.0849(8) 0.9524(8) 0.060(2) Uani 1 1 d . . .
H4 H 1.2444 0.0355 0.9965 0.072 Uiso 1 1 calc R . .
C5 C 1.3732(11) 0.1809(9) 0.9685(8) 0.059(2) Uani 1 1 d . . .
H5 H 1.4642 0.1958 1.0229 0.071 Uiso 1 1 calc R . .
C6 C 1.3702(10) 0.2558(8) 0.9046(7) 0.052(2) Uani 1 1 d . . .
H6 H 1.4604 0.3196 0.9156 0.062 Uiso 1 1 calc R . .
C7 C 1.4356(9) 0.3763(7) 0.7267(7) 0.0408(19) Uani 1 1 d . . .
C8 C 1.4851(9) 0.2814(7) 0.6431(7) 0.0430(19) Uani 1 1 d . . .
C9 C 1.6409(10) 0.3087(9) 0.6265(8) 0.060(2) Uani 1 1 d . . .
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H9 H 1.6749 0.2461 0.5711 0.072 Uiso 1 1 calc R . .
C10 C 1.7448(10) 0.4263(10) 0.6904(9) 0.068(3) Uani 1 1 d . . .
H10 H 1.8481 0.4424 0.6783 0.082 Uiso 1 1 calc R . .
C11 C 1.6960(10) 0.5202(8) 0.7724(8) 0.057(2) Uani 1 1 d . . .
H11 H 1.7658 0.5999 0.8157 0.068 Uiso 1 1 calc R . .
C12 C 1.5434(9) 0.4948(8) 0.7896(7) 0.048(2) Uani 1 1 d . . .
H12 H 1.5109 0.5587 0.8448 0.057 Uiso 1 1 calc R . .
C13 C 1.2078(9) 0.4940(7) 0.8429(7) 0.0428(19) Uani 1 1 d . . .
C14 C 1.1855(9) 0.5845(8) 0.7977(8) 0.053(2) Uani 1 1 d . . .
H14 H 1.1860 0.5656 0.7206 0.064 Uiso 1 1 calc R . .
C15 C 1.1625(11) 0.7033(8) 0.8658(9) 0.062(3) Uani 1 1 d . . .
H15 H 1.1515 0.7649 0.8354 0.074 Uiso 1 1 calc R . .
C16 C 1.1562(11) 0.7281(9) 0.9780(10) 0.067(3) Uani 1 1 d . . .
H16 H 1.1405 0.8071 1.0242 0.081 Uiso 1 1 calc R . .
C17 C 1.1729(11) 0.6373(9) 1.0231(9) 0.067(3) Uani 1 1 d . . .
H17 H 1.1660 0.6544 1.0991 0.080 Uiso 1 1 calc R . .
C18 C 1.2002(9) 0.5195(8) 0.9555(7) 0.051(2) Uani 1 1 d . . .
H18 H 1.2132 0.4587 0.9864 0.061 Uiso 1 1 calc R . .
C19 C 0.9650(13) 0.2301(11) 0.4208(8) 0.076(3) Uani 1 1 d . . .
H19A H 0.9571 0.1548 0.3519 0.092 Uiso 1 1 calc R . .
H19B H 0.8687 0.2604 0.4119 0.092 Uiso 1 1 calc R . .
C20 C 1.0977(19) 0.3280(16) 0.4303(14) 0.164(7) Uani 1 1 d . . .
H20A H 1.0846 0.3475 0.3630 0.246 Uiso 1 1 calc R . .
H20B H 1.1937 0.2984 0.4375 0.246 Uiso 1 1 calc R . .
H20C H 1.1046 0.4042 0.4967 0.246 Uiso 1 1 calc R . .
C21 C 1.5155(16) -0.0901(12) 0.7615(10) 0.100(4) Uani 1 1 d . . .
H21A H 1.6149 -0.0377 0.8142 0.119 Uiso 1 1 calc R . .
H21B H 1.4370 -0.0998 0.8072 0.119 Uiso 1 1 calc R . .
C22 C 1.539(2) -0.2127(15) 0.7006(13) 0.164(8) Uani 1 1 d . . .
H22A H 1.5721 -0.2500 0.7534 0.246 Uiso 1 1 calc R . .
H22B H 1.6196 -0.2048 0.6572 0.246 Uiso 1 1 calc R . .
H22C H 1.4408 -0.2670 0.6493 0.246 Uiso 1 1 calc R . .

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Hg2 0.0800(3) 0.0478(2) 0.0609(3) 0.02389(19) 0.0144(2) 0.01636(19)
S1 0.0452(12) 0.0731(17) 0.0759(17) 0.0385(14) 0.0016(11) -0.0058(12)
S2 0.0631(13) 0.0402(12) 0.0489(13) 0.0088(10) 0.0046(11) 0.0142(10)
P1 0.0417(11) 0.0357(11) 0.0401(12) 0.0139(9) 0.0054(9) 0.0046(9)
C1 0.046(4) 0.037(4) 0.041(5) 0.013(4) 0.011(4) 0.008(4)
C2 0.048(5) 0.038(4) 0.042(5) 0.015(4) 0.010(4) 0.011(4)
C3 0.072(6) 0.045(5) 0.055(6) 0.021(5) 0.018(5) 0.005(5)
C4 0.079(7) 0.048(5) 0.055(6) 0.023(5) 0.012(5) 0.018(5)
C5 0.066(6) 0.063(6) 0.050(6) 0.025(5) 0.002(5) 0.020(5)
C6 0.054(5) 0.042(5) 0.050(5) 0.011(4) -0.001(4) 0.009(4)
C7 0.052(5) 0.034(4) 0.042(5) 0.017(4) 0.018(4) 0.014(4)
C8 0.046(4) 0.042(5) 0.042(5) 0.016(4) 0.005(4) 0.015(4)
C9 0.057(5) 0.065(6) 0.065(6) 0.026(5) 0.018(5) 0.027(5)
C10 0.043(5) 0.072(7) 0.092(8) 0.035(6) 0.015(5) 0.014(5)
C11 0.058(5) 0.042(5) 0.067(6) 0.026(5) 0.002(5) -0.001(4)
C12 0.048(5) 0.039(5) 0.044(5) 0.008(4) 0.002(4) 0.001(4)
C13 0.038(4) 0.034(4) 0.049(5) 0.013(4) 0.000(4) 0.004(3)
C14 0.051(5) 0.057(6) 0.057(6) 0.026(5) 0.016(4) 0.013(4)
C15 0.074(6) 0.040(5) 0.080(7) 0.029(5) 0.020(5) 0.020(5)
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C16 0.071(6) 0.038(5) 0.089(8) 0.012(5) 0.027(6) 0.021(5)
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C18 0.055(5) 0.047(5) 0.056(6) 0.023(4) 0.022(4) 0.011(4)
C19 0.083(7) 0.103(9) 0.050(6) 0.041(6) 0.007(5) 0.021(7)
C20 0.152(14) 0.22(2) 0.168(16) 0.164(16) 0.013(12) 0.004(13)
C21 0.145(11) 0.101(10) 0.084(9) 0.059(8) 0.027(8) 0.054(9)
C22 0.30(2) 0.152(15) 0.146(14) 0.111(13) 0.112(15) 0.158(16)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Hg1 S1 2.386(3) . ?
