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#  
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#  
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# Allen and I. D. Brown [Acta Cryst. (1991), A47, 655-685]. #

#  
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#  
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data\_l  
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\_journal\_name\_full 'Acta Crystallographica, Section E'  
\_journal\_year 2015  
\_journal\_volume 71

\_journal\_issue 9  
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\_journal\_page\_last 1076  
\_journal\_paper\_category GM  
\_journal\_paper\_doi 10.1107/S2056989015015340  
\_journal\_coeditor\_code ZL2640

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\_publ\_contact\_author\_phone ?

\_publ\_section\_title

;

Crystal structure of  
dichlorido(4,11-dimethyl-1,4,8,11-tetraazabicyclo[6.6.2]hexadecane)iron(III)  
hexafluoridophosphate

;

loop\_

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;

In contrast to other similar compounds,  $[\text{FeCl}_2(\text{C}_{14}\text{H}_{30}\text{N}_4)]\text{PF}_6$  is a monomer. Comparison with the mononuclear  $\text{Fe}^{2+}$  complex of the same ligand shows that the smaller  $\text{Fe}^{3+}$  ion is more fully engulfed by the cavity of the bicyclic ligand. Comparison with the  $\mu$ -oxo dinuclear complex of an unsubstituted ligand of the same size demonstrates that the methyl groups of 4,11-dimethyl-1,4,8,11-tetraazabicyclo[6.6.2]hexadecane prevent dimerization upon oxidation.

;

\_chemical\_name\_systematic

;

Dichlorido(4,11-dimethyl-1,4,8,11-tetraazabicyclo[6.6.2]hexadecane)iron(III)  
hexafluoridophosphate

;

\_chemical\_name\_common ?

\_chemical\_formula\_moiety 'C14 H30 Cl2 Fe N4 +, P F6 -'

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_chemical_melting_point ?  
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The symmetry employed for this shelxl refinement is uniquely defined by the following loop, which should always be used as a source of symmetry information in preference to the above space-group names. They are only intended as comments.

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'-x+1/2, y+1/2, z+1/2'  
'x+1/2, -y+1/2, z'  
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_cell_angle_gamma 90  
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Refined as a two-component inversion twin.

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;
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_refine_ls_R_factor_all 0.0934
_refine_ls_R_factor_gt 0.0500
_refine_ls_wR_factor_gt 0.1011
_refine_ls_wR_factor_ref 0.1091
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_refine_ls_restrained_S_all 0.835
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_refine_ls_number_parameters 254
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_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
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_atom_sites_solution_hydrogens geom
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
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Refined as a two-component inversion twin

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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'

'F' 'F' 0.0171 0.0103

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Fe' 'Fe' 0.3463 0.8444

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'N' 'N' 0.0061 0.0033

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'P' 'P' 0.1023 0.0942

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X-AREA (Stoe & Cie, 2002)  
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\_computing\_structure\_solution  
;  
SHELXS97 (Sheldrick, 2008)  
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\_computing\_structure\_refinement  
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SHELXL-2014/7 (Sheldrick, 2015)  
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\_computing\_molecular\_graphics  
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ORTEP3 for Windows (Farrugia, 2012)  
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\_computing\_publication\_material  
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pubCIF (Westrip, 2010)  
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Cl Cl1 0.71279(10) 0.2523(4) 0.3803(3) 0.0471(6) Uani d 1 . .  
Cl Cl2 0.69285(9) -0.0987(3) 0.2182(3) 0.0493(6) Uani d 1 . .  
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N N2 0.5950(3) 0.0889(10) 0.3401(7) 0.043(2) Uani d 1 . .  
N N3 0.6144(3) 0.0869(10) 0.0162(8) 0.042(2) Uani d 1 . .  
N N4 0.7148(3) 0.2294(12) 0.0366(8) 0.045(2) Uani d 1 . .  
C C1 0.5844(5) 0.3692(15) 0.3148(11) 0.058(3) Uani d 1 . .  
H H1A 0.6066 0.3876 0.3990 0.069 Uiso calc 1 . .  
H H1B 0.5593 0.4558 0.3087 0.069 Uiso calc 1 . .  
C C2 0.5569(4) 0.2208(13) 0.3320(11) 0.057(3) Uani d 1 . .  
H H2A 0.5335 0.2044 0.2502 0.069 Uiso calc 1 . .  
H H2B 0.5360 0.2236 0.4201 0.069 Uiso calc 1 . .  
C C3 0.5698(4) -0.0588(14) 0.2979(10) 0.056(3) Uani d 1 . .  
H H3A 0.5409 -0.0765 0.3645 0.067 Uiso calc 1 . .  
H H3B 0.5949 -0.1440 0.3138 0.067 Uiso calc 1 . .  
C C4 0.5490(4) -0.0768(14) 0.1479(10) 0.059(3) Uani d 1 . .  
H H4A 0.5320 -0.1799 0.1407 0.071 Uiso calc 1 . .  
H H4B 0.5222 0.0036 0.1328 0.071 Uiso calc 1 . .  
C C5 0.5867(4) -0.0642(13) 0.0324(11) 0.055(3) Uani d 1 . .  
H H5A 0.5689 -0.0866 -0.0585 0.066 Uiso calc 1 . .  
H H5B 0.6128 -0.1471 0.0463 0.066 Uiso calc 1 . .  
C C6 0.6538(4) 0.0671(13) -0.0993(10) 0.060(3) Uani d 1 . .

