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#     2 = compound (3)
#     3 = compound (4)
#     4 = compound (5)
#     5 = compound (6)
#     separated by #===END
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_publ_contact_author
;
  Dr. Enrique O\~nate
  Departamento de Qu\'imica Inorg\'anica - I.C.M.A.
  Facultad de Ciencias
  Universidad de Zaragoza - C.S.I.C.
  50009 Zaragoza, Spain
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_publ_contact_author_email        enriqueo@unizar.es

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#Publication details

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                      'Castro-Rodrigo, R.'
                      'Esteruelas, M. A.'
                      'L\'opez, A. M.'
                      'Oliv\'an, M.'
                      'O\~nate, E.'

 _publ_requested_journal            'Organometallics'
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;
Organometallics
;
_publ_section_title
;
Structure, and Theoretical Investigation of Hydride-, Dihydrogen-,
and Acetone-OsTp Complexes: A Hydridotris(pyrazolyl)borate
 - Cyclopentadienyl Comparison
;
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May ##, 2007
Please consider this CIF submission as supplementary material of
the structures contained in the paper:

Structure, and Theoretical Investigation of Hydride-, Dihydrogen-,
and Acetone-OsTp Complexes: A Hydridotris(pyrazolyl)borate
 - Cyclopentadienyl Comparison

that is submitted to Organometallics for publication.
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_journal_page_last   ?
_journal_year        ?



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method of Blessing: Blessing, R. H., Acta Crystallogr., Sect. A 1995, 51, 33.

SADABS: Area-Detector Absorption Correction. Bruker-AXS
within SAINT package, v. 6.1 (2000).
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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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H1B H 0.269(4) 0.223(3) 0.5922(13) 0.050 Uiso 1 1 d D . .
H1C H 0.139(2) 0.246(3) 0.538(3) 0.043(15) Uiso 1 1 d D . .
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P2 P 0.23862(11) 0.12097(8) 0.46576(9) 0.0186(3) Uani 1 1 d . D .
B B 0.2313(4) 0.2543(4) 0.2462(3) 0.0200(12) Uani 1 1 d . . .
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N2 N 0.3387(3) 0.2842(2) 0.2950(3) 0.0180(10) Uani 1 1 d . . .
N3 N 0.1229(3) 0.2832(2) 0.3816(3) 0.0183(10) Uani 1 1 d . . .
N4 N 0.1350(3) 0.2922(2) 0.2894(3) 0.0196(10) Uani 1 1 d . . .
N5 N 0.2231(4) 0.3394(3) 0.1058(3) 0.0315(12) Uani 1 1 d . . .
N6 N 0.2292(3) 0.2692(2) 0.1438(3) 0.0214(11) Uani 1 1 d . . .
C1 C 0.4676(4) 0.2932(3) 0.4034(4) 0.0224(12) Uani 1 1 d . . .
H1 H 0.5065 0.2920 0.4624 0.027 Uiso 1 1 calc R . .
C2 C 0.5117(4) 0.3125(3) 0.3218(3) 0.0244(13) Uani 1 1 d . . .
H2 H 0.5836 0.3269 0.3139 0.029 Uiso 1 1 calc R . .
C3 C 0.4273(4) 0.3061(3) 0.2557(3) 0.0238(13) Uani 1 1 d . . .
H3 H 0.4308 0.3156 0.1919 0.029 Uiso 1 1 calc R . .
C4 C 0.0234(4) 0.3066(3) 0.3933(4) 0.0235(13) Uani 1 1 d . . .
H4 H -0.0073 0.3071 0.4508 0.028 Uiso 1 1 calc R . .
C5 C -0.0288(4) 0.3300(3) 0.3112(4) 0.0287(14) Uani 1 1 d . . .
H5 H -0.1001 0.3487 0.3010 0.034 Uiso 1 1 calc R . .
C6 C 0.0445(4) 0.3204(3) 0.2475(4) 0.0266(13) Uani 1 1 d . . .
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C7 C 0.2492(4) 0.2170(4) 0.0793(4) 0.0307(14) Uani 1 1 d . . .
H7 H 0.2570 0.1646 0.0891 0.037 Uiso 1 1 calc R . .
C8 C 0.2377(4) 0.3292(4) 0.0177(4) 0.0391(17) Uani 1 1 d . . .
H8 H 0.2358 0.3684 -0.0264 0.047 Uiso 1 1 calc R . .
C9 C 0.2561(4) 0.2546(5) -0.0031(3) 0.0455(17) Uani 1 1 d . . .
H9 H 0.2703 0.2339 -0.0609 0.055 Uiso 1 1 calc R . .
C10 C 0.1954(6) 0.4473(3) 0.4771(4) 0.057(2) Uani 1 1 d D . .
H10 H 0.1253 0.4237 0.4548 0.069 Uiso 1 1 calc R A 1
C11A C 0.2426(12) 0.4655(9) 0.3890(8) 0.022(3) Uiso 0.50 1 d PD B 1
H11A H 0.3068 0.4967 0.4020 0.033 Uiso 0.50 1 calc PR B 1
H11B H 0.1896 0.4927 0.3482 0.033 Uiso 0.50 1 calc PR B 1
H11C H 0.2626 0.4190 0.3590 0.033 Uiso 0.50 1 calc PR B 1
C11B C 0.2687(13) 0.4646(12) 0.4014(10) 0.054(6) Uiso 0.50 1 d PD B 2
H11D H 0.2852 0.4182 0.3696 0.080 Uiso 0.50 1 calc PR B 2
H11E H 0.3356 0.4872 0.4287 0.080 Uiso 0.50 1 calc PR B 2
H11F H 0.2325 0.4996 0.3572 0.080 Uiso 0.50 1 calc PR B 2
C12A C 0.1582(16) 0.5136(8) 0.5399(10) 0.070 Uiso 0.50 1 d PD B 1
H12A H 0.1292 0.4927 0.5947 0.105 Uiso 0.50 1 calc PR B 1
H12B H 0.1026 0.5432 0.5050 0.105 Uiso 0.50 1 calc PR B 1
H12C H 0.2200 0.5456 0.5586 0.105 Uiso 0.50 1 calc PR B 1
C12B C 0.1581(14) 0.5248(6) 0.5116(9) 0.048 Uiso 0.50 1 d PD B 2
H12D H 0.1103 0.5174 0.5608 0.072 Uiso 0.50 1 calc PR B 2
H12E H 0.1195 0.5519 0.4604 0.072 Uiso 0.50 1 calc PR B 2
H12F H 0.2210 0.5540 0.5354 0.072 Uiso 0.50 1 calc PR B 2
C13 C 0.4011(5) 0.4113(4) 0.5757(5) 0.0503(19) Uani 1 1 d . . .
H13 H 0.4331 0.4116 0.5151 0.060 Uiso 1 1 calc R B .
C14 C 0.4736(5) 0.3592(4) 0.6392(4) 0.0457(18) Uani 1 1 d . B .
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H14A H 0.5492 0.3687 0.6298 0.069 Uiso 1 1 calc R . .
H14B H 0.4560 0.3069 0.6243 0.069 Uiso 1 1 calc R . .
H14C H 0.4614 0.3691 0.7036 0.069 Uiso 1 1 calc R . .
C15 C 0.4089(6) 0.4923(4) 0.6111(6) 0.076(3) Uani 1 1 d . B .
H15A H 0.3721 0.4964 0.6677 0.060 Uiso 1 1 calc R . .
H15B H 0.3749 0.5260 0.5642 0.060 Uiso 1 1 calc R . .
H15C H 0.4847 0.5060 0.6241 0.060 Uiso 1 1 calc R . .
C16 C 0.1950(5) 0.3849(4) 0.6611(4) 0.060(2) Uani 1 1 d D . .
H16 H 0.2071 0.4379 0.6818 0.072 Uiso 1 1 calc R B 1
C17A C 0.0698(7) 0.3752(11) 0.6336(13) 0.055(6) Uiso 0.60 1 d PD B 1
H17A H 0.0510 0.3220 0.6349 0.082 Uiso 0.60 1 calc PR B 1
H17B H 0.0520 0.3950 0.5714 0.082 Uiso 0.60 1 calc PR B 1
H17C H 0.0292 0.4026 0.6774 0.082 Uiso 0.60 1 calc PR B 1
C17B C 0.0735(8) 0.3644(13) 0.6521(16) 0.029(5) Uiso 0.40 1 d PD B 2
H17D H 0.0651 0.3111 0.6370 0.044 Uiso 0.40 1 calc PR B 2
H17E H 0.0359 0.3945 0.6032 0.044 Uiso 0.40 1 calc PR B 2
H17F H 0.0429 0.3745 0.7106 0.044 Uiso 0.40 1 calc PR B 2
C18A C 0.2364(12) 0.3338(8) 0.7418(8) 0.028(4) Uiso 0.50 1 d PD B 1
H18A H 0.1923 0.3412 0.7936 0.042 Uiso 0.50 1 calc PR B 1
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H18C H 0.2317 0.2814 0.7220 0.042 Uiso 0.50 1 calc PR B 1
C18B C 0.2669(14) 0.3371(10) 0.7355(11) 0.063(7) Uiso 0.50 1 d PD B 2
H18D H 0.2577 0.3563 0.7973 0.094 Uiso 0.50 1 calc PR B 2
H18E H 0.3427 0.3410 0.7233 0.094 Uiso 0.50 1 calc PR B 2
H18F H 0.2445 0.2845 0.7316 0.094 Uiso 0.50 1 calc PR B 2
C19 C 0.1300(4) 0.0834(3) 0.3816(4) 0.0259(13) Uani 1 1 d . . .
H19 H 0.1370 0.1112 0.3229 0.031 Uiso 1 1 calc R . .
C20 C 0.1354(4) 0.0000(3) 0.3566(4) 0.0289(14) Uani 1 1 d . . .
H20A H 0.1186 -0.0304 0.4095 0.043 Uiso 1 1 calc R . .
H20B H 0.2079 -0.0122 0.3402 0.043 Uiso 1 1 calc R . .
H20C H 0.0831 -0.0107 0.3041 0.043 Uiso 1 1 calc R . .
C21 C 0.0166(4) 0.1016(3) 0.4094(4) 0.0343(15) Uani 1 1 d . . .
H21A H -0.0367 0.0905 0.3578 0.051 Uiso 1 1 calc R . .
H21B H 0.0127 0.1548 0.4254 0.051 Uiso 1 1 calc R . .
H21C H 0.0017 0.0711 0.4628 0.051 Uiso 1 1 calc R . .
C22 C 0.3617(4) 0.0733(3) 0.4297(3) 0.0203(12) Uani 1 1 d . . .
H22 H 0.3527 0.0185 0.4408 0.024 Uiso 1 1 calc R . .
C23 C 0.4639(4) 0.0977(3) 0.4859(4) 0.0292(14) Uani 1 1 d . . .
H23A H 0.5248 0.0684 0.4672 0.044 Uiso 1 1 calc R . .
H23B H 0.4562 0.0893 0.5515 0.044 Uiso 1 1 calc R . .
H23C H 0.4766 0.1510 0.4752 0.044 Uiso 1 1 calc R . .
C24 C 0.3780(4) 0.0831(3) 0.3268(3) 0.0318(15) Uani 1 1 d . . .
H24A H 0.3955 0.1354 0.3147 0.048 Uiso 1 1 calc R . .
H24B H 0.3119 0.0691 0.2897 0.048 Uiso 1 1 calc R . .
H24C H 0.4371 0.0508 0.3107 0.048 Uiso 1 1 calc R . .
C25 C 0.2109(5) 0.0651(3) 0.5711(4) 0.0356(16) Uani 1 1 d D . .
H25 H 0.1520 0.0368 0.5354 0.043 Uiso 1 1 calc R C 1
C26 C 0.1304(5) 0.1019(3) 0.6308(4) 0.0350(16) Uani 1 1 d . D .
H26A H 0.1024 0.0643 0.6714 0.053 Uiso 1 1 calc R . .
H26B H 0.0709 0.1234 0.5910 0.053 Uiso 1 1 calc R . .
H26C H 0.1665 0.1417 0.6681 0.053 Uiso 1 1 calc R . .
