Reconsideration of the Crystal Structure Refinement of the Complex $[Nb(\eta\text{-}C_5H_4SiMe_3)_2Cl_2]$ *

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The *X*-ray crystal-structure determination of the complex $[Nb(\eta\text{-}C_5H_4SiMe_3)_2Cl_2]$ has been reconsidered in terms of the centrosymmetric space group $P\bar{1}$, instead of that previously employed, non-centrosymmetric $P1$.

The crystal-structure refinement of the complex $[Nb(\eta\text{-}C_5H_4SiMe_3)_2Cl_2]$ has been previously carried out in the non-centrosymmetric space group $P1$ on the basis of two crystallographically independent, but practically identical, molecules.[1] However, a redefinition of the unit-cell origin has shown that these two molecules are related by a crystallographic inversion centre. A re-refinement of the structure in space group $P\bar{1}$ with 2 889 unique reflections $[I > 2\sigma(I)]$ converged at R and R' values of 0.0324 and 0.0394 respectively without significant variations in the molecular parameters. The fractional atomic co-ordinates of the non-hydrogen atoms are given in Table 1 and selected bond distances and angles in Table 2.

Additional material available from the Cambridge Crystallographic Data Centre comprises H-atom co-ordinates, thermal parameters, and remaining bond distances and angles.

Table 1. Fractional atomic co-ordinates ($\times 10^4$) with estimated standard deviations (e.s.d.s) in parentheses for the non-hydrogen atoms

Atom	*X/a*	*Y/b*	*Z/c*
Nb	2 647(1)	−2 500(1)	1 413(1)
Cl(1)	3 892(1)	−3 215(1)	−1 098(2)
Cl(2)	1 062(1)	−1 767(1)	−1 534(2)
Si(1)	5 616(1)	−2 147(1)	3 010(3)
Si(2)	−173(1)	−2 822(1)	1 865(2)
C(1)	3 480(5)	−1 679(4)	4 451(8)
C(2)	2 277(5)	−1 020(4)	4 011(10)
C(3)	2 050(5)	−507(4)	2 235(11)
C(4)	3 088(4)	−860(4)	1 528(9)
C(5)	4 003(4)	−1 582(4)	2 932(7)
C(6)	2 099(4)	−4 099(4)	661(9)
C(7)	3 275(5)	−4 511(4)	1 594(10)
C(8)	3 400(5)	−4 055(4)	3 552(10)
C(9)	2 280(4)	−3 391(4)	3 868(8)
C(10)	1 439(4)	−3 400(4)	2 088(7)
C(11)	5 903(7)	−1 897(9)	619(13)
C(12)	6 252(6)	−3 645(5)	3 623(14)
C(13)	6 279(6)	−1 352(6)	5 107(13)
C(14)	−899(6)	−3 044(8)	−763(11)
C(15)	−677(5)	−1 338(5)	2 763(11)
C(16)	−427(7)	−3 650(7)	3 599(13)

Table 2. Selected bond distances (Å) and angles (°) for $[Nb(\eta\text{-}C_5H_4SiMe_3)_2Cl_2]$ *

Nb–Cl(1)	2.461(2)	Si(1)–C(12)	1.858(7)
Nb–Cl(2)	2.462(2)	Si(1)–C(13)	1.862(8)
Nb–c_{g1}	2.082(6)	C(6)–C(7)	1.392(7)
Nb–c_{g2}	2.075(7)	C(7)–C(8)	1.379(9)
C(1)–C(2)	1.417(7)	C(8)–C(9)	1.407(7)
C(2)–C(3)	1.374(10)	C(9)–C(10)	1.406(7)
C(3)–C(4)	1.404(9)	C(6)–C(10)	1.431(7)
C(4)–C(5)	1.418(6)	C(10)–Si(2)	1.867(5)
C(1)–C(5)	1.400(9)	Si(2)–C(14)	1.839(7)
C(5)–Si(1)	1.883(5)	Si(2)–C(15)	1.846(6)
Si(1)–C(11)	1.846(11)	Si(2)–C(16)	1.853(11)
Cl(1)–Nb–Cl(2)	84.8(1)	C(4)–C(5)–C(1)	105.3(5)
Cl(1)–Nb–c_{g1}	108.7(2)	C(1)–C(5)–Si(1)	125.5(4)
Cl(1)–Nb–c_{g2}	105.9(2)	C(4)–C(5)–Si(1)	128.7(4)
Cl(2)–Nb–c_{g1}	106.8(1)	C(7)–C(6)–C(10)	109.5(5)
Cl(2)–Nb–c_{g2}	108.9(2)	C(6)–C(7)–C(8)	108.4(5)
c_{g1}–Nb–c_{g2}	131.7(2)	C(7)–C(8)–C(9)	107.5(6)
C(2)–C(1)–C(5)	109.6(5)	C(8)–C(9)–C(10)	110.1(5)
C(1)–C(2)–C(3)	107.5(6)	C(9)–C(10)–C(6)	104.4(5)
C(2)–C(3)–C(4)	108.2(6)	C(6)–C(10)–Si(2)	128.9(4)
C(3)–C(4)–C(5)	109.3(5)	C(9)–C(10)–Si(2)	125.9(4)

* c_{g1} = Centroid of the C(1)—C(5) ring, c_{g2} that of the C(6)—C(10) ring.

References

1 A. Antiñolo, J. Martínez de Ilarduja, A. Otero, P. Royo, A. M. Manotti Lanfredi, and A. Tiripicchio, *J. Chem. Soc., Dalton Trans.*, 1988, 2685.

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* Dichlorobis[η-(trimethylsilyl)cyclopentadienyl]niobium(IV).

Supplementary data available: see Instructions for Authors, *J. Chem. Soc., Dalton Trans.*, 1990, Issue 1, pp. xix—xxii.