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Electronic Supplementary Information

Conformation Versus Cohesion in the Relative Stabilities of Gabapentin Polymorphs

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Table 1. Single-crystal X-ray diffraction data for gabapentin Form II, taken at 90 K.

Table 2. Single-crystal X-ray diffraction data for gabapentin Form III, taken at 90 K.

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Table 1. Single-crystal X-ray diffraction data for gabapentin Form II, taken at 90 K.

```
data_mo_data_0m

_audit_creation_method            SHELXL-97
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;
 ?
;
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_Hall   -P2ybc

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

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_cell_length_c                    22.207(10)
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_cell_angle_beta                  90.199(8)
_cell_angle_gamma                 90.00
_cell_volume                      903.1(7)
_cell_formula_units_Z             4
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;
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;

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_computing_structure_solution     'SHELXS-97 (Sheldrick, 2008)'
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_computing_molecular_graphics     'CrystalMaker (Palmer, 2010)'
_computing_publication_material   'Bruker SHELXTL (Bruker, 2011)'

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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_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
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 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
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O2 O 0.67223(17) 0.22265(14) 0.52208(4) 0.0153(3) Uani 1 1 d . . .
N1 N 0.7760(2) 0.83476(19) 0.51471(6) 0.0129(3) Uani 1 1 d . . .
C1 C 0.6759(2) 0.9156(2) 0.72856(7) 0.0167(3) Uani 1 1 d . . .
H13 H 0.5664 0.8381 0.7522 0.020 Uiso 1 1 calc R . .
H12 H 0.7192 1.0298 0.7528 0.020 Uiso 1 1 calc R . .
C2 C 0.8883(2) 0.7943(2) 0.71542(7) 0.0169(3) Uani 1 1 d . . .
H15 H 0.9546 0.7479 0.7538 0.020 Uiso 1 1 calc R . .
H14 H 1.0035 0.8757 0.6952 0.020 Uiso 1 1 calc R . .
C3 C 0.8305(2) 0.6206(2) 0.67523(6) 0.0143(3) Uani 1 1 d . . .
H16 H 0.7342 0.5300 0.6984 0.017 Uiso 1 1 calc R . .
H17 H 0.9736 0.5525 0.6651 0.017 Uiso 1 1 calc R . .
C4 C 0.7053(2) 0.6733(2) 0.61608(6) 0.0126(3) Uani 1 1 d . . .
C5 C 0.8770(2) 0.7715(2) 0.57376(6) 0.0133(3) Uani 1 1 d . . .
H4 H 0.9420 0.8855 0.5944 0.016 Uiso 1 1 calc R . .
H5 H 1.0034 0.6805 0.5657 0.016 Uiso 1 1 calc R . .
C6 C 0.7634(2) 0.3383(2) 0.55967(6) 0.0126(3) Uani 1 1 d . . .
C7 C 0.6040(2) 0.4903(2) 0.58644(6) 0.0129(3) Uani 1 1 d . . .
H6 H 0.5090 0.4250 0.6170 0.016 Uiso 1 1 calc R . .
H7 H 0.5002 0.5332 0.5539 0.016 Uiso 1 1 calc R . .
C8 C 0.5633(2) 0.9813(2) 0.67012(7) 0.0160(3) Uani 1 1 d . . .
H10 H 0.6684 1.0674 0.6480 0.019 Uiso 1 1 calc R . .
H11 H 0.4236 1.0554 0.6795 0.019 Uiso 1 1 calc R . .
C9 C 0.5021(2) 0.8081(2) 0.63063(6) 0.0133(3) Uani 1 1 d . . .
H8 H 0.4365 0.8560 0.5923 0.016 Uiso 1 1 calc R . .
H9 H 0.3829 0.7318 0.6512 0.016 Uiso 1 1 calc R . .
H1 H 0.761(3) 0.970(3) 0.5145(7) 0.016 Uiso 1 1 d . . .
H2 H 0.633(3) 0.786(2) 0.5070(7) 0.016 Uiso 1 1 d . . .
H3 H 0.874(3) 0.794(2) 0.4825(8) 0.016 Uiso 1 1 d . . .

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 _atom_site_aniso_U_23
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 _atom_site_aniso_U_12
O1 0.0125(5) 0.0204(6) 0.0196(6) -0.0054(5) -0.0018(4) 0.0030(4)
O2 0.0159(5) 0.0125(5) 0.0176(5) -0.0029(4) -0.0017(4) 0.0003(4)
N1 0.0119(6) 0.0114(7) 0.0154(7) -0.0005(5) 0.0009(5) 0.0004(5)
C1 0.0190(8) 0.0152(8) 0.0159(8) -0.0038(6) 0.0005(6) -0.0003(6)
C2 0.0176(8) 0.0186(8) 0.0146(8) -0.0012(6) -0.0018(6) -0.0002(6)
C3 0.0134(7) 0.0138(7) 0.0156(8) -0.0001(6) 0.0000(6) 0.0011(6)
C4 0.0111(7) 0.0125(7) 0.0143(7) -0.0005(6) 0.0009(6) 0.0003(6)
```