C27A C 0.268(2) -0.0073(11) 0.600(2) 0.038(8) Uiso 0.20 1 d PD D 1
H27A H 0.2387 -0.0272 0.6550 0.057 Uiso 0.20 1 calc PR D 1
H27B H 0.3454 0.0026 0.6135 0.057 Uiso 0.20 1 calc PR D 1
H27C H 0.2582 -0.0439 0.5498 0.057 Uiso 0.20 1 calc PR D 1
C27B C 0.3053(5) 0.0412(4) 0.6332(5) 0.0332(19) Uiso 0.80 1 d PD D 2
H27D H 0.2808 0.0121 0.6845 0.050 Uiso 0.80 1 calc PR D 2
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N3 0.022(3) 0.018(2) 0.015(2) 0.0020(18) 0.0031(18) 0.002(2)
N4 0.021(2) 0.020(3) 0.019(2) 0.0029(19) 0.0036(18) 0.001(2)
N5 0.041(3) 0.030(3) 0.023(3) 0.010(2) 0.004(2) -0.001(3)
N6 0.027(3) 0.020(3) 0.018(2) 0.0012(17) 0.0041(18) -0.0029(19)
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C2 0.022(3) 0.025(3) 0.027(3) 0.000(2) 0.010(2) -0.007(3)
C3 0.031(3) 0.023(3) 0.019(3) 0.002(2) 0.013(2) -0.002(3)
C4 0.018(3) 0.027(3) 0.026(3) -0.001(2) 0.009(2) -0.002(3)
C5 0.018(3) 0.035(4) 0.032(3) 0.008(3) -0.004(2) 0.008(3)
C6 0.025(3) 0.027(4) 0.026(3) 0.006(2) -0.003(2) 0.002(3)
C7 0.023(3) 0.040(4) 0.029(3) -0.010(3) 0.002(3) 0.000(3)
C8 0.029(4) 0.065(5) 0.025(3) 0.020(3) 0.008(3) 0.001(3)
C9 0.034(3) 0.081(5) 0.022(3) -0.002(4) 0.005(2) 0.011(5)
C10 0.066(6) 0.027(4) 0.079(6) -0.009(4) 0.009(4) 0.006(4)
C13 0.049(5) 0.035(4) 0.070(5) -0.018(4) 0.021(4) -0.006(4)
C14 0.040(4) 0.044(5) 0.049(4) -0.004(3) -0.019(3) -0.003(4)
C15 0.055(5) 0.053(6) 0.126(8) -0.040(5) 0.034(5) -0.022(5)
C16 0.067(6) 0.054(5) 0.061(5) -0.022(4) 0.023(4) -0.016(4)
C19 0.024(3) 0.022(3) 0.032(3) 0.001(2) 0.008(2) -0.003(3)
C20 0.030(3) 0.028(4) 0.028(3) -0.001(3) 0.004(3) -0.003(3)
C21 0.021(3) 0.033(4) 0.049(4) 0.004(3) 0.009(3) 0.000(3)
C22 0.021(3) 0.018(3) 0.023(3) 0.002(2) 0.007(2) 0.005(2)
C23 0.020(3) 0.024(4) 0.045(4) -0.002(3) 0.007(3) 0.003(3)
C24 0.032(4) 0.032(4) 0.033(3) 0.005(3) 0.016(3) 0.016(3)
C25 0.041(4) 0.039(4) 0.030(3) 0.009(3) 0.021(3) 0.009(3)
C26 0.043(4) 0.026(4) 0.040(4) 0.010(3) 0.023(3) 0.002(3)

_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_
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 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
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Os N1 2.197(4) . ?
Os P2 2.3471(16) . ?
Os P1 2.3662(16) . ?
Os H1A 1.572(10) . ?
Os H1B 1.582(10) . ?
Os H1C 1.588(10) . ?
P1 C10 1.847(7) . ?
P1 C16 1.862(6) . ?
P1 C13 1.900(7) . ?
P2 C22 1.871(5) . ?
P2 C19 1.873(5) . ?
P2 C25 1.887(5) . ?
B N6 1.513(6) . ?
B N2 1.556(7) . ?
B N4 1.560(7) . ?
B H1D 1.13(5) . ?
N1 C1 1.335(6) . ?
N1 N2 1.362(5) . ?
N2 C3 1.346(6) . ?
N3 C4 1.335(6) . ?
N3 N4 1.373(5) . ?
N4 C6 1.335(6) . ?
N5 C8 1.325(6) . ?
N5 N6 1.371(6) . ?
N6 C7 1.362(6) . ?
C1 C2 1.397(7) . ?
C1 H1 0.9500 . ?
C2 C3 1.369(7) . ?
C2 H2 0.9500 . ?
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C4 H4 0.9500 . ?
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C6 H6 0.9500 . ?
C7 C9 1.385(8) . ?
C7 H7 0.9500 . ?
C8 C9 1.390(9) . ?
C8 H8 0.9500 . ?
C9 H9 0.9500 . ?
C10 C11A 1.493(8) . ?
C10 C11B 1.524(9) . ?
C10 C12B 1.557(9) . ?
C10 C12A 1.589(9) . ?
C10 H10 1.0000 . ?
C11A H11A 0.9800 . ?
C11A H11B 0.9800 . ?
C11A H11C 0.9800 . ?
C11B H11D 0.9800 . ?
C11B H11E 0.9800 . ?
C11B H11F 0.9800 . ?
C12A H12A 0.9800 . ?
C12A H12B 0.9800 . ?
```

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C13 C14 1.548(9) . ?
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C14 H14C 0.9800 . ?
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C15 H15B 0.9800 . ?
C15 H15C 0.9800 . ?
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C17A H17C 0.9800 . ?
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C17B H17E 0.9800 . ?
C17B H17F 0.9800 . ?
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C18A H18B 0.9800 . ?
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C20 H20B 0.9800 . ?
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C24 H24B 0.9800 . ?
C24 H24C 0.9800 . ?
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C25 C26 1.534(7) . ?
C25 H25 1.0000 . ?
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C26 H26B 0.9800 . ?
C26 H26C 0.9800 . ?
C27A H27A 0.9800 . ?
C27A H27B 0.9800 . ?
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N1 Os P1 92.63(11) . . ?
P2 Os P1 165.75(5) . . ?
N3 Os H1A 169.1(16) . . ?
N1 Os H1A 83.0(16) . . ?
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P1 Os H1A 87.5(16) . . ?
N3 Os H1B 144(2) . . ?
N1 Os H1B 130(2) . . ?
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P1 Os H1B 85.5(19) . . ?
H1A Os H1B 47(2) . . ?
N3 Os H1C 75.3(17) . . ?
N1 Os H1C 160.9(18) . . ?
P2 Os H1C 89(2) . . ?
P1 Os H1C 84(2) . . ?
H1A Os H1C 115(2) . . ?
H1B Os H1C 69(3) . . ?
C10 P1 C16 103.1(3) . . ?
C10 P1 C13 101.6(3) . . ?
C16 P1 C13 105.3(3) . . ?
C10 P1 Os 115.4(2) . . ?
C16 P1 Os 114.7(2) . . ?
C13 P1 Os 115.1(2) . . ?
C22 P2 C19 102.6(2) . . ?
C22 P2 C25 101.5(2) . . ?
C19 P2 C25 99.8(3) . . ?
C22 P2 Os 117.19(18) . . ?
C19 P2 Os 118.34(19) . . ?
C25 P2 Os 114.6(2) . . ?
N6 B N2 109.3(4) . . ?
N6 B N4 111.9(4) . . ?
N2 B N4 109.2(4) . . ?
N6 B H1D 110(2) . . ?
N2 B H1D 105(2) . . ?
N4 B H1D 111(2) . . ?
C1 N1 N2 106.5(4) . . ?
C1 N1 Os 127.7(3) . . ?
N2 N1 Os 125.6(3) . . ?
C3 N2 N1 109.0(4) . . ?
C3 N2 B 127.7(4) . . ?
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N4 N3 Os 126.6(3) . . ?
C6 N4 N3 109.3(4) . . ?
C6 N4 B 129.1(4) . . ?
N3 N4 B 119.9(4) . . ?
C8 N5 N6 104.9(5) . . ?
C7 N6 N5 110.8(4) . . ?
C7 N6 B 124.8(5) . . ?
N5 N6 B 123.7(5) . . ?
N1 C1 C2 110.8(5) . . ?
N1 C1 H1 124.6 . . ?
C2 C1 H1 124.6 . . ?
C3 C2 C1 104.0(5) . . ?
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C1 C2 H2 128.0 . . ?
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C2 C3 H3 125.2 . . ?
N3 C4 C5 111.0(5) . . ?
N3 C4 H4 124.5 . . ?
C5 C4 H4 124.5 . . ?
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C4 C5 H5 127.5 . . ?
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C5 C6 H6 125.5 . . ?
N6 C7 C9 107.2(6) . . ?
N6 C7 H7 126.4 . . ?
C9 C7 H7 126.4 . . ?
N5 C8 C9 112.5(5) . . ?
N5 C8 H8 123.7 . . ?
C9 C8 H8 123.7 . . ?
C7 C9 C8 104.6(5) . . ?
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C8 C9 H9 127.7 . . ?
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C11B C10 P1 108.3(8) . . ?
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P1 C10 H10 102.1 . . ?
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C10 C11A H11B 109.5 . . ?
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C10 C11B H11D 109.5 . . ?
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H12E C12B H12F 109.5 . . ?
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C15 C13 P1 115.5(5) . . ?
C14 C13 P1 112.5(5) . . ?
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P1 C13 H13 105.9 . . ?
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C13 C14 H14B 109.5 . . ?
H14A C14 H14B 109.5 . . ?
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H14A C14 H14C 109.5 . . ?
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C13 C15 H15B 109.5 . . ?
H15A C15 H15B 109.5 . . ?
C13 C15 H15C 109.5 . . ?
H15A C15 H15C 109.5 . . ?
H15B C15 H15C 109.5 . . ?
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C17B C16 C18B 114.7(12) . . ?
C17A C16 C18B 126.6(11) . . ?
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C17B C16 H16 111.7 . . ?
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C16 C17A H17A 109.5 . . ?
C16 C17A H17B 109.5 . . ?
C16 C17A H17C 109.5 . . ?
C16 C17B H17D 109.5 . . ?
C16 C17B H17E 109.5 . . ?
H17D C17B H17E 109.5 . . ?
C16 C17B H17F 109.5 . . ?
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H17E C17B H17F 109.5 . . ?
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C16 C18A H18B 109.5 . . ?
C16 C18A H18C 109.5 . . ?
C16 C18B H18D 109.5 . . ?
C16 C18B H18E 109.5 . . ?
H18D C18B H18E 109.5 . . ?
C16 C18B H18F 109.5 . . ?
H18D C18B H18F 109.5 . . ?
H18E C18B H18F 109.5 . . ?
C20 C19 C21 109.1(5) . . ?
C20 C19 P2 117.3(4) . . ?
C21 C19 P2 112.4(4) . . ?
C20 C19 H19 105.7 . . ?
C21 C19 H19 105.7 . . ?
P2 C19 H19 105.7 . . ?
C19 C20 H20A 109.5 . . ?
C19 C20 H20B 109.5 . . ?
H20A C20 H20B 109.5 . . ?
C19 C20 H20C 109.5 . . ?
H20A C20 H20C 109.5 . . ?
H20B C20 H20C 109.5 . . ?
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C19 C21 H21C 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
C23 C22 C24 108.5(4) . . ?
C23 C22 P2 113.0(4) . . ?
C24 C22 P2 113.7(3) . . ?
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C24 C22 H22 107.1 . . ?
P2 C22 H22 107.1 . . ?
C22 C23 H23A 109.5 . . ?
C22 C23 H23B 109.5 . . ?
H23A C23 H23B 109.5 . . ?
C22 C23 H23C 109.5 . . ?
H23A C23 H23C 109.5 . . ?
H23B C23 H23C 109.5 . . ?
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C22 C24 H24B 109.5 . . ?
H24A C24 H24B 109.5 . . ?
C22 C24 H24C 109.5 . . ?
H24A C24 H24C 109.5 . . ?
H24B C24 H24C 109.5 . . ?
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C27B C25 C26 107.6(5) . . ?
C27A C25 C26 121.7(12) . . ?
C27B C25 P2 117.2(5) . . ?
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P2 C25 H25 91.3 . . ?
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H26B C26 H26C 109.5 . . ?
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_diffrn_measured_fraction_theta_full   0.999
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_refine_diff_density_min   -0.988
_refine_diff_density_rms    0.131


#===END

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# Data for compound 3 (local labelling mae235as)



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;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
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_chemical_formula_weight          566.49

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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'B'  'B'   0.0013   0.0007
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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 'P'  'P'   0.1023   0.0942
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Os'  'Os'  -1.2165   7.6030
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'P2(1)/n'

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

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_cell_length_b                    14.3048(19)
_cell_length_c                    14.1995(18)
_cell_angle_alpha                 90.00
_cell_angle_beta                  107.577(2)
_cell_angle_gamma                 90.00
_cell_volume                      2164.0(5)
_cell_formula_units_Z             4
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used     4005
_cell_measurement_theta_min       2
_cell_measurement_theta_max       23

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_exptl_crystal_size_max           0.10
_exptl_crystal_size_mid           0.06
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_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.739
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1120
_exptl_absorpt_coefficient_mu     5.982
_exptl_absorpt_correction_type    'multi-scan'
_exptl_absorpt_correction_T_min   0.548
_exptl_absorpt_correction_T_max   0.746
_exptl_absorpt_process_details
;
Absorption correction performed with SADABS program. This is based on the
method of Blessing: Blessing, R. H., Acta Crystallogr., Sect. A 1995, 51, 33.

SADABS: Area-Detector Absorption Correction. Bruker-AXS
within SAINT package, v. 6.1 (2000).
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_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Bruker SMART APEX CCD system'
_diffrn_measurement_method        '\w rotations with narrow frames'
_diffrn_detector_area_resol_mean  8.26
_diffrn_standards_decay_%         'no decay'
_diffrn_reflns_number             26930
_diffrn_reflns_av_R_equivalents   0.0621
_diffrn_reflns_av_sigmaI/netI     0.0797
_diffrn_reflns_limit_h_min        -15
_diffrn_reflns_limit_h_max        14
_diffrn_reflns_limit_k_min        -19
_diffrn_reflns_limit_k_max        19
_diffrn_reflns_limit_l_min        -18
_diffrn_reflns_limit_l_max        18
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_diffrn_reflns_theta_max          29.11
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_reflns_number_gt                 4053
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        'SAINT v. 6.1 (Bruker AXS, 2000)'
_computing_data_reduction         'SAINT v. 6.1 (Bruker AXS, 2000)'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'XP, SHELXTL v. 6.1 (Bruker, 2000)'
_computing_publication_material   'XCIF, SHELXTL v. 6.1 (Bruker, 2000)'

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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^)(0.0056P)^2^.0000P] where P=(Fo^2^"^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          5428
_refine_ls_number_parameters      265
_refine_ls_number_restraints      3
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_refine_ls_wR_factor_gt          0.0426
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_refine_ls_restrained_S_all      0.827
_refine_ls_shift/su_max          0.001
_refine_ls_shift/su_mean         0.000

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 _atom_site_symmetry_multiplicity
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 _atom_site_refinement_flags
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 _atom_site_disorder_group
Os Os 0.566028(16) 0.137619(12) 0.341282(12) 0.01379(4) Uani 1 1 d D . .
H1A H 0.6912(19) 0.182(2) 0.334(2) 0.019(11) Uiso 1 1 d D . .
