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μ -Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]chromium(III)} bis(hexafluorodiphosphate)

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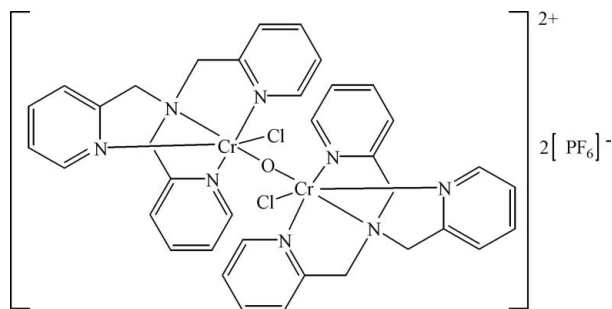
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.032; wR factor = 0.089; data-to-parameter ratio = 13.5.

The title compound, $[\text{Cr}_2\text{Cl}_2\text{O}(\text{C}_{18}\text{H}_{18}\text{N}_4)_2](\text{PF}_6)_2$, is isostructural with the V^{III} analogue. Each Cr^{III} atom is chelated by the tetradentate tris(2-pyridylmethyl)amine ligand *via* four N atoms, and further coordinated by one Cl atom and one bridging O atom, giving a slightly distorted octahedral coordination geometry. The dinuclear complex is centrosymmetric, with the bridging O atom lying on a centre of inversion.

Related literature

For the isostructural V^{III} analogue, see: Tajika *et al.* (2005). For more general related literature, see: Butler & Carrano (1991); Crans *et al.* (1989); Dey (1974); Chen & Zubieta (1990).



Experimental

Crystal data

$[\text{Cr}_2\text{Cl}_2\text{O}(\text{C}_{18}\text{H}_{18}\text{N}_4)_2](\text{PF}_6)_2$
 $M_r = 1061.57$
 Triclinic, $P\bar{1}$
 $a = 8.6107$ (17) Å
 $b = 11.302$ (2) Å
 $c = 12.798$ (3) Å
 $\alpha = 115.50$ (3)°
 $\beta = 107.45$ (3)°

$\gamma = 91.50$ (3)°
 $V = 1054.8$ (4) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 0.81$ mm⁻¹
 $T = 293$ (2) K
 $0.28 \times 0.22 \times 0.18$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\text{min}} = 0.804$, $T_{\text{max}} = 0.867$

8686 measured reflections
 3877 independent reflections
 3594 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.089$
 $S = 1.00$
 3877 reflections

287 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.51$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.33$ e Å⁻³

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: B12257).

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supplementary materials

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μ -Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]chromium(III)} bis(hexafluoridophosphate)

S. Li, S.-B. Wang, F.-L. Zhang and K. Tang

Comment

A classical but nevertheless rapidly developing field of application for related metal-Schiff compounds is their use as catalysts in polymerization, oxidation reactions, and model examples for the interaction of metal ions within the active sites of enzymes (Butler & Carrano, 1991; Crans *et al.*, 1989; Dey, 1974; Chen & Zubieta, 1990). In the dinuclear title compound (Fig. 1), each Cr^{III} atom is chelated by the tetradentate ligand tris(2-pyridylmethyl)amine *via* four N atoms, and further coordinated by one Cl atom and one bridging O atom to give a slightly distorted octahedral coordination geometry.

Experimental

A mixture of chromium(III) trichloride (1 mmol) and tris(2-pyridylmethyl)amine (1 mmol) in 20 ml methanol was refluxed for two hours. After cooling, the solution was filtered and the filtrate was evaporated naturally at room temperature. Blue blocks of the title compound were obtained after a few days with a yield of 31%. Elemental analysis calculated: C 40.39, H 3.35, N 10.44%; found: C 40.35, H 3.39, N 10.42%.

Refinement

All H atoms were placed in calculated positions with C—H = 0.93 or 0.97 Å and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

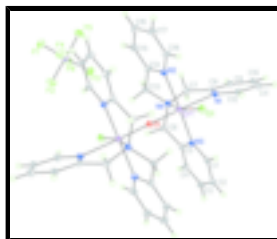


Fig. 1. The molecular structure drawn with 30% probability displacement ellipsoids for the non-H atoms.

