CSIRO Publishing

AUSTRALIAN JOURNAL OF CHEMISTRY

AN INTERNATIONAL JOURNAL FOR CHEMICAL SCIENCE

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

Volume 54, 2001

All enquiries and manuscripts should be directed to:

Dr Alison Green

Australian Journal of Chemistry – an International Journal for Chemical Science

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

Telephone: +61 3 9662 7630
Fax: +61 3 9662 7611
E-mail: ajc@publish.csiro.au

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

www.publish.csiro.au/journals/ajc

10.1071/CH01140_AC

Accessory Publication: *Aust. J. Chem.*, 2001, **54**(11), 711-716.

```
##############################################################################

data_Cd_Persulf_Bipy

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
Bis (2,2'-pyridyl)-mu-peroxodisulfato cadmium(II), monohydrate
;
_chemical_formula_moiety   '[(Cd 2+), 2(C10 H8 N2), (O8 S2 2-)]. (H2 O)'
_chemical_formula_sum      'C20 H18 Cd N4 O9 S2'
_chemical_formula_weight          634.90

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0033   0.0016
 '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'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cd'  'Cd'  -0.8075   1.2024
 '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'

_symmetry_cell_setting            triclinic
_symmetry_space_group_name_H-M    'P -1 '

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, -y, -z'

_cell_length_a                    7.213(3)
_cell_length_b                    9.841(6)
_cell_length_c                    16.371(5)
_cell_angle_alpha                 82.94(4)
_cell_angle_beta                  82.31(3)
_cell_angle_gamma                 86.32(4)
_cell_volume                      1141.6(9)
_cell_formula_units_Z             2
_cell_measurement_temperature     293(2)
_cell_measurement_reflns_used     30
_cell_measurement_theta_min       7.5
_cell_measurement_theta_max       15

_exptl_crystal_description        blocks
_exptl_crystal_colour             colorless
_exptl_crystal_size_max           0.28
_exptl_crystal_size_mid           0.22
_exptl_crystal_size_min           0.18
```

```
_exptl_crystal_density_diffrn     1.847
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              636
_exptl_absorpt_coefficient_mu     1.201
_exptl_absorpt_correction_type    psi_scan
_exptl_absorpt_process_details   ' SHELXTL/PC (Sheldrick,1994)   '
_exptl_absorpt_correction_T_min   0.74
_exptl_absorpt_correction_T_max   0.79

_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   'Siemens R3m'
_diffrn_measurement_method        \w/2\q
_diffrn_standards_number          2
_diffrn_standards_interval_count  98
_diffrn_standards_decay_%         <2
_diffrn_reflns_number             4369
_diffrn_reflns_av_R_equivalents   0.0182
_diffrn_reflns_av_sigmaI/netI     0.0279
_diffrn_reflns_limit_h_min        0
_diffrn_reflns_limit_h_max        8
_diffrn_reflns_limit_k_min        -11
_diffrn_reflns_limit_k_max        11
_diffrn_reflns_limit_l_min        -19
_diffrn_reflns_limit_l_max        19
_diffrn_reflns_theta_min          2.09
_diffrn_reflns_theta_max          25.00
_reflns_number_total              4019
_reflns_number_gt                 3589
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'Siemens P3/P4-PC version V4.27 (1991)'
_computing_cell_refinement        'Siemens P3/P4-PC version V4.27 (1991)'
_computing_data_reduction         'XDISK in SHELXTL/PC(Sheldrick,1994)'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1997)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'XP in SHELXTL/PC(Sheldrick,1994)'
_computing_publication_material
;
CIFTAB (Sheldrick, 1993), PARST (Nardelli, 1983) and
CSD (Allen, Kennard & Taylor, 1983)
;


_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
   'w=1/[\s^2^(Fo^2^)+(0.0441P)^2^+1.3646P] 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     mixed
_refine_ls_extinction_method      none
_refine_ls_number_reflns          4019
_refine_ls_number_parameters      334
_refine_ls_number_restraints      3
_refine_ls_R_factor_all           0.0379
```

```
_refine_ls_R_factor_gt            0.0315
_refine_ls_wR_factor_ref          0.0841
_refine_ls_wR_factor_gt           0.0790
_refine_ls_goodness_of_fit_ref    1.038
_refine_ls_restrained_S_all       1.038
_refine_ls_shift/su_max           <0.01
_refine_ls_shift/su_mean          <0.01

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_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Cd Cd -0.32055(4) -0.00382(3) 0.231436(14) 0.03529(10) Uani 1 d . . .
S1 S 0.18724(12) 0.03119(8) 0.26352(5) 0.02987(19) Uani 1 d . . .
S2 S 0.11697(15) 0.41725(10) 0.22763(6) 0.0451(2) Uani 1 d . . .
O1 O 0.0361(4) -0.0068(3) 0.22274(16) 0.0415(6) Uani 1 d . . .
O2 O 0.3563(3) 0.0601(3) 0.20669(16) 0.0431(6) Uani 1 d . . .
O3 O 0.2190(5) -0.0524(3) 0.33894(17) 0.0520(7) Uani 1 d . . .
O4 O 0.1083(6) 0.4575(3) 0.3086(2) 0.0777(11) Uani 1 d . . .
O5 O 0.3027(5) 0.3992(4) 0.1863(2) 0.0720(10) Uani 1 d . . .
O6 O -0.0150(6) 0.4841(3) 0.1767(3) 0.0916(14) Uani 1 d . . .
O7 O 0.0259(4) 0.2636(3) 0.24039(19) 0.0504(7) Uani 1 d . . .
O8 O 0.1157(4) 0.1724(3) 0.30346(15) 0.0412(6) Uani 1 d . . .
N1A N -0.2569(4) -0.1354(3) 0.35244(17) 0.0324(6) Uani 1 d . . .
N2A N -0.3632(4) 0.1355(3) 0.33309(17) 0.0331(6) Uani 1 d . . .
C1A C -0.1994(6) -0.2686(4) 0.3595(2) 0.0431(9) Uani 1 d . . .
H1AA H -0.1982 -0.3165 0.3139 0.052 Uiso 1 calc R . .
C2A C -0.1427(6) -0.3369(4) 0.4305(3) 0.0465(9) Uani 1 d . . .
H2AA H -0.1046 -0.4292 0.4331 0.056 Uiso 1 calc R . .
C3A C -0.1432(6) -0.2662(4) 0.4983(2) 0.0463(9) Uani 1 d . . .
H3AA H -0.1075 -0.3105 0.5477 0.056 Uiso 1 calc R . .
C4A C -0.1974(5) -0.1290(4) 0.4917(2) 0.0397(8) Uani 1 d . . .