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```
C5 0.0121(7) 0.0135(7) 0.0144(7) -0.0004(6) -0.0006(6) 0.0004(6)
C6 0.0145(7) 0.0102(7) 0.0130(7) 0.0020(6) 0.0019(6) -0.0008(6)
C7 0.0109(7) 0.0132(7) 0.0146(8) 0.0004(6) 0.0001(6) -0.0001(6)
C8 0.0152(8) 0.0131(8) 0.0197(8) -0.0010(6) 0.0028(6) 0.0019(6)
C9 0.0124(7) 0.0139(8) 0.0137(7) -0.0002(6) 0.0005(6) 0.0005(6)

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;
 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
;

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O2 C6 1.2735(18) . ?
N1 C5 1.5027(19) . ?
N1 H1B' 0.938(18) . ?
N1 H1A' 0.920(18) . ?
N1 H1C' 0.962(17) . ?
C1 C8 1.524(2) . ?
C1 C2 1.532(2) . ?
C1 H1A 0.9900 . ?
C1 H1B 0.9900 . ?
C2 C3 1.535(2) . ?
C2 H2A 0.9900 . ?
C2 H2B 0.9900 . ?
C3 C4 1.547(2) . ?
C3 H3A 0.9900 . ?
C3 H3B 0.9900 . ?
C4 C5 1.539(2) . ?
C4 C7 1.547(2) . ?
C4 C9 1.550(2) . ?
C5 H5A 0.9900 . ?
C5 H5B 0.9900 . ?
C6 C7 1.530(2) . ?
C7 H7A 0.9900 . ?
C7 H7B 0.9900 . ?
```

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```
C8 C9 1.529(2) . ?
C8 H8A 0.9900 . ?
C8 H8B 0.9900 . ?
C9 H9A 0.9900 . ?
C9 H9B 0.9900 . ?

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H1B' N1 H1A' 106.3(14) . . ?
C5 N1 H1C' 109.2(9) . . ?
H1B' N1 H1C' 110.1(14) . . ?
H1A' N1 H1C' 107.5(14) . . ?
C8 C1 C2 110.64(12) . . ?
C8 C1 H1A 109.5 . . ?
C2 C1 H1A 109.5 . . ?
C8 C1 H1B 109.5 . . ?
C2 C1 H1B 109.5 . . ?
H1A C1 H1B 108.1 . . ?
C1 C2 C3 111.24(12) . . ?
C1 C2 H2A 109.4 . . ?
C3 C2 H2A 109.4 . . ?
C1 C2 H2B 109.4 . . ?
C3 C2 H2B 109.4 . . ?
H2A C2 H2B 108.0 . . ?
C2 C3 C4 114.35(12) . . ?
C2 C3 H3A 108.7 . . ?
C4 C3 H3A 108.7 . . ?
C2 C3 H3B 108.7 . . ?
C4 C3 H3B 108.7 . . ?
H3A C3 H3B 107.6 . . ?
C5 C4 C3 108.20(12) . . ?
C5 C4 C7 110.73(12) . . ?
C3 C4 C7 110.42(12) . . ?
C5 C4 C9 111.55(12) . . ?
C3 C4 C9 109.21(12) . . ?
C7 C4 C9 106.74(11) . . ?
N1 C5 C4 113.87(12) . . ?
N1 C5 H5A 108.8 . . ?
C4 C5 H5A 108.8 . . ?
N1 C5 H5B 108.8 . . ?
C4 C5 H5B 108.8 . . ?
H5A C5 H5B 107.7 . . ?
O1 C6 O2 123.48(13) . . ?
O1 C6 C7 120.96(13) . . ?
```

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```
O2 C6 C7 115.54(12) . . ?
C6 C7 C4 119.67(12) . . ?
C6 C7 H7A 107.4 . . ?
C4 C7 H7A 107.4 . . ?
C6 C7 H7B 107.4 . . ?
C4 C7 H7B 107.4 . . ?
H7A C7 H7B 106.9 . . ?
C1 C8 C9 110.74(12) . . ?
C1 C8 H8A 109.5 . . ?
C9 C8 H8A 109.5 . . ?
C1 C8 H8B 109.5 . . ?
C9 C8 H8B 109.5 . . ?
H8A C8 H8B 108.1 . . ?
C8 C9 C4 114.41(12) . . ?
C8 C9 H9A 108.7 . . ?
C4 C9 H9A 108.7 . . ?
C8 C9 H9B 108.7 . . ?
C4 C9 H9B 108.7 . . ?
H9A C9 H9B 107.6 . . ?