H1B H 0.689(2) 0.129(3) 0.4308(19) 0.049(14) Uiso 1 1 d D . .
H1C H 0.572(4) 0.075(2) 0.4334(18) 0.039(13) Uiso 1 1 d D . .
P P 0.62222(11) 0.00631(8) 0.27394(8) 0.0156(2) Uani 1 1 d . . .
N1 N 0.4957(3) 0.2201(2) 0.2066(2) 0.0153(8) Uani 1 1 d . . .
N2 N 0.3933(3) 0.2755(2) 0.1954(2) 0.0143(8) Uani 1 1 d . . .
N3 N 0.3693(3) 0.1057(2) 0.3143(2) 0.0153(8) Uani 1 1 d . . .
N4 N 0.2821(3) 0.1750(2) 0.2842(2) 0.0148(8) Uani 1 1 d . . .
N5 N 0.5219(3) 0.2583(2) 0.4131(2) 0.0138(8) Uani 1 1 d . . .
N6 N 0.4135(3) 0.3068(2) 0.3717(2) 0.0147(8) Uani 1 1 d . . .
C1 C 0.5306(4) 0.2321(3) 0.1255(3) 0.0181(10) Uani 1 1 d . . .
H1 H 0.6003 0.2021 0.1134 0.022 Uiso 1 1 calc R . .
C2 C 0.4511(4) 0.2945(3) 0.0612(3) 0.0206(10) Uani 1 1 d . . .
H2 H 0.4549 0.3146 -0.0015 0.025 Uiso 1 1 calc R . .
C3 C 0.3661(4) 0.3205(3) 0.1080(3) 0.0174(10) Uani 1 1 d . . .
H3 H 0.2990 0.3633 0.0832 0.021 Uiso 1 1 calc R . .
C4 C 0.3043(4) 0.0295(3) 0.3227(3) 0.0170(10) Uani 1 1 d . . .
H4 H 0.3410 -0.0299 0.3433 0.020 Uiso 1 1 calc R . .
C5 C 0.1775(4) 0.0476(3) 0.2980(3) 0.0200(10) Uani 1 1 d . . .
H5 H 0.1120 0.0051 0.2975 0.024 Uiso 1 1 calc R . .
C6 C 0.1672(4) 0.1412(3) 0.2740(3) 0.0180(9) Uani 1 1 d . . .
H6 H 0.0913 0.1759 0.2536 0.022 Uiso 1 1 calc R . .
C7 C 0.5800(4) 0.3021(3) 0.4968(3) 0.0175(10) Uani 1 1 d . . .
H7 H 0.6588 0.2839 0.5408 0.021 Uiso 1 1 calc R . .
C8 C 0.5111(4) 0.3773(3) 0.5114(3) 0.0196(10) Uani 1 1 d . . .
H8 H 0.5311 0.4190 0.5660 0.023 Uiso 1 1 calc R . .
C9 C 0.4071(4) 0.3788(3) 0.4300(3) 0.0186(10) Uani 1 1 d . . .
H9 H 0.3413 0.4236 0.4171 0.022 Uiso 1 1 calc R . .
C10 C 0.4883(4) -0.0557(3) 0.1848(3) 0.0186(10) Uani 1 1 d . . .
H10 H 0.4303 -0.0728 0.2236 0.022 Uiso 1 1 calc R . .
C11 C 0.4123(4) 0.0096(3) 0.1032(3) 0.0213(10) Uani 1 1 d . . .
H11A H 0.4666 0.0341 0.0661 0.032 Uiso 1 1 calc R . .
H11B H 0.3793 0.0616 0.1328 0.032 Uiso 1 1 calc R . .
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H11C H 0.3425 -0.0251 0.0584 0.032 Uiso 1 1 calc R . .
C12 C 0.5154(4) -0.1473(3) 0.1397(3) 0.0254(11) Uani 1 1 d . . .
H12A H 0.4362 -0.1792 0.1069 0.038 Uiso 1 1 calc R . .
H12B H 0.5676 -0.1875 0.1920 0.038 Uiso 1 1 calc R . .
H12C H 0.5599 -0.1340 0.0914 0.038 Uiso 1 1 calc R . .
C13 C 0.6927(4) -0.0884(3) 0.3624(3) 0.0202(10) Uani 1 1 d . . .
H13 H 0.7215 -0.1385 0.3252 0.024 Uiso 1 1 calc R . .
C14 C 0.6000(4) -0.1326(3) 0.4098(3) 0.0276(11) Uani 1 1 d . . .
H14A H 0.6418 -0.1830 0.4544 0.041 Uiso 1 1 calc R . .
H14B H 0.5282 -0.1580 0.3581 0.041 Uiso 1 1 calc R . .
H14C H 0.5707 -0.0849 0.4473 0.041 Uiso 1 1 calc R . .
C15 C 0.8075(4) -0.0533(3) 0.4436(3) 0.0258(11) Uani 1 1 d . . .
H15A H 0.7818 -0.0048 0.4822 0.039 Uiso 1 1 calc R . .
H15B H 0.8685 -0.0271 0.4136 0.039 Uiso 1 1 calc R . .
H15C H 0.8460 -0.1054 0.4870 0.039 Uiso 1 1 calc R . .
C16 C 0.7374(4) 0.0180(3) 0.2016(3) 0.0186(10) Uani 1 1 d . . .
H16 H 0.6852 0.0318 0.1323 0.022 Uiso 1 1 calc R . .
C18 C 0.8145(4) -0.0691(3) 0.1938(3) 0.0268(11) Uani 1 1 d . . .
H18A H 0.8584 -0.0581 0.1446 0.040 Uiso 1 1 calc R . .
H18B H 0.7583 -0.1229 0.1737 0.040 Uiso 1 1 calc R . .
H18C H 0.8760 -0.0817 0.2582 0.040 Uiso 1 1 calc R . .
C17 C 0.8277(4) 0.1003(3) 0.2317(3) 0.0237(11) Uani 1 1 d . . .
H17A H 0.8831 0.0906 0.2991 0.036 Uiso 1 1 calc R . .
H17B H 0.7797 0.1581 0.2292 0.036 Uiso 1 1 calc R . .
H17C H 0.8781 0.1052 0.1862 0.036 Uiso 1 1 calc R . .
B B 0.3228(5) 0.2750(3) 0.2730(4) 0.0154(11) Uani 1 1 d . . .
H19 H 0.240(3) 0.321(2) 0.249(2) 0.019 Uiso 1 1 d . . .

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 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
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P 0.0175(6) 0.0149(6) 0.0156(6) -0.0007(5) 0.0068(5) 0.0012(5)
N1 0.015(2) 0.012(2) 0.0182(19) -0.0005(15) 0.0055(16) -0.0015(16)
N2 0.015(2) 0.0114(19) 0.0153(19) -0.0009(15) 0.0024(16) -0.0007(15)
N3 0.020(2) 0.012(2) 0.0138(18) 0.0000(15) 0.0054(16) 0.0017(16)
N4 0.016(2) 0.015(2) 0.0138(18) -0.0005(15) 0.0046(16) 0.0013(16)
N5 0.014(2) 0.0122(19) 0.0140(18) 0.0008(15) 0.0030(15) 0.0003(16)
N6 0.015(2) 0.0116(19) 0.0174(19) 0.0000(15) 0.0050(16) 0.0015(15)
C1 0.019(2) 0.017(2) 0.021(2) -0.0022(19) 0.010(2) -0.004(2)
C2 0.027(3) 0.017(3) 0.015(2) 0.0025(19) 0.004(2) -0.007(2)
C3 0.023(3) 0.012(2) 0.013(2) 0.0005(18) -0.0010(19) -0.0045(19)
C4 0.023(3) 0.013(2) 0.017(2) -0.0011(18) 0.008(2) 0.000(2)
C5 0.017(2) 0.022(3) 0.022(2) -0.002(2) 0.008(2) -0.007(2)
C6 0.015(2) 0.021(2) 0.019(2) 0.003(2) 0.0059(18) 0.001(2)
C7 0.020(2) 0.014(2) 0.018(2) 0.0028(19) 0.005(2) -0.0014(19)
C8 0.024(2) 0.019(3) 0.015(2) -0.0044(19) 0.0056(19) -0.004(2)
C9 0.021(2) 0.009(3) 0.027(2) 0.0002(19) 0.009(2) 0.0046(19)
C10 0.023(3) 0.016(2) 0.021(2) -0.0046(19) 0.013(2) -0.008(2)
C11 0.019(2) 0.024(3) 0.020(2) -0.004(2) 0.005(2) -0.004(2)
C12 0.034(3) 0.018(3) 0.026(2) -0.005(2) 0.012(2) -0.005(2)
C13 0.027(3) 0.015(2) 0.020(2) 0.000(2) 0.009(2) 0.007(2)
```

```
C14 0.041(3) 0.020(3) 0.028(2) 0.006(2) 0.021(2) 0.006(3)
C15 0.031(3) 0.027(3) 0.021(2) 0.001(2) 0.009(2) 0.014(2)
C16 0.022(3) 0.018(3) 0.017(2) 0.0011(19) 0.008(2) 0.003(2)
C18 0.028(3) 0.028(3) 0.030(3) 0.000(2) 0.016(2) 0.006(2)
C17 0.019(3) 0.024(3) 0.030(3) -0.003(2) 0.011(2) -0.004(2)
B 0.015(3) 0.013(3) 0.017(3) 0.000(2) 0.003(2) 0.000(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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Os N3 2.163(3) . ?
Os N1 2.182(3) . ?
Os P 2.2803(11) . ?
Os H1A 1.570(10) . ?
Os H1B 1.570(10) . ?
Os H1C 1.572(10) . ?
P C13 1.854(4) . ?
P C10 1.866(4) . ?
P C16 1.881(4) . ?
N1 C1 1.333(4) . ?
N1 N2 1.361(4) . ?
N2 C3 1.349(4) . ?
N2 B 1.536(5) . ?
N3 C4 1.335(5) . ?
N3 N4 1.365(4) . ?
N4 C6 1.338(5) . ?
N4 B 1.524(6) . ?
N5 C7 1.326(5) . ?
N5 N6 1.366(4) . ?
N6 C9 1.337(5) . ?
N6 B 1.530(6) . ?
C1 C2 1.389(5) . ?
C1 H1 0.9500 . ?
C2 C3 1.365(5) . ?
C2 H2 0.9500 . ?
C3 H3 0.9500 . ?
C4 C5 1.377(5) . ?
C4 H4 0.9500 . ?
C5 C6 1.378(5) . ?
C5 H5 0.9500 . ?
C6 H6 0.9500 . ?
C7 C8 1.375(5) . ?
C7 H7 0.9500 . ?
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C8 C9 1.370(5) . ?
C8 H8 0.9500 . ?
C9 H9 0.9500 . ?
C10 C12 1.529(5) . ?
C10 C11 1.530(5) . ?
C10 H10 1.0000 . ?
C11 H11A 0.9800 . ?
C11 H11B 0.9800 . ?
C11 H11C 0.9800 . ?
C12 H12A 0.9800 . ?
C12 H12B 0.9800 . ?
C12 H12C 0.9800 . ?
C13 C15 1.527(5) . ?
C13 C14 1.532(5) . ?
C13 H13 1.0000 . ?
C14 H14A 0.9800 . ?
C14 H14B 0.9800 . ?
C14 H14C 0.9800 . ?
C15 H15A 0.9800 . ?
C15 H15B 0.9800 . ?
C15 H15C 0.9800 . ?
C16 C17 1.526(5) . ?
C16 C18 1.537(5) . ?
C16 H16 1.0000 . ?
C18 H18A 0.9800 . ?
C18 H18B 0.9800 . ?
C18 H18C 0.9800 . ?
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C17 H17B 0.9800 . ?
C17 H17C 0.9800 . ?
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N5 Os N3 83.49(12) . . ?
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N5 Os P 176.34(9) . . ?
N3 Os P 98.38(9) . . ?
N1 Os P 98.62(9) . . ?
N5 Os H1A 92.3(12) . . ?
N3 Os H1A 162.2(13) . . ?
N1 Os H1A 79.3(13) . . ?
P Os H1A 86.9(12) . . ?
N5 Os H1B 87.1(15) . . ?
N3 Os H1B 136.2(15) . . ?
N1 Os H1B 138.4(16) . . ?
P Os H1B 89.4(15) . . ?
H1A Os H1B 60.4(17) . . ?
N5 Os H1C 91.4(14) . . ?
N3 Os H1C 79.3(15) . . ?
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N1 Os H1C 162.4(15) . . ?
P Os H1C 85.9(14) . . ?
H1A Os H1C 118.1(19) . . ?
H1B Os H1C 58.2(18) . . ?
C13 P C10 101.68(19) . . ?
C13 P C16 102.37(18) . . ?
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C13 P Os 115.60(13) . . ?
C10 P Os 114.18(14) . . ?
C16 P Os 118.45(14) . . ?
C1 N1 N2 106.2(3) . . ?
C1 N1 Os 134.8(3) . . ?
N2 N1 Os 119.0(2) . . ?
C3 N2 N1 109.4(3) . . ?
C3 N2 B 129.8(4) . . ?
N1 N2 B 120.6(3) . . ?
C4 N3 N4 105.3(3) . . ?
C4 N3 Os 135.1(3) . . ?
N4 N3 Os 119.6(2) . . ?
C6 N4 N3 110.1(3) . . ?
C6 N4 B 129.4(4) . . ?
N3 N4 B 120.4(3) . . ?
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C7 N5 Os 133.5(3) . . ?
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C3 C2 C1 104.9(4) . . ?
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C6 C5 H5 127.8 . . ?
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C5 C6 H6 125.7 . . ?
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C9 C8 H8 127.6 . . ?
C7 C8 H8 127.6 . . ?
N6 C9 C8 108.7(4) . . ?
N6 C9 H9 125.7 . . ?
C8 C9 H9 125.7 . . ?
