Supporting Information

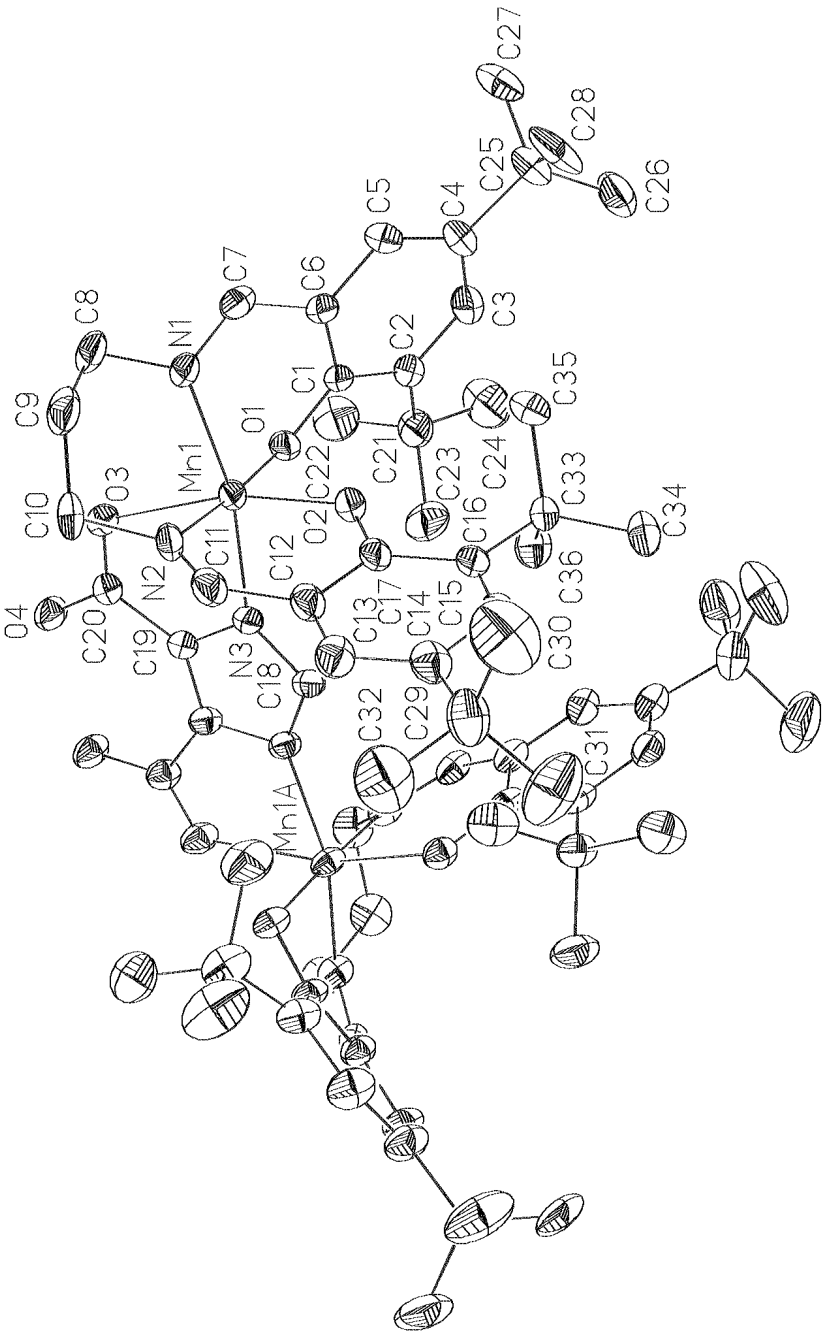


Figure S1

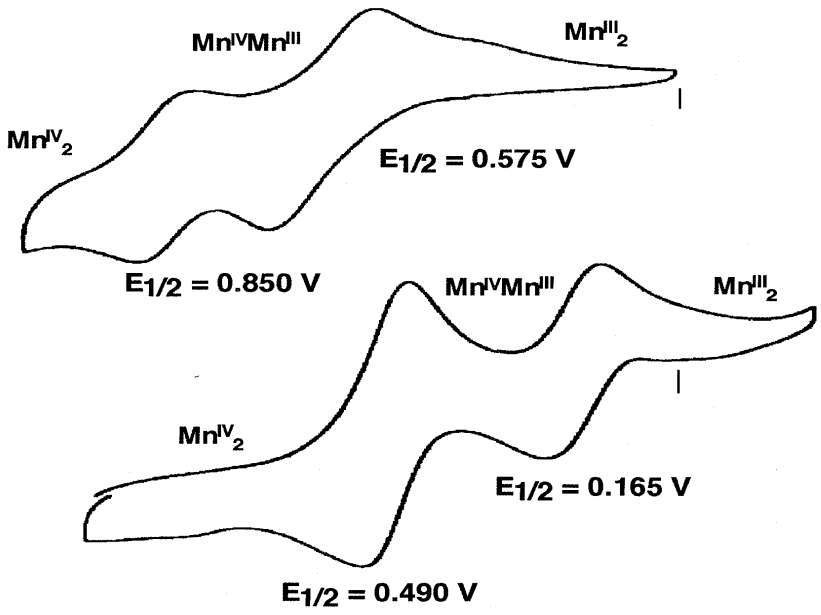
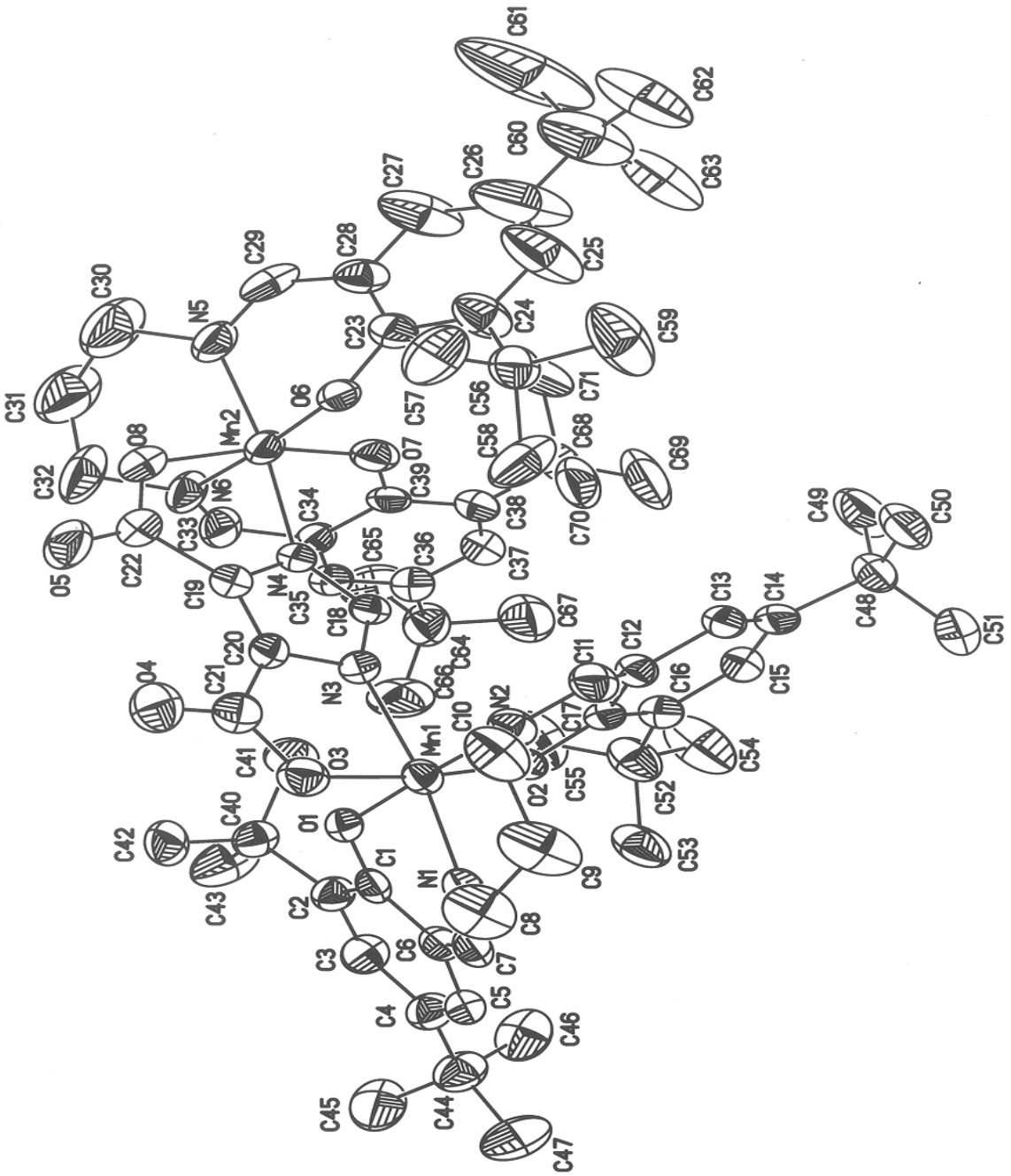


