Vanadocene-Mediated Ionization of Water in the Aqua-Species $[H_2O•B(C_6F_5)_3]$: Structural Characterization of the Hydride $[Cp_2V(\mu\text{-}H)B(C_6F_5)_3]$ and the Hydroxide $[Cp_2V(\mu\text{-}OH)B(C_6F_5)_3]$ Complexes.

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Supplementary Material

1. Full X-ray Data

2. Theoretical studies

1. X-ray data

Data collection were collected at low temperature on a Xcalibur Oxford Diffraction diffractometer using a graphite-monochromated Mo-Kα radiation (λ = 0.71073Å) and equipped with an Oxford Cryosystems Cryostream Cooler Device. The final unit cell parameters have been obtained by means of a least-squares refinement performed on a set of 5000 well measured reflections. The structures have been solved by Direct Methods using SIR92,[1] and refined by means of least-squares procedures on a F^2 with the aid of the program SHELXL97[2] include in the softwares package WinGX version 1.63[3]. The Atomic Scattering Factors were taken from International tables for X-Ray Crystallography.[4] Only the hydride (in **1**) and the hydroxide (in **2**) hydrogen atoms were located on a difference Fourier maps, and refined by using a riding model. Other hydrogen atoms were geometrically placed. All non-hydrogens atoms were anisotropically refined, and in the last cycles of refinement a weighting scheme was used, where weights are calculated from the following formula: $w=1/[\sigma^2(Fo^2)+(aP)^2+bP]$ where $P=(Fo^2+2Fc^2)/3$. Drawing of molecule are performed with the program ORTEP32 [5] with 50% probability displacement ellipsoids for non-hydrogen atoms.

For 1. The structure contains disordered molecule of Toluene. It was difficult to model the atoms positions and distribution reliably. The anisotropic displacement parameters of these atoms were very large. Several trials at defining additional sites or using lower site-occupation factors for these atoms yielded inferior results. Therefore, it was assumed that the Toluene molecule is highly disordered within its cavity, which results in smeared-out electron density. As an alternative strategy, the SQUEEZE function of PLATON (van der Sluis & Spek, 1990; Spek, 2001) was used to eliminate the contribution of the electron density in the solvent region from the intensity data. The use of this strategy and the subsequent solvent-free model produced slightly better refinement results, and hence more precise geometric parameters, than the attempt to model the solvent atoms. Therefore, the solvent-free model and intensity data were used for the final results reported here. PLATON estimated that each cavity contains approximately 50 electrons, which is equivalent to a Toluene molecule.

References:

1 SIR92 - A program for crystal structure solution. A. Altomare, G. Cascarano, C. Giacovazzo and A. Guagliardi, J. Appl. Crystallogr. 1993, 26, 343-350.

2 SHELX97 [Includes SHELXS97, SHELXL97, CIFTAB] - Programs for Crystal Structure Analysis (Release 97-2). G. M. Sheldrick, Institüt für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany, 1998.