C12 C10 C11 109.9(3) . . ?
C12 C10 P 118.1(3) . . ?
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P C10 H10 105.3 . . ?
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H11B C11 H11C 109.5 . . ?
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C10 C12 H12B 109.5 . . ?
H12A C12 H12B 109.5 . . ?
C10 C12 H12C 109.5 . . ?
H12A C12 H12C 109.5 . . ?
H12B C12 H12C 109.5 . . ?
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C15 C13 P 111.1(3) . . ?
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H15A C15 H15C 109.5 . . ?
H15B C15 H15C 109.5 . . ?
C17 C16 C18 107.9(4) . . ?
C17 C16 P 114.8(3) . . ?
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C18 C16 H16 105.2 . . ?
P C16 H16 105.2 . . ?
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H18B C18 H18C 109.5 . . ?
C16 C17 H17A 109.5 . . ?
C16 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
C16 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
N4 B N6 108.7(3) . . ?
N4 B N2 108.3(3) . . ?
N6 B N2 108.3(4) . . ?
N4 B H19 110.0(19) . . ?
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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'B'  'B'   0.0013   0.0007
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 'N'  'N'   0.0061   0.0033
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 'F'  'F'   0.0171   0.0103
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 'P'  'P'   0.1023   0.0942
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Os'  'Os'  -1.2165   7.6030
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'P-1'

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 'x, y, z'
 '-x, -y, -z'
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_cell_length_c                    15.333(10)
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_cell_angle_beta                  100.268(16)
_cell_angle_gamma                 92.698(13)
_cell_volume                      2447(3)
_cell_formula_units_Z             4
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used     1919
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_cell_measurement_theta_max       18

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_exptl_crystal_density_diffrn     1.776
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_exptl_crystal_F_000              1288
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Absorption correction performed with SADABS program. This is based on the
method of Blessing: Blessing, R. H., Acta Crystallogr., Sect. A 1995, 51, 33.

SADABS: Area-Detector Absorption Correction. Bruker-AXS
within SAINT package, v. 6.1 (2000).
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_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Bruker SMART APEX CCD system'
_diffrn_measurement_method        '\w rotations with narrow frames'
_diffrn_detector_area_resol_mean  8.26
_diffrn_standards_decay_%         'no decay'
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_diffrn_reflns_limit_h_max        15
_diffrn_reflns_limit_k_min        -19
_diffrn_reflns_limit_k_max        18
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_diffrn_reflns_theta_min          1.47
_diffrn_reflns_theta_max          28.99
_reflns_number_total              11724
_reflns_number_gt                 6013
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'SMART v. 5.625 (Bruker AXS, 2000)'
_computing_cell_refinement        'SAINT v. 6.1 (Bruker AXS, 2000)'
_computing_data_reduction         'SAINT v. 6.1 (Bruker AXS, 2000)'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'XP, SHELXTL v. 6.1 (Bruker, 2000)'
_computing_publication_material   'XCIF, SHELXTL v. 6.1 (Bruker, 2000)'

_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^)(0.0108P)^2^.0000P] where P=(Fo^2^▪^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_extinction_coef        ?
_refine_ls_number_reflns          11724
_refine_ls_number_parameters      620
_refine_ls_number_restraints      28
_refine_ls_R_factor_all           0.1224
_refine_ls_R_factor_gt            0.0535
_refine_ls_wR_factor_ref          0.0907
_refine_ls_wR_factor_gt           0.0771
_refine_ls_goodness_of_fit_ref    0.730
_refine_ls_restrained_S_all       0.745
_refine_ls_shift/su_max           0.008
_refine_ls_shift/su_mean          0.000

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Os1 Os 0.44337(3) 0.26533(3) 0.35621(3) 0.01941(11) Uani 1 1 d D . .
H01 H 0.355(5) 0.341(5) 0.352(6) 0.040 Uiso 1 1 d D . .
H02 H 0.417(6) 0.367(3) 0.349(6) 0.040 Uiso 1 1 d D . .
H03 H 0.334(5) 0.199(6) 0.280(5) 0.04(3) Uiso 1 1 d D . .
H04 H 0.366(6) 0.206(7) 0.252(3) 0.05(4) Uiso 1 1 d D . .
Os2 Os 1.00993(3) 0.77377(3) 0.29524(3) 0.02070(11) Uani 1 1 d D . .
H05 H 0.928(5) 0.857(4) 0.318(6) 0.040 Uiso 1 1 d D . .
H07 H 1.109(5) 0.816(7) 0.389(4) 0.040 Uiso 1 1 d D . .
H08 H 1.125(4) 0.835(6) 0.366(4) 0.02(3) Uiso 1 1 d D . .
H06 H 0.956(6) 0.840(5) 0.382(4) 0.040 Uiso 1 1 d D . .
P1 P 0.5245(2) 0.26734(19) 0.22762(18) 0.0238(6) Uani 1 1 d . . .
P2 P 1.01986(19) 0.88433(18) 0.21612(17) 0.0202(6) Uani 1 1 d . . .
N1 N 0.5810(6) 0.3545(6) 0.4654(5) 0.0214(19) Uani 1 1 d . . .
N2 N 0.6315(6) 0.3257(6) 0.5348(5) 0.028(2) Uani 1 1 d . . .
N3 N 0.5145(6) 0.1411(6) 0.3627(5) 0.026(2) Uani 1 1 d . . .
N4 N 0.5663(6) 0.1411(5) 0.4527(6) 0.0234(19) Uani 1 1 d . . .
N5 N 0.3801(6) 0.2681(5) 0.4777(5) 0.0225(18) Uani 1 1 d . . .
N6 N 0.4488(6) 0.2553(5) 0.5526(5) 0.0236(19) Uani 1 1 d . . .
N7 N 0.8638(6) 0.6834(6) 0.1966(5) 0.025(2) Uani 1 1 d . . .
N8 N 0.8632(6) 0.5810(6) 0.1555(5) 0.0231(19) Uani 1 1 d . . .
N9 N 1.1086(6) 0.6726(6) 0.2154(5) 0.0253(19) Uani 1 1 d . . .
N10 N 1.0753(6) 0.5712(6) 0.1753(5) 0.026(2) Uani 1 1 d . . .
N11 N 0.9968(6) 0.6714(5) 0.3598(5) 0.0185(18) Uani 1 1 d . . .
N12 N 0.9731(6) 0.5703(5) 0.3031(5) 0.0202(18) Uani 1 1 d . . .
C1 C 0.4348(9) 0.1978(8) 0.1060(7) 0.040(3) Uani 1 1 d . . .
H1 H 0.4808 0.2030 0.0597 0.048 Uiso 1 1 calc R . .
C2 C 0.4050(8) 0.0888(8) 0.0777(7) 0.046(3) Uani 1 1 d . . .
H2A H 0.3484 0.0786 0.1126 0.070 Uiso 1 1 calc R . .
H2B H 0.4731 0.0601 0.0942 0.070 Uiso 1 1 calc R . .
H2C H 0.3740 0.0561 0.0079 0.070 Uiso 1 1 calc R . .
C3 C 0.3261(8) 0.2478(9) 0.0879(7) 0.051(3) Uani 1 1 d . . .
H3A H 0.2865 0.2137 0.0200 0.077 Uiso 1 1 calc R . .
H3B H 0.3480 0.3182 0.1027 0.077 Uiso 1 1 calc R . .
H3C H 0.2758 0.2426 0.1298 0.077 Uiso 1 1 calc R . .
C4 C 0.6550(8) 0.2060(7) 0.2209(6) 0.030(2) Uani 1 1 d . . .
H4 H 0.6309 0.1364 0.2125 0.036 Uiso 1 1 calc R . .
C5 C 0.7474(7) 0.2477(7) 0.3112(7) 0.033(3) Uani 1 1 d . . .
H5A H 0.8115 0.2093 0.3009 0.049 Uiso 1 1 calc R . .
H5B H 0.7185 0.2434 0.3654 0.049 Uiso 1 1 calc R . .
H5C H 0.7723 0.3176 0.3259 0.049 Uiso 1 1 calc R . .
C6 C 0.7021(8) 0.1938(7) 0.1276(7) 0.036(3) Uani 1 1 d . . .
H6A H 0.7229 0.2598 0.1290 0.054 Uiso 1 1 calc R . .
H6B H 0.6435 0.1556 0.0695 0.054 Uiso 1 1 calc R . .
H6C H 0.7690 0.1586 0.1266 0.054 Uiso 1 1 calc R . .
C7 C 0.5585(8) 0.3907(8) 0.2195(8) 0.045(3) Uani 1 1 d . . .
H7 H 0.5428 0.3751 0.1486 0.053 Uiso 1 1 calc R . .
C8 C 0.4783(8) 0.4636(7) 0.2595(8) 0.047(3) Uani 1 1 d . . .
H8A H 0.4985 0.4917 0.3304 0.071 Uiso 1 1 calc R . .
H8B H 0.4007 0.4292 0.2373 0.071 Uiso 1 1 calc R . .
H8C H 0.4836 0.5174 0.2370 0.071 Uiso 1 1 calc R . .
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C9 C 0.6825(9) 0.4388(8) 0.2574(9) 0.070(4) Uani 1 1 d . . .
H9A H 0.6917 0.4985 0.2440 0.105 Uiso 1 1 calc R . .
H9B H 0.7315 0.3912 0.2251 0.105 Uiso 1 1 calc R . .
H9C H 0.7034 0.4574 0.3274 0.105 Uiso 1 1 calc R . .
C10 C 0.6423(8) 0.4422(7) 0.4865(7) 0.025(2) Uani 1 1 d . . .
H10 H 0.6269 0.4825 0.4511 0.030 Uiso 1 1 calc R . .
C11 C 0.7294(8) 0.4662(8) 0.5652(7) 0.032(3) Uani 1 1 d . . .
H11 H 0.7845 0.5236 0.5940 0.038 Uiso 1 1 calc R . .
C12 C 0.7192(8) 0.3909(8) 0.5924(7) 0.033(3) Uani 1 1 d . . .
H12 H 0.7680 0.3850 0.6453 0.040 Uiso 1 1 calc R . .
C13 C 0.5121(8) 0.0454(7) 0.3000(7) 0.028(3) Uani 1 1 d . . .
H13 H 0.4806 0.0211 0.2326 0.034 Uiso 1 1 calc R . .
C14 C 0.5599(7) -0.0122(8) 0.3446(7) 0.034(3) Uani 1 1 d . . .
H14 H 0.5689 -0.0808 0.3156 0.041 Uiso 1 1 calc R . .
C15 C 0.5920(8) 0.0512(8) 0.4403(7) 0.032(3) Uani 1 1 d . . .
H15 H 0.6276 0.0330 0.4905 0.039 Uiso 1 1 calc R . .
C16 C 0.2831(7) 0.2901(6) 0.5081(6) 0.024(2) Uani 1 1 d . . .
H16 H 0.2185 0.3033 0.4717 0.028 Uiso 1 1 calc R . .
C17 C 0.2902(8) 0.2909(7) 0.5998(6) 0.029(2) Uani 1 1 d . . .
H17 H 0.2332 0.3046 0.6368 0.035 Uiso 1 1 calc R . .
C18 C 0.3932(8) 0.2686(7) 0.6254(6) 0.030(3) Uani 1 1 d . . .
H18 H 0.4227 0.2630 0.6846 0.035 Uiso 1 1 calc R . .
C19 C 1.0854(8) 0.8345(7) 0.1091(6) 0.026(2) Uani 1 1 d . . .
H19 H 1.1562 0.8099 0.1312 0.032 Uiso 1 1 calc R . .
C20 C 1.0113(8) 0.7427(7) 0.0297(7) 0.037(3) Uani 1 1 d . . .
H20A H 0.9406 0.7624 0.0039 0.055 Uiso 1 1 calc R . .
H20B H 0.9938 0.6945 0.0567 0.055 Uiso 1 1 calc R . .
H20C H 1.0516 0.7123 -0.0224 0.055 Uiso 1 1 calc R . .
C21 C 1.1230(7) 0.9075(7) 0.0672(6) 0.029(2) Uani 1 1 d . . .
H21A H 1.1966 0.8939 0.0502 0.044 Uiso 1 1 calc R . .
H21B H 1.1295 0.9760 0.1156 0.044 Uiso 1 1 calc R . .
H21C H 1.0668 0.8992 0.0092 0.044 Uiso 1 1 calc R . .
C22 C 1.1084(7) 1.0043(6) 0.2971(6) 0.024(2) Uani 1 1 d . . .
H22 H 1.0947 1.0525 0.2659 0.029 Uiso 1 1 calc R . .
C23 C 1.2355(7) 0.9935(7) 0.3106(7) 0.034(3) Uani 1 1 d . . .
H23A H 1.2797 1.0591 0.3496 0.051 Uiso 1 1 calc R . .
H23B H 1.2558 0.9656 0.2472 0.051 Uiso 1 1 calc R . .
H23C H 1.2520 0.9488 0.3437 0.051 Uiso 1 1 calc R . .
C24 C 1.0795(8) 1.0497(7) 0.3970(7) 0.040(3) Uani 1 1 d . . .
H24A H 1.1084 1.0121 0.4350 0.059 Uiso 1 1 calc R . .
H24B H 0.9970 1.0468 0.3898 0.059 Uiso 1 1 calc R . .
H24C H 1.1143 1.1194 0.4304 0.059 Uiso 1 1 calc R . .
C25 C 0.8815(7) 0.9181(7) 0.1704(7) 0.026(2) Uani 1 1 d . . .
H25 H 0.8351 0.8532 0.1256 0.031 Uiso 1 1 calc R . .
C26 C 0.8119(8) 0.9673(7) 0.2471(7) 0.041(3) Uani 1 1 d . . .
H26A H 0.8500 1.0341 0.2910 0.061 Uiso 1 1 calc R . .
H26B H 0.8051 0.9267 0.2842 0.061 Uiso 1 1 calc R . .