μ -Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]chromium(III)} dihexafluoridophosphate

Crystal data

$[\text{Cr}_2\text{Cl}_2\text{O}(\text{C}_{18}\text{H}_{18}\text{N}_4)_2](\text{PF}_6)_2$

$M_r = 1061.57$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.6107(17)$ Å

$Z = 1$

$F_{000} = 536$

$D_x = 1.671$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3877 reflections

supplementary materials

$b = 11.302$ (2) Å	$\theta = 3.0\text{--}25.5^\circ$
$c = 12.798$ (3) Å	$\mu = 0.81$ mm ⁻¹
$\alpha = 115.50$ (3)°	$T = 293$ (2) K
$\beta = 107.45$ (3)°	Block, blue
$\gamma = 91.50$ (3)°	$0.28 \times 0.22 \times 0.18$ mm
$V = 1054.8$ (4) Å ³	

Data collection

Bruker APEX II CCD diffractometer	3877 independent reflections
Radiation source: fine-focus sealed tube	3594 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.021$
$T = 293$ (2) K	$\theta_{\text{max}} = 25.5^\circ$
φ and ω scans	$\theta_{\text{min}} = 3.0^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -8 \rightarrow 10$
$T_{\text{min}} = 0.804$, $T_{\text{max}} = 0.867$	$k = -13 \rightarrow 13$
8686 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.3428P]$
$wR(F^2) = 0.089$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3877 reflections	$\Delta\rho_{\text{max}} = 0.51$ e Å ⁻³
287 parameters	$\Delta\rho_{\text{min}} = -0.33$ e Å ⁻³
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL, $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.042 (3)

Special details

Geometry. 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.

Refinement. 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 $F^2 > \sigma(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cr1	1.03745 (3)	0.34679 (3)	0.39271 (2)	0.0408 (4)
C1	0.9871 (3)	0.1897 (2)	0.53070 (18)	0.0447 (4)
H1	1.1018	0.1984	0.5573	0.054*
C2	0.8992 (3)	0.1306 (2)	0.5741 (2)	0.0534 (5)
H2	0.9533	0.0998	0.6296	0.064*
C3	0.7284 (3)	0.1173 (3)	0.5340 (2)	0.0605 (6)
H3	0.6662	0.0779	0.5626	0.073*
C4	0.6514 (3)	0.1630 (2)	0.4513 (2)	0.0552 (5)
H4	0.5367	0.1537	0.4226	0.066*
C5	0.7464 (2)	0.22306 (19)	0.41135 (18)	0.0425 (4)
C6	0.6721 (2)	0.2874 (2)	0.3310 (2)	0.0490 (5)
H6A	0.5643	0.2353	0.2730	0.059*
H6B	0.6563	0.3757	0.3822	0.059*
C7	0.7467 (3)	0.1753 (2)	0.1450 (2)	0.0573 (6)
H7A	0.7443	0.2004	0.0811	0.069*
H7B	0.6381	0.1253	0.1216	0.069*
C8	0.8712 (2)	0.08565 (19)	0.14924 (17)	0.0414 (4)
C9	0.8351 (3)	-0.0448 (2)	0.0588 (2)	0.0528 (5)
H9	0.7315	-0.0793	-0.0028	0.063*
C10	0.9546 (3)	-0.1237 (2)	0.0606 (2)	0.0617 (6)
H10	0.9327	-0.2119	0.0003	0.074*
C11	1.1069 (3)	-0.0697 (2)	0.1532 (2)	0.0607 (6)
H11	1.1894	-0.1208	0.1564	0.073*
C12	1.1346 (3)	0.0605 (2)	0.2404 (2)	0.0526 (5)
H12	1.2374	0.0964	0.3028	0.063*
C13	0.7605 (3)	0.4147 (2)	0.23723 (19)	0.0475 (5)
H13A	0.7430	0.4881	0.3059	0.057*
H13B	0.6651	0.3917	0.1639	0.057*
C14	0.9146 (3)	0.4574 (2)	0.21891 (17)	0.0471 (5)
C15	0.9138 (4)	0.5296 (2)	0.1547 (2)	0.0606 (6)
H15	0.8154	0.5482	0.1149	0.073*
C16	1.0629 (4)	0.5734 (3)	0.1512 (2)	0.0728 (8)
H16	1.0650	0.6237	0.1100	0.087*
C17	1.2075 (4)	0.5435 (3)	0.2077 (3)	0.0715 (7)
H17	1.3076	0.5721	0.2047	0.086*
C18	1.2007 (3)	0.4704 (3)	0.2686 (2)	0.0610 (6)
H18	1.2978	0.4490	0.3069	0.073*
Cl1	1.31398 (6)	0.35078 (6)	0.48445 (5)	0.05507 (17)
F1	0.5115 (2)	0.90789 (16)	0.13882 (17)	0.0825 (5)
F2	0.4878 (2)	0.8490 (2)	0.27945 (15)	0.0893 (5)
F3	0.5830 (3)	0.6607 (2)	0.1912 (2)	0.1078 (7)
F4	0.7325 (2)	0.8610 (2)	0.24906 (17)	0.0999 (6)
F5	0.6040 (2)	0.72005 (19)	0.04870 (17)	0.0929 (6)
F6	0.36012 (19)	0.71102 (16)	0.08031 (14)	0.0726 (4)
N1	1.0192 (2)	0.13917 (16)	0.23969 (15)	0.0436 (4)