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C2 C3 C4 C7 -166.42(12) . . . . ?
C2 C3 C4 C9 -49.35(16) . . . . ?
C3 C4 C5 N1 -178.67(11) . . . . ?
C7 C4 C5 N1 60.19(15) . . . . ?
C9 C4 C5 N1 -58.53(16) . . . . ?
O1 C6 C7 C4 20.3(2) . . . . ?
O2 C6 C7 C4 -161.00(12) . . . . ?
C5 C4 C7 C6 51.03(17) . . . . ?
C3 C4 C7 C6 -68.78(16) . . . . ?
C9 C4 C7 C6 172.63(12) . . . . ?
C2 C1 C8 C9 57.14(16) . . . . ?
C1 C8 C9 C4 -55.64(16) . . . . ?
C5 C4 C9 C8 -69.14(16) . . . . ?
C3 C4 C9 C8 50.42(16) . . . . ?
C7 C4 C9 C8 169.79(12) . . . . ?

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_refine_diff_density_min   -0.189
_refine_diff_density_rms    0.042
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Table 2. Single-crystal X-ray diffraction data for gabapentin Form III, taken at 90 K.

```
data_cu_data_0ma

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common            'Gabapentin Form III'
_chemical_melting_point           ?
_chemical_formula_moiety          'C9 H17 N O2'
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 'C9 H17 N O2'
_chemical_formula_weight          171.24

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 _atom_type_scat_dispersion_imag
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 'C'  'C'   0.0181   0.0091
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0311   0.0180
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0492   0.0322
 '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)/c
_symmetry_space_group_name_Hall   -P2ybc

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

_cell_length_a                    14.5052(8)
_cell_length_b                    6.6423(4)
_cell_length_c                    9.8052(5)
_cell_angle_alpha                 90.00
_cell_angle_beta                  105.719(3)
_cell_angle_gamma                 90.00
_cell_volume                      909.38(9)
_cell_formula_units_Z             4
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_cell_measurement_temperature     90(2)
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_cell_measurement_theta_max       67.74

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_exptl_absorpt_process_details    'SADABS SHELXL-97 (Sheldrick, 2008)'

_exptl_special_details
;
 ?
;

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_computing_structure_solution     'SHELXS-97 (Sheldrick, 2008)'
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_computing_molecular_graphics     'CrystalMaker (Palmer, 2010)'
_computing_publication_material   'Bruker SHELXTL(Bruker,2011)'

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

_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^)+(0.0851P)^2^+0.2218P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
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_refine_ls_number_reflns          1580
_refine_ls_number_parameters      110
_refine_ls_number_restraints      100
_refine_ls_R_factor_all           0.0548
_refine_ls_R_factor_gt            0.0518
_refine_ls_wR_factor_ref          0.1428
_refine_ls_wR_factor_gt           0.1392
_refine_ls_goodness_of_fit_ref    1.037
_refine_ls_restrained_S_all       1.004
_refine_ls_shift/su_max           0.000
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 _atom_site_U_iso_or_equiv
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 _atom_site_symmetry_multiplicity