3 WINGX - 1.63 Integrated System of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data. L.Farrugia,

J. Appl. Crystallogr.1999, 32, 837 - 838.

4 INTERNATIONAL tables for X-Ray crystallography, 1974, Vol IV, Kynoch press, Birmingham, England.

5 ORTEP3 for Windows - L. J. Farrugia, J. Appl. Crystallogr. 1997, 30, 565.

Data for 1

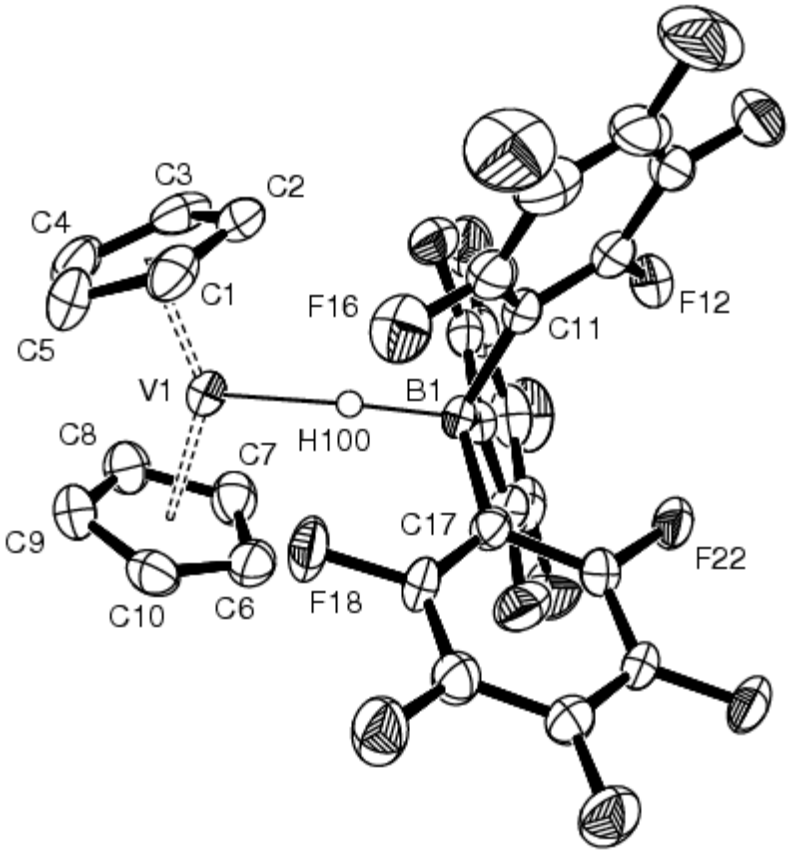

Table 1. Crystal data and structure refinement for **1**.

Identification code	rc040504
Empirical formula	C56 H22 B2 F30 V2
Formula weight	1388.24
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 18.733(2) A alpha = 90 deg. b = 15.9994(17) A beta = 95.807(9) deg. c = 19.453(2) A gamma = 90 deg.
Volume	5800.3(11) A^3
Z, Calculated density	4, 1.590 Mg/m^3
Absorption coefficient	0.456 mm^-1
F(000)	2736
Crystal size	0.375 x 0.1 x 0.075 mm
Theta range for data collection	3.18 to 32.09 deg.
Limiting indices	-27<=h<=27, -20<=k<=23, -27<=l<=23
Reflections collected / unique	29734 / 9503 [R(int) = 0.0762]
Completeness to theta = 32.09	93.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9706 and 0.9236
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9503 / 0 / 410
Goodness-of-fit on F^2	0.743
Final R indices [I>2sigma(I)]	R1 = 0.0493, wR2 = 0.1052
R indices (all data)	R1 = 0.1973, wR2 = 0.1345
Largest diff. peak and hole	0.375 and -0.300 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6404(2)	1527(2)	3508(2)	44(1)
C(2)	5956(2)	952(2)	3115(2)	43(1)
C(3)	5957(2)	198(2)	3479(2)	48(1)
C(4)	6417(2)	307(3)	4099(2)	58(1)
C(5)	6682(2)	1128(3)	4115(2)	52(1)
C(6)	8129(2)	54(2)	2806(2)	42(1)
C(7)	7741(2)	-683(2)	2935(2)	42(1)
C(8)	7680(2)	-697(2)	3653(2)	44(1)
C(9)	8027(2)	24(2)	3958(2)	47(1)
C(10)	8305(2)	480(2)	3433(2)	45(1)
C(11)	6190(2)	1425(2)	1364(2)	33(1)
C(12)	5706(2)	1204(2)	809(2)	39(1)
C(13)	5128(2)	1687(3)	560(2)	49(1)
C(14)	5011(2)	2436(3)	869(2)	56(1)
C(15)	5479(2)	2686(3)	1409(2)	53(1)
C(16)	6044(2)	2188(2)	1639(2)	40(1)
C(17)	7581(2)	1478(2)	1432(2)	29(1)
C(18)	7999(2)	2014(2)	1867(2)	34(1)
C(19)	8500(2)	2550(2)	1653(2)	37(1)
C(20)	8616(2)	2579(2)	966(2)	37(1)
C(21)	8231(2)	2060(2)	512(2)	33(1)
C(22)	7718(2)	1548(2)	743(2)	31(1)
C(23)	6907(2)	-80(2)	1424(2)	32(1)
C(24)	6325(2)	-581(2)	1525(2)	35(1)
C(25)	6249(2)	-1406(2)	1349(2)	41(1)
C(26)	6792(2)	-1791(2)	1049(2)	49(1)
C(27)	7398(2)	-1344(2)	943(2)	45(1)
C(28)	7437(2)	-515(2)	1132(2)	35(1)
F(12)	5778(1)	476(1)	460(1)	50(1)
F(13)	4673(1)	1416(2)	17(1)	69(1)
F(14)	4442(1)	2909(2)	628(1)	87(1)
F(15)	5381(1)	3428(2)	1721(1)	84(1)
F(16)	6495(1)	2497(1)	2169(1)	52(1)
F(18)	7920(1)	2037(1)	2557(1)	46(1)
F(19)	8868(1)	3073(1)	2105(1)	55(1)
F(20)	9104(1)	3109(1)	750(1)	54(1)
F(21)	8336(1)	2077(1)	-166(1)	45(1)
F(22)	7321(1)	1086(1)	260(1)	40(1)
F(24)	5768(1)	-242(1)	1819(1)	45(1)
F(25)	5661(1)	-1836(1)	1455(1)	60(1)
F(26)	6745(1)	-2596(1)	858(1)	69(1)
F(27)	7937(1)	-1713(1)	651(1)	65(1)
F(28)	8068(1)	-131(1)	1021(1)	50(1)
V(1)	7090(1)	450(1)	3210(1)	32(1)
B(1)	6918(2)	902(3)	1642(2)	31(1)