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N2	1.0566 (2)	0.42848 (18)	0.27454 (16)	0.0482 (4)
N3	0.91312 (19)	0.23567 (15)	0.45104 (15)	0.0406 (3)
N4	0.7776 (2)	0.29834 (16)	0.26214 (15)	0.0424 (4)
O1	1.0000	0.5000	0.5000	0.0420 (4)
P1	0.54870 (7)	0.78424 (6)	0.16549 (5)	0.05276 (17)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0378 (11)	0.0424 (10)	0.0424 (10)	0.0088 (8)	0.0112 (8)	0.0212 (8)
C1	0.0415 (10)	0.0468 (10)	0.0459 (10)	0.0095 (8)	0.0121 (8)	0.0233 (8)
C2	0.0597 (14)	0.0546 (12)	0.0513 (12)	0.0109 (10)	0.0179 (10)	0.0300 (10)
C3	0.0606 (14)	0.0666 (14)	0.0669 (14)	0.0057 (11)	0.0281 (11)	0.0381 (12)
C4	0.0395 (11)	0.0606 (13)	0.0695 (14)	0.0063 (9)	0.0206 (10)	0.0324 (11)
C5	0.0351 (9)	0.0412 (9)	0.0456 (10)	0.0057 (7)	0.0117 (8)	0.0166 (8)
C6	0.0302 (9)	0.0572 (12)	0.0614 (12)	0.0093 (8)	0.0107 (8)	0.0322 (10)
C7	0.0517 (13)	0.0499 (12)	0.0462 (11)	0.0099 (9)	-0.0011 (9)	0.0127 (9)
C8	0.0424 (10)	0.0438 (10)	0.0403 (9)	0.0052 (8)	0.0153 (8)	0.0207 (8)
C9	0.0562 (13)	0.0484 (11)	0.0497 (11)	0.0027 (9)	0.0185 (10)	0.0189 (9)
C10	0.0769 (17)	0.0441 (11)	0.0634 (14)	0.0138 (11)	0.0334 (13)	0.0178 (10)
C11	0.0653 (15)	0.0551 (13)	0.0714 (15)	0.0256 (11)	0.0342 (12)	0.0297 (11)
C12	0.0460 (12)	0.0572 (12)	0.0570 (12)	0.0167 (9)	0.0199 (10)	0.0265 (10)
C13	0.0504 (11)	0.0490 (11)	0.0410 (10)	0.0162 (9)	0.0097 (8)	0.0224 (9)
C14	0.0599 (13)	0.0426 (10)	0.0358 (9)	0.0112 (9)	0.0152 (9)	0.0162 (8)
C15	0.0864 (18)	0.0503 (12)	0.0451 (12)	0.0140 (11)	0.0197 (11)	0.0237 (10)
C16	0.114 (2)	0.0544 (13)	0.0572 (14)	0.0012 (14)	0.0362 (15)	0.0288 (12)
C17	0.084 (2)	0.0710 (16)	0.0683 (16)	-0.0005 (14)	0.0357 (14)	0.0343 (13)
C18	0.0612 (14)	0.0666 (14)	0.0615 (14)	0.0042 (11)	0.0280 (11)	0.0307 (12)
Cl1	0.0334 (3)	0.0609 (3)	0.0596 (3)	0.0131 (2)	0.0101 (2)	0.0215 (2)
F1	0.0810 (11)	0.0724 (10)	0.0988 (12)	0.0060 (8)	0.0208 (9)	0.0507 (9)
F2	0.0836 (12)	0.1141 (14)	0.0632 (9)	0.0059 (10)	0.0336 (8)	0.0300 (9)
F3	0.1008 (15)	0.1236 (16)	0.163 (2)	0.0524 (12)	0.0641 (14)	0.1074 (16)
F4	0.0483 (9)	0.1549 (19)	0.0854 (12)	-0.0063 (10)	0.0024 (8)	0.0605 (12)
F5	0.0973 (13)	0.0965 (12)	0.0873 (12)	0.0083 (10)	0.0563 (10)	0.0288 (10)
F6	0.0571 (9)	0.0710 (9)	0.0731 (9)	-0.0042 (7)	0.0144 (7)	0.0248 (7)
N1	0.0425 (9)	0.0456 (9)	0.0444 (9)	0.0116 (7)	0.0164 (7)	0.0210 (7)
N2	0.0526 (10)	0.0497 (9)	0.0451 (9)	0.0087 (8)	0.0187 (8)	0.0231 (8)
N3	0.0348 (8)	0.0421 (8)	0.0447 (8)	0.0082 (6)	0.0125 (7)	0.0205 (7)
N4	0.0376 (8)	0.0442 (8)	0.0411 (8)	0.0101 (7)	0.0077 (6)	0.0195 (7)
O1	0.0384 (10)	0.0430 (10)	0.0424 (10)	0.0081 (8)	0.0119 (8)	0.0190 (8)
P1	0.0429 (3)	0.0665 (4)	0.0529 (3)	0.0075 (3)	0.0151 (2)	0.0321 (3)