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O1 O 0.48142(7) 0.78610(15) 0.58242(10) 0.0196(3) Uani 1 1 d U . .
O2 O 0.36082(8) 0.56550(16) 0.55220(13) 0.0311(3) Uani 1 1 d U . .
N1 N 0.41912(8) 1.18867(17) 0.64848(12) 0.0167(3) Uani 1 1 d U . .
H15 H 0.4506 1.1175 0.5957 0.025 Uiso 1 1 calc R . .
H17 H 0.4586 1.2085 0.7369 0.025 Uiso 1 1 calc R . .
H16 H 0.4008 1.3099 0.6066 0.025 Uiso 1 1 calc R . .
C7 C 0.06786(11) 0.9813(2) 0.32785(16) 0.0247(4) Uani 1 1 d U . .
H10 H 0.0234 0.9322 0.2387 0.030 Uiso 1 1 calc R . .
H9 H 0.0303 1.0620 0.3788 0.030 Uiso 1 1 calc R . .
C6 C 0.14433(10) 1.1144(2) 0.29292(14) 0.0197(4) Uani 1 1 d U . .
H7 H 0.1764 1.0392 0.2316 0.024 Uiso 1 1 calc R . .
H8 H 0.1137 1.2349 0.2403 0.024 Uiso 1 1 calc R . .
C5 C 0.21860(10) 1.1801(2) 0.42786(14) 0.0168(4) Uani 1 1 d U . .
H6 H 0.1868 1.2630 0.4858 0.020 Uiso 1 1 calc R . .
H5 H 0.2675 1.2648 0.4021 0.020 Uiso 1 1 calc R . .
C4 C 0.26836(9) 1.0003(2) 0.51672(13) 0.0153(4) Uani 1 1 d U . .
C3 C 0.33274(10) 1.0741(2) 0.65874(13) 0.0169(4) Uani 1 1 d U . .
H4 H 0.2943 1.1611 0.7044 0.020 Uiso 1 1 calc R . .
H3 H 0.3540 0.9562 0.7211 0.020 Uiso 1 1 calc R . .
C1 C 0.39526(10) 0.7294(2) 0.52900(14) 0.0172(4) Uani 1 1 d U . .
C2 C 0.32839(10) 0.8807(2) 0.43452(13) 0.0162(4) Uani 1 1 d U . .
H2 H 0.2845 0.8084 0.3545 0.019 Uiso 1 1 calc R . .
H1 H 0.3667 0.9762 0.3948 0.019 Uiso 1 1 calc R . .
C8 C 0.11267(11) 0.8013(2) 0.41940(15) 0.0224(4) Uani 1 1 d U . .
H11 H 0.0620 0.7274 0.4490 0.027 Uiso 1 1 calc R . .
H12 H 0.1406 0.7085 0.3623 0.027 Uiso 1 1 calc R . .
C9 C 0.19066(10) 0.8656(2) 0.55108(13) 0.0185(4) Uani 1 1 d U . .
H14 H 0.2215 0.7437 0.6015 0.022 Uiso 1 1 calc R . .
H13 H 0.1606 0.9396 0.6155 0.022 Uiso 1 1 calc R . .

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 _atom_site_aniso_U_33
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 _atom_site_aniso_U_12
O1 0.0214(6) 0.0193(6) 0.0181(5) 0.0019(4) 0.0053(4) 0.0013(4)
O2 0.0302(6) 0.0136(6) 0.0476(7) 0.0053(5) 0.0075(5) -0.0006(4)
N1 0.0206(6) 0.0142(7) 0.0156(6) -0.0022(4) 0.0053(5) -0.0007(4)
C7 0.0217(8) 0.0258(9) 0.0246(7) 0.0028(6) 0.0030(6) -0.0022(6)
C6 0.0217(7) 0.0186(8) 0.0183(7) 0.0036(5) 0.0046(6) 0.0034(6)
C5 0.0217(8) 0.0131(7) 0.0175(7) 0.0006(5) 0.0084(6) 0.0012(5)
C4 0.0195(7) 0.0136(8) 0.0142(6) -0.0003(5) 0.0066(5) -0.0005(5)
```

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C3 0.0213(7) 0.0166(7) 0.0141(6) 0.0000(5) 0.0072(5) -0.0008(5)
C1 0.0229(8) 0.0133(7) 0.0165(7) -0.0020(5) 0.0070(5) 0.0011(5)
C2 0.0210(7) 0.0146(7) 0.0135(6) -0.0016(5) 0.0056(5) 0.0011(5)
C8 0.0231(8) 0.0210(8) 0.0234(7) 0.0011(5) 0.0068(6) -0.0068(6)
C9 0.0220(8) 0.0179(8) 0.0167(7) 0.0027(5) 0.0070(6) -0.0022(6)

_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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O1 C1 1.2741(18) . ?
O2 C1 1.2443(18) . ?
N1 C3 1.4924(18) . ?
N1 H1A 0.9100 . ?
N1 H1B 0.9100 . ?
N1 H1C 0.9100 . ?
C7 C6 1.528(2) . ?
C7 C8 1.530(2) . ?
C7 H7A 0.9900 . ?
C7 H7B 0.9900 . ?
C6 C5 1.5261(19) . ?
C6 H6A 0.9900 . ?
C6 H6B 0.9900 . ?
C5 C4 1.5379(18) . ?
C5 H5A 0.9900 . ?
C5 H5B 0.9900 . ?
C4 C3 1.5320(17) . ?
C4 C9 1.5460(18) . ?
C4 C2 1.5555(18) . ?
C3 H3A 0.9900 . ?
C3 H3B 0.9900 . ?
C1 C2 1.5236(19) . ?
C2 H2A 0.9900 . ?
C2 H2B 0.9900 . ?
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C8 C9 1.5290(19) . ?
C8 H8A 0.9900 . ?
C8 H8B 0.9900 . ?
C9 H9A 0.9900 . ?
C9 H9B 0.9900 . ?