Figure S2. Cyclic voltammograms of **1** (top) and after one equivalent of base addition to **1** (bottom)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C62
C60
C63
C27
C26
C28
C25
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C24
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N5
C23
C59
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C57
C56
C71
C58
C68
O8
Mn2
O7
C69
C32
N6
C39
C38
C70
C34
C49
C50
C33
C65
C36
C37
O5
C22
C19
N4
C35
C18
C67
C13
C14
C48
C51
C20
C12
C64
O4
C21
N3
C66
C11
C16
C15
C10
N2
C17
Mn1
C54
C41
O3
O2
C55
C52
C40
O1
C53
C42
C1
N1
C9
C43
C2
C8
C3
C6
C7
C5
C4
C46
C45
C44
C47

Figure S3

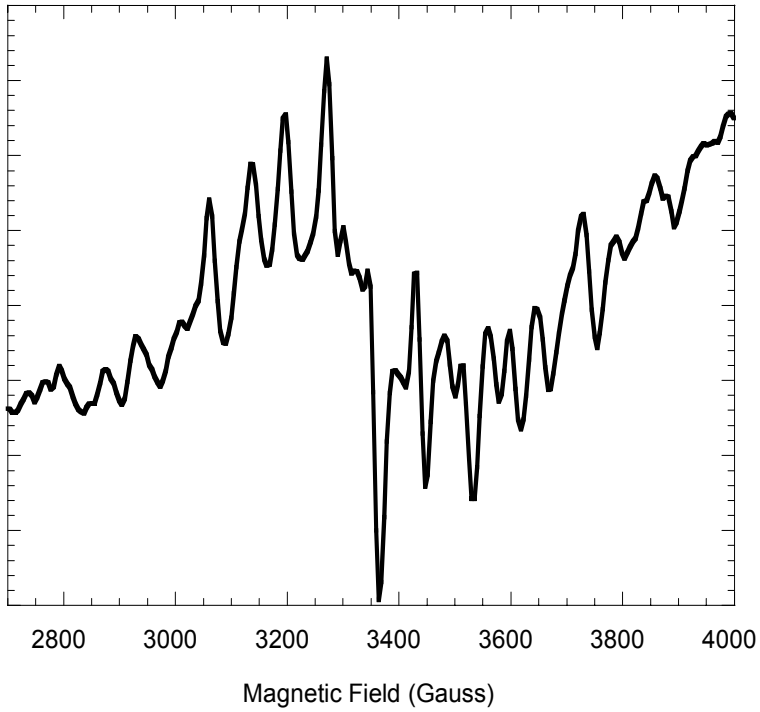

Figure S4. g=2 region of the 53K EPR spectrum of **2**

Data of Mn2(III)(dtsalpn)HDCBI (2)

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

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   occupancies of 0.65/0.35.  One of the t-butyl
   groups (C26-C28) is also disordered and refined at occupancies of 0.58 and
   0.42 for 2 orientations rotated approx. 60 deg. with respect to one another.
   All hydrogens were placed in calculated positions except for the hydrogen on
   O4 which was refined isotropically.  O4-H4OX, 0.86(2) A; O4A..H4OX, 1.61A.