Hg1 P1 2.807(2) . ?
Hg2 C21 2.100(11) . ?
Hg2 S2 2.368(2) . ?
S1 C2 1.760(8) . ?
S2 C8 1.778(8) . ?
P1 C1 1.815(8) . ?
P1 C7 1.818(8) . ?
P1 C13 1.835(8) . ?
C1 C6 1.402(11) . ?
C1 C2 1.408(10) . ?
C2 C3 1.391(11) . ?
C3 C4 1.390(12) . ?
C4 C5 1.366(12) . ?
C5 C6 1.379(12) . ?
C7 C12 1.394(10) . ?
C7 C8 1.399(10) . ?
C8 C9 1.397(11) . ?
C9 C10 1.375(12) . ?
C10 C11 1.377(12) . ?
C11 C12 1.372(11) . ?
C13 C18 1.373(11) . ?
C13 C14 1.381(11) . ?
C14 C15 1.391(12) . ?
C15 C16 1.367(13) . ?
C16 C17 1.374(13) . ?
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C19 C20 1.419(16) . ?
C21 C22 1.402(16) . ?
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C19 Hg1 P1 111.6(3) . . ?
S1 Hg1 P1 80.27(7) . . ?
C21 Hg2 S2 178.7(3) . . ?
C2 S1 Hg1 107.2(3) . . ?
C8 S2 Hg2 98.0(3) . . ?
C1 P1 C7 103.0(4) . . ?
C1 P1 C13 105.2(4) . . ?
C7 P1 C13 103.2(3) . . ?
C1 P1 Hg1 97.9(2) . . ?
C7 P1 Hg1 123.9(3) . . ?
C13 P1 Hg1 120.4(2) . . ?
C6 C1 C2 118.6(8) . . ?
C6 C1 P1 121.1(6) . . ?
C2 C1 P1 120.3(6) . . ?
C3 C2 C1 118.1(8) . . ?
C3 C2 S1 115.9(6) . . ?
C1 C2 S1 126.0(6) . . ?
C4 C3 C2 122.5(8) . . ?
C5 C4 C3 118.8(9) . . ?
C4 C5 C6 120.4(9) . . ?
C5 C6 C1 121.4(8) . . ?
C12 C7 C8 118.6(7) . . ?
C12 C7 P1 123.9(6) . . ?
C8 C7 P1 117.5(6) . . ?
C9 C8 C7 118.7(7) . . ?
C9 C8 S2 119.8(6) . . ?
C7 C8 S2 121.5(6) . . ?
C10 C9 C8 121.3(8) . . ?
C9 C10 C11 120.0(8) . . ?
C12 C11 C10 119.3(8) . . ?
C11 C12 C7 122.0(8) . . ?
C18 C13 C14 119.5(8) . . ?
C18 C13 P1 124.0(7) . . ?
C14 C13 P1 116.2(7) . . ?
C13 C14 C15 121.0(9) . . ?
C16 C15 C14 119.0(9) . . ?
C15 C16 C17 120.6(9) . . ?
C16 C17 C18 120.3(9) . . ?
C13 C18 C17 119.5(9) . . ?
C20 C19 Hg1 114.3(8) . . ?
C22 C21 Hg2 116.7(9) . . ?

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Compound (10*)

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;
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 'Si'  'Si'   0.0817   0.0704
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 'O'  'O'   0.0106   0.0060
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 'x, y, z'
 '-x, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y-1/2, z-1/2'

_cell_length_a                    12.472(3)
_cell_length_b                    19.760(5)
_cell_length_c                    14.774(4)
_cell_angle_alpha                 90.00
_cell_angle_beta                  111.260(4)
_cell_angle_gamma                 90.00
_cell_volume                      3393.0(15)
_cell_formula_units_Z             4
_cell_measurement_temperature     293(2)
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_exptl_crystal_description        'Prism'
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_exptl_crystal_density_diffrn     1.848
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1800
_exptl_absorpt_coefficient_mu     9.298
_exptl_absorpt_correction_type    'multi-scan'
_exptl_absorpt_correction_T_min   0.0197
_exptl_absorpt_correction_T_max   0.0463
_exptl_absorpt_process_details    ?

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;
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_diffrn_ambient_temperature       293(2)
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_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Smart-CCD-1000 BRUKER'
_diffrn_measurement_method        'omega scans'
_diffrn_detector_area_resol_mean  ?
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_diffrn_reflns_theta_min          1.80
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_reflns_number_total              6923
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_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
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_computing_publication_material   ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
```

```
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0545P)^2^+0.0000P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     'constr'
_refine_ls_extinction_method      none
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_refine_ls_number_parameters      325
_refine_ls_number_restraints      0
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Hg1 Hg 0.30030(3) 0.262439(17) 0.94285(2) 0.05349(12) Uani 1 1 d . . .
Hg2 Hg 0.53230(3) 0.102068(19) 1.07595(3) 0.06247(13) Uani 1 1 d . . .
S1 S 0.22682(18) 0.23830(12) 1.06797(14) 0.0550(5) Uani 1 1 d . . .
S2 S 0.45531(17) -0.00350(10) 1.09662(15) 0.0523(5) Uani 1 1 d . . .
P1 P 0.22317(16) 0.08734(10) 0.97608(13) 0.0395(4) Uani 1 1 d . . .
Si1 Si -0.0127(2) 0.32077(13) 1.0365(2) 0.0720(8) Uani 1 1 d . . .
Si2 Si 0.5003(2) -0.05956(13) 1.31470(17) 0.0627(7) Uani 1 1 d . . .
O1 O 0.3144(4) 0.1237(3) 0.9530(3) 0.0446(12) Uani 1 1 d . . .