H4AA H -0.1964 -0.0792 0.5364 0.048 Uiso 1 calc R . .
C5A C -0.2537(5) -0.0651(4) 0.4175(2) 0.0309(7) Uani 1 d . . .
C6A C -0.3110(4) 0.0836(4) 0.4072(2) 0.0293(7) Uani 1 d . . .
C7A C -0.3101(5) 0.1664(4) 0.4694(2) 0.0395(8) Uani 1 d . . .
H7AA H -0.2733 0.1301 0.5203 0.047 Uiso 1 calc R . .
C8A C -0.3646(6) 0.3036(4) 0.4554(3) 0.0493(10) Uani 1 d . . .
H8AA H -0.3640 0.3605 0.4967 0.059 Uiso 1 calc R . .
C9A C -0.4192(6) 0.3552(4) 0.3805(3) 0.0474(10) Uani 1 d . . .
H9AA H -0.4560 0.4473 0.3700 0.057 Uiso 1 calc R . .
C10A C -0.4185(6) 0.2681(4) 0.3213(2) 0.0429(9) Uani 1 d . . .
H10A H -0.4581 0.3026 0.2707 0.052 Uiso 1 calc R . .
N1B N -0.2509(4) 0.1156(3) 0.10287(17) 0.0309(6) Uani 1 d . . .
N2B N -0.3373(4) -0.1532(3) 0.13607(17) 0.0329(6) Uani 1 d . . .
C1B C -0.2059(5) 0.2469(4) 0.0889(3) 0.0428(9) Uani 1 d . . .
H1BA H -0.2065 0.2958 0.1341 0.051 Uiso 1 calc R . .
C2B C -0.1586(6) 0.3127(4) 0.0104(3) 0.0492(10) Uani 1 d . . .
H2BA H -0.1291 0.4044 0.0027 0.059 Uiso 1 calc R . .
C3B C -0.1559(6) 0.2402(4) -0.0563(3) 0.0497(10) Uani 1 d . . .
H3BA H -0.1236 0.2818 -0.1101 0.060 Uiso 1 calc R . .
C4B C -0.2015(6) 0.1055(4) -0.0425(2) 0.0425(9) Uani 1 d . . .
```

```
H4BA H -0.2002 0.0548 -0.0870 0.051 Uiso 1 calc R . .
C5B C -0.2495(4) 0.0450(3) 0.0380(2) 0.0307(7) Uani 1 d . . .
C6B C -0.2993(5) -0.1019(4) 0.0558(2) 0.0303(7) Uani 1 d . . .
C7B C -0.3080(5) -0.1828(4) -0.0070(2) 0.0403(9) Uani 1 d . . .
H7BA H -0.2821 -0.1463 -0.0623 0.048 Uiso 1 calc R . .
C8B C -0.3553(6) -0.3178(4) 0.0126(3) 0.0450(9) Uani 1 d . . .
H8BA H -0.3601 -0.3731 -0.0292 0.054 Uiso 1 calc R . .
C9B C -0.3950(6) -0.3690(4) 0.0940(3) 0.0476(10) Uani 1 d . . .
H9BA H -0.4276 -0.4595 0.1087 0.057 Uiso 1 calc R . .
C10B C -0.3856(6) -0.2834(4) 0.1542(2) 0.0414(9) Uani 1 d . . .
H10B H -0.4142 -0.3179 0.2096 0.050 Uiso 1 calc R . .
O1W O -0.6518(5) -0.3397(4) 0.3430(3) 0.0692(10) Uani 1 d D . .
H1WA H -0.690(6) -0.258(4) 0.337(3) 0.064(15) Uiso 1 d D . .
H1WB H -0.732(6) -0.392(4) 0.334(3) 0.073(18) Uiso 1 d D . .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
Cd 0.04288(17) 0.04245(16) 0.02149(14) -0.00614(10) -0.00748(10) 0.00259(11)
S1 0.0318(4) 0.0330(4) 0.0247(4) -0.0040(3) -0.0042(3) 0.0025(3)
S2 0.0516(6) 0.0346(5) 0.0502(6) 0.0012(4) -0.0144(5) -0.0054(4)
O1 0.0339(14) 0.0548(16) 0.0378(14) -0.0097(12) -0.0067(11) -0.0048(12)
O2 0.0285(13) 0.0660(18) 0.0359(14) -0.0132(12) -0.0040(11) 0.0022(12)
O3 0.080(2) 0.0401(15) 0.0363(14) 0.0004(12) -0.0189(14) 0.0088(14)
O4 0.121(3) 0.0525(19) 0.062(2) -0.0206(16) -0.009(2) -0.0055(19)
O5 0.066(2) 0.081(2) 0.064(2) 0.0080(18) 0.0029(17) -0.0180(18)
O6 0.106(3) 0.0448(18) 0.132(4) 0.019(2) -0.071(3) -0.0021(19)
O7 0.0455(16) 0.0394(15) 0.0683(19) 0.0026(13) -0.0242(14) 0.0009(12)
O8 0.0527(16) 0.0380(14) 0.0319(13) -0.0050(10) -0.0052(11) 0.0073(12)
N1A 0.0335(16) 0.0371(15) 0.0264(14) -0.0036(12) -0.0035(12) -0.0016(12)
N2A 0.0314(15) 0.0386(16) 0.0298(15) -0.0046(12) -0.0063(12) 0.0011(12)
C1A 0.047(2) 0.043(2) 0.041(2) -0.0099(17) -0.0072(17) 0.0013(17)
C2A 0.053(2) 0.038(2) 0.047(2) 0.0007(17) -0.0095(19) 0.0036(18)
C3A 0.048(2) 0.052(2) 0.036(2) 0.0068(17) -0.0085(17) 0.0028(19)
C4A 0.044(2) 0.048(2) 0.0278(18) -0.0028(15) -0.0091(15) 0.0017(17)
C5A 0.0264(17) 0.0397(18) 0.0254(16) -0.0017(14) 0.0007(13) -0.0041(14)
C6A 0.0222(16) 0.0408(18) 0.0257(16) -0.0045(14) -0.0035(13) -0.0049(13)
C7A 0.040(2) 0.051(2) 0.0288(18) -0.0073(16) -0.0083(15) -0.0022(17)
C8A 0.056(3) 0.049(2) 0.046(2) -0.0196(18) -0.0052(19) -0.0003(19)
C9A 0.049(2) 0.038(2) 0.055(2) -0.0081(18) -0.0081(19) 0.0050(17)
C10A 0.045(2) 0.046(2) 0.037(2) -0.0016(16) -0.0096(17) 0.0060(17)
N1B 0.0260(14) 0.0373(15) 0.0300(14) -0.0044(12) -0.0067(11) 0.0022(12)
N2B 0.0353(16) 0.0362(15) 0.0275(14) -0.0045(12) -0.0054(12) 0.0014(12)
C1B 0.040(2) 0.041(2) 0.050(2) -0.0062(17) -0.0139(17) -0.0017(16)
C2B 0.037(2) 0.039(2) 0.068(3) 0.0095(19) -0.0093(19) -0.0025(17)
C3B 0.046(2) 0.055(2) 0.041(2) 0.0132(19) 0.0038(18) 0.0010(19)
C4B 0.047(2) 0.051(2) 0.0270(18) -0.0010(16) -0.0013(16) 0.0071(18)
C5B 0.0219(16) 0.0387(18) 0.0316(17) -0.0030(14) -0.0072(13) 0.0051(14)
C6B 0.0241(16) 0.0402(18) 0.0266(16) -0.0065(14) -0.0052(13) 0.0071(14)
C7B 0.040(2) 0.051(2) 0.0318(18) -0.0137(16) -0.0061(15) 0.0070(17)
C8B 0.042(2) 0.049(2) 0.049(2) -0.0214(18) -0.0107(18) 0.0047(18)
C9B 0.050(2) 0.036(2) 0.059(3) -0.0085(18) -0.014(2) -0.0013(17)
C10B 0.047(2) 0.041(2) 0.0358(19) -0.0032(16) -0.0064(17) -0.0015(17)
O1W 0.076(3) 0.052(2) 0.084(3) -0.0192(19) -0.020(2) 0.0065(19)

_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.
;

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_distance
 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
Cd N2A 2.262(3) . ?
Cd N1B 2.291(3) . ?
Cd N2B 2.292(3) . ?
Cd N1A 2.313(3) . ?
Cd O2 2.448(3) 1_455 ?
Cd O1 2.556(3) . ?
S1 O3 1.434(3) . ?
S1 O1 1.443(3) . ?
S1 O2 1.452(3) . ?
S1 O8 1.633(3) . ?
S2 O4 1.421(4) . ?
S2 O6 1.425(4) . ?
S2 O5 1.428(4) . ?
S2 O7 1.666(3) . ?
O7 O8 1.472(4) . ?
N1A C5A 1.344(4) . ?
N1A C1A 1.344(5) . ?
N2A C10A 1.338(5) . ?
N2A C6A 1.349(4) . ?
C1A C2A 1.368(5) . ?
C1A H1AA 0.9300 . ?
C2A C3A 1.380(6) . ?
C2A H2AA 0.9300 . ?
C3A C4A 1.376(6) . ?
C3A H3AA 0.9300 . ?
C4A C5A 1.395(5) . ?
C4A H4AA 0.9300 . ?
C5A C6A 1.490(5) . ?
C6A C7A 1.381(5) . ?
C7A C8A 1.383(6) . ?
C7A H7AA 0.9300 . ?
C8A C9A 1.366(6) . ?
C8A H8AA 0.9300 . ?
C9A C10A 1.371(6) . ?
C9A H9AA 0.9300 . ?
C10A H10A 0.9300 . ?
N1B C5B 1.337(4) . ?
N1B C1B 1.338(5) . ?
N2B C10B 1.337(5) . ?
N2B C6B 1.347(4) . ?
C1B C2B 1.376(6) . ?
C1B H1BA 0.9300 . ?
C2B C3B 1.374(6) . ?
C2B H2BA 0.9300 . ?
C3B C4B 1.371(6) . ?
C3B H3BA 0.9300 . ?