 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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O2 O 0.45707(18) 0.62397(6) 0.60137(10) 0.0281(5) Uani 1 1 d . . .
O3 O 0.45576(19) 0.50138(6) 0.60756(10) 0.0320(6) Uani 1 1 d . . .
O4 O 0.4840(2) 0.45841(6) 0.68864(11) 0.0354(6) Uani 1 1 d . . .
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C6 C 0.5944(3) 0.59674(9) 0.49170(15) 0.0277(7) Uani 1 1 d . . .
C7 C 0.5037(3) 0.57549(9) 0.46187(15) 0.0288(8) Uani 1 1 d . . .
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C8 C 0.3621(3) 0.53318(10) 0.45732(17) 0.0374(9) Uani 1 1 d . . .
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C14 C 0.2290(3) 0.69594(10) 0.64630(17) 0.0339(8) Uani 1 1 d . . .
C15 C 0.3308(3) 0.70839(9) 0.64389(16) 0.0339(8) Uani 1 1 d . . .
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C16 C 0.4102(3) 0.68574(9) 0.63102(15) 0.0294(8) Uani 1 1 d . . .
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H18 H 0.5000 0.6077 0.7500 0.034(3) Uiso 1 2 calc SR . .
C19 C 0.4887(2) 0.52324(9) 0.71603(14) 0.0244(7) Uani 1 1 d . . .
C20 C 0.4751(3) 0.49289(9) 0.66715(16) 0.0279(7) Uani 1 1 d . . .
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H37B H 0.2565 0.0548 0.2311 0.126 Uiso 0.65 1 calc PR D 1
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H44C H 0.8701 0.1060 0.2786 0.126 Uiso 0.65 1 calc PR F 1
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H48 H 0.6109 0.1568 0.4507 0.101 Uiso 0.65 1 calc PR F 1
C49 C 0.7648(5) 0.15677(19) 0.4464(2) 0.0841(7) Uiso 0.65 1 d PG F 1
H49 H 0.7884 0.1657 0.4903 0.101 Uiso 0.65 1 calc PR F 1
C50 C 0.8357(3) 0.14903(19) 0.4058(3) 0.0841(7) Uiso 0.65 1 d PG F 1
H50 H 0.9077 0.1526 0.4219 0.101 Uiso 0.65 1 calc PR F 1
C37A C 0.4216(8) 0.0541(3) 0.4560(6) 0.0963(16) Uiso 0.35 1 d PG F 2
H37D H 0.4967 0.0560 0.4717 0.144 Uiso 0.35 1 calc PR F 2
H37E H 0.3953 0.0317 0.4754 0.144 Uiso 0.35 1 calc PR F 2
H37F H 0.3876 0.0766 0.4694 0.144 Uiso 0.35 1 calc PR F 2
C38A C 0.4009(10) 0.0511(4) 0.3881(4) 0.0963(16) Uiso 0.35 1 d PG F 2
C39A C 0.2988(9) 0.0475(4) 0.3551(6) 0.0963(16) Uiso 0.35 1 d PG F 2
H39A H 0.2441 0.0470 0.3795 0.116 Uiso 0.35 1 calc PR F 2
C40A C 0.2766(7) 0.0447(4) 0.2865(6) 0.0963(16) Uiso 0.35 1 d PG F 2
H40A H 0.2068 0.0422 0.2640 0.116 Uiso 0.35 1 calc PR F 2
C41A C 0.3566(10) 0.0454(3) 0.2508(4) 0.0963(16) Uiso 0.35 1 d PG F 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
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 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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_exptl_crystal_colour             green
_exptl_crystal_size_max           0.20
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_exptl_crystal_size_mid          0.30
_exptl_crystal_size_min          0.40
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.109
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             3068
_exptl_absorpt_coefficient_mu    0.347
_exptl_absorpt_correction_type   multi-scan
_exptl_absorpt_correction_T_min  0.8735
_exptl_absorpt_correction_T_max  0.9338
_exptl_absorpt_process_details   'Blessing, Acta Cryst. (1995) A51 33-38.'

_exptl_special_details
;
 hemisphere of 1321 frames x 30 sec. @ 4.109 cm; 0.3 deg. steps in omega & phi
;

_diffrn_ambient_temperature      158(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  'CCD area detector'
_diffrn_measurement_method       'phi and omega scans'
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number         ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        ?
_diffrn_reflns_number            55447
_diffrn_reflns_av_R_equivalents  0.0502
_diffrn_reflns_av_sigmaI/netI    0.0588
_diffrn_reflns_limit_h_min       -20
_diffrn_reflns_limit_h_max       20
_diffrn_reflns_limit_k_min       0
_diffrn_reflns_limit_k_max       27
_diffrn_reflns_limit_l_min       0
_diffrn_reflns_limit_l_max       30
_diffrn_reflns_theta_min         1.27
_diffrn_reflns_theta_max         26.41
_reflns_number_total             17626
_reflns_number_gt                10096
_reflns_threshold_expression     >2sigma(I)

_computing_data_collection       'Bruker SMART'
_computing_cell_refinement       'Bruker SMART'
_computing_data_reduction        'Bruker SHELXTL'
_computing_structure_solution    'Bruker SHELXTL'
_computing_structure_refinement  'Bruker SHELXTL'
_computing_molecular_graphics    'Bruker SHELXTL'
_computing_publication_material  'Bruker SHELXTL'