C1 C 0.0938(6) 0.2022(4) 0.9888(5) 0.0411(17) Uani 1 1 d . . .
C2 C 0.0914(6) 0.1379(4) 0.9472(5) 0.0386(16) Uani 1 1 d . . .
C3 C -0.0133(6) 0.1120(4) 0.8846(5) 0.0470(19) Uani 1 1 d . . .
H3 H -0.0159 0.0701 0.8554 0.056 Uiso 1 1 calc R . .
```

```
C4 C -0.1126(7) 0.1485(4) 0.8664(6) 0.054(2) Uani 1 1 d . . .
H4 H -0.1825 0.1312 0.8249 0.065 Uiso 1 1 calc R . .
C5 C -0.1092(7) 0.2102(4) 0.9089(6) 0.054(2) Uani 1 1 d . . .
H5 H -0.1777 0.2339 0.8953 0.065 Uiso 1 1 calc R . .
C6 C -0.0084(7) 0.2391(4) 0.9715(5) 0.0498(19) Uani 1 1 d . . .
C7 C -0.1672(10) 0.3478(6) 0.9941(9) 0.115(4) Uani 1 1 d . . .
H7A H -0.1952 0.3553 0.9252 0.173 Uiso 1 1 calc R . .
H7B H -0.1734 0.3889 1.0264 0.173 Uiso 1 1 calc R . .
H7C H -0.2121 0.3130 1.0088 0.173 Uiso 1 1 calc R . .
C8 C 0.0358(11) 0.3051(6) 1.1679(7) 0.115(4) Uani 1 1 d . . .
H8A H -0.0089 0.2692 1.1802 0.173 Uiso 1 1 calc R . .
H8B H 0.0261 0.3455 1.2002 0.173 Uiso 1 1 calc R . .
H8C H 0.1156 0.2925 1.1918 0.173 Uiso 1 1 calc R . .
C9 C 0.0695(10) 0.3897(5) 1.0072(9) 0.108(4) Uani 1 1 d . . .
H9A H 0.0421 0.3962 0.9382 0.163 Uiso 1 1 calc R . .
H9B H 0.1496 0.3780 1.0303 0.163 Uiso 1 1 calc R . .
H9C H 0.0594 0.4308 1.0380 0.163 Uiso 1 1 calc R . .
C10 C 0.3511(6) 0.0184(3) 1.1487(5) 0.0387(16) Uani 1 1 d . . .
C11 C 0.2548(6) 0.0574(3) 1.1000(5) 0.0370(16) Uani 1 1 d . . .
C12 C 0.1756(6) 0.0698(4) 1.1438(5) 0.0491(19) Uani 1 1 d . . .
H12 H 0.1122 0.0970 1.1122 0.059 Uiso 1 1 calc R . .
C13 C 0.1885(7) 0.0427(4) 1.2338(5) 0.053(2) Uani 1 1 d . . .
H13 H 0.1338 0.0507 1.2616 0.064 Uiso 1 1 calc R . .
C14 C 0.2830(6) 0.0039(4) 1.2807(5) 0.0486(19) Uani 1 1 d . . .
H14 H 0.2914 -0.0142 1.3410 0.058 Uiso 1 1 calc R . .
C15 C 0.3684(6) -0.0097(3) 1.2417(5) 0.0409(17) Uani 1 1 d . . .
C16 C 0.4782(9) -0.0912(5) 1.4256(6) 0.090(3) Uani 1 1 d . . .
H16A H 0.5442 -0.1168 1.4645 0.135 Uiso 1 1 calc R . .
H16B H 0.4112 -0.1196 1.4069 0.135 Uiso 1 1 calc R . .
H16C H 0.4677 -0.0536 1.4626 0.135 Uiso 1 1 calc R . .
C17 C 0.6263(7) -0.0015(6) 1.3531(7) 0.093(3) Uani 1 1 d . . .
H17A H 0.6942 -0.0262 1.3908 0.140 Uiso 1 1 calc R . .
H17B H 0.6135 0.0345 1.3916 0.140 Uiso 1 1 calc R . .
H17C H 0.6364 0.0171 1.2967 0.140 Uiso 1 1 calc R . .
C18 C 0.5257(11) -0.1350(5) 1.2501(8) 0.114(4) Uani 1 1 d . . .
H18A H 0.5936 -0.1581 1.2911 0.172 Uiso 1 1 calc R . .
H18B H 0.5358 -0.1209 1.1915 0.172 Uiso 1 1 calc R . .
H18C H 0.4608 -0.1649 1.2342 0.172 Uiso 1 1 calc R . .
C19 C 0.1812(6) 0.0115(4) 0.9031(5) 0.0415(17) Uani 1 1 d . . .
C20 C 0.1849(7) 0.0130(4) 0.8096(6) 0.059(2) Uani 1 1 d . . .
H20 H 0.2112 0.0515 0.7880 0.070 Uiso 1 1 calc R . .
C21 C 0.1493(8) -0.0426(5) 0.7493(7) 0.074(3) Uani 1 1 d . . .
H21 H 0.1504 -0.0411 0.6867 0.089 Uiso 1 1 calc R . .
C22 C 0.1125(7) -0.0999(4) 0.7815(7) 0.063(2) Uani 1 1 d . . .
H22 H 0.0901 -0.1374 0.7410 0.076 Uiso 1 1 calc R . .
C23 C 0.1085(6) -0.1021(4) 0.8730(7) 0.061(2) Uani 1 1 d . . .
H23 H 0.0822 -0.1408 0.8942 0.073 Uiso 1 1 calc R . .
C24 C 0.1439(6) -0.0464(4) 0.9338(5) 0.0468(18) Uani 1 1 d . . .
H24 H 0.1424 -0.0484 0.9962 0.056 Uiso 1 1 calc R . .
C25 C 0.3481(12) 0.2880(6) 0.8242(7) 0.100(4) Uani 1 1 d . . .
H25A H 0.3507 0.2461 0.7908 0.120 Uiso 1 1 calc R . .
H25B H 0.2856 0.3146 0.7800 0.120 Uiso 1 1 calc R . .
C26 C 0.4508(10) 0.3232(6) 0.8364(8) 0.104(4) Uani 1 1 d . . .
H26A H 0.4567 0.3306 0.7741 0.156 Uiso 1 1 calc R . .
H26B H 0.5154 0.2970 0.8764 0.156 Uiso 1 1 calc R . .
H26C H 0.4502 0.3660 0.8670 0.156 Uiso 1 1 calc R . .