H26C H 0.7362 0.9725 0.2151 0.061 Uiso 1 1 calc R . .
C27 C 0.8854(8) 0.9786(7) 0.1088(7) 0.040(3) Uani 1 1 d . . .
H27A H 0.8104 0.9982 0.0937 0.061 Uiso 1 1 calc R . .
H27B H 0.9077 0.9379 0.0484 0.061 Uiso 1 1 calc R . .
H27C H 0.9408 1.0384 0.1447 0.061 Uiso 1 1 calc R . .
C28 C 0.7598(8) 0.6998(7) 0.1639(6) 0.025(2) Uani 1 1 d . . .
H28 H 0.7341 0.7634 0.1814 0.030 Uiso 1 1 calc R . .
C29 C 0.6957(8) 0.6114(7) 0.1016(7) 0.031(3) Uani 1 1 d . . .
H29 H 0.6197 0.6030 0.0675 0.037 Uiso 1 1 calc R . .
C30 C 0.7614(7) 0.5386(7) 0.0979(6) 0.028(2) Uani 1 1 d . . .
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H30 H 0.7392 0.4692 0.0609 0.033 Uiso 1 1 calc R . .
C31 C 1.2158(7) 0.6805(7) 0.1986(6) 0.024(2) Uani 1 1 d . . .
H31 H 1.2632 0.7417 0.2191 0.029 Uiso 1 1 calc R . .
C32 C 1.2454(8) 0.5893(7) 0.1490(6) 0.026(2) Uani 1 1 d . . .
H32 H 1.3143 0.5752 0.1280 0.032 Uiso 1 1 calc R . .
C33 C 1.1542(8) 0.5213(8) 0.1355(6) 0.033(3) Uani 1 1 d . . .
H33 H 1.1491 0.4508 0.1032 0.040 Uiso 1 1 calc R . .
C34 C 0.9977(7) 0.6790(7) 0.4490(6) 0.022(2) Uani 1 1 d . . .
H34 H 1.0122 0.7404 0.5043 0.027 Uiso 1 1 calc R . .
C35 C 0.9752(8) 0.5871(8) 0.4519(7) 0.034(3) Uani 1 1 d . . .
H35 H 0.9707 0.5729 0.5066 0.041 Uiso 1 1 calc R . .
C36 C 0.9611(8) 0.5221(8) 0.3582(7) 0.031(3) Uani 1 1 d . . .
H36 H 0.9448 0.4518 0.3355 0.038 Uiso 1 1 calc R . .
B1 B 0.5727(10) 0.2351(9) 0.5438(9) 0.029(3) Uani 1 1 d . . .
H1D H 0.627(7) 0.225(6) 0.606(6) 0.04(3) Uiso 1 1 d . . .
B2 B 0.9605(9) 0.5333(8) 0.1920(8) 0.024(3) Uani 1 1 d . . .
H2D H 0.940(6) 0.454(6) 0.157(5) 0.03(2) Uiso 1 1 d . . .
B3 B 0.4505(11) 0.7716(10) 0.1120(9) 0.034(3) Uani 1 1 d . . .
B4 B 0.0740(6) 0.2623(6) 0.2474(5) 0.047(4) Uani 1 1 d D . .
F1 F 0.4660(5) 0.7443(5) 0.1887(4) 0.070(2) Uani 1 1 d . . .
F2 F 0.4218(5) 0.6870(5) 0.0270(4) 0.0600(19) Uani 1 1 d . . .
F3 F 0.3679(5) 0.8319(5) 0.1186(5) 0.069(2) Uani 1 1 d . . .
F4 F 0.5516(5) 0.8218(5) 0.1153(4) 0.0576(19) Uani 1 1 d . . .
F5A F 0.0363(11) 0.2245(10) 0.3163(8) 0.055(5) Uiso 0.40 1 d PD A 1
F6A F 0.1058(12) 0.1801(8) 0.1793(9) 0.039(6) Uiso 0.40 1 d PD A 1
F7A F 0.1546(9) 0.3395(8) 0.3016(10) 0.072(5) Uiso 0.40 1 d PD A 1
F8A F -0.0255(9) 0.2887(11) 0.2068(10) 0.035(6) Uiso 0.40 1 d PD A 1
F5B F 0.0893(8) 0.2923(7) 0.3439(5) 0.061(3) Uiso 0.60 1 d PD A 2
F6B F 0.1186(8) 0.1752(5) 0.2030(7) 0.037(4) Uiso 0.60 1 d PD A 2
F7B F 0.1444(6) 0.3411(5) 0.2343(6) 0.037(2) Uiso 0.60 1 d PD A 2
F8B F -0.0337(6) 0.2620(8) 0.2004(7) 0.037(4) Uiso 0.60 1 d PD A 2

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Os2 0.0205(2) 0.0208(3) 0.0207(2) 0.00764(19) 0.00607(18) 0.00138(19)
P1 0.0183(14) 0.0277(16) 0.0262(14) 0.0119(12) 0.0051(11) 0.0021(12)
P2 0.0169(13) 0.0185(14) 0.0221(13) 0.0051(11) 0.0038(10) 0.0014(11)
N1 0.029(5) 0.027(5) 0.017(4) 0.014(4) 0.014(4) 0.013(4)
N2 0.025(5) 0.031(5) 0.025(5) 0.004(4) 0.010(4) 0.012(4)
N3 0.024(5) 0.034(5) 0.011(4) 0.001(4) 0.003(3) -0.005(4)
N4 0.027(5) 0.014(5) 0.036(5) 0.014(4) 0.013(4) 0.008(4)
N5 0.025(5) 0.019(5) 0.022(4) 0.011(4) -0.004(4) 0.004(4)
N6 0.025(5) 0.020(5) 0.029(5) 0.011(4) 0.014(4) 0.005(4)
N7 0.022(5) 0.036(6) 0.021(4) 0.014(4) 0.008(4) 0.009(4)
N8 0.016(4) 0.020(5) 0.027(5) 0.003(4) 0.005(4) 0.001(4)
N9 0.023(5) 0.025(5) 0.031(5) 0.015(4) 0.005(4) 0.004(4)
N10 0.038(5) 0.023(5) 0.020(4) 0.009(4) 0.012(4) 0.003(4)
N11 0.020(4) 0.020(5) 0.020(4) 0.008(3) 0.015(3) 0.002(4)
N12 0.024(4) 0.018(5) 0.022(4) 0.010(4) 0.005(3) 0.004(4)
C1 0.039(7) 0.061(9) 0.030(6) 0.025(6) 0.016(5) 0.008(6)
```

```
C2 0.048(8) 0.051(8) 0.021(6) -0.001(5) -0.001(5) -0.002(6)
C3 0.038(7) 0.087(10) 0.034(7) 0.030(7) 0.007(5) 0.009(7)
C4 0.034(6) 0.038(7) 0.026(6) 0.020(5) 0.010(5) 0.003(5)
C5 0.029(6) 0.039(7) 0.042(7) 0.023(5) 0.018(5) 0.015(5)
C6 0.030(6) 0.042(7) 0.043(7) 0.022(6) 0.014(5) 0.010(5)
C7 0.028(6) 0.042(8) 0.056(8) 0.015(6) -0.001(6) 0.008(6)
C8 0.037(7) 0.038(7) 0.077(9) 0.035(7) 0.007(6) 0.011(6)
C9 0.068(10) 0.052(9) 0.089(11) 0.022(8) 0.033(8) -0.005(8)
C10 0.032(6) 0.018(6) 0.029(6) 0.008(5) 0.019(5) 0.005(5)
C11 0.021(6) 0.026(6) 0.043(7) 0.007(5) 0.008(5) 0.002(5)
C12 0.021(6) 0.047(8) 0.023(6) 0.007(5) 0.000(4) 0.000(5)
C13 0.024(6) 0.023(6) 0.039(6) 0.011(5) 0.016(5) -0.004(5)
C14 0.027(6) 0.030(6) 0.048(7) 0.014(6) 0.019(5) 0.008(5)
C15 0.029(6) 0.045(7) 0.033(6) 0.024(5) 0.009(5) 0.012(5)
C16 0.021(5) 0.019(6) 0.027(5) 0.009(4) 0.000(4) -0.003(4)
C17 0.037(6) 0.038(7) 0.026(6) 0.021(5) 0.021(5) 0.006(5)
C18 0.032(6) 0.040(7) 0.018(5) 0.014(5) 0.009(5) -0.007(5)
C19 0.034(6) 0.023(6) 0.029(6) 0.016(5) 0.012(5) 0.007(5)
C20 0.050(7) 0.029(7) 0.026(6) 0.004(5) 0.010(5) 0.002(6)
C21 0.037(6) 0.026(6) 0.032(6) 0.016(5) 0.015(5) 0.006(5)
C22 0.018(5) 0.021(6) 0.031(6) 0.008(4) 0.007(4) -0.004(4)
C23 0.023(6) 0.031(7) 0.038(6) 0.009(5) -0.003(5) -0.004(5)
C24 0.036(6) 0.026(6) 0.044(7) 0.000(5) 0.013(5) -0.004(5)
C25 0.024(6) 0.019(6) 0.036(6) 0.012(5) 0.007(5) 0.002(5)
C26 0.030(6) 0.032(7) 0.059(8) 0.017(6) 0.011(6) 0.006(5)
C27 0.026(6) 0.042(7) 0.063(8) 0.037(6) -0.002(5) -0.001(5)
C28 0.033(6) 0.023(6) 0.027(6) 0.016(5) 0.011(5) 0.002(5)
C29 0.018(5) 0.039(7) 0.033(6) 0.018(5) -0.002(5) -0.007(5)
C30 0.025(6) 0.028(6) 0.022(5) 0.001(5) 0.005(4) 0.003(5)
C31 0.023(6) 0.034(6) 0.019(5) 0.012(5) 0.007(4) 0.009(5)
C32 0.018(5) 0.032(6) 0.029(6) 0.012(5) 0.007(4) 0.007(5)
C33 0.043(7) 0.034(7) 0.021(5) 0.006(5) 0.014(5) 0.012(6)
C34 0.017(5) 0.026(6) 0.024(5) 0.008(5) 0.006(4) 0.007(5)
C35 0.038(7) 0.041(7) 0.039(7) 0.026(6) 0.020(5) 0.012(6)
C36 0.034(6) 0.030(7) 0.036(6) 0.017(5) 0.013(5) 0.005(5)
B1 0.026(7) 0.032(8) 0.038(7) 0.024(6) 0.005(6) 0.014(6)
B2 0.029(7) 0.019(7) 0.026(6) 0.013(5) 0.004(5) -0.008(5)
B3 0.043(8) 0.034(8) 0.032(7) 0.016(6) 0.013(6) 0.009(7)
B4 0.037(8) 0.060(11) 0.048(9) 0.022(8) 0.019(7) 0.016(8)
F1 0.064(5) 0.103(6) 0.049(4) 0.048(4) -0.010(4) -0.009(4)
F2 0.074(5) 0.056(5) 0.039(4) 0.012(4) 0.003(4) -0.003(4)
F3 0.048(4) 0.077(6) 0.081(5) 0.027(4) 0.014(4) 0.026(4)
F4 0.048(4) 0.067(5) 0.052(4) 0.017(4) 0.017(3) -0.009(4)

_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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C1 C3 H3B 109.5 . . ?
H3A C3 H3B 109.5 . . ?
C1 C3 H3C 109.5 . . ?
H3A C3 H3C 109.5 . . ?
H3B C3 H3C 109.5 . . ?
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_diffrn_reflns_theta_full              27.50
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;
_chemical_name_common             ?
_chemical_melting_point           ?
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_chemical_formula_sum
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loop_
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 _atom_type_description
 _atom_type_scat_dispersion_real
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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'B'  'B'   0.0013   0.0007
 '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'
 'F'  'F'   0.0171   0.0103
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 'P'  'P'   0.1023   0.0942
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Os'  'Os'  -1.2165   7.6030
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_cell_angle_gamma                 90.00
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 Absorption correction performed with SADABS program. This is based on the
 method of Blessing: Blessing, R. H., Acta Crystallogr., Sect. A 1995, 51, 33.

 SADABS: Area-Detector Absorption Correction. Bruker-AXS
  within SAINT package, v. 6.1 (2000).
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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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H02 H 0.193(8) 0.235(5) 0.261(3) 0.030 Uiso 1 1 d D . .
P P 0.11212(19) 0.31599(12) 0.41968(12) 0.0167(4) Uani 1 1 d . . .
F1 F 0.5777(7) 0.3075(4) 0.6222(4) 0.064(2) Uani 1 1 d . . .
F2 F 0.7213(6) 0.3083(5) 0.7360(5) 0.089(3) Uani 1 1 d . . .
F3 F 0.5572(5) 0.2255(3) 0.7323(3) 0.0445(14) Uani 1 1 d . . .
F4 F 0.7111(5) 0.2035(4) 0.6424(3) 0.0493(15) Uani 1 1 d . . .
O1 O 0.4031(5) 0.2769(3) 0.3957(3) 0.0189(11) Uani 1 1 d . . .
N1 N 0.0838(6) 0.1327(4) 0.3533(4) 0.0176(13) Uani 1 1 d . . .
N2 N 0.0936(6) 0.0577(4) 0.3892(4) 0.0187(14) Uani 1 1 d . . .
N3 N 0.3331(6) 0.1115(4) 0.3236(4) 0.0205(14) Uani 1 1 d . . .
N4 N 0.3134(6) 0.0353(4) 0.3545(4) 0.0228(15) Uani 1 1 d . . .
N5 N 0.2718(6) 0.1586(4) 0.4944(4) 0.0163(13) Uani 1 1 d . . .
N6 N 0.2689(6) 0.0777(4) 0.5023(4) 0.0177(13) Uani 1 1 d . . .
B1 B 0.6446(10) 0.2614(7) 0.6825(7) 0.032(2) Uani 1 1 d . . .