```
C4B C5B 1.386(5) . ?
C4B H4BA 0.9300 . ?
C5B C6B 1.497(5) . ?
C6B C7B 1.386(5) . ?
C7B C8B 1.382(6) . ?
C7B H7BA 0.9300 . ?
C8B C9B 1.365(6) . ?
C8B H8BA 0.9300 . ?
C9B C10B 1.383(6) . ?
C9B H9BA 0.9300 . ?
C10B H10B 0.9300 . ?
O1W H1WA 0.83(3) . ?
O1W H1WB 0.84(3) . ?

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
N2A Cd N1B 111.99(11) . . ?
N2A Cd N2B 168.90(10) . . ?
N1B Cd N2B 73.12(11) . . ?
N2A Cd N1A 72.94(11) . . ?
N1B Cd N1A 156.07(10) . . ?
N2B Cd N1A 106.60(11) . . ?
N2A Cd O2 87.46(10) . 1_455 ?
N1B Cd O2 83.11(10) . 1_455 ?
N2B Cd O2 83.34(10) . 1_455 ?
N1A Cd O2 120.81(10) . 1_455 ?
N2A Cd O1 92.91(10) . . ?
N1B Cd O1 80.14(10) . . ?
N2B Cd O1 97.76(10) . . ?
N1A Cd O1 76.18(10) . . ?
O3 S1 O1 115.91(18) . . ?
O3 S1 O2 114.17(18) . . ?
O1 S1 O2 112.97(15) . . ?
O3 S1 O8 98.04(15) . . ?
O1 S1 O8 106.55(15) . . ?
O2 S1 O8 107.39(16) . . ?
O4 S2 O6 116.6(3) . . ?
O4 S2 O5 114.3(2) . . ?
O6 S2 O5 115.0(3) . . ?
O4 S2 O7 105.85(19) . . ?
O6 S2 O7 96.32(19) . . ?
O5 S2 O7 106.03(19) . . ?
S1 O1 Cd 143.34(15) . . ?
O8 O7 S2 109.9(2) . . ?
O7 O8 S1 107.66(19) . . ?
C5A N1A C1A 118.4(3) . . ?
C5A N1A Cd 115.0(2) . . ?
C1A N1A Cd 125.9(2) . . ?
C10A N2A C6A 119.0(3) . . ?
C10A N2A Cd 123.8(2) . . ?
C6A N2A Cd 116.9(2) . . ?
N1A C1A C2A 123.2(4) . . ?
N1A C1A H1AA 118.4 . . ?
C2A C1A H1AA 118.4 . . ?
C1A C2A C3A 118.7(4) . . ?
```

```
C1A C2A H2AA 120.6 . . ?
C3A C2A H2AA 120.6 . . ?
C4A C3A C2A 119.0(4) . . ?
C4A C3A H3AA 120.5 . . ?
C2A C3A H3AA 120.5 . . ?
C3A C4A C5A 119.6(3) . . ?
C3A C4A H4AA 120.2 . . ?
C5A C4A H4AA 120.2 . . ?
N1A C5A C4A 121.0(3) . . ?
N1A C5A C6A 117.5(3) . . ?
C4A C5A C6A 121.4(3) . . ?
N2A C6A C7A 120.7(3) . . ?
N2A C6A C5A 116.8(3) . . ?
C7A C6A C5A 122.5(3) . . ?
C6A C7A C8A 119.4(3) . . ?
C6A C7A H7AA 120.3 . . ?
C8A C7A H7AA 120.3 . . ?
C9A C8A C7A 119.6(4) . . ?
C9A C8A H8AA 120.2 . . ?
C7A C8A H8AA 120.2 . . ?
C8A C9A C10A 118.5(4) . . ?
C8A C9A H9AA 120.8 . . ?
C10A C9A H9AA 120.8 . . ?
N2A C10A C9A 122.8(4) . . ?
N2A C10A H10A 118.6 . . ?
C9A C10A H10A 118.6 . . ?
C5B N1B C1B 118.7(3) . . ?
C5B N1B Cd 116.3(2) . . ?
C1B N1B Cd 125.0(2) . . ?
C10B N2B C6B 118.8(3) . . ?
C10B N2B Cd 125.2(2) . . ?
C6B N2B Cd 115.9(2) . . ?
N1B C1B C2B 122.7(4) . . ?
N1B C1B H1BA 118.6 . . ?
C2B C1B H1BA 118.6 . . ?
C3B C2B C1B 118.6(4) . . ?
C3B C2B H2BA 120.7 . . ?
C1B C2B H2BA 120.7 . . ?
C4B C3B C2B 119.0(4) . . ?
C4B C3B H3BA 120.5 . . ?
C2B C3B H3BA 120.5 . . ?
C3B C4B C5B 119.8(4) . . ?
C3B C4B H4BA 120.1 . . ?
C5B C4B H4BA 120.1 . . ?
N1B C5B C4B 121.1(3) . . ?
N1B C5B C6B 117.4(3) . . ?
C4B C5B C6B 121.5(3) . . ?
N2B C6B C7B 120.8(3) . . ?
N2B C6B C5B 117.3(3) . . ?
C7B C6B C5B 122.0(3) . . ?
C8B C7B C6B 119.8(4) . . ?
C8B C7B H7BA 120.1 . . ?
C6B C7B H7BA 120.1 . . ?
C9B C8B C7B 119.2(4) . . ?
C9B C8B H8BA 120.4 . . ?
C7B C8B H8BA 120.4 . . ?
C8B C9B C10B 118.6(4) . . ?
C8B C9B H9BA 120.7 . . ?
C10B C9B H9BA 120.7 . . ?
N2B C10B C9B 122.8(4) . . ?
N2B C10B H10B 118.6 . . ?
```

```
C9B C10B H10B 118.6 . . ?
H1WA O1W H1WB 111.4(18) . . ?

loop_
 _geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag
O3 S1 O1 Cd 73.7(3) . . . . ?
O2 S1 O1 Cd -151.8(2) . . . . ?
O8 S1 O1 Cd -34.1(3) . . . . ?
N2A Cd O1 S1 10.5(3) . . . . ?
N1B Cd O1 S1 122.3(3) . . . . ?
N2B Cd O1 S1 -166.4(3) . . . . ?
N1A Cd O1 S1 -61.1(3) . . . . ?
O2 Cd O1 S1 101.2(3) 1_455 . . . ?
O3 S1 O2 Cd -4.8(2) . . . 1_655 ?
O1 S1 O2 Cd -140.11(18) . . . 1_655 ?
O8 S1 O2 Cd 102.69(19) . . . 1_655 ?
O4 S2 O7 O8 -50.8(3) . . . . ?
O6 S2 O7 O8 -170.7(3) . . . . ?
O5 S2 O7 O8 71.0(3) . . . . ?
S2 O7 O8 S1 -128.33(19) . . . . ?
O3 S1 O8 O7 -164.9(2) . . . . ?
O1 S1 O8 O7 -44.8(2) . . . . ?
O2 S1 O8 O7 76.6(2) . . . . ?
N2A Cd N1A C5A -7.6(2) . . . . ?
N1B Cd N1A C5A 98.4(3) . . . . ?
N2B Cd N1A C5A -176.0(2) . . . . ?
O2 Cd N1A C5A -83.8(2) 1_455 . . . ?
O1 Cd N1A C5A 89.9(2) . . . . ?
N2A Cd N1A C1A -178.0(3) . . . . ?
N1B Cd N1A C1A -72.1(4) . . . . ?
N2B Cd N1A C1A 13.6(3) . . . . ?
O2 Cd N1A C1A 105.7(3) 1_455 . . . ?
O1 Cd N1A C1A -80.5(3) . . . . ?
N1B Cd N2A C10A 26.0(3) . . . . ?
N2B Cd N2A C10A -89.6(6) . . . . ?
N1A Cd N2A C10A -178.9(3) . . . . ?
O2 Cd N2A C10A -55.6(3) 1_455 . . . ?
O1 Cd N2A C10A 106.5(3) . . . . ?
N1B Cd N2A C6A -147.1(2) . . . . ?
N2B Cd N2A C6A 97.3(5) . . . . ?
N1A Cd N2A C6A 8.0(2) . . . . ?
O2 Cd N2A C6A 131.4(2) 1_455 . . . ?
O1 Cd N2A C6A -66.6(2) . . . . ?
C5A N1A C1A C2A 1.8(6) . . . . ?
Cd N1A C1A C2A 172.0(3) . . . . ?
N1A C1A C2A C3A -0.4(6) . . . . ?
C1A C2A C3A C4A -1.2(6) . . . . ?
C2A C3A C4A C5A 1.2(6) . . . . ?
C1A ?1A C5A C4A -1.8(5) . . . . ?
Cd ?1A C5A C4A -173.0(3) . . . . ?
C1A N1A C5A C6A 177.7(3) . . . . ?
Cd N1A C5A C6A 6.5(4) . . . . ?
```