C27 C 0.6097(9) 0.1932(5) 1.0678(9) 0.097(4) Uani 1 1 d . . .
H27A H 0.6686 0.1850 1.0407 0.117 Uiso 1 1 calc R . .
H27B H 0.5524 0.2227 1.0232 0.117 Uiso 1 1 calc R . .
C28 C 0.6631(14) 0.2293(7) 1.1623(13) 0.160(6) Uani 1 1 d . . .
H28A H 0.6973 0.2707 1.1521 0.240 Uiso 1 1 calc R . .
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H28B H 0.7213 0.2011 1.2067 0.240 Uiso 1 1 calc R . .
H28C H 0.6051 0.2392 1.1889 0.240 Uiso 1 1 calc R . .

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0.00850(16)
Hg2 0.0508(2) 0.0696(3) 0.0668(2) 0.00752(17) 0.02101(16) -0.00253(17)
S1 0.0558(12) 0.0673(14) 0.0369(11) -0.0099(10) 0.0109(9) -0.0081(11)
S2 0.0590(12) 0.0533(13) 0.0564(13) 0.0085(10) 0.0351(10) 0.0131(10)
P1 0.0436(10) 0.0455(12) 0.0316(10) 0.0028(8) 0.0162(8) 0.0000(9)
Si1 0.0795(18) 0.0570(16) 0.0763(19) -0.0092(13) 0.0242(15) 0.0148(14)
Si2 0.0800(16) 0.0615(16) 0.0484(14) 0.0156(12) 0.0255(12) 0.0288(14)
O1 0.045(3) 0.052(3) 0.038(3) 0.006(2) 0.017(2) -0.002(2)
C1 0.047(4) 0.047(5) 0.028(4) 0.004(3) 0.012(3) -0.001(4)
C2 0.042(4) 0.045(4) 0.030(4) 0.003(3) 0.015(3) -0.003(3)
C3 0.047(4) 0.045(5) 0.046(4) 0.005(4) 0.013(4) -0.005(4)
C4 0.045(5) 0.060(6) 0.051(5) 0.000(4) 0.008(4) -0.004(4)
C5 0.046(5) 0.059(6) 0.053(5) 0.011(4) 0.013(4) 0.010(4)
C6 0.058(5) 0.047(5) 0.043(4) 0.009(4) 0.016(4) 0.004(4)
C7 0.114(9) 0.085(8) 0.145(11) -0.014(8) 0.045(8) 0.042(7)
C8 0.140(11) 0.138(11) 0.076(8) -0.024(7) 0.050(7) 0.020(9)
C9 0.112(9) 0.054(7) 0.128(10) -0.008(6) 0.006(8) 0.006(6)
C10 0.044(4) 0.038(4) 0.038(4) -0.006(3) 0.020(3) -0.006(3)
C11 0.040(4) 0.043(4) 0.031(4) 0.003(3) 0.017(3) 0.004(3)
C12 0.045(4) 0.065(5) 0.039(4) 0.004(4) 0.017(3) 0.005(4)
C13 0.053(5) 0.065(6) 0.053(5) 0.007(4) 0.032(4) 0.005(4)
C14 0.062(5) 0.053(5) 0.035(4) 0.008(4) 0.023(4) 0.001(4)
C15 0.047(4) 0.037(4) 0.042(4) -0.001(3) 0.020(3) -0.001(3)
C16 0.116(9) 0.090(8) 0.058(6) 0.034(5) 0.023(6) 0.036(6)
C17 0.057(6) 0.142(11) 0.071(7) 0.005(7) 0.012(5) 0.006(6)
C18 0.193(13) 0.068(7) 0.101(9) 0.032(6) 0.076(9) 0.062(8)
C19 0.044(4) 0.041(4) 0.042(4) 0.003(3) 0.018(3) -0.001(3)
C20 0.076(6) 0.059(6) 0.048(5) -0.003(4) 0.031(4) -0.015(5)
C21 0.078(6) 0.088(8) 0.059(6) -0.021(5) 0.029(5) -0.013(6)
C22 0.062(5) 0.057(6) 0.071(6) -0.021(5) 0.025(5) -0.005(5)
C23 0.044(5) 0.055(6) 0.084(7) 0.004(5) 0.025(4) 0.002(4)
C24 0.049(4) 0.050(5) 0.048(5) 0.003(4) 0.025(4) 0.005(4)
C25 0.168(12) 0.082(8) 0.055(6) 0.001(5) 0.048(7) -0.007(8)
C26 0.135(10) 0.120(10) 0.082(8) -0.012(7) 0.070(7) -0.047(8)
C27 0.071(7) 0.064(7) 0.126(10) 0.006(7) -0.001(6) -0.012(6)
C28 0.174(15) 0.083(10) 0.215(19) -0.001(11) 0.060(14) 0.013(10)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
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 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Hg1 S1 2.390(2) . ?
Hg2 C27 2.067(10) . ?
Hg2 S2 2.362(2) . ?
S1 C1 1.795(7) . ?
S2 C10 1.787(7) . ?
P1 O1 1.486(5) . ?
P1 C19 1.809(7) . ?
P1 C11 1.825(7) . ?
P1 C2 1.837(7) . ?
Si1 C8 1.837(11) . ?
Si1 C9 1.848(11) . ?
Si1 C7 1.875(11) . ?
Si1 C6 1.887(8) . ?
Si2 C18 1.858(10) . ?
Si2 C17 1.860(10) . ?
Si2 C16 1.866(9) . ?
Si2 C15 1.886(7) . ?
C1 C2 1.407(10) . ?
C1 C6 1.409(10) . ?
C2 C3 1.395(9) . ?
C3 C4 1.373(10) . ?
C4 C5 1.364(11) . ?
C5 C6 1.385(10) . ?
C10 C11 1.388(9) . ?
C10 C15 1.425(9) . ?
C11 C12 1.385(9) . ?
C12 C13 1.387(10) . ?
C13 C14 1.365(10) . ?
C14 C15 1.408(10) . ?
C19 C24 1.373(10) . ?
C19 C20 1.399(10) . ?
C20 C21 1.383(11) . ?
C21 C22 1.369(12) . ?
C22 C23 1.371(12) . ?
C23 C24 1.388(11) . ?
C25 C26 1.411(14) . ?
C27 C28 1.491(17) . ?

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C25 Hg1 S1 174.0(4) . . ?
C27 Hg2 S2 175.7(3) . . ?
C1 S1 Hg1 95.6(2) . . ?
C10 S2 Hg2 103.6(2) . . ?