B2 B 0.2228(8) 0.0257(5) 0.4252(6) 0.0200(19) Uani 1 1 d . . .
H03 H 0.227(7) -0.039(5) 0.450(5) 0.024 Uiso 1 1 d . . .
C1 C -0.0338(7) 0.1376(5) 0.3152(4) 0.0178(16) Uani 1 1 d . . .
H1 H -0.0675 0.1828 0.2843 0.021 Uiso 1 1 calc R . .
C2 C -0.0982(7) 0.0672(5) 0.3277(5) 0.0225(17) Uani 1 1 d . . .
H2 H -0.1828 0.0552 0.3081 0.027 Uiso 1 1 calc R . .
C3 C -0.0158(8) 0.0183(5) 0.3738(5) 0.0228(18) Uani 1 1 d . . .
H3 H -0.0329 -0.0347 0.3920 0.027 Uiso 1 1 calc R . .
C4 C 0.4102(7) 0.1025(5) 0.2601(5) 0.0244(18) Uani 1 1 d . . .
H4 H 0.4399 0.1454 0.2269 0.029 Uiso 1 1 calc R . .
C5 C 0.4412(8) 0.0226(5) 0.2490(5) 0.0265(19) Uani 1 1 d . . .
H5 H 0.4941 0.0007 0.2084 0.032 Uiso 1 1 calc R . .
C6 C 0.3785(8) -0.0182(5) 0.3101(5) 0.0274(19) Uani 1 1 d . . .
H6 H 0.3806 -0.0745 0.3193 0.033 Uiso 1 1 calc R . .
C7 C 0.3211(7) 0.1888(5) 0.5698(5) 0.0197(17) Uani 1 1 d . . .
H7 H 0.3348 0.2440 0.5819 0.024 Uiso 1 1 calc R . .
C8 C 0.3490(8) 0.1260(5) 0.6275(5) 0.0260(18) Uani 1 1 d . . .
H8 H 0.3828 0.1300 0.6855 0.031 Uiso 1 1 calc R . .
C9 C 0.3171(7) 0.0568(5) 0.5823(5) 0.0221(17) Uani 1 1 d . . .
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H9 H 0.3271 0.0037 0.6035 0.026 Uiso 1 1 calc R . .
C10 C 0.5152(7) 0.2627(5) 0.4167(4) 0.0186(16) Uani 1 1 d . . .
C11 C 0.6059(8) 0.3315(5) 0.4226(6) 0.031(2) Uani 1 1 d . . .
H11A H 0.5665 0.3784 0.3941 0.047 Uiso 1 1 calc R . .
H11B H 0.6820 0.3170 0.3944 0.047 Uiso 1 1 calc R . .
H11C H 0.6285 0.3440 0.4832 0.047 Uiso 1 1 calc R . .
C12 C 0.5699(8) 0.1821(5) 0.4379(5) 0.0275(19) Uani 1 1 d . . .
H12A H 0.5016 0.1438 0.4450 0.041 Uiso 1 1 calc R . .
H12B H 0.6239 0.1854 0.4916 0.041 Uiso 1 1 calc R . .
H12C H 0.6201 0.1643 0.3912 0.041 Uiso 1 1 calc R . .
C13 C 0.0372(7) 0.2914(5) 0.5212(4) 0.0217(16) Uani 1 1 d . . .
H13 H 0.1084 0.2799 0.5650 0.026 Uiso 1 1 calc R . .
C14 C -0.0406(8) 0.2132(5) 0.5126(5) 0.0240(17) Uani 1 1 d . . .
H14A H -0.0796 0.2028 0.5665 0.036 Uiso 1 1 calc R . .
H14B H 0.0149 0.1685 0.5002 0.036 Uiso 1 1 calc R . .
H14C H -0.1065 0.2188 0.4656 0.036 Uiso 1 1 calc R . .
C15 C -0.0413(8) 0.3569(5) 0.5607(5) 0.0257(18) Uani 1 1 d . . .
H15A H -0.1216 0.3631 0.5262 0.039 Uiso 1 1 calc R . .
H15B H 0.0050 0.4077 0.5615 0.039 Uiso 1 1 calc R . .
H15C H -0.0577 0.3418 0.6196 0.039 Uiso 1 1 calc R . .
C16 C -0.0237(7) 0.3471(5) 0.3436(5) 0.0188(16) Uani 1 1 d . . .
H16 H -0.0931 0.3084 0.3532 0.023 Uiso 1 1 calc R . .
C17 C -0.0006(8) 0.3403(5) 0.2462(5) 0.0220(17) Uani 1 1 d . . .
H17A H -0.0746 0.3605 0.2116 0.033 Uiso 1 1 calc R . .
H17B H 0.0136 0.2840 0.2316 0.033 Uiso 1 1 calc R . .
H17C H 0.0735 0.3720 0.2342 0.033 Uiso 1 1 calc R . .
C18 C -0.0793(8) 0.4307(5) 0.3576(5) 0.0246(18) Uani 1 1 d . . .
H18A H -0.0194 0.4717 0.3415 0.037 Uiso 1 1 calc R . .
H18B H -0.0954 0.4372 0.4183 0.037 Uiso 1 1 calc R . .
H18C H -0.1585 0.4366 0.3218 0.037 Uiso 1 1 calc R . .
C19 C 0.1902(7) 0.4130(5) 0.4464(5) 0.0202(17) Uani 1 1 d . . .
H19 H 0.1230 0.4520 0.4597 0.024 Uiso 1 1 calc R . .
C20 C 0.2863(8) 0.4091(5) 0.5263(5) 0.0260(19) Uani 1 1 d . . .
H20A H 0.3554 0.3728 0.5144 0.039 Uiso 1 1 calc R . .
H20B H 0.2441 0.3891 0.5759 0.039 Uiso 1 1 calc R . .
H20C H 0.3201 0.4627 0.5390 0.039 Uiso 1 1 calc R . .
C21 C 0.2573(7) 0.4469(5) 0.3689(5) 0.0228(17) Uani 1 1 d . . .
H21A H 0.2973 0.4982 0.3850 0.034 Uiso 1 1 calc R . .
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H21C H 0.3216 0.4089 0.3527 0.034 Uiso 1 1 calc R . .

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P 0.0174(10) 0.0197(10) 0.0129(8) 0.0009(7) 0.0005(7) 0.0015(8)
F1 0.086(5) 0.073(5) 0.034(3) 0.017(3) 0.021(3) 0.040(4)
F2 0.050(4) 0.126(7) 0.091(5) -0.063(5) 0.005(4) -0.038(4)
F3 0.051(4) 0.044(4) 0.041(3) -0.007(3) 0.019(3) -0.012(3)
F4 0.047(3) 0.062(4) 0.041(3) -0.001(3) 0.014(3) 0.018(3)
O1 0.018(3) 0.021(3) 0.018(2) 0.003(2) 0.006(2) -0.003(2)
N1 0.023(3) 0.018(3) 0.012(3) 0.000(3) 0.002(2) 0.000(3)
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N2 0.021(3) 0.017(3) 0.019(3) -0.006(3) 0.004(3) 0.001(3)
N3 0.017(3) 0.026(4) 0.019(3) 0.002(3) 0.003(3) 0.003(3)
N4 0.024(4) 0.020(4) 0.024(3) 0.004(3) -0.001(3) -0.002(3)
N5 0.017(3) 0.014(3) 0.017(3) -0.002(2) -0.003(3) -0.002(3)
N6 0.017(3) 0.020(3) 0.016(3) 0.001(3) 0.000(3) -0.002(3)
B1 0.024(5) 0.041(6) 0.031(5) -0.005(5) 0.004(4) 0.004(5)
B2 0.013(4) 0.017(4) 0.030(5) -0.004(4) 0.003(4) -0.004(3)
C1 0.020(4) 0.019(4) 0.014(3) -0.005(3) -0.002(3) -0.003(3)
C2 0.017(4) 0.034(5) 0.016(4) 0.001(3) -0.004(3) -0.007(3)
C3 0.027(4) 0.028(5) 0.014(4) -0.010(3) 0.004(3) -0.010(4)
C4 0.023(4) 0.033(5) 0.018(4) -0.004(3) 0.004(3) -0.005(4)
C5 0.019(4) 0.038(5) 0.024(4) -0.005(4) 0.005(3) 0.001(4)
C6 0.028(5) 0.026(5) 0.028(4) -0.007(4) -0.006(4) 0.003(4)
C7 0.014(4) 0.025(4) 0.020(4) -0.004(3) -0.002(3) 0.000(3)
C8 0.024(4) 0.036(5) 0.018(4) -0.001(4) 0.000(3) 0.000(4)
C9 0.014(4) 0.031(5) 0.020(4) 0.011(3) -0.001(3) 0.006(3)
C10 0.016(4) 0.031(4) 0.009(3) -0.002(3) 0.002(3) -0.004(3)
C11 0.027(5) 0.036(5) 0.030(5) -0.003(4) -0.001(4) -0.002(4)
C12 0.030(5) 0.032(5) 0.020(4) -0.004(3) -0.006(3) -0.002(4)
C13 0.024(4) 0.026(4) 0.015(3) -0.001(3) 0.000(3) 0.000(4)
C14 0.032(5) 0.025(4) 0.016(3) -0.002(3) 0.006(3) -0.004(4)
C15 0.034(5) 0.027(5) 0.017(4) -0.002(3) 0.013(3) 0.005(4)
C16 0.017(4) 0.023(4) 0.015(3) 0.000(3) -0.003(3) 0.000(3)
C17 0.030(5) 0.022(4) 0.014(3) 0.000(3) -0.004(3) 0.007(3)
C18 0.025(5) 0.024(4) 0.024(4) 0.003(3) -0.001(3) 0.005(4)
C19 0.018(4) 0.019(4) 0.023(4) -0.002(3) 0.003(3) 0.007(3)
C20 0.029(5) 0.027(5) 0.020(4) 0.001(3) -0.005(3) -0.003(4)
C21 0.022(5) 0.020(4) 0.026(4) 0.001(3) 0.006(3) -0.004(3)

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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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Os N3 2.111(6) . ?
Os N5 2.113(6) . ?
Os O1 2.121(5) . ?
Os P 2.356(2) . ?
Os H01 1.79(5) . ?
Os H02 1.79(5) . ?
P C19 1.852(8) . ?
P C13 1.868(7) . ?
P C16 1.873(7) . ?
F1 B1 1.373(12) . ?
F2 B1 1.368(12) . ?
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F4 B1 1.374(11) . ?
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N1 N2 1.372(8) . ?
N2 C3 1.342(9) . ?
N2 B2 1.541(11) . ?
N3 C4 1.339(9) . ?
N3 N4 1.381(9) . ?
N4 C6 1.352(10) . ?
N4 B2 1.525(11) . ?
N5 C7 1.349(9) . ?
N5 N6 1.355(8) . ?
N6 C9 1.357(9) . ?
N6 B2 1.533(10) . ?
B2 H03 1.15(8) . ?
C1 C2 1.381(11) . ?
C1 H1 0.9500 . ?
C2 C3 1.362(11) . ?
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C3 H3 0.9500 . ?
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C8 H8 0.9500 . ?
C9 H9 0.9500 . ?
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C11 H11B 0.9800 . ?
C11 H11C 0.9800 . ?
C12 H12A 0.9800 . ?
C12 H12B 0.9800 . ?
C12 H12C 0.9800 . ?
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C14 H14B 0.9800 . ?
C14 H14C 0.9800 . ?
C15 H15A 0.9800 . ?
C15 H15B 0.9800 . ?
C15 H15C 0.9800 . ?
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C17 H17B 0.9800 . ?
C17 H17C 0.9800 . ?
C18 H18A 0.9800 . ?
C18 H18B 0.9800 . ?
C18 H18C 0.9800 . ?
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C19 C20 1.552(10) . ?
C19 C21 1.555(10) . ?
C19 H19 1.0000 . ?
C20 H20A 0.9800 . ?
C20 H20B 0.9800 . ?
C20 H20C 0.9800 . ?
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O1 Os P 91.57(15) . . ?
N1 Os H01 107(3) . . ?
N3 Os H01 91(3) . . ?
N5 Os H01 164(3) . . ?
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P Os H01 89(3) . . ?
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N2 N1 Os 118.7(5) . . ?
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C4 N3 N4 105.7(6) . . ?
C4 N3 Os 133.9(6) . . ?
N4 N3 Os 120.1(5) . . ?
C6 N4 N3 109.4(7) . . ?
C6 N4 B2 132.5(7) . . ?
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N3 N4 B2 118.0(6) . . ?
C7 N5 N6 107.6(6) . . ?
C7 N5 Os 132.4(5) . . ?
N6 N5 Os 118.9(4) . . ?
N5 N6 C9 109.3(6) . . ?
N5 N6 B2 120.0(6) . . ?
C9 N6 B2 130.6(7) . . ?
F2 B1 F1 110.6(10) . . ?
F2 B1 F4 112.0(8) . . ?
F1 B1 F4 109.9(8) . . ?
F2 B1 F3 107.5(8) . . ?
F1 B1 F3 106.8(8) . . ?
F4 B1 F3 109.9(9) . . ?
N4 B2 N6 108.9(6) . . ?
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N4 B2 H03 109(4) . . ?
N6 B2 H03 106(4) . . ?
N2 B2 H03 118(4) . . ?
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C2 C1 H1 125.1 . . ?
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C1 C2 H2 126.9 . . ?
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C2 C3 H3 125.8 . . ?
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C4 C5 H5 127.6 . . ?
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C5 C6 H6 125.7 . . ?
N5 C7 C8 109.3(7) . . ?
N5 C7 H7 125.3 . . ?
C8 C7 H7 125.4 . . ?
C9 C8 C7 105.4(7) . . ?
C9 C8 H8 127.3 . . ?
C7 C8 H8 127.3 . . ?
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C8 C9 H9 125.8 . . ?
O1 C10 C12 125.7(7) . . ?