Geometric parameters (\AA , $^\circ$)

Cr1—O1	1.7986 (7)	C9—H9	0.930
Cr1—N3	2.1206 (18)	C10—C11	1.378 (4)
Cr1—N2	2.1238 (18)	C10—H10	0.930
Cr1—N4	2.2370 (19)	C11—C12	1.370 (3)
Cr1—N1	2.2814 (19)	C11—H11	0.930

Cr1—C11	2.3070 (9)	C12—N1	1.351 (3)
O1—Cr1 ⁱ	1.7986 (7)	C12—H12	0.930
C1—N3	1.341 (3)	C13—N4	1.482 (3)
C1—C2	1.369 (3)	C13—C14	1.516 (3)
C1—H1	0.930	C13—H13A	0.970
C2—C3	1.386 (4)	C13—H13B	0.970
C2—H2	0.930	C14—N2	1.345 (3)
C3—C4	1.376 (4)	C14—C15	1.383 (3)
C3—H3	0.930	C15—C16	1.384 (4)
C4—C5	1.382 (3)	C15—H15	0.930
C4—H4	0.930	C16—C17	1.371 (4)
C5—N3	1.352 (3)	C16—H16	0.930
C5—C6	1.506 (3)	C17—C18	1.369 (4)
C6—N4	1.479 (3)	C17—H17	0.930
C6—H6A	0.970	C18—N2	1.351 (3)
C6—H6B	0.970	C18—H18	0.930
C7—N4	1.483 (3)	F1—P1	1.5939 (17)
C7—C8	1.499 (3)	F2—P1	1.5803 (18)
C7—H7A	0.970	F3—P1	1.582 (2)
C7—H7B	0.970	F4—P1	1.5859 (18)
C8—N1	1.342 (3)	F5—P1	1.5804 (18)
C8—C9	1.379 (3)	F6—P1	1.6129 (17)
C9—C10	1.380 (4)		
O1—Cr1—N3	91.01 (5)	N1—C12—H12	118.5
O1—Cr1—N2	92.46 (5)	C11—C12—H12	118.5
N3—Cr1—N2	154.67 (7)	N4—C13—C14	110.48 (16)
O1—Cr1—N4	91.36 (6)	N4—C13—H13A	109.6
N3—Cr1—N4	78.03 (7)	C14—C13—H13A	109.6
N2—Cr1—N4	76.81 (7)	N4—C13—H13B	109.6
O1—Cr1—N1	166.58 (5)	C14—C13—H13B	109.6
N3—Cr1—N1	81.87 (7)	H13A—C13—H13B	108.1
N2—Cr1—N1	89.30 (7)	N2—C14—C15	120.7 (2)
N4—Cr1—N1	76.09 (7)	N2—C14—C13	116.67 (18)
O1—Cr1—C11	103.29 (5)	C15—C14—C13	122.5 (2)
N3—Cr1—C11	104.03 (5)	C14—C15—C16	118.4 (3)
N2—Cr1—C11	99.56 (6)	C14—C15—H15	120.8
N4—Cr1—C11	165.11 (5)	C16—C15—H15	120.8
N1—Cr1—C11	89.52 (6)	C17—C16—C15	120.8 (2)
N3—C1—C2	122.1 (2)	C17—C16—H16	119.6
N3—C1—H1	118.9	C15—C16—H16	119.6
C2—C1—H1	119.0	C16—C17—C18	118.2 (3)
C3—C2—C1	118.8 (2)	C16—C17—H17	120.9
C3—C2—H2	120.6	C18—C17—H17	120.9
C1—C2—H2	120.6	N2—C18—C17	121.8 (3)
C2—C3—C4	119.4 (2)	N2—C18—H18	119.1
C2—C3—H3	120.3	C17—C18—H18	119.1
C4—C3—H3	120.3	C12—N1—C8	117.79 (18)
C3—C4—C5	119.3 (2)	C12—N1—Cr1	126.02 (15)