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O1 P1 C19 110.1(3) . . ?
O1 P1 C11 118.8(3) . . ?
C19 P1 C11 103.9(3) . . ?
O1 P1 C2 112.3(3) . . ?
C19 P1 C2 105.7(3) . . ?
C11 P1 C2 105.0(3) . . ?
C8 Si1 C9 111.9(6) . . ?
C8 Si1 C7 107.8(6) . . ?
C9 Si1 C7 107.6(5) . . ?
C8 Si1 C6 109.5(5) . . ?
C9 Si1 C6 113.0(5) . . ?
C7 Si1 C6 106.8(4) . . ?
C18 Si2 C17 111.6(6) . . ?
C18 Si2 C16 106.8(5) . . ?
C17 Si2 C16 108.5(5) . . ?
C18 Si2 C15 113.7(4) . . ?
C17 Si2 C15 108.5(4) . . ?
C16 Si2 C15 107.5(4) . . ?
C2 C1 C6 120.9(7) . . ?
C2 C1 S1 120.8(5) . . ?
C6 C1 S1 118.3(6) . . ?
C3 C2 C1 119.1(7) . . ?
C3 C2 P1 119.9(6) . . ?
C1 C2 P1 121.0(5) . . ?
C4 C3 C2 119.9(7) . . ?
C5 C4 C3 120.2(7) . . ?
C4 C5 C6 123.1(8) . . ?
C5 C6 C1 116.7(7) . . ?
C5 C6 Si1 120.4(6) . . ?
C1 C6 Si1 122.7(6) . . ?
C11 C10 C15 121.1(6) . . ?
C11 C10 S2 122.6(5) . . ?
C15 C10 S2 116.2(5) . . ?
C12 C11 C10 119.0(6) . . ?
C12 C11 P1 118.7(5) . . ?
C10 C11 P1 122.1(5) . . ?
C11 C12 C13 121.6(7) . . ?
C14 C13 C12 118.9(7) . . ?
C13 C14 C15 122.8(7) . . ?
C14 C15 C10 116.6(6) . . ?
C14 C15 Si2 119.9(5) . . ?
C10 C15 Si2 123.4(5) . . ?
C24 C19 C20 118.7(7) . . ?
C24 C19 P1 123.6(6) . . ?
C20 C19 P1 117.7(6) . . ?
C21 C20 C19 120.1(8) . . ?
C22 C21 C20 120.2(9) . . ?
C21 C22 C23 120.4(8) . . ?
C22 C23 C24 119.7(8) . . ?
C19 C24 C23 120.9(7) . . ?
C26 C25 Hg1 121.9(8) . . ?
C28 C27 Hg2 114.9(9) . . ?

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Compound (11)

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
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 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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P1 P 0.3352(3) 0.08007(11) 0.04719(16) 0.0503(8) Uani 1 1 d . . .
P2 P 0.8006(3) 0.20678(13) 0.22207(19) 0.0636(10) Uani 1 1 d . . .
Si1 Si 0.1255(3) -0.06501(13) 0.1748(2) 0.0747(12) Uani 1 1 d . . .
Si2 Si 0.2483(4) 0.27522(14) 0.0576(2) 0.0805(13) Uani 1 1 d . . .
Si3 Si 0.8112(4) 0.39034(16) 0.1200(2) 0.0834(13) Uani 1 1 d . . .
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Si4 Si 0.3947(4) 0.17650(14) 0.3323(2) 0.0796(13) Uani 1 1 d . . .
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C4 C 0.1568(14) -0.0380(6) -0.0174(8) 0.090(5) Uani 1 1 d . . .
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C5 C 0.1312(12) -0.0563(5) 0.0392(8) 0.077(4) Uani 1 1 d . . .
H5 H 0.0895 -0.0840 0.0363 0.092 Uiso 1 1 calc R . .
C6 C 0.1651(10) -0.0351(4) 0.1016(7) 0.058(3) Uani 1 1 d . . .
C7 C 0.0090(15) -0.0329(6) 0.2039(9) 0.121(7) Uani 1 1 d . . .
H7A H -0.0569 -0.0283 0.1680 0.181 Uiso 1 1 calc R . .
H7B H 0.0390 -0.0033 0.2210 0.181 Uiso 1 1 calc R . .
H7C H -0.0161 -0.0502 0.2381 0.181 Uiso 1 1 calc R . .
C8 C 0.2569(14) -0.0756(6) 0.2408(9) 0.126(7) Uani 1 1 d . . .
H8A H 0.3145 -0.0927 0.2232 0.189 Uiso 1 1 calc R . .
H8B H 0.2344 -0.0931 0.2756 0.189 Uiso 1 1 calc R . .
H8C H 0.2899 -0.0464 0.2579 0.189 Uiso 1 1 calc R . .
C9 C 0.0696(16) -0.1245(6) 0.1474(9) 0.121(6) Uani 1 1 d . . .
H9A H 0.1307 -0.1416 0.1330 0.181 Uiso 1 1 calc R . .
H9B H 0.0024 -0.1218 0.1118 0.181 Uiso 1 1 calc R . .
H9C H 0.0472 -0.1404 0.1836 0.181 Uiso 1 1 calc R . .
C10 C 0.2785(11) 0.1745(5) 0.0533(6) 0.059(3) Uani 1 1 d . . .
C11 C 0.2378(11) 0.1286(4) 0.0540(6) 0.052(3) Uani 1 1 d . . .
C12 C 0.1216(12) 0.1200(5) 0.0573(6) 0.062(4) Uani 1 1 d . . .
H12 H 0.0950 0.0896 0.0587 0.075 Uiso 1 1 calc R . .
C13 C 0.0461(12) 0.1562(5) 0.0584(7) 0.073(4) Uani 1 1 d . . .
H13 H -0.0323 0.1504 0.0598 0.087 Uiso 1 1 calc R . .
C14 C 0.0846(13) 0.2012(5) 0.0574(6) 0.068(4) Uani 1 1 d . . .
H14 H 0.0314 0.2252 0.0586 0.081 Uiso 1 1 calc R . .
C15 C 0.2001(12) 0.2122(4) 0.0547(6) 0.056(3) Uani 1 1 d . . .
C16 C 0.3261(16) 0.2925(5) -0.0107(8) 0.107(6) Uani 1 1 d . . .
H16A H 0.2760 0.2858 -0.0526 0.160 Uiso 1 1 calc R . .
H16B H 0.3983 0.2753 -0.0063 0.160 Uiso 1 1 calc R . .