_refine_special_details
;
 Use of the PLATON/SQUEEZE subroutine revealed the presence of six solvent
 accessible voids of total volume 1392.3 A^3 and containing an extimated
 222 electrons per unit cell due to diffuse solvent scattering.  This has
```

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 been included in all derived crystal quantities as 10 additional acetonitrile
 solvate molecules per unit cell.
 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^)+(0.1276P)^2^+0.0000P] 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      SHELXL
_refine_ls_extinction_coef        0.00057(17)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          17626
_refine_ls_number_parameters      924
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.1226
_refine_ls_R_factor_gt            0.0692
_refine_ls_wR_factor_ref          0.2277
_refine_ls_wR_factor_gt           0.2029
_refine_ls_goodness_of_fit_ref    1.097
_refine_ls_restrained_S_all       1.097
_refine_ls_shift/su_max           0.002
_refine_ls_shift/su_mean          0.000

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
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Mn1 Mn 0.02727(3) 0.38891(2) 0.42436(2) 0.03275(16) Uani 1 1 d . . .
Mn2 Mn 0.09065(3) 0.10403(2) 0.45122(2) 0.04233(17) Uani 1 1 d . . .
O1 O 0.12423(13) 0.40236(9) 0.47646(9) 0.0326(5) Uani 1 1 d . . .
O2 O 0.08545(13) 0.38744(9) 0.36493(9) 0.0353(5) Uani 1 1 d . . .
O3 O -0.03397(15) 0.37991(11) 0.48629(10) 0.0444(6) Uani 1 1 d . . .
O4 O -0.07261(18) 0.31611(13) 0.54815(12) 0.0609(8) Uani 1 1 d . . .
O5 O -0.0289(2) 0.17760(13) 0.56891(12) 0.0667(8) Uani 1 1 d . . .
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O6 O -0.00959(14) 0.09583(10) 0.40049(10) 0.0403(6) Uani 1 1 d . . .
O7 O 0.15127(16) 0.11270(10) 0.39052(11) 0.0487(6) Uani 1 1 d . . .
O8 O 0.03284(16) 0.11316(11) 0.51904(11) 0.0484(6) Uani 1 1 d . . .
N1 N 0.00460(17) 0.47960(14) 0.42220(11) 0.0392(7) Uani 1 1 d . . .
N2 N -0.07723(16) 0.37912(13) 0.36902(12) 0.0387(7) Uani 1 1 d . . .
N3 N 0.03979(16) 0.29717(12) 0.43886(11) 0.0327(6) Uani 1 1 d . . .
N4 N 0.07126(17) 0.19880(12) 0.45343(11) 0.0353(6) Uani 1 1 d . . .
N5 N 0.0948(2) 0.01183(16) 0.45966(15) 0.0563(9) Uani 1 1 d . . .
N6 N 0.1983(2) 0.10616(15) 0.50535(13) 0.0556(9) Uani 1 1 d . . .
C1 C 0.17671(19) 0.44752(15) 0.47253(12) 0.0323(7) Uani 1 1 d . . .
C2 C 0.2601(2) 0.43953(16) 0.49841(15) 0.0390(8) Uani 1 1 d . . .
C3 C 0.3121(2) 0.48715(17) 0.49270(16) 0.0471(9) Uani 1 1 d . . .
H3A H 0.3688 0.4814 0.5079 0.057 Uiso 1 1 calc R . .
C4 C 0.2880(2) 0.54394(17) 0.46607(16) 0.0460(9) Uani 1 1 d . . .
C5 C 0.2062(2) 0.55152(16) 0.44415(14) 0.0396(8) Uani 1 1 d . . .
H5A H 0.1871 0.5898 0.4273 0.048 Uiso 1 1 calc R . .
C6 C 0.1500(2) 0.50344(15) 0.44614(13) 0.0350(7) Uani 1 1 d . . .
C7 C 0.0640(2) 0.51826(16) 0.42814(13) 0.0386(8) Uani 1 1 d . . .
H7A H 0.0504 0.5603 0.4200 0.046 Uiso 1 1 calc R . .
C8 C -0.0789(2) 0.5050(2) 0.4183(2) 0.0672(13) Uani 1 1 d . . .
H8A H -0.0930 0.5019 0.4558 0.081 Uiso 1 1 calc R . .
H8B H -0.0777 0.5494 0.4089 0.081 Uiso 1 1 calc R . .
C9 C -0.1448(3) 0.4755(2) 0.3771(2) 0.0789(15) Uani 1 1 d . . .
H9A H -0.1361 0.4850 0.3390 0.095 Uiso 1 1 calc R . .
H9B H -0.1977 0.4942 0.3807 0.095 Uiso 1 1 calc R . .
C10 C -0.1517(2) 0.4051(2) 0.38258(18) 0.0576(11) Uani 1 1 d . . .
H10A H -0.1560 0.3938 0.4213 0.069 Uiso 1 1 calc R . .
H10B H -0.2008 0.3895 0.3562 0.069 Uiso 1 1 calc R . .
C11 C -0.0822(2) 0.35876(16) 0.31819(15) 0.0419(8) Uani 1 1 d . . .
H11A H -0.1359 0.3507 0.2973 0.050 Uiso 1 1 calc R . .
C12 C -0.0164(2) 0.34706(15) 0.29019(14) 0.0365(8) Uani 1 1 d . . .
C13 C -0.0386(2) 0.32621(15) 0.23430(14) 0.0401(8) Uani 1 1 d . . .
H13A H -0.0935 0.3137 0.2199 0.048 Uiso 1 1 calc R . .
C14 C 0.0166(2) 0.32365(15) 0.20065(15) 0.0421(9) Uani 1 1 d . . .
C15 C 0.0976(2) 0.34219(15) 0.22377(15) 0.0433(8) Uani 1 1 d . . .
H15A H 0.1369 0.3400 0.2005 0.052 Uiso 1 1 calc R . .
C16 C 0.1237(2) 0.36328(15) 0.27814(15) 0.0403(8) Uani 1 1 d . . .
C17 C 0.0652(2) 0.36526(14) 0.31301(14) 0.0351(8) Uani 1 1 d . . .