```
C3A C4A C5A N1A 0.3(5) . . . . ?
C3A C4A C5A C6A -179.2(3) . . . . ?
C10A N2A C6A C7A -1.5(5) . . . . ?
Cd N2A C6A C7A 171.9(3) . . . . ?
C10A N2A C6A C5A 179.0(3) . . . . ?
Cd N2A C6A C5A -7.6(4) . . . . ?
N1A C5A C6A N2A 0.6(4) . . . . ?
C4A C5A C6A N2A -179.9(3) . . . . ?
N1A C5A C6A C7A -178.9(3) . . . . ?
C4A C5A C6A C7A 0.6(5) . . . . ?
N2A C6A C7A C8A 0.4(5) . . . . ?
C5A C6A C7A C8A 179.8(3) . . . . ?
C6A C7A C8A C9A 0.3(6) . . . . ?
C7A C8A C9A C10A 0.1(6) . . . . ?
C6A N2A C10A C9A 2.0(6) . . . . ?
Cd N2A C10A C9A -170.9(3) . . . . ?
C8A C9A C10A N2A -1.3(6) . . . . ?
N2A Cd N1B C5B -170.8(2) . . . . ?
N2B Cd N1B C5B -1.3(2) . . . . ?
N1A Cd N1B C5B 91.7(3) . . . . ?
O2 Cd N1B C5B -86.4(2) 1_455 . . . ?
O1 Cd N1B C5B 100.0(2) . . . . ?
N2A Cd N1B C1B 11.7(3) . . . . ?
N2B Cd N1B C1B -178.7(3) . . . . ?
N1A Cd N1B C1B -85.8(4) . . . . ?
O2 Cd N1B C1B 96.1(3) 1_455 . . . ?
O1 Cd N1B C1B -77.4(3) . . . . ?
N2A Cd N2B C10B -58.8(6) . . . . ?
N1B Cd N2B C10B -177.8(3) . . . . ?
N1A Cd N2B C10B 27.2(3) . . . . ?
O2 Cd N2B C10B -93.0(3) 1_455 . . . ?
O1 Cd N2B C10B 105.0(3) . . . . ?
N2A Cd N2B C6B 119.5(5) . . . . ?
N1B Cd N2B C6B 0.4(2) . . . . ?
N1A Cd N2B C6B -154.6(2) . . . . ?
O2 Cd N2B C6B 85.2(2) 1_455 . . . ?
O1 Cd N2B C6B -76.8(2) . . . . ?
C5B N1B C1B C2B 0.2(5) . . . . ?
Cd N1B C1B C2B 177.6(3) . . . . ?
N1B C1B C2B C3B -0.6(6) . . . . ?
C1B C2B C3B C4B 0.5(6) . . . . ?
C2B C3B C4B C5B 0.1(6) . . . . ?
C1B N1B C5B C4B 0.3(5) . . . . ?
Cd N1B C5B C4B -177.3(3) . . . . ?
C1B N1B C5B C6B 179.6(3) . . . . ?
Cd N1B C5B C6B 2.0(4) . . . . ?
C3B C4B C5B N1B -0.5(5) . . . . ?
C3B C4B C5B C6B -179.7(3) . . . . ?
C10B N2B C6B C7B -0.7(5) . . . . ?
Cd N2B C6B C7B -179.0(3) . . . . ?
C10B N2B C6B C5B 178.8(3) . . . . ?
Cd N2B C6B C5B 0.5(4) . . . . ?
N1B C5B C6B N2B -1.6(4) . . . . ?
C4B C5B C6B N2B 177.6(3) . . . . ?
N1B C5B C6B C7B 177.8(3) . . . . ?
C4B C5B C6B C7B -2.9(5) . . . . ?
N2B C6B C7B C8B -0.3(5) . . . . ?
C5B C6B C7B C8B -179.8(3) . . . . ?
C6B C7B C8B C9B 0.7(6) . . . . ?
C7B C8B C9B C10B -0.2(6) . . . . ?
C6B N2B C10B C9B 1.3(6) . . . . ?
```

```
Cd N2B C10B C9B 179.4(3) . . . . ?
C8B C9B C10B N2B -0.8(6) . . . . ?

_diffrn_measured_fraction_theta_max    0.999
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.999
_refine_diff_density_max    1.040
_refine_diff_density_min   -0.381
_refine_diff_density_rms    0.075

################################################################################

data_Hg_Persulf_Terp

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
catena(bis((mu!2$-Acetato-O,O,O')-(terpyridyne-N,N',N"))-
(mu!2$-Peroxodisulfato-O,O') mercury(ii) )
;
_chemical_formula_moiety '[2(Hg 2+), 2(C15 H11 N3), (O8 S2 2-), 2(C2 O2 H3)]'
_chemical_formula_sum    'C34 H28 Hg2 N6 O12 S2'
_chemical_formula_weight          1177.92

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0033   0.0016
 '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'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 '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'

_symmetry_cell_setting            triclinic
_symmetry_space_group_name_H-M    'P -1 '


loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, -y, -z'

_cell_length_a                    10.653(2)
_cell_length_b                    12.195(3)
_cell_length_c                    14.641(3)
_cell_angle_alpha                 88.295(19)
_cell_angle_beta                  83.553(18)
_cell_angle_gamma                 73.921(19)
_cell_volume                      1816.0(7)
_cell_formula_units_Z             2
_cell_measurement_temperature     293(2)
```

```
_cell_measurement_reflns_used     30
_cell_measurement_theta_min       7.5
_cell_measurement_theta_max       15

_exptl_crystal_description        plates
_exptl_crystal_colour             colorless
_exptl_crystal_size_max           0.80
_exptl_crystal_size_mid           0.30
_exptl_crystal_size_min           0.15
_exptl_crystal_density_diffrn     2.154
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1124
_exptl_absorpt_coefficient_mu     8.632
_exptl_absorpt_correction_type    psi_scan
_exptl_absorpt_process_details   ' SHELXTL/PC (Sheldrick,1994)   '
_exptl_absorpt_correction_T_min   0.04
_exptl_absorpt_correction_T_max   0.18

_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   'Siemens R3m'
_diffrn_measurement_method        \w/2\q
_diffrn_standards_number          2
_diffrn_standards_interval_count  98
_diffrn_standards_decay_%         <2
_diffrn_reflns_number             6396
_diffrn_reflns_av_R_equivalents   0.052
_diffrn_reflns_av_sigmaI/netI     0.0784
_diffrn_reflns_limit_h_min        -11
_diffrn_reflns_limit_h_max        11
_diffrn_reflns_limit_k_min        -14
_diffrn_reflns_limit_k_max        14
_diffrn_reflns_limit_l_min        0
_diffrn_reflns_limit_l_max        17
_diffrn_reflns_theta_min          1.74
_diffrn_reflns_theta_max          25.00
_reflns_number_total              6179
_reflns_number_gt                 3940
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'Siemens P3/P4-PC version V4.27 (1991)'
_computing_cell_refinement        'Siemens P3/P4-PC version V4.27 (1991)'
_computing_data_reduction         'XDISK in SHELXTL/PC(Sheldrick,1994)'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1997)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'XP in SHELXTL/PC(Sheldrick,1994)'
_computing_publication_material
;
CIFTAB (Sheldrick, 1993), PARST (Nardelli, 1983) and
CSD (Allen, Kennard & Taylor, 1983)
;


_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'w=1/[\s^2^(Fo^2^)+(0.0849P)^2^+0.5293P] 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     mixed
_refine_ls_extinction_method      none
_refine_ls_number_reflns          6179
_refine_ls_number_parameters      507
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0943
_refine_ls_R_factor_gt            0.0498
_refine_ls_wR_factor_ref          0.1306
_refine_ls_wR_factor_gt           0.1101
_refine_ls_goodness_of_fit_ref    0.963
_refine_ls_restrained_S_all       0.963
_refine_ls_shift/su_max           <0.01
_refine_ls_shift/su_mean          <0.01