H16C H 0.3434 0.3251 -0.0077 0.160 Uiso 1 1 calc R . .
C17 C 0.1132(16) 0.3120(5) 0.0466(8) 0.106(6) Uani 1 1 d . . .
H17A H 0.0639 0.3060 0.0042 0.159 Uiso 1 1 calc R . .
H17B H 0.1354 0.3442 0.0495 0.159 Uiso 1 1 calc R . .
H17C H 0.0705 0.3049 0.0804 0.159 Uiso 1 1 calc R . .
C18 C 0.3406(14) 0.2872(5) 0.1387(8) 0.100(5) Uani 1 1 d . . .
H18A H 0.4114 0.2690 0.1444 0.149 Uiso 1 1 calc R . .
H18B H 0.2980 0.2794 0.1723 0.149 Uiso 1 1 calc R . .
H18C H 0.3608 0.3195 0.1418 0.149 Uiso 1 1 calc R . .
C19 C 0.3724(10) 0.0848(4) -0.0324(6) 0.049(3) Uani 1 1 d . . .
C20 C 0.2971(13) 0.1023(5) -0.0854(7) 0.074(4) Uani 1 1 d . . .
H20 H 0.2221 0.1116 -0.0810 0.089 Uiso 1 1 calc R . .
C21 C 0.3285(16) 0.1068(4) -0.1461(7) 0.077(4) Uani 1 1 d . . .
H21 H 0.2776 0.1204 -0.1816 0.093 Uiso 1 1 calc R . .
C22 C 0.4389(17) 0.0903(6) -0.1519(9) 0.090(5) Uani 1 1 d . . .
H22 H 0.4611 0.0920 -0.1925 0.108 Uiso 1 1 calc R . .
C23 C 0.5148(13) 0.0718(5) -0.0995(9) 0.086(5) Uani 1 1 d . . .
H23 H 0.5887 0.0613 -0.1038 0.103 Uiso 1 1 calc R . .
C24 C 0.4804(12) 0.0690(5) -0.0394(7) 0.066(4) Uani 1 1 d . . .
H24 H 0.5316 0.0561 -0.0033 0.079 Uiso 1 1 calc R . .
C25 C 0.6452(14) 0.0208(5) 0.2352(10) 0.120(7) Uani 1 1 d . . .
H25A H 0.6765 0.0400 0.2731 0.144 Uiso 1 1 calc R . .
H25B H 0.6620 -0.0114 0.2477 0.144 Uiso 1 1 calc R . .
C26 C 0.7077(16) 0.0335(7) 0.1775(11) 0.135(8) Uani 1 1 d . . .
H26A H 0.7912 0.0289 0.1914 0.203 Uiso 1 1 calc R . .
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H26B H 0.6921 0.0654 0.1655 0.203 Uiso 1 1 calc R . .
H26C H 0.6779 0.0140 0.1402 0.203 Uiso 1 1 calc R . .
C27 C 0.8235(11) 0.2945(5) 0.1732(6) 0.063(4) Uani 1 1 d . . .
C28 C 0.8801(12) 0.2599(5) 0.2100(7) 0.061(4) Uani 1 1 d . . .
C29 C 0.9989(12) 0.2635(5) 0.2373(6) 0.068(4) Uani 1 1 d . . .
H29 H 1.0388 0.2385 0.2599 0.082 Uiso 1 1 calc R . .
C30 C 1.0586(13) 0.3041(6) 0.2314(7) 0.077(4) Uani 1 1 d . . .
H30 H 1.1380 0.3069 0.2512 0.093 Uiso 1 1 calc R . .
C31 C 1.0024(13) 0.3391(5) 0.1973(7) 0.071(4) Uani 1 1 d . . .
H31 H 1.0448 0.3661 0.1938 0.085 Uiso 1 1 calc R . .
C32 C 0.8803(12) 0.3380(5) 0.1656(6) 0.066(4) Uani 1 1 d . . .
C33 C 0.7601(17) 0.3761(6) 0.0312(7) 0.126(7) Uani 1 1 d . . .
H33A H 0.8249 0.3640 0.0141 0.189 Uiso 1 1 calc R . .
H33B H 0.7307 0.4037 0.0074 0.189 Uiso 1 1 calc R . .
H33C H 0.6984 0.3534 0.0263 0.189 Uiso 1 1 calc R . .
C34 C 0.6933(14) 0.4139(5) 0.1562(7) 0.105(6) Uani 1 1 d . . .
H34A H 0.6601 0.4407 0.1317 0.158 Uiso 1 1 calc R . .
H34B H 0.7246 0.4226 0.2011 0.158 Uiso 1 1 calc R . .
H34C H 0.6331 0.3908 0.1551 0.158 Uiso 1 1 calc R . .
C35 C 0.9269(17) 0.4356(6) 0.1261(9) 0.129(7) Uani 1 1 d . . .
H35A H 0.9904 0.4241 0.1072 0.193 Uiso 1 1 calc R . .
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C36 C 0.6122(11) 0.1954(4) 0.2883(6) 0.058(3) Uani 1 1 d . . .
C37 C 0.7025(11) 0.2242(4) 0.2767(6) 0.058(3) Uani 1 1 d . . .
C38 C 0.7253(12) 0.2657(5) 0.3110(7) 0.075(4) Uani 1 1 d . . .
H38 H 0.7897 0.2838 0.3064 0.090 Uiso 1 1 calc R . .
C39 C 0.6542(14) 0.2799(5) 0.3511(9) 0.093(5) Uani 1 1 d . . .
H39 H 0.6678 0.3080 0.3735 0.111 Uiso 1 1 calc R . .
C40 C 0.5626(15) 0.2525(5) 0.3582(8) 0.090(5) Uani 1 1 d . . .
H40 H 0.5139 0.2630 0.3857 0.108 Uiso 1 1 calc R . .
C41 C 0.5359(12) 0.2094(5) 0.3271(7) 0.071(4) Uani 1 1 d . . .
C42 C 0.2951(12) 0.1726(6) 0.2492(8) 0.099(5) Uani 1 1 d . . .
H42A H 0.3331 0.1550 0.2203 0.148 Uiso 1 1 calc R . .
H42B H 0.2783 0.2033 0.2316 0.148 Uiso 1 1 calc R . .
H42C H 0.2228 0.1576 0.2530 0.148 Uiso 1 1 calc R . .
C43 C 0.4301(15) 0.1182(5) 0.3718(8) 0.106(6) Uani 1 1 d . . .
H43A H 0.4808 0.1221 0.4143 0.159 Uiso 1 1 calc R . .