H H6A 0.6364 0.0548 -0.1924 0.072 Uiso calc 1 . .  
H H6B 0.6743 -0.0283 -0.0810 0.072 Uiso calc 1 . .  
C C7 0.6900(5) 0.2105(14) -0.1046(11) 0.067(3) Uani d 1 . .  
H H7A 0.7166 0.1952 -0.1789 0.081 Uiso calc 1 . .  
H H7B 0.6701 0.3053 -0.1286 0.081 Uiso calc 1 . .  
C C8 0.7315(4) 0.4001(13) 0.0555(11) 0.059(3) Uani d 1 . .  
H H8A 0.7520 0.4078 0.1442 0.071 Uiso calc 1 . .  
H H8B 0.7545 0.4280 -0.0247 0.071 Uiso calc 1 . .  
C C9 0.6882(5) 0.5214(14) 0.0628(13) 0.073(4) Uani d 1 . .  
H H9A 0.7043 0.6258 0.0699 0.088 Uiso calc 1 . .  
H H9B 0.6693 0.5179 -0.0287 0.088 Uiso calc 1 . .  
C C10 0.6499(4) 0.5070(11) 0.1805(13) 0.067(3) Uani d 1 . .  
H H10A 0.6685 0.5103 0.2724 0.080 Uiso calc 1 . .  
H H10B 0.6269 0.5990 0.1773 0.080 Uiso calc 1 . .  
C C11 0.5873(5) 0.3684(14) 0.0505(12) 0.064(4) Uani d 1 . .  
H H11A 0.6044 0.4357 -0.0209 0.077 Uiso calc 1 . .  
H H11B 0.5537 0.4166 0.0735 0.077 Uiso calc 1 . .  
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H H12A 0.5430 0.1728 0.0135 0.072 Uiso calc 1 . .  
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C C13 0.6132(4) 0.0676(13) 0.4876(9) 0.058(3) Uani d 1 . .  
H H13A 0.6302 0.1632 0.5200 0.087 Uiso calc 1 . .  
H H13B 0.5838 0.0450 0.5497 0.087 Uiso calc 1 . .  
H H13C 0.6376 -0.0194 0.4911 0.087 Uiso calc 1 . .  
C C14 0.7641(4) 0.1488(14) 0.0423(11) 0.058(3) Uani d 1 . .  
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H H14B 0.7588 0.0373 0.0246 0.088 Uiso calc 1 . .  
H H14C 0.7871 0.1917 -0.0306 0.088 Uiso calc 1 . .  
P P1 0.58082(9) 0.6220(4) 0.6714(2) 0.0514(7) Uani d 1 . .  
F F1 0.5510(2) 0.7847(7) 0.6576(6) 0.0737(19) Uani d 1 . .  
F F2 0.5482(3) 0.5900(10) 0.8133(7) 0.097(3) Uani d 1 . .

F F3 0.6235(3) 0.7031(11) 0.7626(8) 0.117(3) Uani d 1 . .

F F4 0.6122(2) 0.6531(8) 0.5300(6) 0.0635(17) Uani d 1 . .

F F5 0.5377(3) 0.5381(11) 0.5818(8) 0.094(3) Uani d 1 . .