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_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Hg1A Hg 0.57163(5) 0.82216(4) 0.48033(3) 0.0399(2) Uani 1 d . . .
Hg1B Hg 1.10236(6) 0.86345(5) 0.05888(3) 0.0474(2) Uani 1 d . . .
C1C C 0.6980(15) 0.9854(13) 0.4105(10) 0.049(4) Uani 1 d . . .
C2C C 0.7790(16) 1.0492(13) 0.3491(12) 0.071(5) Uani 1 d . . .
H2CA H 0.7534 1.1282 0.3665 0.106 Uiso 1 calc R . .
H2CB H 0.7643 1.0427 0.2862 0.106 Uiso 1 calc R . .
H2CC H 0.8705 1.0168 0.3557 0.106 Uiso 1 calc R . .
O1C O 0.6778(11) 0.8994(9) 0.3735(7) 0.061(3) Uani 1 d . . .
O2C O 0.6606(10) 1.0104(10) 0.4906(7) 0.063(3) Uani 1 d . . .
C1D C 1.2461(16) 1.0078(11) -0.0187(11) 0.051(4) Uani 1 d . . .
C2D C 1.3346(16) 1.0739(15) -0.0668(12) 0.079(6) Uani 1 d . . .
H2DA H 1.2832 1.1495 -0.0802 0.118 Uiso 1 calc R . .
H2DB H 1.3774 1.0359 -0.1230 0.118 Uiso 1 calc R . .
H2DC H 1.3996 1.0785 -0.0277 0.118 Uiso 1 calc R . .
O1D O 1.2654(14) 0.9714(11) 0.0611(8) 0.089(4) Uani 1 d . . .
O2D O 1.1558(12) 0.9889(10) -0.0598(9) 0.085(4) Uani 1 d . . .
S1E S 0.8659(4) 0.6336(3) 0.5577(2) 0.0442(8) Uani 1 d . . .
O1E O 0.7925(10) 0.6526(8) 0.4798(6) 0.052(2) Uani 1 d . . .
O2E O 0.8138(12) 0.5762(10) 0.6292(6) 0.077(4) Uani 1 d . . .
O3E O 0.9102(11) 0.7292(9) 0.5828(7) 0.067(3) Uani 1 d . . .
O4E O 1.0105(11) 0.5534(9) 0.5159(8) 0.076(3) Uani 1 d . . .
S1F S 1.3256(4) 0.5963(4) -0.0224(2) 0.0515(9) Uani 1 d . . .
O1F O 1.3223(11) 0.7120(10) -0.0051(7) 0.073(3) Uani 1 d . . .
O2F O 1.3138(13) 0.5698(10) -0.1144(6) 0.076(4) Uani 1 d . . .
O3F O 1.2481(12) 0.5520(10) 0.0456(6) 0.072(3) Uani 1 d . . .
O4F O 1.4821(17) 0.5617(5) -0.0058(15) 0.178(9) Uani 1 d D . .
N1A N 0.4857(11) 0.7490(10) 0.3547(7) 0.045(3) Uani 1 d . . .
N2A N 0.4567(10) 0.6920(9) 0.5352(7) 0.038(3) Uani 1 d . . .
N3A N 0.5571(12) 0.8167(9) 0.6403(7) 0.043(3) Uani 1 d . . .
C1A C 0.5080(15) 0.7743(13) 0.2661(9) 0.053(4) Uani 1 d . . .
```

```
H1AA H 0.5583 0.8246 0.2499 0.064 Uiso 1 calc R . .
C2A C 0.4594(18) 0.7288(17) 0.1983(10) 0.076(6) Uani 1 d . . .
H2AA H 0.4741 0.7493 0.1371 0.091 Uiso 1 calc R . .
C3A C 0.3884(16) 0.6521(15) 0.2226(9) 0.064(5) Uani 1 d . . .
H3AA H 0.3544 0.6206 0.1773 0.077 Uiso 1 calc R . .
C4A C 0.3671(14) 0.6213(12) 0.3116(9) 0.048(4) Uani 1 d . . .
H4AA H 0.3214 0.5676 0.3281 0.058 Uiso 1 calc R . .
C5A C 0.4168(13) 0.6736(11) 0.3777(7) 0.038(3) Uani 1 d . . .
C6A C 0.3952(13) 0.6478(11) 0.4775(8) 0.037(3) Uani 1 d . . .
C7A C 0.3119(15) 0.5823(13) 0.5095(9) 0.055(4) Uani 1 d . . .
H7AA H 0.2697 0.5508 0.4693 0.066 Uiso 1 calc R . .
C8A C 0.2935(15) 0.5653(13) 0.6039(9) 0.057(4) Uani 1 d . . .
H8AA H 0.2370 0.5231 0.6279 0.069 Uiso 1 calc R . .
C9A C 0.3596(15) 0.6114(11) 0.6619(9) 0.047(4) Uani 1 d . . .
H9AA H 0.3504 0.5983 0.7249 0.057 Uiso 1 calc R . .
C10A C 0.4406(12) 0.6782(10) 0.6244(7) 0.031(3) Uani 1 d . . .
C11A C 0.5061(14) 0.7383(13) 0.6827(8) 0.043(3) Uani 1 d . . .
C12A C 0.5092(15) 0.7198(14) 0.7753(9) 0.058(4) Uani 1 d . . .
H12A H 0.4728 0.6643 0.8028 0.070 Uiso 1 calc R . .
C13A C 0.562(2) 0.7787(18) 0.8270(11) 0.087(6) Uani 1 d . . .
H13A H 0.5634 0.7657 0.8898 0.104 Uiso 1 calc R . .
C14A C 0.6180(18) 0.8623(17) 0.7825(10) 0.076(6) Uani 1 d . . .
H14A H 0.6560 0.9069 0.8149 0.091 Uiso 1 calc R . .
C15A C 0.6128(16) 0.8737(14) 0.6897(11) 0.065(5) Uani 1 d . . .
H15A H 0.6519 0.9260 0.6594 0.078 Uiso 1 calc R . .
N1B N 1.0236(12) 0.7838(11) -0.0620(7) 0.052(3) Uani 1 d . . .
N2B N 0.9855(11) 0.7397(9) 0.1202(7) 0.039(3) Uani 1 d . . .
N3B N 1.0907(10) 0.8626(10) 0.2219(7) 0.042(3) Uani 1 d . . .
C1B C 1.0506(18) 0.8074(16) -0.1494(10) 0.075(5) Uani 1 d . . .
H1BA H 1.1013 0.8575 -0.1650 0.090 Uiso 1 calc R . .
C2B C 1.0032(17) 0.7568(15) -0.2201(10) 0.065(5) Uani 1 d . . .
H2BA H 1.0168 0.7774 -0.2813 0.079 Uiso 1 calc R . .
C3B C 0.938(2) 0.6780(16) -0.1954(10) 0.077(6) Uani 1 d . . .
H3BA H 0.9107 0.6404 -0.2406 0.092 Uiso 1 calc R . .
C4B C 0.9110(17) 0.6529(13) -0.1046(9) 0.061(4) Uani 1 d . . .
H4BA H 0.8641 0.6002 -0.0879 0.073 Uiso 1 calc R . .
C5B C 0.9559(13) 0.7084(12) -0.0369(9) 0.044(3) Uani 1 d . . .
C6B C 0.9331(15) 0.6865(12) 0.0632(9) 0.045(3) Uani 1 d . . .
C7B C 0.8568(15) 0.6144(13) 0.0977(9) 0.053(4) Uani 1 d . . .
H7BA H 0.8200 0.5767 0.0583 0.064 Uiso 1 calc R . .
C8B C 0.8381(18) 0.6010(14) 0.1906(10) 0.071(5) Uani 1 d . . .
H8BA H 0.7883 0.5531 0.2149 0.085 Uiso 1 calc R . .
C9B C 0.8919(17) 0.6572(14) 0.2486(9) 0.062(5) Uani 1 d . . .
H9BA H 0.8780 0.6489 0.3120 0.074 Uiso 1 calc R . .
C10B C 0.9676(15) 0.7268(12) 0.2107(9) 0.045(4) Uani 1 d . . .
C11B C 1.0319(13) 0.7911(12) 0.2669(8) 0.041(3) Uani 1 d . . .
C12B C 1.0281(15) 0.7800(13) 0.3615(9) 0.055(4) Uani 1 d . . .
H12B H 0.9882 0.7279 0.3911 0.066 Uiso 1 calc R . .
C13B C 1.0808(16) 0.8428(14) 0.4114(9) 0.057(4) Uani 1 d . . .
H13B H 1.0734 0.8375 0.4752 0.068 Uiso 1 calc R . .
C14B C 1.1460(15) 0.9156(14) 0.3667(9) 0.055(4) Uani 1 d . . .
H14B H 1.1873 0.9577 0.3988 0.066 Uiso 1 calc R . .
C15B C 1.1476(15) 0.9234(13) 0.2699(9) 0.054(4) Uani 1 d . . .
H15B H 1.1898 0.9728 0.2385 0.065 Uiso 1 calc R . .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
```