O1 C10 C11 118.2(7) . . ?
C12 C10 C11 116.0(7) . . ?
C10 C11 H11A 109.5 . . ?
C10 C11 H11B 109.5 . . ?
H11A C11 H11B 109.5 . . ?
C10 C11 H11C 109.5 . . ?
H11A C11 H11C 109.5 . . ?
H11B C11 H11C 109.5 . . ?
C10 C12 H12A 109.5 . . ?
C10 C12 H12B 109.5 . . ?
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H12A C12 H12B 109.5 . . ?
C10 C12 H12C 109.5 . . ?
H12A C12 H12C 109.5 . . ?
H12B C12 H12C 109.5 . . ?
C15 C13 C14 109.4(6) . . ?
C15 C13 P 117.6(6) . . ?
C14 C13 P 111.8(5) . . ?
C15 C13 H13 105.7 . . ?
C14 C13 H13 105.7 . . ?
P C13 H13 105.7 . . ?
C13 C14 H14A 109.5 . . ?
C13 C14 H14B 109.5 . . ?
H14A C14 H14B 109.5 . . ?
C13 C14 H14C 109.5 . . ?
H14A C14 H14C 109.5 . . ?
H14B C14 H14C 109.5 . . ?
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C13 C15 H15B 109.5 . . ?
H15A C15 H15B 109.5 . . ?
C13 C15 H15C 109.5 . . ?
H15A C15 H15C 109.5 . . ?
H15B C15 H15C 109.5 . . ?
C18 C16 C17 107.1(6) . . ?
C18 C16 P 116.6(5) . . ?
C17 C16 P 115.2(5) . . ?
C18 C16 H16 105.6 . . ?
C17 C16 H16 105.6 . . ?
P C16 H16 105.6 . . ?
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C16 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
C16 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
C16 C18 H18A 109.5 . . ?
C16 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
C16 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
C20 C19 C21 109.0(6) . . ?
C20 C19 P 113.7(5) . . ?
C21 C19 P 111.5(5) . . ?
C20 C19 H19 107.5 . . ?
C21 C19 H19 107.5 . . ?
P C19 H19 107.5 . . ?
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C19 C20 H20B 109.5 . . ?
H20A C20 H20B 109.5 . . ?
C19 C20 H20C 109.5 . . ?
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H20B C20 H20C 109.5 . . ?
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C19 C21 H21B 109.5 . . ?
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C19 C21 H21C 109.5 . . ?
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H21B C21 H21C 109.5 . . ?

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# Data for compound 6 (local labelling mae248as)


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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'B'  'B'   0.0013   0.0007
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 'N'  'N'   0.0061   0.0033
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 'O'  'O'   0.0106   0.0060
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 'P'  'P'   0.1023   0.0942
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 'Os'  'Os'  -1.2165   7.6030
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 'x, y, z'
 '-x□, y□, -z□'
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 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

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_cell_length_c                    18.658(2)
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_cell_angle_beta                  91.351(2)
_cell_angle_gamma                 90.00
_cell_volume                      4632.9(9)
_cell_formula_units_Z             4
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used     3354
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;
Absorption correction performed with SADABS program. This is based on the
method of Blessing: Blessing, R. H., Acta Crystallogr., Sect. A 1995, 51, 33.

SADABS: Area-Detector Absorption Correction. Bruker-AXS
within SAINT package, v. 6.1 (2000).
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_diffrn_radiation_monochromator   graphite
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_diffrn_measurement_method        '\w rotations with narrow frames'
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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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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
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_refine_ls_number_parameters      554
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_refine_ls_R_factor_gt            0.0447
_refine_ls_wR_factor_ref          0.0784
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P1 P 0.13330(10) 0.93210(6) 0.22145(7) 0.0202(3) Uani 1 1 d . . .
N1 N 0.4355(3) 1.03362(18) 0.1738(2) 0.0172(9) Uani 1 1 d . . .
N2 N 0.4415(3) 1.08109(18) 0.1207(2) 0.0180(9) Uani 1 1 d . . .
N3 N 0.2737(3) 0.97434(18) 0.0871(2) 0.0176(9) Uani 1 1 d . . .
N4 N 0.2999(3) 1.02828(18) 0.0440(2) 0.0188(9) Uani 1 1 d . . .
N5 N 0.2268(3) 1.08028(19) 0.1852(2) 0.0173(9) Uani 1 1 d . . .
N6 N 0.2570(3) 1.12187(19) 0.1293(2) 0.0175(9) Uani 1 1 d . . .
O1 O 0.3347(2) 0.99801(15) 0.30453(16) 0.0210(8) Uani 1 1 d . . .
O2 O 0.3887(2) 0.90011(15) 0.21768(17) 0.0200(8) Uani 1 1 d . . .
C1 C 0.5318(4) 1.0332(2) 0.2061(3) 0.0203(11) Uani 1 1 d . . .
H1 H 0.5516 1.0047 0.2454 0.024 Uiso 1 1 calc R . .
C2 C 0.5972(4) 1.0798(2) 0.1744(3) 0.0220(12) Uani 1 1 d . . .
H2 H 0.6684 1.0895 0.1872 0.026 Uiso 1 1 calc R . .
C3 C 0.5383(4) 1.1091(2) 0.1208(3) 0.0240(12) Uani 1 1 d . . .
H3 H 0.5615 1.1436 0.0888 0.029 Uiso 1 1 calc R . .
C4 C 0.2837(4) 1.0112(3) -0.0256(2) 0.0257(12) Uani 1 1 d . . .
H4 H 0.2964 1.0398 -0.0657 0.031 Uiso 1 1 calc R . .
C5 C 0.2460(4) 0.9458(3) -0.0287(3) 0.0270(13) Uani 1 1 d . . .
H5 H 0.2273 0.9202 -0.0704 0.032 Uiso 1 1 calc R . .
C6 C 0.2409(4) 0.9247(2) 0.0421(3) 0.0234(12) Uani 1 1 d . . .
H6 H 0.2173 0.8809 0.0569 0.028 Uiso 1 1 calc R . .
C7 C 0.2108(4) 1.1833(2) 0.1348(3) 0.0231(12) Uani 1 1 d . . .
H7 H 0.2182 1.2204 0.1023 0.028 Uiso 1 1 calc R . .
C8 C 0.1512(4) 1.1838(2) 0.1951(3) 0.0230(12) Uani 1 1 d . . .
H8 H 0.1099 1.2204 0.2127 0.028 Uiso 1 1 calc R . .
C9 C 0.1643(4) 1.1197(2) 0.2244(3) 0.0221(12) Uani 1 1 d . . .
H9 H 0.1326 1.1051 0.2675 0.027 Uiso 1 1 calc R . .
C10 C 0.0153(4) 0.9804(2) 0.1880(3) 0.0223(11) Uani 1 1 d . . .
H10 H 0.0204 1.0262 0.2116 0.027 Uiso 1 1 calc R . .
C11 C 0.0197(4) 0.9949(2) 0.1073(2) 0.0275(13) Uani 1 1 d . . .
H11A H 0.0188 0.9515 0.0808 0.041 Uiso 1 1 calc R . .
H11B H 0.0844 1.0199 0.0970 0.041 Uiso 1 1 calc R . .
H11C H -0.0414 1.0225 0.0924 0.041 Uiso 1 1 calc R . .
C12 C -0.0937(4) 0.9532(3) 0.2062(3) 0.0298(13) Uani 1 1 d . . .
H12A H -0.1469 0.9879 0.1941 0.045 Uiso 1 1 calc R . .
H12B H -0.0957 0.9430 0.2576 0.045 Uiso 1 1 calc R . .
H12C H -0.1083 0.9115 0.1787 0.045 Uiso 1 1 calc R . .
C13 C 0.1081(4) 0.9196(2) 0.3175(3) 0.0258(12) Uani 1 1 d . . .
H13 H 0.0408 0.8935 0.3210 0.031 Uiso 1 1 calc R . .
C14 C 0.0943(4) 0.9870(3) 0.3578(3) 0.0314(13) Uani 1 1 d . . .
H14A H 0.0745 0.9774 0.4072 0.047 Uiso 1 1 calc R . .
H14B H 0.0390 1.0142 0.3339 0.047 Uiso 1 1 calc R . .
H14C H 0.1606 1.0126 0.3581 0.047 Uiso 1 1 calc R . .
C15 C 0.1957(4) 0.8757(3) 0.3527(3) 0.0354(14) Uani 1 1 d . . .
H15A H 0.2643 0.8914 0.3364 0.053 Uiso 1 1 calc R . .
H15B H 0.1854 0.8277 0.3393 0.053 Uiso 1 1 calc R . .
H15C H 0.1931 0.8802 0.4050 0.053 Uiso 1 1 calc R . .
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C16 C 0.1072(4) 0.8443(2) 0.1834(3) 0.0260(13) Uani 1 1 d . . .
H16 H 0.0775 0.8516 0.1338 0.031 Uiso 1 1 calc R . .
C17 C 0.0277(4) 0.8005(3) 0.2219(3) 0.0384(15) Uani 1 1 d . . .
H17A H 0.0067 0.7619 0.1913 0.058 Uiso 1 1 calc R . .
H17B H -0.0343 0.8282 0.2326 0.058 Uiso 1 1 calc R . .
H17C H 0.0595 0.7832 0.2667 0.058 Uiso 1 1 calc R . .
C18 C 0.2071(4) 0.8007(2) 0.1749(3) 0.0323(14) Uani 1 1 d . . .
H18A H 0.2340 0.7867 0.2223 0.048 Uiso 1 1 calc R . .
H18B H 0.2607 0.8277 0.1507 0.048 Uiso 1 1 calc R . .
H18C H 0.1901 0.7600 0.1462 0.048 Uiso 1 1 calc R . .
C19 C 0.3731(4) 1.0415(3) 0.3462(3) 0.0237(12) Uani 1 1 d . . .
C20 C 0.4014(4) 1.0190(3) 0.4210(2) 0.0364(14) Uani 1 1 d . . .
H20A H 0.3853 0.9703 0.4263 0.055 Uiso 1 1 calc R . .
H20B H 0.3606 1.0456 0.4552 0.055 Uiso 1 1 calc R . .
H20C H 0.4767 1.0266 0.4303 0.055 Uiso 1 1 calc R . .
C21 C 0.3909(4) 1.1136(2) 0.3279(3) 0.0316(14) Uani 1 1 d . . .
H21A H 0.3700 1.1215 0.2777 0.047 Uiso 1 1 calc R . .
H21B H 0.4656 1.1246 0.3349 0.047 Uiso 1 1 calc R . .
H21C H 0.3489 1.1428 0.3589 0.047 Uiso 1 1 calc R . .
C22 C 0.4647(4) 0.8716(2) 0.1897(3) 0.0215(12) Uani 1 1 d . . .
C23 C 0.5356(4) 0.8294(2) 0.2363(3) 0.0310(14) Uani 1 1 d . . .
H23A H 0.6048 0.8513 0.2403 0.046 Uiso 1 1 calc R . .
H23B H 0.5430 0.7838 0.2152 0.046 Uiso 1 1 calc R . .
H23C H 0.5056 0.8253 0.2840 0.046 Uiso 1 1 calc R . .
C24 C 0.4889(4) 0.8767(2) 0.1121(3) 0.0299(13) Uani 1 1 d . . .
H24A H 0.4614 0.8362 0.0869 0.045 Uiso 1 1 calc R . .
H24B H 0.5652 0.8793 0.1065 0.045 Uiso 1 1 calc R . .
H24C H 0.4558 0.9179 0.0918 0.045 Uiso 1 1 calc R . .
C25 C 0.7956(4) 0.1778(2) 0.2998(2) 0.0165(11) Uani 1 1 d . . .
C26 C 0.8596(4) 0.1410(2) 0.2532(2) 0.0178(11) Uani 1 1 d . . .
H26 H 0.8985 0.1033 0.2722 0.021 Uiso 1 1 calc R . .
C27 C 0.8694(4) 0.1564(2) 0.1812(3) 0.0206(11) Uani 1 1 d . . .
H27 H 0.9163 0.1309 0.1527 0.025 Uiso 1 1 calc R . .
C28 C 0.8104(4) 0.2089(2) 0.1511(3) 0.0219(12) Uani 1 1 d . . .
H28 H 0.8176 0.2207 0.1021 0.026 Uiso 1 1 calc R . .
C29 C 0.7412(4) 0.2438(2) 0.1934(3) 0.0225(12) Uani 1 1 d . . .
H29 H 0.6974 0.2783 0.1728 0.027 Uiso 1 1 calc R . .
C30 C 0.7348(4) 0.2290(2) 0.2658(2) 0.0187(11) Uani 1 1 d . . .
H30 H 0.6872 0.2545 0.2938 0.022 Uiso 1 1 calc R . .
C31 C 0.7847(4) 0.0791(2) 0.3970(2) 0.0178(11) Uani 1 1 d . . .
C32 C 0.8503(4) 0.0380(2) 0.4397(3) 0.0218(12) Uani 1 1 d . . .
H32 H 0.9066 0.0595 0.4655 0.026 Uiso 1 1 calc R . .
C33 C 0.8385(4) -0.0320(2) 0.4470(3) 0.0243(13) Uani 1 1 d . . .
H33 H 0.8866 -0.0572 0.4765 0.029 Uiso 1 1 calc R . .
C34 C 0.7573(4) -0.0651(3) 0.4116(3) 0.0272(13) Uani 1 1 d . . .
H34 H 0.7481 -0.1131 0.4166 0.033 Uiso 1 1 calc R . .
C35 C 0.6891(4) -0.0270(2) 0.3685(3) 0.0290(13) Uani 1 1 d . . .
H35 H 0.6323 -0.0488 0.3437 0.035 Uiso 1 1 calc R . .
C36 C 0.7040(4) 0.0426(3) 0.3618(3) 0.0260(12) Uani 1 1 d . . .