Table 3. Bond lengths [A] and angles [deg] for **1**.

C(1)-C(5)	1.397(5)
C(1)-C(2)	1.414(5)
C(1)-V(1)	2.260(3)
C(1)-H(1)	0.9800
C(2)-C(3)	1.400(5)
C(2)-V(1)	2.261(3)
C(2)-H(2)	0.9800
C(3)-C(4)	1.420(5)
C(3)-V(1)	2.273(3)
C(3)-H(3)	0.9800
C(4)-C(5)	1.402(5)
C(4)-V(1)	2.252(3)
C(4)-H(4)	0.9800
C(5)-V(1)	2.264(3)
C(5)-H(5)	0.9800
C(6)-C(10)	1.406(5)
C(6)-C(7)	1.421(5)
C(6)-V(1)	2.263(3)
C(6)-H(6)	0.9800
C(7)-C(8)	1.413(4)
C(7)-V(1)	2.278(3)
C(7)-H(7)	0.9800
C(8)-C(9)	1.422(5)
C(8)-V(1)	2.269(3)
C(8)-H(8)	0.9800
C(9)-C(10)	1.399(5)
C(9)-V(1)	2.270(3)
C(9)-H(9)	0.9800
C(10)-V(1)	2.274(3)
C(10)-H(10)	0.9800
C(11)-C(16)	1.371(5)
C(11)-C(12)	1.382(4)
C(11)-B(1)	1.645(5)
C(12)-F(12)	1.361(4)
C(12)-C(13)	1.380(5)
C(13)-F(13)	1.357(4)
C(13)-C(14)	1.368(6)
C(14)-F(14)	1.352(4)
C(14)-C(15)	1.357(6)
C(15)-F(15)	1.354(4)
C(15)-C(16)	1.365(5)
C(16)-F(16)	1.357(4)
C(17)-C(18)	1.388(4)
C(17)-C(22)	1.393(4)
C(17)-B(1)	1.632(5)
C(18)-F(18)	1.366(3)
C(18)-C(19)	1.368(4)
C(19)-F(19)	1.350(4)
C(19)-C(20)	1.375(4)
C(20)-F(20)	1.347(3)
C(20)-C(21)	1.362(4)
C(21)-F(21)	1.353(3)
C(21)-C(22)	1.373(4)
C(22)-F(22)	1.355(3)
C(23)-C(28)	1.380(4)
C(23)-C(24)	1.384(4)
C(23)-B(1)	1.626(5)
C(24)-F(24)	1.352(3)
C(24)-C(25)	1.366(5)

C(25)-F(25)	1.331(4)
C(25)-C(26)	1.368(5)
C(26)-F(26)	1.339(4)
C(26)-C(27)	1.375(5)
C(27)-F(27)	1.345(4)
C(27)-C(28)	1.375(5)
C(28)-F(28)	1.368(4)
V(1)-H(100)	1.87(2)
B(1)-H(100)	1.34(2)