```
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
Hg1A 0.0372(4) 0.0423(3) 0.0398(3) -0.0007(2) -0.0026(2) -0.0108(3)
Hg1B 0.0534(5) 0.0514(4) 0.0399(3) 0.0049(3) -0.0068(3) -0.0184(3)
C1C 0.035(10) 0.046(9) 0.066(9) 0.001(7) -0.006(7) -0.007(7)
C2C 0.040(11) 0.049(9) 0.115(14) 0.007(9) 0.009(9) -0.007(8)
O1C 0.070(8) 0.056(7) 0.060(6) 0.001(5) 0.001(5) -0.024(6)
O2C 0.047(7) 0.078(8) 0.059(6) -0.005(5) -0.008(5) -0.008(6)
C1D 0.049(11) 0.030(7) 0.066(9) -0.020(7) 0.014(8) -0.002(7)
C2D 0.042(11) 0.083(13) 0.115(14) 0.041(11) -0.010(10) -0.029(10)
O1D 0.105(11) 0.088(9) 0.062(7) 0.015(7) 0.003(7) -0.012(8)
O2D 0.055(9) 0.063(8) 0.134(11) -0.036(7) -0.014(8) -0.007(7)
S1E 0.046(2) 0.046(2) 0.0397(17) -0.0007(14) -0.0078(15) -0.0090(18)
O1E 0.052(7) 0.053(6) 0.049(5) -0.004(4) -0.015(5) -0.006(5)
O2E 0.107(10) 0.101(9) 0.041(5) 0.013(6) -0.002(6) -0.060(8)
O3E 0.079(9) 0.062(7) 0.063(6) -0.007(5) -0.004(6) -0.028(7)
O4E 0.046(8) 0.057(7) 0.123(9) -0.024(6) -0.029(6) -0.001(6)
S1F 0.038(2) 0.067(3) 0.0438(18) -0.0050(17) -0.0041(16) -0.004(2)
O1F 0.068(9) 0.075(8) 0.074(7) -0.028(6) -0.009(6) -0.012(7)
O2F 0.121(11) 0.074(7) 0.041(5) -0.013(5) 0.004(6) -0.045(8)
O3F 0.087(9) 0.102(9) 0.045(5) 0.001(6) 0.001(5) -0.058(8)
O4F 0.090(13) 0.17(2) 0.25(2) 0.111(18) 0.009(13) -0.031(14)
N1A 0.036(8) 0.054(7) 0.047(6) 0.006(5) -0.006(5) -0.017(6)
N2A 0.029(7) 0.040(6) 0.044(6) 0.008(5) -0.007(5) -0.008(5)
N3A 0.059(8) 0.032(6) 0.042(6) -0.006(5) -0.010(5) -0.018(6)
C1A 0.046(10) 0.072(10) 0.047(8) 0.005(7) -0.007(7) -0.024(9)
C2A 0.090(15) 0.112(15) 0.035(8) 0.010(9) -0.011(8) -0.044(13)
C3A 0.056(12) 0.085(12) 0.042(8) -0.011(8) -0.007(7) -0.003(10)
C4A 0.037(9) 0.049(9) 0.058(8) -0.005(7) -0.012(7) -0.010(7)
C5A 0.032(8) 0.049(8) 0.026(6) -0.010(5) 0.006(5) 0.000(7)
C6A 0.030(8) 0.047(8) 0.035(6) 0.001(6) -0.008(5) -0.011(7)
C7A 0.060(11) 0.068(10) 0.041(7) -0.006(7) -0.008(7) -0.021(9)
C8A 0.059(11) 0.071(11) 0.048(8) 0.003(7) 0.000(7) -0.030(9)
C9A 0.064(11) 0.044(8) 0.039(7) 0.007(6) -0.015(7) -0.018(8)
C10A 0.024(8) 0.033(7) 0.032(6) 0.004(5) -0.003(5) -0.002(6)
C11A 0.031(9) 0.060(9) 0.034(6) -0.003(6) -0.009(6) -0.003(7)
C12A 0.055(11) 0.088(12) 0.043(7) 0.008(8) -0.010(7) -0.038(10)
C13A 0.101(17) 0.123(17) 0.053(9) -0.010(10) -0.013(10) -0.056(15)
C14A 0.083(14) 0.116(16) 0.047(9) -0.003(9) -0.005(8) -0.058(13)
C15A 0.056(12) 0.071(11) 0.076(11) -0.024(9) 0.009(8) -0.037(10)
N1B 0.049(9) 0.065(8) 0.038(6) 0.002(6) -0.008(6) -0.005(7)
N2B 0.034(7) 0.033(6) 0.040(6) -0.004(5) 0.001(5) 0.004(5)
N3B 0.023(7) 0.054(7) 0.049(6) -0.012(5) 0.002(5) -0.011(6)
C1B 0.090(15) 0.104(14) 0.043(8) 0.013(9) -0.010(9) -0.046(12)
C2B 0.056(12) 0.085(13) 0.046(8) 0.005(8) -0.005(8) -0.005(10)
C3B 0.113(17) 0.084(13) 0.044(8) 0.000(8) -0.025(9) -0.038(13)
C4B 0.084(13) 0.059(10) 0.044(8) -0.003(7) -0.014(8) -0.026(10)
C5B 0.031(9) 0.050(9) 0.047(7) 0.004(6) -0.016(6) -0.002(7)
C6B 0.045(10) 0.040(8) 0.048(8) -0.009(6) -0.011(7) -0.004(7)
C7B 0.056(11) 0.055(9) 0.053(8) -0.004(7) -0.011(7) -0.019(8)
C8B 0.108(16) 0.076(12) 0.051(8) 0.012(8) -0.015(9) -0.059(12)
C9B 0.077(13) 0.074(11) 0.039(7) -0.005(7) 0.008(7) -0.035(10)
C10B 0.055(10) 0.041(8) 0.039(7) -0.011(6) -0.011(7) -0.011(7)
C11B 0.023(8) 0.054(9) 0.039(7) -0.001(6) -0.002(6) 0.000(7)
C12B 0.053(11) 0.058(9) 0.049(8) 0.003(7) -0.009(7) -0.006(8)
C13B 0.067(12) 0.075(11) 0.030(6) 0.007(7) -0.011(7) -0.020(9)
C14B 0.037(10) 0.078(11) 0.056(8) -0.014(8) -0.021(7) -0.018(9)
C15B 0.045(10) 0.062(10) 0.056(8) -0.003(7) -0.002(7) -0.018(8)

_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.
;

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_distance
 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
Hg1A O1C 2.172(9) . ?
Hg1A N3A 2.331(10) . ?
Hg1A N2A 2.334(10) . ?
Hg1A N1A 2.438(11) . ?
Hg1B N2B 2.311(11) . ?
Hg1B N3B 2.376(10) . ?
Hg1B N1B 2.380(12) . ?
Hg1B O2D 2.406(13) . ?
Hg1B O1D 2.456(14) . ?
Hg1B O1F 2.644(12) . ?
C1C O2C 1.216(17) . ?
C1C O1C 1.275(17) . ?
C1C C2C 1.521(19) . ?
C1D O1D 1.256(17) . ?
C1D O2D 1.266(18) . ?
C1D C2D 1.508(19) . ?
S1E O2E 1.391(9) . ?
S1E O1E 1.432(9) . ?
S1E O3E 1.444(11) . ?
S1E O4E 1.640(12) . ?
O4E O4E 1.48(2) 2_766 ?
S1F O3F 1.413(10) . ?
S1F O2F 1.421(10) . ?
S1F O1F 1.430(11) . ?
S1F O4F 1.647(19) . ?
O4F O4F 1.455(10) 2_865 ?
N1A C1A 1.334(15) . ?
N1A C5A 1.342(16) . ?
N2A C10A 1.309(14) . ?
N2A C6A 1.334(16) . ?
N3A C15A 1.309(17) . ?
N3A C11A 1.331(16) . ?
C1A C2A 1.37(2) . ?
C2A C3A 1.37(2) . ?
C3A C4A 1.357(19) . ?
C4A C5A 1.400(17) . ?
C5A C6A 1.492(15) . ?
C6A C7A 1.387(18) . ?
C7A C8A 1.391(17) . ?
C8A C9A 1.384(19) . ?
C9A C10A 1.403(17) . ?
C10A C11A 1.486(18) . ?
C11A C12A 1.370(17) . ?
C12A C13A 1.33(2) . ?
C13A C14A 1.42(2) . ?
C14A C15A 1.37(2) . ?
N1B C1B 1.320(17) . ?
```

```
N1B C5B 1.337(17) . ?
N2B C10B 1.327(15) . ?
N2B C6B 1.329(16) . ?
N3B C11B 1.328(16) . ?
N3B C15B 1.337(17) . ?
C1B C2B 1.43(2) . ?
C2B C3B 1.35(2) . ?
C3B C4B 1.37(2) . ?
C4B C5B 1.412(19) . ?
C5B C6B 1.487(18) . ?
C6B C7B 1.403(19) . ?
C7B C8B 1.364(18) . ?
C8B C9B 1.37(2) . ?
C9B C10B 1.389(19) . ?
C10B C11B 1.492(18) . ?
C11B C12B 1.384(17) . ?
C12B C13B 1.34(2) . ?
C13B C14B 1.38(2) . ?
C14B C15B 1.415(18) . ?