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loop\_

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\_atom\_site\_aniso\_U\_13

\_atom\_site\_aniso\_U\_23

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Cl1 0.0505(14) 0.0455(15) 0.0452(12) -0.0004(14) -0.0107(12) -0.0074(12)

Cl2 0.0602(13) 0.0356(11) 0.0522(13) 0.0070(10) -0.0035(13) 0.0016(13)

N1 0.053(4) 0.054(5) 0.036(5) 0.008(4) 0.005(4) 0.003(4)

N2 0.048(5) 0.045(5) 0.037(4) 0.002(4) -0.002(4) 0.003(4)

N3 0.039(5) 0.045(5) 0.042(4) -0.006(4) -0.009(4) -0.004(4)

N4 0.041(5) 0.048(6) 0.047(4) -0.001(5) -0.002(4) -0.009(4)

C1 0.066(8) 0.055(9) 0.052(6) -0.002(7) 0.001(5) -0.006(6)

C2 0.054(7) 0.059(8) 0.058(7) 0.005(6) 0.024(5) 0.011(6)

C3 0.061(8) 0.056(8) 0.049(6) -0.022(6) 0.012(5) -0.002(5)

C4 0.067(7) 0.052(7) 0.058(6) -0.012(6) -0.004(6) -0.002(5)

C5 0.059(7) 0.055(8) 0.051(6) -0.007(6) 0.002(6) -0.008(5)

C6 0.072(8) 0.067(8) 0.040(5) -0.008(6) -0.009(5) 0.000(5)

C7 0.086(8) 0.070(8) 0.046(6) -0.011(6) 0.007(6) 0.004(6)

C8 0.076(8) 0.044(7) 0.058(6) 0.003(6) 0.007(5) 0.006(5)

C9 0.086(9) 0.047(7) 0.086(8) 0.002(7) 0.032(7) 0.002(6)

C10 0.092(8) 0.030(5) 0.079(9) -0.005(5) 0.005(8) 0.007(6)

C11 0.067(9) 0.052(9) 0.073(7) 0.025(7) -0.008(6) 0.003(6)

C12 0.068(7) 0.053(8) 0.059(6) -0.004(6) -0.022(6) 0.004(6)

C13 0.071(8) 0.068(8) 0.035(5) -0.021(6) 0.007(5) 0.014(5)  
C14 0.053(7) 0.059(8) 0.064(6) 0.010(6) 0.013(5) -0.003(6)  
P1 0.0442(14) 0.0654(18) 0.0445(16) 0.0126(13) 0.0024(11) 0.0086(13)  
F1 0.069(4) 0.063(4) 0.090(5) 0.024(3) 0.029(3) 0.022(3)  
F2 0.123(7) 0.094(6) 0.075(4) 0.050(5) 0.058(4) 0.038(4)  
F3 0.073(5) 0.171(9) 0.107(5) 0.025(5) -0.027(4) -0.090(5)  
F4 0.060(4) 0.077(5) 0.054(3) 0.004(3) 0.012(3) 0.000(3)  
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\_geom\_special\_details

;

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

planes.

;

loop\_

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Fe1 N1 . 2.197(7) ?

Fe1 N3 . 2.223(7) ?

Fe1 N2 . 2.229(8) ?

Fe1 Cl2 . 2.278(3) ?

Fe1 Cl1 . 2.288(3) ?

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N1 C10 . 1.461(11) ?  
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N3 C12 . 1.453(13) ?  
N3 C5 . 1.490(13) ?  
N3 C6 . 1.501(12) ?  
N4 C14 . 1.458(12) ?  
N4 C7 . 1.482(13) ?  
N4 C8 . 1.538(15) ?  
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C1 H1B . 0.9900 ?  
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C2 H2B . 0.9900 ?  
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N4 Fe1 N3 . . 81.8(3) ?

N1 Fe1 N3 . . 79.8(3) ?

N4 Fe1 N2 . . 166.8(3) ?

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N4 Fe1 Cl2 . . 96.7(3) ?

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N3 Fe1 Cl2 . . 90.9(2) ?

N2 Fe1 Cl2 . . 91.2(2) ?

N4 Fe1 Cl1 . . 92.4(2) ?

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N3 Fe1 Cl1 . . 171.0(2) ?

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C10 N1 C1 . . 106.8(8) ?

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C2 C1 N1 . . 110.6(9) ?  
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C1 C2 N2 . . 109.6(9) ?  
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C5 C4 C3 . . 116.1(9) ?  
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H9A C9 H9B . . 107.2 ?  
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H13B C13 H13C . . 109.5 ?  
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N4 C14 H14C . . 109.5 ?  
H14A C14 H14C . . 109.5 ?  
H14B C14 H14C . . 109.5 ?