C(5)-C(1)-C(2)	107.9(4)
C(5)-C(1)-V(1)	72.1(2)
C(2)-C(1)-V(1)	71.8(2)
C(5)-C(1)-H(1)	125.9
C(2)-C(1)-H(1)	125.9
V(1)-C(1)-H(1)	125.9
C(3)-C(2)-C(1)	108.5(3)
C(3)-C(2)-V(1)	72.5(2)
C(1)-C(2)-V(1)	71.7(2)
C(3)-C(2)-H(2)	125.6
C(1)-C(2)-H(2)	125.6
V(1)-C(2)-H(2)	125.6
C(2)-C(3)-C(4)	107.1(3)
C(2)-C(3)-V(1)	71.56(19)
C(4)-C(3)-V(1)	70.9(2)
C(2)-C(3)-H(3)	126.4
C(4)-C(3)-H(3)	126.4
V(1)-C(3)-H(3)	126.4
C(5)-C(4)-C(3)	108.4(3)
C(5)-C(4)-V(1)	72.4(2)
C(3)-C(4)-V(1)	72.52(19)
C(5)-C(4)-H(4)	125.7
C(3)-C(4)-H(4)	125.7
V(1)-C(4)-H(4)	125.7
C(1)-C(5)-C(4)	108.1(3)
C(1)-C(5)-V(1)	71.88(19)
C(4)-C(5)-V(1)	71.5(2)
C(1)-C(5)-H(5)	125.9
C(4)-C(5)-H(5)	125.9
V(1)-C(5)-H(5)	125.9
C(10)-C(6)-C(7)	109.0(3)
C(10)-C(6)-V(1)	72.4(2)
C(7)-C(6)-V(1)	72.34(19)
C(10)-C(6)-H(6)	125.4
C(7)-C(6)-H(6)	125.4
V(1)-C(6)-H(6)	125.4
C(8)-C(7)-C(6)	106.5(3)
C(8)-C(7)-V(1)	71.6(2)
C(6)-C(7)-V(1)	71.18(19)
C(8)-C(7)-H(7)	126.6
C(6)-C(7)-H(7)	126.6
V(1)-C(7)-H(7)	126.6
C(7)-C(8)-C(9)	108.5(3)
C(7)-C(8)-V(1)	72.23(19)
C(9)-C(8)-V(1)	71.8(2)
C(7)-C(8)-H(8)	125.7
C(9)-C(8)-H(8)	125.7
V(1)-C(8)-H(8)	125.7
C(10)-C(9)-C(8)	107.9(3)
C(10)-C(9)-V(1)	72.2(2)
C(8)-C(9)-V(1)	71.7(2)
C(10)-C(9)-H(9)	125.9

C(8)-C(9)-H(9)	125.9
V(1)-C(9)-H(9)	125.9
C(9)-C(10)-C(6)	108.0(3)
C(9)-C(10)-V(1)	71.9(2)
C(6)-C(10)-V(1)	71.50(19)
C(9)-C(10)-H(10)	125.9
C(6)-C(10)-H(10)	125.9
V(1)-C(10)-H(10)	125.9
C(16)-C(11)-C(12)	112.9(3)
C(16)-C(11)-B(1)	121.1(3)
C(12)-C(11)-B(1)	125.8(3)
F(12)-C(12)-C(13)	114.8(3)
F(12)-C(12)-C(11)	121.0(3)
C(13)-C(12)-C(11)	124.2(4)
F(13)-C(13)-C(14)	120.3(4)
F(13)-C(13)-C(12)	120.3(4)
C(14)-C(13)-C(12)	119.4(4)
F(14)-C(14)-C(15)	121.9(4)
F(14)-C(14)-C(13)	119.5(4)
C(15)-C(14)-C(13)	118.5(4)
F(15)-C(15)-C(14)	119.8(4)
F(15)-C(15)-C(16)	120.1(4)
C(14)-C(15)-C(16)	120.1(4)
F(16)-C(16)-C(15)	116.0(4)
F(16)-C(16)-C(11)	119.1(3)
C(15)-C(16)-C(11)	124.8(4)
C(18)-C(17)-C(22)	112.9(3)
C(18)-C(17)-B(1)	126.2(3)
C(22)-C(17)-B(1)	120.4(3)
F(18)-C(18)-C(19)	115.4(3)
F(18)-C(18)-C(17)	120.4(3)
C(19)-C(18)-C(17)	124.2(3)
F(19)-C(19)-C(18)	120.7(3)
F(19)-C(19)-C(20)	119.4(3)
C(18)-C(19)-C(20)	119.9(3)
F(20)-C(20)-C(21)	120.8(3)
F(20)-C(20)-C(19)	120.3(3)
C(21)-C(20)-C(19)	118.9(3)
F(21)-C(21)-C(20)	119.9(3)
F(21)-C(21)-C(22)	120.6(3)
C(20)-C(21)-C(22)	119.5(3)
F(22)-C(22)-C(21)	116.7(3)
F(22)-C(22)-C(17)	118.7(3)
C(21)-C(22)-C(17)	124.5(3)
C(28)-C(23)-C(24)	112.1(3)
C(28)-C(23)-B(1)	127.1(3)
C(24)-C(23)-B(1)	120.8(3)
F(24)-C(24)-C(25)	115.3(3)
F(24)-C(24)-C(23)	118.7(3)
C(25)-C(24)-C(23)	125.9(3)
F(25)-C(25)-C(24)	121.7(3)
F(25)-C(25)-C(26)	119.7(4)
C(24)-C(25)-C(26)	118.6(4)
F(26)-C(26)-C(25)	121.3(4)
F(26)-C(26)-C(27)	119.3(4)
C(25)-C(26)-C(27)	119.4(4)
F(27)-C(27)-C(26)	120.2(4)
F(27)-C(27)-C(28)	120.9(4)
C(26)-C(27)-C(28)	118.9(4)
F(28)-C(28)-C(27)	114.5(3)
F(28)-C(28)-C(23)	120.4(3)
C(27)-C(28)-C(23)	125.1(3)