C18 C 0.07797(19) 0.24831(14) 0.42281(13) 0.0321(7) Uani 1 1 d . . .
H18A H 0.1067 0.2490 0.3929 0.038 Uiso 1 1 calc R . .
C19 C 0.0259(2) 0.21650(15) 0.49217(14) 0.0380(8) Uani 1 1 d . . .
C20 C 0.0066(2) 0.27770(15) 0.48381(13) 0.0364(8) Uani 1 1 d . . .
C21 C -0.0368(2) 0.32533(17) 0.50961(16) 0.0444(9) Uani 1 1 d . . .
C22 C 0.0079(2) 0.16689(17) 0.53089(16) 0.0476(9) Uani 1 1 d . . .
C23 C -0.0226(2) 0.05525(17) 0.35880(15) 0.0444(9) Uani 1 1 d . . .
C24 C -0.0807(2) 0.06907(19) 0.30897(17) 0.0589(11) Uani 1 1 d . . .
C25 C -0.0852(3) 0.0298(2) 0.2644(2) 0.109(2) Uani 1 1 d . . .
H25A H -0.1198 0.0421 0.2301 0.131 Uiso 1 1 calc R . .
C26 C -0.0464(8) -0.0238(6) 0.2638(6) 0.142(7) Uani 1 1 d . . .
C27 C 0.0051(2) -0.0424(2) 0.3199(2) 0.0883(18) Uani 1 1 d . . .
H27A H 0.0296 -0.0821 0.3242 0.106 Uiso 1 1 calc R . .
C28 C 0.0172(2) -0.00232(16) 0.36513(17) 0.0469(9) Uani 1 1 d . . .
C29 C 0.0663(3) -0.0218(3) 0.4174(3) 0.0566(17) Uani 1 1 d . . .
H29A H 0.0790 -0.0646 0.4210 0.068 Uiso 1 1 calc R . .
C30 C 0.1199(4) -0.0194(3) 0.5145(3) 0.113(2) Uani 1 1 d . . .
H30A H 0.1377 -0.0619 0.5080 0.136 Uiso 1 1 calc R . .
H30B H 0.0717 -0.0225 0.5323 0.136 Uiso 1 1 calc R . .
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C31 C 0.1877(5) 0.0125(4) 0.5543(3) 0.145(3) Uani 1 1 d . . .
H31A H 0.1836 -0.0025 0.5921 0.174 Uiso 1 1 calc R . .
H31B H 0.2389 -0.0053 0.5465 0.174 Uiso 1 1 calc R . .
C32 C 0.2025(3) 0.0765(3) 0.5607(2) 0.0905(18) Uani 1 1 d . . .
H32A H 0.2574 0.0834 0.5846 0.109 Uiso 1 1 calc R . .
H32B H 0.1613 0.0953 0.5796 0.109 Uiso 1 1 calc R . .
C33 C 0.2646(3) 0.12657(19) 0.49442(16) 0.0555(11) Uani 1 1 d . . .
H33A H 0.3097 0.1289 0.5254 0.067 Uiso 1 1 calc R . .
C34 C 0.2807(2) 0.14680(16) 0.44120(15) 0.0462(9) Uani 1 1 d . . .
C35 C 0.3600(3) 0.16950(17) 0.44078(17) 0.0537(10) Uani 1 1 d . . .
H35A H 0.3966 0.1768 0.4756 0.064 Uiso 1 1 calc R . .
C36 C 0.3858(3) 0.18133(18) 0.39213(17) 0.0569(11) Uani 1 1 d . . .
C37 C 0.3277(3) 0.17067(18) 0.34201(17) 0.0605(11) Uani 1 1 d . . .
H37A H 0.3442 0.1790 0.3076 0.073 Uiso 1 1 calc R . .
C38 C 0.2493(3) 0.14923(17) 0.33888(16) 0.0530(10) Uani 1 1 d . . .
C39 C 0.2241(2) 0.13610(15) 0.39042(15) 0.0465(9) Uani 1 1 d . . .
C40 C 0.2897(2) 0.38097(16) 0.53332(16) 0.0431(9) Uani 1 1 d . . .
C41 C 0.2751(2) 0.32294(18) 0.49728(17) 0.0570(11) Uani 1 1 d . . .
H41A H 0.2876 0.2865 0.5213 0.086 Uiso 1 1 calc R . .
H41B H 0.3106 0.3236 0.4698 0.086 Uiso 1 1 calc R . .
H41C H 0.2176 0.3215 0.4776 0.086 Uiso 1 1 calc R . .
C42 C 0.2457(3) 0.37565(19) 0.58183(16) 0.0578(11) Uani 1 1 d . . .
H42A H 0.2569 0.4124 0.6056 0.087 Uiso 1 1 calc R . .
H42B H 0.2651 0.3389 0.6041 0.087 Uiso 1 1 calc R . .
H42C H 0.1866 0.3722 0.5672 0.087 Uiso 1 1 calc R . .
C43 C 0.3820(3) 0.3849(2) 0.5587(2) 0.0827(17) Uani 1 1 d . . .
H43A H 0.3932 0.4223 0.5816 0.124 Uiso 1 1 calc R . .
H43B H 0.4127 0.3863 0.5284 0.124 Uiso 1 1 calc R . .
H43C H 0.3988 0.3486 0.5823 0.124 Uiso 1 1 calc R . .
C44 C 0.3516(3) 0.59281(19) 0.46093(19) 0.0582(11) Uani 1 1 d . . .
C45 C 0.4110(3) 0.6026(2) 0.5166(2) 0.0948(19) Uani 1 1 d . . .
H45A H 0.3806 0.6155 0.5451 0.142 Uiso 1 1 calc R . .
H45B H 0.4507 0.6347 0.5122 0.142 Uiso 1 1 calc R . .
H45C H 0.4401 0.5640 0.5283 0.142 Uiso 1 1 calc R . .
C46 C 0.3996(3) 0.5722(2) 0.4168(2) 0.0736(14) Uani 1 1 d . . .
H46A H 0.4274 0.5331 0.4285 0.110 Uiso 1 1 calc R . .
H46B H 0.4403 0.6036 0.4130 0.110 Uiso 1 1 calc R . .
H46C H 0.3617 0.5665 0.3806 0.110 Uiso 1 1 calc R . .
C47 C 0.3100(3) 0.6548(2) 0.4411(2) 0.0818(15) Uani 1 1 d . . .
H47A H 0.2735 0.6668 0.4661 0.123 Uiso 1 1 calc R . .
H47B H 0.2782 0.6503 0.4027 0.123 Uiso 1 1 calc R . .
H47C H 0.3520 0.6866 0.4419 0.123 Uiso 1 1 calc R . .
C48 C -0.0066(2) 0.30516(18) 0.13838(15) 0.0514(10) Uani 1 1 d . . .
C49 C 0.0419(3) 0.2487(2) 0.12772(19) 0.0758(14) Uani 1 1 d . . .
H49A H 0.1006 0.2574 0.1390 0.114 Uiso 1 1 calc R . .
H49B H 0.0285 0.2384 0.0877 0.114 Uiso 1 1 calc R . .
H49C H 0.0278 0.2139 0.1496 0.114 Uiso 1 1 calc R . .