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F4 P1 F6 . . 88.7(4) ?  
F3 P1 F1 . . 90.0(4) ?  
F5 P1 F1 . . 90.6(4) ?  
F4 P1 F1 . . 92.0(3) ?  
F6 P1 F1 . . 179.2(4) ?  
F3 P1 F2 . . 89.8(5) ?  
F5 P1 F2 . . 89.4(4) ?  
F4 P1 F2 . . 179.2(4) ?  
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F1 P1 F2 . . 87.8(3) ?

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C13 N2 C2 C1 . . . . 85.8(10) ?

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Fe1 N3 C5 C4 . . . . 62.3(11) ?  
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C5 N3 C6 C7 . . . . -170.6(8) ?  
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Fe1 N4 C7 C6 . . . . -31.9(11) ?  
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N4 C8 C9 C10 . . . . 60.6(14) ?  
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Fe1 N1 C10 C9 . . . . 63.5(11) ?  
C8 C9 C10 N1 . . . . -64.2(14) ?  
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Fe1 N1 C11 C12 . . . . 17.9(12) ?  
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Fe1 N3 C12 C11 . . . . 16.2(12) ?

N1 C11 C12 N3 . . . . -23.2(15) ?

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C2 H2A F1 2\_664 0.99 2.36 3.249(12) 148.3

C3 H3B Cl2 . 0.99 2.73 3.304(11) 117.4

C5 H5B Cl2 . 0.99 2.67 3.277(11) 120.1

C6 H6B Cl2 . 0.99 2.91 3.453(10) 115.3

C8 H8A Cl1 . 0.99 2.78 3.337(10) 116.1

C8 H8B Cl2 3\_654 0.99 2.78 3.726(11) 159.4

C9 H9A Cl2 1\_565 0.99 2.76 3.571(12) 139.7

C10 H10A Cl1 . 0.99 2.69 3.311(11) 121.0

C11 H11A F2 1\_554 0.99 2.51 3.097(13) 117.7

C11 H11B F5 2\_664 0.99 2.41 3.360(15) 160.8

C13 H13A Cl1 . 0.98 2.63 3.198(10) 117.2

C13 H13B F1 1\_545 0.98 2.59 3.323(11) 131.2

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C14 H14B Cl1 3\_644 0.98 2.89 3.772(11) 150.3

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0 -1 -32 33.18 31.84 0
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_shelx_hkl_checksum 77692
_shelx_res_file
;
shelx.res created by SHELXL-2014/7
TITL New: Pna21
CELL 0.71073 26.0020 8.5752 9.3829 90.000 90.000 90.000
ZERR 4.00 0.0040 0.0015 0.0016 0.000 0.000 0.000
LATT -1
SYMM -X, -Y, 1/2 + Z
SYMM 1/2 - X, 1/2 + Y, 1/2 + Z
SYMM 1/2 + X, 1/2 - Y, Z
SFAC C H CL F FE N P
UNIT 56 120 8 24 4 16 4
MERG 2
TWIN
equiv $1 x, -1+y, z
equiv $2 1.5-x, y-0.5, z+0.5
equiv $3 1.5-x, y+0.5, z+0.5
rtab cl Cl2 h9a_$1
rtab cl cl2 h8b_$2
rtab cl cl2 h14c_$2
rtab cl cl1 h8b_$2
rtab cl Cl1 h9a_$2
rtab cl cl1 h14b_$3
shel 15 0.5
FMAP 2
PLAN 20
SIZE 0.070 0.090 0.120
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ACTA