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C3—C4—H4	120.4	C8—N1—Cr1	115.61 (13)
C5—C4—H4	120.4	C14—N2—C18	120.1 (2)
N3—C5—C4	120.95 (19)	C14—N2—Cr1	114.45 (14)
N3—C5—C6	116.79 (18)	C18—N2—Cr1	124.62 (17)
C4—C5—C6	122.07 (19)	C1—N3—C5	119.42 (18)
N4—C6—C5	112.19 (16)	C1—N3—Cr1	125.22 (14)
N4—C6—H6A	109.2	C5—N3—Cr1	115.07 (13)
C5—C6—H6A	109.2	C6—N4—C7	112.30 (18)
N4—C6—H6B	109.2	C6—N4—C13	112.63 (16)
C5—C6—H6B	109.2	C7—N4—C13	109.74 (17)
H6A—C6—H6B	107.9	C6—N4—Cr1	105.11 (12)
N4—C7—C8	114.97 (17)	C7—N4—Cr1	112.78 (13)
N4—C7—H7A	108.5	C13—N4—Cr1	103.96 (12)
C8—C7—H7A	108.5	Cr1—O1—Cr1 ⁱ	180.0
N4—C7—H7B	108.5	F5—P1—F3	90.59 (12)
C8—C7—H7B	108.5	F5—P1—F2	178.06 (11)
H7A—C7—H7B	107.5	F3—P1—F2	90.59 (13)
N1—C8—C9	122.2 (2)	F5—P1—F4	90.15 (11)
N1—C8—C7	117.57 (17)	F3—P1—F4	91.62 (13)
C9—C8—C7	120.13 (19)	F2—P1—F4	91.35 (11)
C10—C9—C8	119.3 (2)	F5—P1—F1	89.58 (11)
C10—C9—H9	120.4	F3—P1—F1	179.22 (11)
C8—C9—H9	120.4	F2—P1—F1	89.22 (11)
C11—C10—C9	118.9 (2)	F4—P1—F1	89.14 (11)
C11—C10—H10	120.5	F5—P1—F6	90.19 (10)
C9—C10—H10	120.5	F3—P1—F6	90.39 (12)
C10—C11—C12	118.9 (2)	F2—P1—F6	88.26 (10)
C10—C11—H11	120.6	F4—P1—F6	177.95 (11)
C12—C11—H11	120.6	F1—P1—F6	88.85 (10)
N1—C12—C11	122.9 (2)		

Symmetry codes: (i) $-x+2, -y+1, -z+1$.

Fig. 1