C50 C -0.0982(3) 0.2885(2) 0.12123(17) 0.0629(12) Uani 1 1 d . . .
H50A H -0.1314 0.3246 0.1260 0.094 Uiso 1 1 calc R . .
H50B H -0.1107 0.2548 0.1450 0.094 Uiso 1 1 calc R . .
H50C H -0.1107 0.2754 0.0818 0.094 Uiso 1 1 calc R . .
C51 C 0.0098(3) 0.3599(2) 0.10282(18) 0.0774(14) Uani 1 1 d . . .
H51A H 0.0678 0.3714 0.1132 0.116 Uiso 1 1 calc R . .
H51B H -0.0241 0.3950 0.1094 0.116 Uiso 1 1 calc R . .
H51C H -0.0037 0.3486 0.0630 0.116 Uiso 1 1 calc R . .
C52 C 0.2112(2) 0.3857(2) 0.29913(18) 0.0593(11) Uani 1 1 d . . .
C53 C 0.2107(3) 0.4550(2) 0.31293(19) 0.0753(15) Uani 1 1 d . . .
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H53A H 0.1854 0.4780 0.2791 0.113 Uiso 1 1 calc R . .
H53B H 0.2670 0.4693 0.3262 0.113 Uiso 1 1 calc R . .
H53C H 0.1792 0.4618 0.3423 0.113 Uiso 1 1 calc R . .
C54 C 0.2646(3) 0.3779(3) 0.2552(2) 0.0939(19) Uani 1 1 d . . .
H54A H 0.2401 0.4007 0.2211 0.141 Uiso 1 1 calc R . .
H54B H 0.2681 0.3340 0.2461 0.141 Uiso 1 1 calc R . .
H54C H 0.3196 0.3939 0.2702 0.141 Uiso 1 1 calc R . .
C55 C 0.2511(3) 0.3507(3) 0.3524(2) 0.0875(17) Uani 1 1 d . . .
H55A H 0.2532 0.3066 0.3439 0.131 Uiso 1 1 calc R . .
H55B H 0.2188 0.3569 0.3813 0.131 Uiso 1 1 calc R . .
H55C H 0.3069 0.3662 0.3659 0.131 Uiso 1 1 calc R . .
C56 C -0.1363(2) 0.12583(18) 0.30375(17) 0.0521(10) Uani 1 1 d . . .
C57 C -0.1912(3) 0.1198(2) 0.3450(2) 0.0756(14) Uani 1 1 d . . .
H57A H -0.2172 0.0790 0.3411 0.113 Uiso 1 1 calc R . .
H57B H -0.2336 0.1518 0.3376 0.113 Uiso 1 1 calc R . .
H57C H -0.1589 0.1246 0.3832 0.113 Uiso 1 1 calc R . .
C58 C -0.0883(3) 0.1870(2) 0.3153(2) 0.0832(16) Uani 1 1 d . . .
H58A H -0.1268 0.2217 0.3105 0.125 Uiso 1 1 calc R . .
H58B H -0.0514 0.1913 0.2889 0.125 Uiso 1 1 calc R . .
H58C H -0.0561 0.1869 0.3539 0.125 Uiso 1 1 calc R . .
C59 C -0.1924(3) 0.1311(3) 0.2454(2) 0.105(2) Uani 1 1 d . . .
H59A H -0.2313 0.0966 0.2397 0.157 Uiso 1 1 calc R . .
H59B H -0.1592 0.1299 0.2165 0.157 Uiso 1 1 calc R . .
H59C H -0.2226 0.1701 0.2427 0.157 Uiso 1 1 calc R . .
C60 C -0.0493(4) -0.0672(3) 0.2142(3) 0.130(3) Uani 1 1 d . . .
C61 C -0.0233(6) -0.1354(3) 0.2338(4) 0.236(6) Uani 1 1 d . . .
H61A H -0.0319 -0.1627 0.2010 0.354 Uiso 1 1 calc R . .
H61B H -0.0567 -0.1497 0.2601 0.354 Uiso 1 1 calc R . .
H61C H 0.0347 -0.1360 0.2523 0.354 Uiso 1 1 calc R . .
C62 C -0.1329(3) -0.0673(4) 0.1798(3) 0.135(3) Uani 1 1 d . . .
H62A H -0.1567 -0.0259 0.1798 0.203 Uiso 1 1 calc R . .
H62B H -0.1668 -0.0969 0.1953 0.203 Uiso 1 1 calc R . .
H62C H -0.1310 -0.0791 0.1412 0.203 Uiso 1 1 calc R . .
C63 C 0.0040(6) -0.0386(5) 0.1752(4) 0.118(4) Uani 1 1 d . . .
H63A H -0.0202 0.0006 0.1601 0.176 Uiso 1 1 calc R . .
H63B H 0.0060 -0.0671 0.1442 0.176 Uiso 1 1 calc R . .
H63C H 0.0596 -0.0314 0.1968 0.176 Uiso 1 1 calc R . .
C64 C 0.4708(3) 0.2047(2) 0.39130(19) 0.0678(12) Uani 1 1 d . . .
C65 C 0.5261(8) 0.1531(7) 0.4157(8) 0.096(6) Uani 0.400(9) 1 d P B 1
H65A H 0.5138 0.1165 0.3918 0.144 Uiso 0.400(9) 1 calc PR B 1
H65B H 0.5176 0.1436 0.4534 0.144 Uiso 0.400(9) 1 calc PR B 1
H65C H 0.5832 0.1653 0.4178 0.144 Uiso 0.400(9) 1 calc PR B 1
C65A C 0.5283(5) 0.2118(5) 0.4522(3) 0.078(3) Uani 0.600(9) 1 d P B 2
H65D H 0.5334 0.1718 0.4714 0.117 Uiso 0.600(9) 1 calc PR B 2
H65E H 0.5042 0.2419 0.4741 0.117 Uiso 0.600(9) 1 calc PR B 2
H65F H 0.5827 0.2260 0.4483 0.117 Uiso 0.600(9) 1 calc PR B 2
C66 C 0.4822(8) 0.2624(6) 0.4229(7) 0.090(5) Uani 0.400(9) 1 d P B 1
H66A H 0.4711 0.2555 0.4605 0.134 Uiso 0.400(9) 1 calc PR B 1
H66B H 0.4443 0.2936 0.4033 0.134 Uiso 0.400(9) 1 calc PR B 1
H66C H 0.5387 0.2767 0.4262 0.134 Uiso 0.400(9) 1 calc PR B 1
C66A C 0.4667(6) 0.2707(5) 0.3674(5) 0.109(5) Uani 0.600(9) 1 d P B 2
H66D H 0.4338 0.2708 0.3291 0.164 Uiso 0.600(9) 1 calc PR B 2
H66E H 0.5222 0.2852 0.3669 0.164 Uiso 0.600(9) 1 calc PR B 2
H66F H 0.4414 0.2981 0.3910 0.164 Uiso 0.600(9) 1 calc PR B 2
C67 C 0.4773(11) 0.2144(9) 0.3265(6) 0.096(6) Uani 0.400(9) 1 d P B 1
H67A H 0.4656 0.1754 0.3062 0.143 Uiso 0.400(9) 1 calc PR B 1
H67B H 0.5327 0.2282 0.3248 0.143 Uiso 0.400(9) 1 calc PR B 1
```