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
O1C Hg1A N3A 134.8(4) . . ?
O1C Hg1A N2A 153.6(4) . . ?
N3A Hg1A N2A 70.5(4) . . ?
O1C Hg1A N1A 85.6(4) . . ?
N3A Hg1A N1A 139.5(4) . . ?
N2A Hg1A N1A 69.4(4) . . ?
N2B Hg1B N3B 69.6(4) . . ?
N2B Hg1B N1B 70.7(4) . . ?
N3B Hg1B N1B 140.2(4) . . ?
N2B Hg1B O2D 152.3(4) . . ?
N3B Hg1B O2D 134.5(4) . . ?
N1B Hg1B O2D 83.8(4) . . ?
N2B Hg1B O1D 153.8(4) . . ?
N3B Hg1B O1D 86.5(4) . . ?
N1B Hg1B O1D 133.0(4) . . ?
O2D Hg1B O1D 53.8(4) . . ?
N2B Hg1B O1F 99.0(4) . . ?
N3B Hg1B O1F 108.0(4) . . ?
N1B Hg1B O1F 80.6(4) . . ?
O2D Hg1B O1F 86.6(4) . . ?
O1D Hg1B O1F 77.9(4) . . ?
O2C C1C O1C 121.8(14) . . ?
O2C C1C C2C 122.8(15) . . ?
O1C C1C C2C 115.2(14) . . ?
C1C O1C Hg1A 106.1(9) . . ?
O1D C1D O2D 121.6(15) . . ?
O1D C1D C2D 118.8(16) . . ?
O2D C1D C2D 119.5(15) . . ?
C1D O1D Hg1B 91.0(10) . . ?
C1D O2D Hg1B 93.1(10) . . ?
O2E S1E O1E 113.5(7) . . ?
O2E S1E O3E 116.7(6) . . ?
O1E S1E O3E 114.9(6) . . ?
```

```
O2E S1E O4E 109.4(7) . . ?
O1E S1E O4E 103.2(6) . . ?
O3E S1E O4E 96.5(6) . . ?
O4E O4E S1E 106.6(11) 2_766 . ?
O3F S1F O2F 114.9(7) . . ?
O3F S1F O1F 112.9(7) . . ?
O2F S1F O1F 116.2(6) . . ?
O3F S1F O4F 113.0(8) . . ?
O2F S1F O4F 109.4(9) . . ?
O1F S1F O4F 87.2(6) . . ?
S1F O1F Hg1B 121.5(7) . . ?
O4F O4F S1F 104.5(17) 2_865 . ?
C1A N1A C5A 118.8(11) . . ?
C1A N1A Hg1A 124.9(9) . . ?
C5A N1A Hg1A 116.2(8) . . ?
C10A N2A C6A 122.6(11) . . ?
C10A N2A Hg1A 117.2(9) . . ?
C6A N2A Hg1A 119.5(8) . . ?
C15A N3A C11A 117.7(12) . . ?
C15A N3A Hg1A 124.0(9) . . ?
C11A N3A Hg1A 117.5(8) . . ?
N1A C1A C2A 122.3(14) . . ?
C1A C2A C3A 118.4(13) . . ?
C4A C3A C2A 121.2(15) . . ?
C3A C4A C5A 117.3(14) . . ?
N1A C5A C4A 121.9(11) . . ?
N1A C5A C6A 116.8(11) . . ?
C4A C5A C6A 121.3(12) . . ?
N2A C6A C7A 121.1(11) . . ?
N2A C6A C5A 117.7(11) . . ?
C7A C6A C5A 121.2(11) . . ?
C6A C7A C8A 117.7(13) . . ?
C9A C8A C7A 119.9(13) . . ?
C8A C9A C10A 119.0(11) . . ?
N2A C10A C9A 119.7(12) . . ?
N2A C10A C11A 118.1(11) . . ?
C9A C10A C11A 122.2(10) . . ?
N3A C11A C12A 121.1(13) . . ?
N3A C11A C10A 115.8(10) . . ?
C12A C11A C10A 123.1(13) . . ?
C13A C12A C11A 122.0(15) . . ?
C12A C13A C14A 117.5(15) . . ?
C15A C14A C13A 116.6(16) . . ?
N3A C15A C14A 125.0(15) . . ?
C1B N1B C5B 121.4(13) . . ?
C1B N1B Hg1B 122.4(11) . . ?
C5B N1B Hg1B 116.1(8) . . ?
C10B N2B C6B 121.6(12) . . ?
C10B N2B Hg1B 119.9(9) . . ?
C6B N2B Hg1B 118.4(8) . . ?
C11B N3B C15B 118.5(11) . . ?
C11B N3B Hg1B 117.4(8) . . ?
C15B N3B Hg1B 123.9(9) . . ?
N1B C1B C2B 120.8(15) . . ?
C3B C2B C1B 118.1(14) . . ?
C2B C3B C4B 120.8(16) . . ?
C3B C4B C5B 118.9(15) . . ?
N1B C5B C4B 119.9(12) . . ?
N1B C5B C6B 117.0(12) . . ?
C4B C5B C6B 123.1(13) . . ?
N2B C6B C7B 120.3(12) . . ?
```

```
N2B C6B C5B 117.8(12) . . ?
C7B C6B C5B 121.9(13) . . ?
C8B C7B C6B 118.2(13) . . ?
C7B C8B C9B 120.8(14) . . ?
C8B C9B C10B 118.6(13) . . ?
N2B C10B C9B 120.5(13) . . ?
N2B C10B C11B 116.2(12) . . ?
C9B C10B C11B 123.3(12) . . ?
N3B C11B C12B 121.1(13) . . ?
N3B C11B C10B 116.5(11) . . ?
C12B C11B C10B 122.3(13) . . ?
C13B C12B C11B 121.4(14) . . ?
C12B C13B C14B 119.0(12) . . ?
C13B C14B C15B 117.3(13) . . ?
N3B C15B C14B 122.6(13) . . ?

loop_
 _geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag
O2C C1C O1C Hg1A 0.2(18) . . . . ?
C2C C1C O1C Hg1A 176.5(10) . . . . ?
N3A Hg1A O1C C1C -26.2(12) . . . . ?
N2A Hg1A O1C C1C 173.3(9) . . . . ?
N1A Hg1A O1C C1C 154.4(10) . . . . ?
O2D C1D O1D Hg1B 6.6(15) . . . . ?
C2D C1D O1D Hg1B -172.4(12) . . . . ?
N2B Hg1B O1D C1D 176.8(8) . . . . ?
N3B Hg1B O1D C1D -159.7(9) . . . . ?
N1B Hg1B O1D C1D 26.4(12) . . . . ?
O2D Hg1B O1D C1D -3.7(8) . . . . ?
O1F Hg1B O1D C1D 91.0(9) . . . . ?
O1D C1D O2D Hg1B -6.8(15) . . . . ?
C2D C1D O2D Hg1B 172.2(12) . . . . ?
N2B Hg1B O2D C1D -176.8(8) . . . . ?
N3B Hg1B O2D C1D 38.2(11) . . . . ?
N1B Hg1B O2D C1D -154.7(9) . . . . ?
O1D Hg1B O2D C1D 3.7(8) . . . . ?
O1F Hg1B O2D C1D -73.8(9) . . . . ?
O2E S1E O4E O4E 59.0(13) . . . 2_766 ?
O1E S1E O4E O4E -62.2(12) . . . 2_766 ?
O3E S1E O4E O4E -179.7(11) . . . 2_766 ?
O3F S1F O1F Hg1B -40.0(9) . . . . ?
O2F S1F O1F Hg1B 95.9(9) . . . . ?
O4F S1F O1F Hg1B -153.9(9) . . . . ?
N2B Hg1B O1F S1F 20.5(7) . . . . ?
N3B Hg1B O1F S1F 91.8(7) . . . . ?
N1B Hg1B O1F S1F -48.1(7) . . . . ?
O2D Hg1B O1F S1F -132.3(7) . . . . ?
O1D Hg1B O1F S1F 174.0(8) . . . . ?
O3F S1F O4F O4F 52(2) . . . 2_865 ?
O2F S1F O4F O4F -78(2) . . . 2_865 ?
O1F S1F O4F O4F 165(2) . . . 2_865 ?
O1C Hg1A N1A C1A -5.0(12) . . . . ?
```