C(4)-V(1)-C(1)	60.28(14)
C(4)-V(1)-C(2)	60.32(13)
C(1)-V(1)-C(2)	36.45(12)
C(4)-V(1)-C(6)	143.75(14)
C(1)-V(1)-C(6)	146.49(14)
C(2)-V(1)-C(6)	154.87(12)
C(4)-V(1)-C(5)	36.18(13)
C(1)-V(1)-C(5)	35.98(12)
C(2)-V(1)-C(5)	60.32(13)
C(6)-V(1)-C(5)	140.71(14)
C(4)-V(1)-C(8)	85.09(14)
C(1)-V(1)-C(8)	141.97(13)
C(2)-V(1)-C(8)	137.45(14)
C(6)-V(1)-C(8)	60.17(13)
C(5)-V(1)-C(8)	106.33(14)
C(4)-V(1)-C(9)	86.20(14)
C(1)-V(1)-C(9)	119.26(14)
C(2)-V(1)-C(9)	144.96(13)
C(6)-V(1)-C(9)	60.10(12)
C(5)-V(1)-C(9)	86.90(14)
C(8)-V(1)-C(9)	36.52(12)
C(4)-V(1)-C(3)	36.57(13)
C(1)-V(1)-C(3)	60.51(14)
C(2)-V(1)-C(3)	35.96(12)
C(6)-V(1)-C(3)	152.50(14)
C(5)-V(1)-C(3)	60.60(14)
C(8)-V(1)-C(3)	101.50(14)
C(9)-V(1)-C(3)	118.60(14)
C(4)-V(1)-C(10)	118.89(14)
C(1)-V(1)-C(10)	121.32(14)
C(2)-V(1)-C(10)	157.21(14)
C(6)-V(1)-C(10)	36.09(12)
C(5)-V(1)-C(10)	104.62(14)
C(8)-V(1)-C(10)	60.28(14)
C(9)-V(1)-C(10)	35.87(12)
C(3)-V(1)-C(10)	154.13(14)
C(4)-V(1)-C(7)	116.96(14)
C(1)-V(1)-C(7)	176.98(14)
C(2)-V(1)-C(7)	141.74(14)
C(6)-V(1)-C(7)	36.48(12)
C(5)-V(1)-C(7)	142.51(13)
C(8)-V(1)-C(7)	36.22(11)
C(9)-V(1)-C(7)	60.81(13)
C(3)-V(1)-C(7)	116.61(14)
C(10)-V(1)-C(7)	60.74(14)
C(4)-V(1)-H(100)	136.3(7)
C(1)-V(1)-H(100)	84.3(7)
C(2)-V(1)-H(100)	76.0(7)
C(6)-V(1)-H(100)	79.7(7)
C(5)-V(1)-H(100)	119.6(7)
C(8)-V(1)-H(100)	133.7(7)
C(9)-V(1)-H(100)	136.0(7)
C(3)-V(1)-H(100)	105.2(7)
C(10)-V(1)-H(100)	100.6(7)
C(7)-V(1)-H(100)	97.6(7)
C(23)-B(1)-C(17)	118.0(3)
C(23)-B(1)-C(11)	114.7(3)
C(17)-B(1)-C(11)	104.8(3)
C(23)-B(1)-H(100)	107.3(10)
C(17)-B(1)-H(100)	104.0(10)
C(11)-B(1)-H(100)	107.0(10)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **1**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	50(2)	47(2)	36(2)	-6(2)	16(2)	7(2)
C(2)	33(2)	64(3)	33(2)	2(2)	12(2)	10(2)
C(3)	34(2)	59(3)	55(3)	4(2)	23(2)	-4(2)
C(4)	53(3)	88(4)	35(2)	23(2)	22(2)	16(2)
C(5)	60(3)	71(3)	27(2)	-5(2)	11(2)	3(2)
C(6)	36(2)	56(3)	36(2)	9(2)	7(2)	13(2)