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H67C H 0.4375 0.2456 0.3093 0.143 Uiso 0.400(9) 1 calc PR B 1
C67A C 0.5181(7) 0.1644(9) 0.3582(7) 0.143(7) Uani 0.600(9) 1 d P B 2
H67D H 0.5251 0.1232 0.3750 0.214 Uiso 0.600(9) 1 calc PR B 2
H67E H 0.5720 0.1828 0.3589 0.214 Uiso 0.600(9) 1 calc PR B 2
H67F H 0.4879 0.1613 0.3193 0.214 Uiso 0.600(9) 1 calc PR B 2
C68 C 0.1908(3) 0.1374(2) 0.28245(17) 0.0672(12) Uani 1 1 d . . .
C69 C 0.2259(4) 0.1565(3) 0.2327(2) 0.107(2) Uani 1 1 d . . .
H69A H 0.2362 0.2011 0.2342 0.161 Uiso 1 1 calc R . .
H69B H 0.1869 0.1464 0.1979 0.161 Uiso 1 1 calc R . .
H69C H 0.2775 0.1345 0.2335 0.161 Uiso 1 1 calc R . .
C70 C 0.1101(3) 0.1719(2) 0.27978(18) 0.0796(15) Uani 1 1 d . . .
H70A H 0.0840 0.1574 0.3100 0.119 Uiso 1 1 calc R . .
H70B H 0.0736 0.1641 0.2434 0.119 Uiso 1 1 calc R . .
H70C H 0.1210 0.2162 0.2842 0.119 Uiso 1 1 calc R . .
C71 C 0.1721(3) 0.0667(2) 0.2774(2) 0.0882(17) Uani 1 1 d . . .
H71A H 0.1413 0.0545 0.3059 0.132 Uiso 1 1 calc R . .
H71B H 0.2237 0.0436 0.2831 0.132 Uiso 1 1 calc R . .
H71C H 0.1395 0.0576 0.2400 0.132 Uiso 1 1 calc R . .
N7 N 0.2506(6) 0.8557(6) 0.4007(5) 0.113(4) Uani 0.50 1 d P . .
C72 C 0.1004(13) 0.5154(6) 0.7919(5) 0.107(6) Uani 0.50 1 d P . .
C73 C 0.0238(9) 0.5012(4) 0.7860(6) 0.093(4) Uani 0.50 1 d P . .
H73A H -0.0087 0.5389 0.7858 0.139 Uiso 0.50 1 calc PR . .
H73B H 0.0162 0.4748 0.8173 0.139 Uiso 0.50 1 calc PR . .
H73C H 0.0056 0.4791 0.7505 0.139 Uiso 0.50 1 calc PR . .
N8 N 0.2246(5) 0.2199(4) 0.8911(4) 0.080(2) Uani 0.50 1 d P . .
C74 C 0.2063(7) 0.8180(6) 0.3805(4) 0.070(3) Uani 0.50 1 d P . .
C75 C 0.1524(6) 0.7729(4) 0.3599(3) 0.057(2) Uani 0.50 1 d P . .
H75A H 0.1271 0.7569 0.3900 0.086 Uiso 0.50 1 calc PR . .
H75B H 0.1812 0.7394 0.3450 0.086 Uiso 0.50 1 calc PR . .
H75C H 0.1098 0.7896 0.3297 0.086 Uiso 0.50 1 calc PR . .
N9 N 0.1685(10) 0.5358(6) 0.7961(6) 0.142(6) Uani 0.50 1 d P . .
C76 C 0.2513(4) 0.2489(4) 0.9275(4) 0.0499(19) Uani 0.50 1 d P . .
C77 C 0.2876(5) 0.2889(4) 0.9752(3) 0.0521(19) Uani 0.50 1 d P . .
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H77B H 0.2453 0.3007 0.9959 0.078 Uiso 0.50 1 calc PR . .
H77C H 0.3102 0.3261 0.9612 0.078 Uiso 0.50 1 calc PR . .