```
N3A Hg1A N1A C1A 175.6(11) . . . . ?
N2A Hg1A N1A C1A -176.2(13) . . . . ?
O1C Hg1A N1A C5A 171.5(10) . . . . ?
N3A Hg1A N1A C5A -7.9(12) . . . . ?
N2A Hg1A N1A C5A 0.3(9) . . . . ?
O1C Hg1A N2A C10A 165.0(9) . . . . ?
N3A Hg1A N2A C10A -0.5(9) . . . . ?
N1A Hg1A N2A C10A -174.8(10) . . . . ?
O1C Hg1A N2A C6A -24.4(15) . . . . ?
N3A Hg1A N2A C6A 170.2(11) . . . . ?
N1A Hg1A N2A C6A -4.1(10) . . . . ?
O1C Hg1A N3A C15A 5.2(15) . . . . ?
N2A Hg1A N3A C15A 176.2(13) . . . . ?
N1A Hg1A N3A C15A -175.6(11) . . . . ?
O1C Hg1A N3A C11A -164.3(9) . . . . ?
N2A Hg1A N3A C11A 6.7(9) . . . . ?
N1A Hg1A N3A C11A 14.9(13) . . . . ?
C5A N1A C1A C2A 2(2) . . . . ?
Hg1A N1A C1A C2A 178.6(13) . . . . ?
N1A C1A C2A C3A -2(3) . . . . ?
C1A C2A C3A C4A 0(3) . . . . ?
C2A C3A C4A C5A 2(2) . . . . ?
C1A N1A C5A C4A 0(2) . . . . ?
Hg1A N1A C5A C4A -177.1(10) . . . . ?
C1A N1A C5A C6A 179.7(13) . . . . ?
Hg1A N1A C5A C6A 3.0(15) . . . . ?
C3A C4A C5A N1A -2(2) . . . . ?
C3A C4A C5A C6A 178.3(13) . . . . ?
C10A N2A C6A C7A -1(2) . . . . ?
Hg1A N2A C6A C7A -171.4(10) . . . . ?
C10A N2A C6A C5A 177.4(11) . . . . ?
Hg1A N2A C6A C5A 7.2(16) . . . . ?
N1A C5A C6A N2A -6.7(18) . . . . ?
C4A C5A C6A N2A 173.3(13) . . . . ?
N1A C5A C6A C7A 171.9(13) . . . . ?
C4A C5A C6A C7A -8(2) . . . . ?
N2A C6A C7A C8A 1(2) . . . . ?
C5A C6A C7A C8A -177.9(14) . . . . ?
C6A C7A C8A C9A -1(2) . . . . ?
C7A C8A C9A C10A 2(2) . . . . ?
C6A N2A C10A C9A 2.2(19) . . . . ?
Hg1A N2A C10A C9A 172.6(9) . . . . ?
C6A N2A C10A C11A -175.5(12) . . . . ?
Hg1A N2A C10A C11A -5.2(15) . . . . ?
C8A C9A C10A N2A -3(2) . . . . ?
C8A C9A C10A C11A 174.9(13) . . . . ?
C15A N3A C11A C12A 2(2) . . . . ?
Hg1A N3A C11A C12A 171.7(11) . . . . ?
C15A N3A C11A C10A 178.3(13) . . . . ?
Hg1A N3A C11A C10A -11.5(15) . . . . ?
N2A C10A C11A N3A 11.2(18) . . . . ?
C9A C10A C11A N3A -166.5(12) . . . . ?
N2A C10A C11A C12A -172.1(13) . . . . ?
C9A C10A C11A C12A 10(2) . . . . ?
N3A C11A C12A C13A 0(3) . . . . ?
C10A C11A C12A C13A -176.5(16) . . . . ?
C11A C12A C13A C14A 0(3) . . . . ?
C12A C13A C14A C15A -1(3) . . . . ?
C11A N3A C15A C14A -3(3) . . . . ?
Hg1A N3A C15A C14A -172.3(14) . . . . ?
C13A C14A C15A N3A 2(3) . . . . ?
```

```
N2B Hg1B N1B C1B -177.7(14) . . . . ?
N3B Hg1B N1B C1B 178.6(12) . . . . ?
O2D Hg1B N1B C1B 13.0(13) . . . . ?
O1D Hg1B N1B C1B -11.0(16) . . . . ?
O1F Hg1B N1B C1B -74.6(13) . . . . ?
N2B Hg1B N1B C5B -1.3(9) . . . . ?
N3B Hg1B N1B C5B -5.0(13) . . . . ?
O2D Hg1B N1B C5B -170.6(10) . . . . ?
O1D Hg1B N1B C5B 165.4(9) . . . . ?
O1F Hg1B N1B C5B 101.8(10) . . . . ?
N3B Hg1B N2B C10B 0.0(10) . . . . ?
N1B Hg1B N2B C10B -177.4(11) . . . . ?
O2D Hg1B N2B C10B -154.0(10) . . . . ?
O1D Hg1B N2B C10B 25.1(15) . . . . ?
O1F Hg1B N2B C10B 106.0(10) . . . . ?
N3B Hg1B N2B C6B 177.3(11) . . . . ?
N1B Hg1B N2B C6B -0.1(10) . . . . ?
O2D Hg1B N2B C6B 23.3(15) . . . . ?
O1D Hg1B N2B C6B -157.6(10) . . . . ?
O1F Hg1B N2B C6B -76.7(10) . . . . ?
N2B Hg1B N3B C11B 3.2(9) . . . . ?
N1B Hg1B N3B C11B 7.0(13) . . . . ?
O2D Hg1B N3B C11B 166.7(9) . . . . ?
O1D Hg1B N3B C11B -166.0(10) . . . . ?
O1F Hg1B N3B C11B -89.9(10) . . . . ?
N2B Hg1B N3B C15B 178.3(12) . . . . ?
N1B Hg1B N3B C15B -177.9(10) . . . . ?
O2D Hg1B N3B C15B -18.2(14) . . . . ?
O1D Hg1B N3B C15B 9.1(11) . . . . ?
O1F Hg1B N3B C15B 85.2(12) . . . . ?
C5B N1B C1B C2B 3(3) . . . . ?
Hg1B N1B C1B C2B 179.1(12) . . . . ?
N1B C1B C2B C3B -5(3) . . . . ?
C1B C2B C3B C4B 4(3) . . . . ?
C2B C3B C4B C5B -2(3) . . . . ?
C1B N1B C5B C4B -1(2) . . . . ?
Hg1B N1B C5B C4B -177.0(11) . . . . ?
C1B N1B C5B C6B 178.8(15) . . . . ?
Hg1B N1B C5B C6B 2.4(16) . . . . ?
C3B C4B C5B N1B 0(2) . . . . ?
C3B C4B C5B C6B -179.5(15) . . . . ?
C10B N2B C6B C7B 0(2) . . . . ?
Hg1B N2B C6B C7B -177.4(10) . . . . ?
C10B N2B C6B C5B 178.6(13) . . . . ?
Hg1B N2B C6B C5B 1.4(16) . . . . ?
N1B C5B C6B N2B -2.5(19) . . . . ?
C4B C5B C6B N2B 176.8(14) . . . . ?
N1B C5B C6B C7B 176.1(13) . . . . ?
C4B C5B C6B C7B -5(2) . . . . ?
N2B C6B C7B C8B 0(2) . . . . ?
C5B C6B C7B C8B -178.5(15) . . . . ?
C6B C7B C8B C9B 0(3) . . . . ?
C7B C8B C9B C10B -1(3) . . . . ?
C6B N2B C10B C9B 0(2) . . . . ?
Hg1B N2B C10B C9B 176.7(11) . . . . ?
C6B N2B C10B C11B 179.9(12) . . . . ?
Hg1B N2B C10B C11B -2.9(17) . . . . ?
C8B C9B C10B N2B 1(2) . . . . ?
C8B C9B C10B C11B -179.4(15) . . . . ?
C15B N3B C11B C12B 1(2) . . . . ?
Hg1B N3B C11B C12B 175.9(11) . . . . ?
```

```
C15B N3B C11B C10B 178.8(13) . . . . ?
Hg1B N3B C11B C10B -5.8(15) . . . . ?
N2B C10B C11B N3B 5.8(19) . . . . ?
C9B C10B C11B N3B -173.8(14) . . . . ?
N2B C10B C11B C12B -175.9(13) . . . . ?
C9B C10B C11B C12B 4(2) . . . . ?
N3B C11B C12B C13B 2(2) . . . . ?
C10B C11B C12B C13B -176.6(14) . . . . ?
C11B C12B C13B C14B -3(2) . . . . ?
C12B C13B C14B C15B 3(2) . . . . ?
C11B N3B C15B C14B -1(2) . . . . ?
Hg1B N3B C15B C14B -175.9(11) . . . . ?
C13B C14B C15B N3B -1(2) . . . . ?

_diffrn_measured_fraction_theta_max    0.926
_diffrn_reflns_theta_full              25.05
_diffrn_measured_fraction_theta_full   0.926
_refine_diff_density_max    1.539
_refine_diff_density_min   -1.495
_refine_diff_density_rms    0.181


################################################################################
```