BOND \$H

CONF

L.S. 12

TEMP -123.00

WGHT 0.037800

BASF 0.02589

FVAR 0.35913

FE1 5 0.662318 0.149821 0.203863 11.00000 0.04154 0.03789 =  
0.03877 -0.00314 -0.00248 0.00115

CL1 3 0.712789 0.252287 0.380333 11.00000 0.05049 0.04551 =  
0.04522 -0.00742 -0.01072 -0.00037

CL2 3 0.692851 -0.098701 0.218175 11.00000 0.06021 0.03562 =  
0.05221 0.00159 -0.00349 0.00700

N1 6 0.618166 0.366412 0.177496 11.00000 0.05332 0.05430 =  
0.03600 0.00298 0.00467 0.00822

N2 6 0.595030 0.088885 0.340069 11.00000 0.04799 0.04531 =  
0.03689 0.00260 -0.00240 0.00174

N3 6 0.614420 0.086923 0.016182 11.00000 0.03882 0.04534 =  
0.04207 -0.00388 -0.00879 -0.00614

N4 6 0.714770 0.229390 0.036610 11.00000 0.04082 0.04809 =  
0.04662 -0.00868 -0.00156 -0.00148

C1 1 0.584445 0.369218 0.314826 11.00000 0.06645 0.05503 =  
0.05192 -0.00581 0.00125 -0.00248

AFIX 23

H1A 2 0.606601 0.387606 0.398971 11.00000 -1.20000

H1B 2 0.559345 0.455767 0.308697 11.00000 -1.20000

AFIX 0

C2 1 0.556895 0.220772 0.331962 11.00000 0.05379 0.05901 =  
0.05847 0.01053 0.02420 0.00464

AFIX 23

H2A 2 0.533458 0.204411 0.250164 11.00000 -1.20000  
H2B 2 0.535974 0.223602 0.420079 11.00000 -1.20000  
AFIX 0  
C3 1 0.569799 -0.058772 0.297889 11.00000 0.06125 0.05595 =  
0.04946 -0.00189 0.01162 -0.02171  
AFIX 23  
H3A 2 0.540869 -0.076515 0.364539 11.00000 -1.20000  
H3B 2 0.594851 -0.143957 0.313758 11.00000 -1.20000  
AFIX 0  
C4 1 0.548979 -0.076803 0.147921 11.00000 0.06744 0.05206 =  
0.05772 -0.00193 -0.00360 -0.01186  
AFIX 23  
H4A 2 0.532027 -0.179877 0.140721 11.00000 -1.20000  
H4B 2 0.522205 0.003590 0.132769 11.00000 -1.20000  
AFIX 0  
C5 1 0.586747 -0.064208 0.032411 11.00000 0.05895 0.05484 =  
0.05056 -0.00759 0.00221 -0.00725  
AFIX 23  
H5A 2 0.568857 -0.086592 -0.058453 11.00000 -1.20000  
H5B 2 0.612779 -0.147067 0.046327 11.00000 -1.20000  
AFIX 0  
C6 1 0.653845 0.067064 -0.099300 11.00000 0.07224 0.06669 =  
0.03995 -0.00024 -0.00928 -0.00783  
AFIX 23  
H6A 2 0.636366 0.054753 -0.192358 11.00000 -1.20000  
H6B 2 0.674279 -0.028277 -0.081033 11.00000 -1.20000  
AFIX 0  
C7 1 0.690033 0.210502 -0.104589 11.00000 0.08562 0.07031 =  
0.04575 0.00371 0.00656 -0.01112  
AFIX 23  
H7A 2 0.716602 0.195174 -0.178853 11.00000 -1.20000