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O2 0.0386(12) 0.0314(12) 0.0320(12) -0.0043(9) -0.0019(10) -0.0057(10)
O3 0.0483(14) 0.0386(14) 0.0452(15) -0.0042(11) 0.0066(12) 0.0035(11)
O4 0.081(2) 0.0596(18) 0.0508(17) -0.0019(13) 0.0332(16) 0.0009(15)
O5 0.106(2) 0.0529(17) 0.0542(18) 0.0093(14) 0.0473(18) 0.0016(16)
O6 0.0468(14) 0.0292(12) 0.0387(13) 0.0069(10) -0.0057(11) -0.0093(10)
O7 0.0546(16) 0.0329(13) 0.0485(15) -0.0014(11) -0.0132(12) -0.0023(12)
O8 0.0664(17) 0.0323(14) 0.0481(15) 0.0061(11) 0.0154(13) -0.0072(12)
N1 0.0370(16) 0.0495(18) 0.0292(15) -0.0059(13) 0.0024(12) 0.0057(14)
N2 0.0350(15) 0.0396(16) 0.0388(17) -0.0056(13) 0.0014(13) 0.0009(12)
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C10 0.0299(19) 0.081(3) 0.058(3) -0.017(2) 0.0004(18) 0.0043(19)
C11 0.0380(19) 0.041(2) 0.041(2) -0.0025(16) -0.0052(16) 0.0017(16)
C12 0.0422(19) 0.0292(17) 0.0335(18) -0.0011(14) -0.0032(15) 0.0001(14)
C13 0.049(2) 0.0298(17) 0.0361(19) -0.0027(14) -0.0044(16) 0.0000(15)
C14 0.057(2) 0.0239(17) 0.040(2) -0.0035(14) -0.0010(17) 0.0041(15)
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C16 0.046(2) 0.0329(18) 0.041(2) -0.0026(15) 0.0051(16) -0.0034(15)
C17 0.048(2) 0.0201(15) 0.0344(18) -0.0003(13) 0.0013(15) 0.0023(14)
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C19 0.047(2) 0.0340(18) 0.0329(18) -0.0018(14) 0.0073(15) -0.0057(15)
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C24 0.051(2) 0.059(3) 0.057(3) -0.016(2) -0.012(2) 0.012(2)
C25 0.103(4) 0.096(4) 0.099(4) -0.050(3) -0.050(3) 0.045(3)
C26 0.126(11) 0.081(7) 0.181(12) -0.053(7) -0.055(8) 0.002(7)
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C32 0.084(3) 0.113(4) 0.060(3) 0.051(3) -0.020(3) -0.035(3)
C33 0.059(3) 0.057(2) 0.039(2) 0.0135(18) -0.0154(19) -0.013(2)
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C36 0.075(3) 0.046(2) 0.046(2) 0.0010(18) 0.004(2) -0.010(2)
C37 0.088(3) 0.047(2) 0.044(2) -0.0035(18) 0.008(2) -0.010(2)
C38 0.075(3) 0.036(2) 0.042(2) -0.0070(16) -0.001(2) -0.0057(19)
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C42 0.073(3) 0.057(3) 0.038(2) 0.0072(18) -0.003(2) 0.017(2)
C43 0.049(3) 0.063(3) 0.120(5) 0.032(3) -0.022(3) 0.002(2)
C44 0.053(2) 0.049(2) 0.069(3) 0.008(2) 0.004(2) -0.0105(19)
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C47 0.078(3) 0.051(3) 0.118(4) 0.014(3) 0.024(3) -0.017(2)
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C55 0.042(3) 0.131(5) 0.079(4) -0.016(3) -0.012(2) -0.006(3)
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C57 0.070(3) 0.067(3) 0.092(4) 0.028(3) 0.022(3) 0.020(2)
C58 0.072(3) 0.061(3) 0.106(4) 0.041(3) -0.006(3) -0.010(2)
C59 0.101(4) 0.127(5) 0.065(3) -0.022(3) -0.033(3) 0.057(4)
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C61 0.176(7) 0.163(7) 0.306(11) -0.174(8) -0.098(7) 0.089(6)
C62 0.104(5) 0.165(7) 0.126(6) -0.088(5) -0.001(4) -0.037(4)
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C65A 0.062(5) 0.101(8) 0.067(6) 0.005(5) 0.005(4) -0.033(5)
C66 0.075(9) 0.071(9) 0.112(13) -0.008(9) -0.006(8) -0.038(7)
C66A 0.092(7) 0.130(9) 0.096(9) 0.048(7) -0.007(6) -0.060(6)
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C69 0.126(5) 0.154(6) 0.038(3) -0.020(3) 0.005(3) -0.030(4)
C70 0.109(4) 0.077(3) 0.039(2) 0.000(2) -0.018(2) 0.016(3)
C71 0.103(4) 0.078(4) 0.079(4) -0.041(3) 0.007(3) -0.019(3)
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C75 0.077(5) 0.061(5) 0.045(4) 0.010(4) 0.036(4) 0.022(4)
N9 0.163(12) 0.108(10) 0.127(10) -0.005(7) -0.033(10) 0.093(10)
C76 0.036(4) 0.038(4) 0.075(6) 0.009(4) 0.009(4) 0.006(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
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C22 O8 Mn2 119.1(2) . . ?
C7 N1 C8 117.3(3) . . ?
C7 N1 Mn1 120.1(2) . . ?
C8 N1 Mn1 122.5(3) . . ?
C11 N2 C10 117.0(3) . . ?
C11 N2 Mn1 124.0(2) . . ?
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C18 N4 C19 106.3(3) . . ?
C18 N4 Mn2 138.9(2) . . ?
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C29 N5 C30 117.2(4) . . ?
C29 N5 Mn2 119.3(3) . . ?
C30 N5 Mn2 123.0(4) . . ?
C33 N6 C32 117.4(3) . . ?
C33 N6 Mn2 125.0(3) . . ?
C32 N6 Mn2 117.3(3) . . ?
O1 C1 C6 121.2(3) . . ?
O1 C1 C2 118.6(3) . . ?
C6 C1 C2 120.1(3) . . ?
C3 C2 C1 116.5(3) . . ?
C3 C2 C40 122.4(3) . . ?
C1 C2 C40 121.1(3) . . ?
C2 C3 C4 125.2(3) . . ?
C5 C4 C3 116.8(3) . . ?
C5 C4 C44 122.7(3) . . ?
C3 C4 C44 120.5(3) . . ?
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N1 C7 C6 125.7(3) . . ?
C9 C8 N1 116.2(4) . . ?
C8 C9 C10 115.5(4) . . ?
N2 C10 C9 106.3(3) . . ?
N2 C11 C12 127.5(3) . . ?
C13 C12 C17 120.7(3) . . ?
C13 C12 C11 116.2(3) . . ?
C17 C12 C11 122.3(3) . . ?
C14 C13 C12 121.3(3) . . ?
C13 C14 C15 117.5(3) . . ?
C13 C14 C48 122.8(3) . . ?
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C16 C15 C14 124.3(3) . . ?
C15 C16 C17 117.6(3) . . ?
C15 C16 C52 121.2(3) . . ?
C17 C16 C52 121.2(3) . . ?
O2 C17 C12 120.7(3) . . ?
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C12 C17 C16 118.7(3) . . ?
N4 C18 N3 112.2(3) . . ?
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N4 C19 C22 116.0(3) . . ?
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N3 C20 C21 115.6(3) . . ?
O4 C21 O3 122.8(3) . . ?
O4 C21 C20 124.7(3) . . ?
O3 C21 C20 112.5(3) . . ?
O5 C22 O8 124.8(3) . . ?
O5 C22 C19 122.1(3) . . ?
O8 C22 C19 113.1(3) . . ?
O6 C23 C28 120.3(3) . . ?
O6 C23 C24 119.3(3) . . ?
C28 C23 C24 120.3(3) . . ?
C25 C24 C23 117.6(4) . . ?
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C23 C24 C56 122.4(3) . . ?
C26 C25 C24 127.1(7) . . ?
C25 C26 C27 114.3(7) . . ?
C25 C26 C60 127.6(14) . . ?
C27 C26 C60 118.1(12) . . ?
C28 C27 C26 120.9(6) . . ?
C27 C28 C23 118.8(4) . . ?
C27 C28 C29 119.1(4) . . ?
C23 C28 C29 122.1(4) . . ?
N5 C29 C28 127.0(5) . . ?
N5 C30 C31 114.2(5) . . ?
C32 C31 C30 128.1(6) . . ?
C31 C32 N6 110.6(5) . . ?
N6 C33 C34 128.6(4) . . ?
C39 C34 C35 120.7(4) . . ?
C39 C34 C33 121.4(3) . . ?
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C36 C35 C34 122.3(4) . . ?
C35 C36 C37 115.8(4) . . ?
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C38 C37 C36 125.4(4) . . ?
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C37 C38 C68 122.0(4) . . ?
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C42 C40 C2 109.8(3) . . ?
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C43 C40 C2 110.7(3) . . ?
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C49 C48 C50 107.3(3) . . ?
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C14 C48 C50 111.3(3) . . ?
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C59 C56 C58 107.5(4) . . ?
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C62 C60 C63 104.2(6) . . ?
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C67A C64 C67 53.9(8) . . ?
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C65A C64 C67 138.0(7) . . ?
C69 C68 C70 108.4(4) . . ?
C69 C68 C38 113.1(4) . . ?
C70 C68 C38 110.5(4) . . ?
C69 C68 C71 108.1(4) . . ?
C70 C68 C71 108.4(4) . . ?
C38 C68 C71 108.3(4) . . ?
N9 C72 C73 172.1(13) . . ?
N7 C74 C75 176.1(10) . . ?
N8 C76 C77 178.5(10) . . ?

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_diffrn_reflns_theta_full              26.41
_diffrn_measured_fraction_theta_full   0.998
_refine_diff_density_max    0.638
_refine_diff_density_min   -0.491
_refine_diff_density_rms    0.080
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