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C3 N1 H1B 109.5 . . ?
H1A N1 H1B 109.5 . . ?
C3 N1 H1C 109.5 . . ?
H1A N1 H1C 109.5 . . ?
H1B N1 H1C 109.5 . . ?
C6 C7 C8 111.40(12) . . ?
C6 C7 H7A 109.3 . . ?
C8 C7 H7A 109.3 . . ?
C6 C7 H7B 109.3 . . ?
C8 C7 H7B 109.3 . . ?
H7A C7 H7B 108.0 . . ?
C5 C6 C7 110.83(11) . . ?
C5 C6 H6A 109.5 . . ?
C7 C6 H6A 109.5 . . ?
C5 C6 H6B 109.5 . . ?
C7 C6 H6B 109.5 . . ?
H6A C6 H6B 108.1 . . ?
C6 C5 C4 112.47(11) . . ?
C6 C5 H5A 109.1 . . ?
C4 C5 H5A 109.1 . . ?
C6 C5 H5B 109.1 . . ?
C4 C5 H5B 109.1 . . ?
H5A C5 H5B 107.8 . . ?
C3 C4 C5 110.08(11) . . ?
C3 C4 C9 106.74(10) . . ?
C5 C4 C9 108.36(11) . . ?
C3 C4 C2 110.22(11) . . ?
C5 C4 C2 110.23(10) . . ?
C9 C4 C2 111.14(11) . . ?
N1 C3 C4 114.72(10) . . ?
N1 C3 H3A 108.6 . . ?
C4 C3 H3A 108.6 . . ?
N1 C3 H3B 108.6 . . ?
C4 C3 H3B 108.6 . . ?
H3A C3 H3B 107.6 . . ?
O2 C1 O1 125.52(13) . . ?
O2 C1 C2 117.85(12) . . ?
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```
O1 C1 C2 116.56(12) . . ?
C1 C2 C4 112.05(10) . . ?
C1 C2 H2A 109.2 . . ?
C4 C2 H2A 109.2 . . ?
C1 C2 H2B 109.2 . . ?
C4 C2 H2B 109.2 . . ?
H2A C2 H2B 107.9 . . ?
C9 C8 C7 112.13(12) . . ?
C9 C8 H8A 109.2 . . ?
C7 C8 H8A 109.2 . . ?
C9 C8 H8B 109.2 . . ?
C7 C8 H8B 109.2 . . ?
H8A C8 H8B 107.9 . . ?
C8 C9 C4 113.19(11) . . ?
C8 C9 H9A 108.9 . . ?
C4 C9 H9A 108.9 . . ?
C8 C9 H9B 108.9 . . ?
C4 C9 H9B 108.9 . . ?
H9A C9 H9B 107.8 . . ?

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C8 C7 C6 C5 -54.68(16) . . . . ?
C7 C6 C5 C4 58.26(15) . . . . ?
C6 C5 C4 C3 -173.07(11) . . . . ?
C6 C5 C4 C9 -56.68(13) . . . . ?
C6 C5 C4 C2 65.14(14) . . . . ?
C5 C4 C3 N1 -69.14(14) . . . . ?
C9 C4 C3 N1 173.47(11) . . . . ?
C2 C4 C3 N1 52.66(15) . . . . ?
O2 C1 C2 C4 80.74(15) . . . . ?
O1 C1 C2 C4 -96.41(14) . . . . ?
C3 C4 C2 C1 46.18(15) . . . . ?
C5 C4 C2 C1 167.90(11) . . . . ?
C9 C4 C2 C1 -71.95(14) . . . . ?
C6 C7 C8 C9 52.45(16) . . . . ?
C7 C8 C9 C4 -53.23(16) . . . . ?
C3 C4 C9 C8 172.59(12) . . . . ?
C5 C4 C9 C8 54.06(15) . . . . ?
C2 C4 C9 C8 -67.20(15) . . . . ?

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_diffrn_reflns_theta_full              66.59
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_refine_diff_density_max    0.340
_refine_diff_density_min   -0.322
_refine_diff_density_rms    0.068
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