H7B 2 0.670092 0.305283 -0.128579 11.00000 -1.20000

AFIX 0

C8 1 0.731523 0.400126 0.055531 11.00000 0.07629 0.04375 =  
0.05823 0.00577 0.00660 0.00341

AFIX 23

H8A 2 0.752012 0.407796 0.144186 11.00000 -1.20000

H8B 2 0.754481 0.427976 -0.024700 11.00000 -1.20000

AFIX 0

C9 1 0.688233 0.521366 0.062770 11.00000 0.08572 0.04732 =  
0.08630 0.00160 0.03154 0.00198

AFIX 23

H9A 2 0.704289 0.625760 0.069855 11.00000 -1.20000

H9B 2 0.669291 0.517905 -0.028702 11.00000 -1.20000

AFIX 0

C10 1 0.649873 0.507047 0.180467 11.00000 0.09183 0.02997 =  
0.07883 0.00682 0.00490 -0.00471

AFIX 23

H10A 2 0.668499 0.510260 0.272444 11.00000 -1.20000

H10B 2 0.626867 0.598969 0.177255 11.00000 -1.20000

AFIX 0

C11 1 0.587266 0.368380 0.050476 11.00000 0.06660 0.05249 =  
0.07268 0.00270 -0.00753 0.02505

AFIX 23

H11A 2 0.604369 0.435704 -0.020941 11.00000 -1.20000

H11B 2 0.553678 0.416554 0.073511 11.00000 -1.20000

AFIX 0

C12 1 0.577488 0.208914 -0.016826 11.00000 0.06840 0.05293 =  
0.05917 0.00403 -0.02245 -0.00417

AFIX 23

H12A 2 0.543021 0.172808 0.013514 11.00000 -1.20000

H12B 2 0.576494 0.222210 -0.121598 11.00000 -1.20000

AFIX 0

C13 1 0.613184 0.067630 0.487558 11.00000 0.07106 0.06846 =  
0.03519 0.01405 0.00697 -0.02133

AFIX 33

H13A 2 0.630239 0.163159 0.520005 11.00000 -1.50000  
H13B 2 0.583815 0.045009 0.549666 11.00000 -1.50000  
H13C 2 0.637572 -0.019415 0.491096 11.00000 -1.50000

AFIX 0

C14 1 0.764105 0.148802 0.042276 11.00000 0.05279 0.05856 =  
0.06401 -0.00265 0.01299 0.01018

AFIX 33

H14A 2 0.779543 0.163265 0.136636 11.00000 -1.50000  
H14B 2 0.758839 0.037300 0.024631 11.00000 -1.50000  
H14C 2 0.787092 0.191678 -0.030630 11.00000 -1.50000

AFIX 0

P1 7 0.580817 0.621987 0.671392 11.00000 0.04422 0.06543 =  
0.04452 0.00863 0.00238 0.01260

F1 4 0.551045 0.784731 0.657617 11.00000 0.06872 0.06288 =  
0.08960 0.02162 0.02878 0.02403

F2 4 0.548229 0.589955 0.813341 11.00000 0.12295 0.09406 =  
0.07481 0.03782 0.05795 0.04959

F3 4 0.623486 0.703109 0.762563 11.00000 0.07281 0.17133 =  
0.10666 -0.08982 -0.02703 0.02517

F4 4 0.612231 0.653074 0.530034 11.00000 0.05997 0.07656 =  
0.05405 -0.00005 0.01172 0.00434

F5 4 0.537691 0.538072 0.581812 11.00000 0.05389 0.13149 =  
0.09725 -0.03243 0.01721 -0.02052

F6 4 0.609684 0.459186 0.686171 11.00000 0.12349 0.08108 =  
0.07885 0.01882 0.03844 0.04588

HKLF 4 1.0 0.00 0.00 1.00 1.00 0.00 0.00 0.00 1.00 0.00

REM New: Pna21

REM R1 = 0.0500 for 2249 Fo > 4sig(Fo) and 0.0934 for all 4186 data

REM 254 parameters refined using 1 restraints

END

WGHT 0.0378 0.0000

REM Highest difference peak 0.391, deepest hole -0.333, 1-sigma level 0.072

Q1 1 0.7307 -0.1058 0.2299 11.00000 0.05 0.39

Q2 1 0.6723 0.2264 0.3543 11.00000 0.05 0.36

Q3 1 0.6765 0.2437 0.4205 11.00000 0.05 0.30

Q4 1 0.7166 0.0627 0.0234 11.00000 0.05 0.28

Q5 1 0.6992 0.3177 0.3684 11.00000 0.05 0.27

Q6 1 0.6161 0.1401 0.2063 11.00000 0.05 0.26

Q7 1 0.5115 0.0283 0.3633 11.00000 0.05 0.26

Q8 1 0.5684 0.3605 0.1845 11.00000 0.05 0.26

Q9 1 0.7077 0.1431 0.1894 11.00000 0.05 0.25

Q10 1 0.5705 0.1654 0.4727 11.00000 0.05 0.25

Q11 1 0.5757 0.7849 0.6684 11.00000 0.05 0.24

Q12 1 0.6215 0.0896 0.2815 11.00000 0.05 0.24

Q13 1 0.6478 -0.1017 0.1960 11.00000 0.05 0.24

Q14 1 0.6694 0.2202 0.0600 11.00000 0.05 0.24

Q15 1 0.5132 0.7861 0.6885 11.00000 0.05 0.24

Q16 1 0.7186 0.2785 0.4395 11.00000 0.05 0.24

Q17 1 0.6148 0.7636 0.7114 11.00000 0.05 0.24

Q18 1 0.6599 -0.0429 0.2068 11.00000 0.05 0.23

Q19 1 0.7623 0.0990 0.0339 11.00000 0.05 0.22

Q20 1 0.4951 0.5273 0.7096 11.00000 0.05 0.22

;

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