Additions and Corrections

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Martin Schubart, Liam O'Dwyer, Lutz H. Gade, Wan-Sheung Li, and Mary McPartlin*: Synthesis and Structures of N-Alkylated Azatitanatranes.

Pages 3893−3898. In the original paper, the crystal structure of $N[CH_2CH_2NEt]_3Ti(OTf)$ (**4**) was reported in the wrong space group $P\bar{1}$ (No. 2), with two independent molecules in the asymmetric unit cell. The data were re-examined, and the structure was fully refined in the monoclinic space group $I2/a$. Attempts to refine the structure in the standard space group $C2/c$ (a = 30.808 Å, b = 8.954 Å, c = 17.010 Å, β = 121.69°) were unsatisfactory because of correlations. Very high thermal parameters for the fluorine atoms were again observed, and it proved possible to resolve each into two components with occupancy factors of 0.5 in this space group. The bond distances and angles are equal within experimental error to those reported originally, and all other conclusions remain unaffected by this change. Revisions of Tables 1, 6, and 7 are included here. The diagram of **4** in Figure 3 was incorrectly labeled, and a revised version is also shown here.

Table 1. Crystal Data for $N[CH_2CH_2NEt]_3Ti(OTf)$ (**4**)

empirical formula	$C_{13}H_{27}N_4F_3O_3STi$	D_{calcd} (g cm^{-3})	1.412
		space group	$I2/a$
fw	424.34	F(000)	1776
crystal system	monoclinic	μ(Mo Kα) (cm^{-1})	5.5
a (Å)	17.010(4)	no. of obsd reflcns	1662
b (Å)	8.954(3)	$I/3\sigma(I)$	
c (Å)	26.229(5)	no. of variables	196
β (deg)	91.81(2)	R; R_w	0.0801; 0.0896
V (Å^3)	3992.88	data/param	8.48
Z	8		

Table 6. Selected Bond Lengths (Å) and Angles (deg) of Molecule **4**

Ti−N(1)	2.216(8)	Ti−O(1)	1.981(7)
Ti−N(2)	1.902(8)	O(1)−S(1)	1.472(7)
Ti−N(3)	1.926(7)	S(1)−C(1s)	1.827(21)
Ti−N(4)	1.902(9)		
N(4)−Ti−N(2)	111.4(4)	N(3)−Ti−N(1)	76.0(3)
S(1)−O(1)−Ti	164.0(4)	N(3)−Ti−N(2)	118.7(3)
N(1)−Ti−O(1)	177.3(3)	N(4)−Ti−O(1)	102.0(3)
N(2)−Ti−O(1)	103.5(3)	N(4)−Ti−N(1)	79.0(3)
N(2)−Ti−N(1)	78.3(3)	N(4)−Ti−N(3)	116.7(4)
N(3)−Ti−O(1)	101.3(3)	C(1s)−S(1)−O(1)	100.0(7)

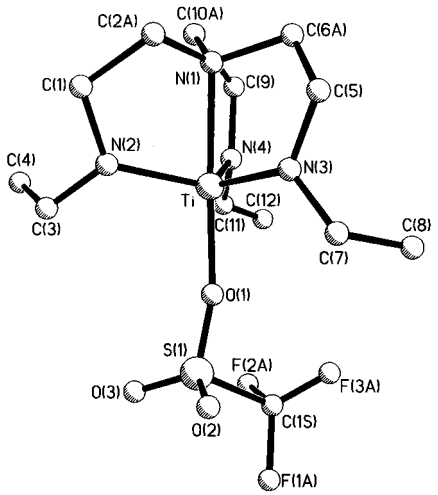

Figure 3.

Table 7. Fractional Atomic Coordinates of **4**

atom	x	y	z
Ti	0.02838(9)	0.11179(17)	0.14649(6)
O(1)	0.1133(4)	0.2575(8)	0.1343(2)
O(2)	0.1451(6)	0.5058(10)	0.1594(4)
O(3)	0.2458(4)	0.3167(12)	0.1624(4)
S(1)	0.1754(1)	0.3711(3)	0.1406(1)
N(1)	−0.0707(4)	−0.0435(8)	0.1586(3)
N(2)	0.0488(5)	0.0496(9)	0.2150(3)
N(3)	−0.0638(4)	0.2306(8)	0.1313(3)
N(4)	0.0513(5)	−0.0427(10)	0.0995(3)
C(1s)	0.1959(11)	0.4076(22)	0.0738(8)
C(1)	−0.0097(7)	−0.0361(15)	0.2430(4)
C(2a)	−0.0926(10)	−0.0340(21)	0.2133(7)
C(2b)	−0.0552(19)	−0.1379(38)	0.2075(13)
C(3)	0.1272(7)	0.0403(13)	0.2382(4)
C(4)	0.1658(9)	−0.1108(19)	0.2343(6)
C(5)	−0.1431(6)	0.1705(12)	0.1290(5)
C(6a)	−0.1408(11)	−0.0013(21)	0.1234(7)
C(6b)	−0.1447(17)	0.0375(33)	0.1706(11)
C(7)	−0.0599(6)	0.3882(11)	0.1155(3)
C(8)	−0.0655(7)	0.4075(15)	0.0579(4)
C(9)	0.0043(7)	−0.1763(14)	0.0952(5)
C(10a)	−0.0458(10)	−0.1980(22)	0.1445(7)
C(10b)	−0.0852(19)	−0.1259(40)	0.1132(13)
C(11)	0.1293(15)	−0.0610(27)	0.0764(12)
C(12)	0.1449(15)	−0.0658(31)	0.0329(8)
F(1a)	0.2436(8)	0.5327(16)	0.0768(5)
F(2a)	0.2415(7)	0.2781(16)	0.0603(5)
F(3a)	0.1438(9)	0.3932(18)	0.0403(6)
F(1b)	0.2479(15)	0.4833(28)	0.0632(9)
F(2b)	0.1898(16)	0.3212(35)	0.0453(10)
F(3b)	0.1269(8)	0.4836(15)	0.0555(5)

We thank Dr. R. E. Marsh (California Institute of Technology) for pointing out these errors.

Supporting Information Available: Complete listings of atomic coordinates, bond distances, bond angles, and anisotropic and isotropic thermal parameters for $N[CH_2CH_2NEt]_3Ti(OTf)$ (10 pages). Ordering information is given on any current masthead page.

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