H36 H 0.6565 0.0673 0.3314 0.031 Uiso 1 1 calc R . .
C37 C 0.7007(4) 0.2032(2) 0.4254(2) 0.0193(11) Uani 1 1 d . . .
C38 C 0.6164(4) 0.1718(3) 0.4586(3) 0.0252(12) Uani 1 1 d . . .
H38 H 0.6140 0.1232 0.4596 0.030 Uiso 1 1 calc R . .
C39 C 0.5361(4) 0.2079(3) 0.4902(3) 0.0305(13) Uani 1 1 d . . .
H39 H 0.4801 0.1839 0.5118 0.037 Uiso 1 1 calc R . .
C40 C 0.5370(4) 0.2787(3) 0.4905(3) 0.0323(14) Uani 1 1 d . . .
H40 H 0.4819 0.3038 0.5117 0.039 Uiso 1 1 calc R . .
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C41 C 0.6198(4) 0.3119(3) 0.4593(3) 0.0284(13) Uani 1 1 d . . .
H41 H 0.6221 0.3605 0.4589 0.034 Uiso 1 1 calc R . .
C42 C 0.6994(4) 0.2748(3) 0.4286(2) 0.0231(12) Uani 1 1 d . . .
H42 H 0.7564 0.2991 0.4086 0.028 Uiso 1 1 calc R . .
C43 C 0.9111(4) 0.1861(2) 0.4235(2) 0.0173(11) Uani 1 1 d . . .
C44 C 1.0075(4) 0.1815(2) 0.3893(3) 0.0218(12) Uani 1 1 d . . .
H44 H 1.0074 0.1682 0.3404 0.026 Uiso 1 1 calc R . .
C45 C 1.1038(4) 0.1953(2) 0.4235(3) 0.0249(12) Uani 1 1 d . . .
H45 H 1.1674 0.1910 0.3982 0.030 Uiso 1 1 calc R . .
C46 C 1.1060(4) 0.2151(2) 0.4943(3) 0.0275(13) Uani 1 1 d . . .
H46 H 1.1711 0.2246 0.5183 0.033 Uiso 1 1 calc R . .
C47 C 1.0129(4) 0.2211(2) 0.5301(3) 0.0259(12) Uani 1 1 d . . .
H47 H 1.0135 0.2344 0.5790 0.031 Uiso 1 1 calc R . .
C48 C 0.9182(4) 0.2076(2) 0.4943(3) 0.0211(11) Uani 1 1 d . . .
H48 H 0.8549 0.2134 0.5196 0.025 Uiso 1 1 calc R . .
B1 B 0.3392(5) 1.0957(3) 0.0767(3) 0.0195(13) Uani 1 1 d . . .
H49 H 0.356(4) 1.129(2) 0.035(3) 0.040 Uiso 1 1 d . . .
B2 B 0.7974(4) 0.1621(3) 0.3866(3) 0.0153(12) Uani 1 1 d . . .

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N1 0.021(2) 0.014(2) 0.016(2) 0.0017(16) -0.0005(18) 0.0025(17)
N2 0.022(2) 0.012(2) 0.020(2) -0.0003(17) 0.0002(19) 0.0018(17)
N3 0.016(2) 0.014(2) 0.023(2) -0.0002(17) 0.0003(18) -0.0004(17)
N4 0.017(2) 0.020(3) 0.019(2) 0.0024(17) 0.0012(18) 0.0021(17)
N5 0.012(2) 0.020(2) 0.020(2) -0.0022(18) -0.0018(18) -0.0021(17)
N6 0.020(2) 0.018(2) 0.014(2) -0.0013(17) -0.0016(18) 0.0005(18)
O1 0.0215(19) 0.018(2) 0.0229(19) 0.0004(14) -0.0017(15) -0.0007(14)
O2 0.0168(19) 0.0199(19) 0.023(2) -0.0008(15) 0.0022(16) -0.0044(15)
C1 0.023(3) 0.020(3) 0.018(3) -0.001(2) -0.004(2) 0.000(2)
C2 0.018(3) 0.023(3) 0.026(3) -0.004(2) 0.002(2) -0.003(2)
C3 0.021(3) 0.019(3) 0.032(3) 0.000(2) 0.003(3) -0.004(2)
C4 0.024(3) 0.038(3) 0.015(3) -0.004(2) -0.001(2) 0.001(3)
C5 0.024(3) 0.032(3) 0.024(3) -0.013(2) 0.002(2) -0.006(2)
C6 0.020(3) 0.020(3) 0.029(3) -0.009(2) -0.001(2) 0.003(2)
C7 0.022(3) 0.017(3) 0.029(3) -0.001(2) -0.007(2) 0.000(2)
C8 0.019(3) 0.019(3) 0.031(3) -0.005(2) -0.004(2) 0.005(2)
C9 0.020(3) 0.022(3) 0.024(3) -0.004(2) 0.001(2) 0.001(2)
C10 0.018(3) 0.020(3) 0.029(3) -0.004(2) 0.000(2) 0.002(2)
C11 0.024(3) 0.028(3) 0.031(3) 0.002(2) -0.003(2) 0.006(2)
C12 0.018(3) 0.030(3) 0.041(4) -0.005(3) 0.003(3) -0.001(2)
C13 0.024(3) 0.026(3) 0.028(3) 0.003(2) 0.008(2) -0.007(2)
C14 0.028(3) 0.044(3) 0.022(3) 0.005(3) 0.006(2) 0.000(3)
C15 0.038(4) 0.036(4) 0.033(3) 0.011(3) 0.008(3) -0.004(3)
C16 0.022(3) 0.015(3) 0.041(4) -0.003(2) 0.000(3) -0.004(2)
C17 0.026(3) 0.026(3) 0.063(4) -0.003(3) 0.005(3) -0.008(3)
C18 0.027(3) 0.023(3) 0.047(4) -0.004(3) 0.002(3) 0.000(2)
C19 0.019(3) 0.028(3) 0.024(3) -0.001(2) 0.007(2) 0.007(2)
C20 0.041(4) 0.050(4) 0.019(3) -0.003(3) -0.002(3) -0.004(3)
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C21 0.028(3) 0.026(3) 0.041(4) -0.008(3) -0.005(3) 0.004(2)
C22 0.019(3) 0.010(3) 0.035(3) 0.000(2) 0.000(2) -0.006(2)
C23 0.022(3) 0.024(3) 0.046(4) -0.001(3) -0.005(3) 0.001(2)
C24 0.027(3) 0.024(3) 0.039(4) -0.003(3) 0.009(3) 0.002(2)
C25 0.011(3) 0.018(3) 0.021(3) -0.004(2) -0.002(2) -0.004(2)
C26 0.017(3) 0.018(3) 0.018(3) -0.002(2) -0.005(2) 0.002(2)
C27 0.016(3) 0.025(3) 0.022(3) -0.005(2) 0.000(2) 0.000(2)
C28 0.025(3) 0.025(3) 0.015(3) 0.000(2) 0.002(2) -0.006(2)
C29 0.023(3) 0.021(3) 0.024(3) 0.004(2) -0.003(2) 0.001(2)
C30 0.013(3) 0.022(3) 0.020(3) -0.006(2) 0.001(2) -0.002(2)
C31 0.016(3) 0.023(3) 0.014(3) -0.001(2) 0.002(2) 0.000(2)
C32 0.023(3) 0.021(3) 0.022(3) 0.000(2) 0.001(2) -0.004(2)
C33 0.025(3) 0.022(3) 0.026(3) 0.004(2) -0.001(2) 0.003(2)
C34 0.038(4) 0.017(3) 0.027(3) 0.003(2) 0.004(3) -0.001(2)
C35 0.035(3) 0.024(4) 0.027(3) -0.002(2) -0.008(3) -0.007(2)
C36 0.029(3) 0.025(3) 0.024(3) 0.002(2) -0.007(2) 0.001(2)
C37 0.019(3) 0.024(3) 0.014(3) 0.001(2) -0.002(2) 0.002(2)
C38 0.027(3) 0.025(3) 0.024(3) -0.001(2) 0.002(2) 0.001(2)
C39 0.023(3) 0.038(4) 0.031(3) -0.005(3) 0.007(3) -0.005(3)
C40 0.022(3) 0.052(4) 0.023(3) -0.011(3) 0.002(3) 0.010(3)
C41 0.031(3) 0.026(3) 0.027(3) -0.005(2) -0.003(3) 0.006(2)
C42 0.026(3) 0.029(3) 0.014(3) -0.001(2) -0.002(2) 0.000(2)
C43 0.023(3) 0.012(2) 0.017(3) 0.000(2) 0.000(2) 0.000(2)
C44 0.027(3) 0.017(3) 0.021(3) 0.001(2) -0.001(2) -0.001(2)
C45 0.017(3) 0.025(3) 0.033(3) -0.002(2) 0.001(2) -0.001(2)
C46 0.021(3) 0.020(3) 0.040(4) 0.006(2) -0.016(3) -0.003(2)
C47 0.037(3) 0.022(3) 0.018(3) -0.002(2) -0.005(3) -0.002(2)
C48 0.024(3) 0.019(3) 0.020(3) 0.002(2) 0.000(2) 0.001(2)
B1 0.023(3) 0.020(3) 0.016(3) -0.001(2) 0.002(3) 0.002(3)
B2 0.016(3) 0.016(3) 0.014(3) 0.000(2) 0.001(2) -0.003(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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P1 C10 1.867(5) . ?
P1 C16 1.883(5) . ?
N1 C1 1.352(5) . ?
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N4 B1 1.531(6) . ?
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C45 H45 0.9500 . ?
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O1 Os P1 93.10(9) . . ?
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C3 N2 N1 110.1(4) . . ?
C3 N2 B1 133.0(4) . . ?
N1 N2 B1 116.8(4) . . ?
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C6 N3 Os 136.5(3) . . ?
N4 N3 Os 118.2(3) . . ?
C4 N4 N3 109.9(4) . . ?
C4 N4 B1 129.5(4) . . ?
N3 N4 B1 120.6(4) . . ?
C9 N5 N6 104.7(4) . . ?
C9 N5 Os 135.9(3) . . ?
N6 N5 Os 119.0(3) . . ?
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C7 N6 B1 130.7(4) . . ?
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C22 O2 Os 136.7(3) . . ?
N1 C1 C2 110.7(4) . . ?
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C16 C18 H18C 109.5 . . ?
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H18B C18 H18C 109.5 . . ?
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C21 C19 C20 117.6(5) . . ?
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C19 C20 H20B 109.5 . . ?
H20A C20 H20B 109.5 . . ?
C19 C20 H20C 109.5 . . ?
H20A C20 H20C 109.5 . . ?
H20B C20 H20C 109.5 . . ?
C19 C21 H21A 109.5 . . ?
C19 C21 H21B 109.5 . . ?
H21A C21 H21B 109.5 . . ?
C19 C21 H21C 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
O2 C22 C23 118.0(5) . . ?
O2 C22 C24 124.0(5) . . ?
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C22 C23 H23B 109.5 . . ?
H23A C23 H23B 109.5 . . ?
C22 C23 H23C 109.5 . . ?
H23A C23 H23C 109.5 . . ?
H23B C23 H23C 109.5 . . ?
C22 C24 H24A 109.5 . . ?
C22 C24 H24B 109.5 . . ?
H24A C24 H24B 109.5 . . ?
C22 C24 H24C 109.5 . . ?
H24A C24 H24C 109.5 . . ?
H24B C24 H24C 109.5 . . ?
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C26 C25 B2 121.2(4) . . ?
C30 C25 B2 124.8(4) . . ?
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C39 C38 C37 123.2(5) . . ?
C39 C38 H38 118.4 . . ?
C37 C38 H38 118.4 . . ?
C38 C39 C40 120.3(5) . . ?
C38 C39 H39 119.9 . . ?
C40 C39 H39 119.9 . . ?
C41 C40 C39 118.4(5) . . ?
C41 C40 H40 120.8 . . ?
C39 C40 H40 120.8 . . ?
C40 C41 C42 120.2(5) . . ?
C40 C41 H41 119.9 . . ?
C42 C41 H41 119.9 . . ?
C41 C42 C37 123.5(5) . . ?
C41 C42 H42 118.3 . . ?
C37 C42 H42 118.3 . . ?
C48 C43 C44 114.6(4) . . ?
C48 C43 B2 121.3(4) . . ?
C44 C43 B2 124.0(4) . . ?
C45 C44 C43 123.3(5) . . ?
C45 C44 H44 118.3 . . ?
C43 C44 H44 118.3 . . ?
C46 C45 C44 119.5(5) . . ?
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C46 C45 H45 120.3 . . ?
C44 C45 H45 120.3 . . ?
C47 C46 C45 119.3(5) . . ?
C47 C46 H46 120.3 . . ?
C45 C46 H46 120.3 . . ?
C46 C47 C48 119.8(5) . . ?
C46 C47 H47 120.1 . . ?
C48 C47 H47 120.1 . . ?
C43 C48 C47 123.5(5) . . ?
C43 C48 H48 118.3 . . ?
C47 C48 H48 118.3 . . ?
N4 B1 N6 108.7(4) . . ?
N4 B1 N2 108.3(4) . . ?
N6 B1 N2 107.3(4) . . ?
N4 B1 H49 108(3) . . ?
N6 B1 H49 115(3) . . ?
N2 B1 H49 109(3) . . ?
C31 B2 C25 107.6(4) . . ?
C31 B2 C37 110.6(4) . . ?
C25 B2 C37 110.3(4) . . ?
C31 B2 C43 108.6(4) . . ?
C25 B2 C43 110.4(4) . . ?
C37 B2 C43 109.3(4) . . ?

_diffrn_measured_fraction_theta_max    0.933
_diffrn_reflns_theta_full              27.50
_diffrn_measured_fraction_theta_full   0.999
_refine_diff_density_max    1.804
_refine_diff_density_min   -1.170
_refine_diff_density_rms    0.133
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