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H43C H 0.3583 0.1032 0.3767 0.159 Uiso 1 1 calc R . .
C44 C 0.3168(16) 0.2108(6) 0.3846(10) 0.127(7) Uani 1 1 d . . .
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H44B H 0.2449 0.1953 0.3881 0.190 Uiso 1 1 calc R . .
H44C H 0.2989 0.2409 0.3655 0.190 Uiso 1 1 calc R . .
C45 C 0.9027(12) 0.1677(5) 0.2707(8) 0.066(4) Uani 1 1 d . . .
C46 C 0.9323(15) 0.1710(6) 0.3363(10) 0.096(5) Uani 1 1 d . . .
H46 H 0.8985 0.1943 0.3575 0.115 Uiso 1 1 calc R . .
C47 C 1.0165(19) 0.1390(9) 0.3756(12) 0.132(7) Uani 1 1 d . . .
H47 H 1.0391 0.1411 0.4212 0.159 Uiso 1 1 calc R . .
C48 C 1.0592(19) 0.1058(9) 0.3400(17) 0.142(9) Uani 1 1 d . . .
H48 H 1.1120 0.0844 0.3632 0.170 Uiso 1 1 calc R . .
C49 C 1.032(2) 0.1013(8) 0.2745(15) 0.136(9) Uani 1 1 d . . .
H49 H 1.0642 0.0780 0.2528 0.163 Uiso 1 1 calc R . .
C50 C 0.9536(16) 0.1327(7) 0.2412(9) 0.100(5) Uani 1 1 d . . .
H50 H 0.9335 0.1303 0.1956 0.120 Uiso 1 1 calc R . .
C51 C 0.6948(18) 0.1902(7) -0.0234(9) 0.120(7) Uani 1 1 d . . .
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H51B H 0.6868 0.1593 -0.0063 0.144 Uiso 1 1 calc R . .
C52 C 0.611(2) 0.1958(8) -0.0814(12) 0.182(11) Uani 1 1 d . . .
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Hg2 0.0904(5) 0.1194(6) 0.0739(4) -0.0084(4) 0.0089(4) -0.0509(4)
Hg3 0.0506(3) 0.0675(4) 0.0721(4) -0.0097(3) 0.0061(3) -0.0128(3)
S1 0.071(3) 0.069(2) 0.072(2) -0.0038(19) 0.0199(19) -0.0074(19)
S2 0.053(2) 0.072(2) 0.082(3) 0.008(2) 0.0141(19) -0.0116(18)
S3 0.053(2) 0.101(3) 0.108(3) -0.014(3) -0.006(2) -0.013(2)
S4 0.068(2) 0.056(2) 0.072(2) -0.0089(18) 0.0105(19) -0.0072(18)
P1 0.044(2) 0.0471(19) 0.057(2) 0.0012(16) 0.0047(16) -0.0013(15)
P2 0.048(2) 0.069(2) 0.075(3) -0.021(2) 0.0172(19) -0.0135(18)
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Si2 0.112(4) 0.051(2) 0.084(3) -0.003(2) 0.033(3) 0.003(2)
Si3 0.093(3) 0.087(3) 0.067(3) -0.010(2) 0.008(2) -0.009(3)
Si4 0.066(3) 0.072(3) 0.110(4) -0.007(3) 0.039(3) -0.007(2)
O1 0.050(5) 0.056(5) 0.052(5) 0.008(4) 0.000(4) 0.000(4)
O2 0.061(6) 0.089(7) 0.071(6) -0.026(5) 0.018(5) -0.020(5)
C1 0.031(7) 0.058(8) 0.067(9) -0.005(7) -0.002(6) -0.003(6)
C2 0.051(8) 0.053(8) 0.047(8) -0.001(7) 0.003(6) -0.007(6)
C3 0.066(10) 0.060(9) 0.084(11) -0.004(8) 0.013(8) -0.017(8)
C4 0.100(13) 0.100(13) 0.065(11) -0.014(9) 0.008(9) -0.019(10)
C5 0.068(10) 0.060(9) 0.099(13) -0.012(9) 0.007(9) -0.033(8)
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C7 0.099(14) 0.126(15) 0.159(18) 0.038(13) 0.077(13) 0.023(11)
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C10 0.049(8) 0.065(9) 0.063(9) -0.004(7) 0.014(7) 0.006(7)
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C13 0.044(8) 0.074(10) 0.100(12) 0.015(9) 0.016(8) 0.003(8)
C14 0.067(10) 0.072(10) 0.065(9) 0.009(8) 0.016(8) 0.027(8)
C15 0.058(9) 0.052(8) 0.060(9) 0.005(6) 0.011(7) -0.002(7)
C16 0.163(18) 0.061(10) 0.106(13) 0.018(9) 0.052(12) -0.001(10)
C17 0.153(17) 0.070(11) 0.101(13) -0.017(9) 0.044(12) 0.023(10)
C18 0.102(13) 0.090(12) 0.112(14) -0.020(10) 0.033(11) -0.010(10)
C19 0.041(8) 0.040(7) 0.061(8) 0.002(6) 0.002(6) 0.002(6)
C20 0.069(10) 0.075(10) 0.080(11) 0.005(8) 0.020(9) 0.031(8)
C21 0.117(14) 0.054(9) 0.058(10) 0.009(7) 0.012(9) 0.009(9)
C22 0.100(14) 0.087(12) 0.092(14) -0.030(10) 0.039(12) -0.006(10)
C23 0.048(10) 0.098(12) 0.112(14) -0.018(11) 0.015(10) 0.006(9)
C24 0.060(10) 0.074(10) 0.069(10) 0.001(8) 0.022(8) 0.006(7)
C25 0.072(12) 0.075(12) 0.19(2) -0.003(12) -0.039(13) 0.025(9)
C26 0.090(14) 0.126(17) 0.20(2) -0.003(15) 0.063(15) 0.024(12)
C27 0.048(9) 0.074(10) 0.064(9) -0.005(8) 0.009(7) -0.014(8)
C28 0.047(9) 0.068(9) 0.072(10) -0.026(8) 0.021(7) -0.015(7)
C29 0.045(9) 0.096(11) 0.067(9) -0.012(8) 0.020(7) -0.011(8)
C30 0.052(10) 0.087(11) 0.088(11) -0.008(9) 0.004(8) 0.001(9)
C31 0.065(10) 0.071(10) 0.082(11) -0.009(9) 0.027(8) -0.018(8)
C32 0.060(9) 0.088(11) 0.054(9) -0.009(7) 0.018(7) -0.013(8)
C33 0.169(19) 0.140(16) 0.058(11) 0.002(10) -0.003(11) 0.019(14)
C34 0.117(15) 0.095(12) 0.095(12) -0.018(10) 0.001(11) 0.001(10)
C35 0.155(19) 0.100(14) 0.130(16) 0.004(12) 0.023(13) -0.006(13)
C36 0.045(8) 0.060(8) 0.071(9) -0.004(7) 0.015(7) 0.009(7)
```

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C37 0.049(8) 0.062(9) 0.069(9) -0.012(7) 0.023(7) 0.000(7)
C38 0.061(10) 0.076(10) 0.092(11) -0.036(9) 0.028(8) -0.027(8)
C39 0.078(12) 0.065(10) 0.145(16) -0.029(10) 0.048(11) -0.018(9)
C40 0.108(14) 0.069(11) 0.105(13) -0.024(9) 0.052(11) 0.013(10)
C41 0.076(10) 0.054(9) 0.089(11) -0.004(8) 0.032(9) 0.003(7)
C42 0.059(10) 0.125(14) 0.117(14) -0.006(11) 0.029(9) -0.016(9)
C43 0.107(14) 0.090(12) 0.136(15) 0.004(11) 0.059(12) -0.016(10)
C44 0.113(15) 0.092(13) 0.20(2) -0.017(13) 0.095(14) -0.006(11)
C45 0.057(9) 0.067(9) 0.078(11) -0.031(8) 0.024(8) -0.005(7)
C46 0.079(12) 0.100(13) 0.109(15) -0.010(11) 0.017(11) 0.005(10)
C47 0.109(18) 0.15(2) 0.139(19) 0.040(17) 0.026(15) 0.006(15)
C48 0.072(15) 0.13(2) 0.23(3) 0.01(2) 0.04(2) 0.015(13)
C49 0.086(17) 0.125(18) 0.20(3) -0.03(2) 0.035(18) 0.026(13)
C50 0.077(13) 0.118(15) 0.112(14) -0.033(13) 0.036(11) -0.011(11)
C51 0.128(17) 0.155(18) 0.077(13) -0.003(12) 0.018(12) -0.056(14)
C52 0.19(3) 0.22(3) 0.15(2) 0.01(2) 0.06(2) -0.10(2)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Hg1 O1 2.622(7) . ?
Hg2 C51 2.131(18) . ?
Hg2 S3 2.380(4) . ?
Hg3 S2 2.326(4) . ?
Hg3 S4 2.328(4) . ?
Hg3 O1 2.617(7) . ?
S1 C1 1.768(12) . ?
S2 C10 1.766(13) . ?
S3 C27 1.771(13) . ?
S4 C36 1.785(13) . ?
P1 O1 1.492(7) . ?
P1 C19 1.796(13) . ?
P1 C2 1.820(12) . ?
P1 C11 1.821(12) . ?
P2 O2 1.502(9) . ?
P2 C45 1.787(15) . ?
P2 C28 1.831(13) . ?
P2 C37 1.832(12) . ?
Si1 C7 1.839(16) . ?
Si1 C8 1.850(15) . ?
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Si1 C9 1.878(16) . ?
Si1 C6 1.883(14) . ?
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Si2 C16 1.894(15) . ?
Si2 C15 1.898(13) . ?
Si3 C34 1.820(16) . ?
Si3 C35 1.855(18) . ?
Si3 C33 1.861(15) . ?
Si3 C32 1.871(15) . ?
Si4 C44 1.836(16) . ?
Si4 C42 1.869(16) . ?
Si4 C43 1.878(16) . ?
Si4 C41 1.913(14) . ?
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C1 C2 1.426(16) . ?
C2 C3 1.366(16) . ?
C3 C4 1.376(18) . ?
C4 C5 1.374(19) . ?
C5 C6 1.410(18) . ?
C10 C11 1.404(16) . ?
C10 C15 1.420(16) . ?
C11 C12 1.384(16) . ?
C12 C13 1.366(17) . ?
C13 C14 1.373(17) . ?
C14 C15 1.387(17) . ?
C19 C20 1.352(16) . ?
C19 C24 1.366(16) . ?
C20 C21 1.387(18) . ?
C21 C22 1.39(2) . ?
C22 C23 1.36(2) . ?
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C25 C26 1.56(2) . ?
C27 C28 1.341(17) . ?
C27 C32 1.440(17) . ?
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S1 Hg1 O1 81.23(19) . . ?
C51 Hg2 S3 178.3(6) . . ?
S2 Hg3 S4 169.45(13) . . ?
S2 Hg3 O1 84.88(18) . . ?
S4 Hg3 O1 99.79(17) . . ?
C1 S1 Hg1 100.4(4) . . ?
C10 S2 Hg3 97.9(4) . . ?
C27 S3 Hg2 97.4(5) . . ?
C36 S4 Hg3 96.9(4) . . ?
O1 P1 C19 109.0(5) . . ?
O1 P1 C2 110.7(5) . . ?
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O1 P1 C11 116.1(5) . . ?
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O2 P2 C37 118.9(5) . . ?
C45 P2 C37 104.2(7) . . ?
C28 P2 C37 104.4(6) . . ?
C7 Si1 C8 112.8(9) . . ?
C7 Si1 C9 109.2(8) . . ?
C8 Si1 C9 104.7(8) . . ?
C7 Si1 C6 110.6(6) . . ?
C8 Si1 C6 111.9(7) . . ?
C9 Si1 C6 107.4(7) . . ?
C18 Si2 C17 108.7(7) . . ?
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C18 Si2 C15 108.8(6) . . ?
C17 Si2 C15 107.9(7) . . ?
C16 Si2 C15 114.2(6) . . ?
C34 Si3 C35 107.6(8) . . ?
C34 Si3 C33 112.3(8) . . ?
C35 Si3 C33 107.5(9) . . ?
C34 Si3 C32 111.8(7) . . ?
C35 Si3 C32 107.7(8) . . ?
C33 Si3 C32 109.8(7) . . ?
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C42 Si4 C43 112.7(8) . . ?
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C6 C1 C2 119.6(11) . . ?
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C12 C13 C14 120.7(13) . . ?
C13 C14 C15 122.3(12) . . ?
C14 C15 C10 116.9(12) . . ?
C14 C15 Si2 119.8(10) . . ?
C10 C15 Si2 123.3(10) . . ?
C20 C19 C24 119.4(13) . . ?
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