C(7)	48(2)	44(3)	35(2)	2(2)	3(2)	12(2)
C(8)	45(2)	49(3)	36(2)	14(2)	1(2)	6(2)
C(9)	45(2)	64(3)	29(2)	7(2)	-3(2)	1(2)
C(10)	31(2)	57(3)	45(2)	4(2)	-3(2)	-8(2)
C(11)	31(2)	44(2)	24(2)	10(2)	7(2)	2(2)
C(12)	34(2)	52(3)	31(2)	10(2)	10(2)	0(2)
C(13)	29(2)	82(3)	37(2)	26(2)	4(2)	-1(2)
C(14)	36(2)	69(3)	63(3)	34(2)	9(2)	15(2)
C(15)	52(3)	45(3)	64(3)	14(2)	23(2)	10(2)
C(16)	35(2)	48(3)	37(2)	11(2)	8(2)	3(2)
C(17)	28(2)	34(2)	24(2)	2(1)	6(2)	6(2)
C(18)	43(2)	41(2)	18(2)	2(2)	7(2)	0(2)
C(19)	39(2)	41(2)	31(2)	-2(2)	2(2)	-8(2)
C(20)	35(2)	43(2)	33(2)	6(2)	5(2)	-8(2)
C(21)	33(2)	47(2)	19(2)	3(2)	6(2)	-3(2)
C(22)	32(2)	39(2)	23(2)	-3(2)	2(2)	0(2)
C(23)	29(2)	45(2)	20(2)	1(2)	-1(1)	0(2)
C(24)	36(2)	46(2)	21(2)	0(2)	1(2)	-3(2)
C(25)	46(2)	51(3)	23(2)	3(2)	-5(2)	-10(2)
C(26)	72(3)	38(3)	33(2)	2(2)	-5(2)	4(2)
C(27)	59(3)	46(3)	31(2)	1(2)	6(2)	18(2)
C(28)	35(2)	44(2)	27(2)	5(2)	5(2)	1(2)
F(12)	42(1)	78(2)	28(1)	1(1)	-2(1)	3(1)
F(13)	40(1)	112(2)	52(1)	32(1)	-8(1)	-3(1)
F(14)	53(2)	93(2)	115(2)	49(2)	4(2)	25(2)
F(15)	92(2)	56(2)	106(2)	8(1)	18(2)	30(2)
F(16)	64(2)	43(1)	49(1)	-2(1)	9(1)	5(1)
F(18)	62(1)	56(1)	20(1)	-2(1)	6(1)	-9(1)
F(19)	64(1)	60(2)	39(1)	-5(1)	3(1)	-24(1)
F(20)	55(1)	62(2)	46(1)	3(1)	12(1)	-23(1)
F(21)	51(1)	61(1)	24(1)	5(1)	13(1)	-8(1)
F(22)	42(1)	58(1)	21(1)	-3(1)	4(1)	-10(1)
F(24)	38(1)	61(2)	39(1)	-1(1)	9(1)	-9(1)
F(25)	65(2)	69(2)	44(1)	2(1)	-2(1)	-30(1)
F(26)	103(2)	45(2)	55(1)	-5(1)	-2(1)	-5(1)
F(27)	78(2)	59(2)	60(2)	-5(1)	20(1)	26(1)
F(28)	45(1)	56(1)	51(1)	1(1)	19(1)	5(1)
V(1)	32(1)	43(1)	23(1)	2(1)	6(1)	0(1)
B(1)	28(2)	49(3)	16(2)	3(2)	4(2)	0(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1**.

	x	y	z	U(eq)
H(1)	6472	2117	3395	52
H(2)	5663	1076	2681	51
H(3)	5664	-297	3348	58
H(4)	6496	-102	4472	69
H(5)	6980	1388	4500	63
H(6)	8285	214	2358	51
H(7)	7587	-1122	2600	51
H(8)	7468	-1150	3904	53
H(9)	8098	151	4453	56
H(10)	8603	983	3497	54
H(100)	6978(11)	937(14)	2332(11)	8(6)

Data for 2

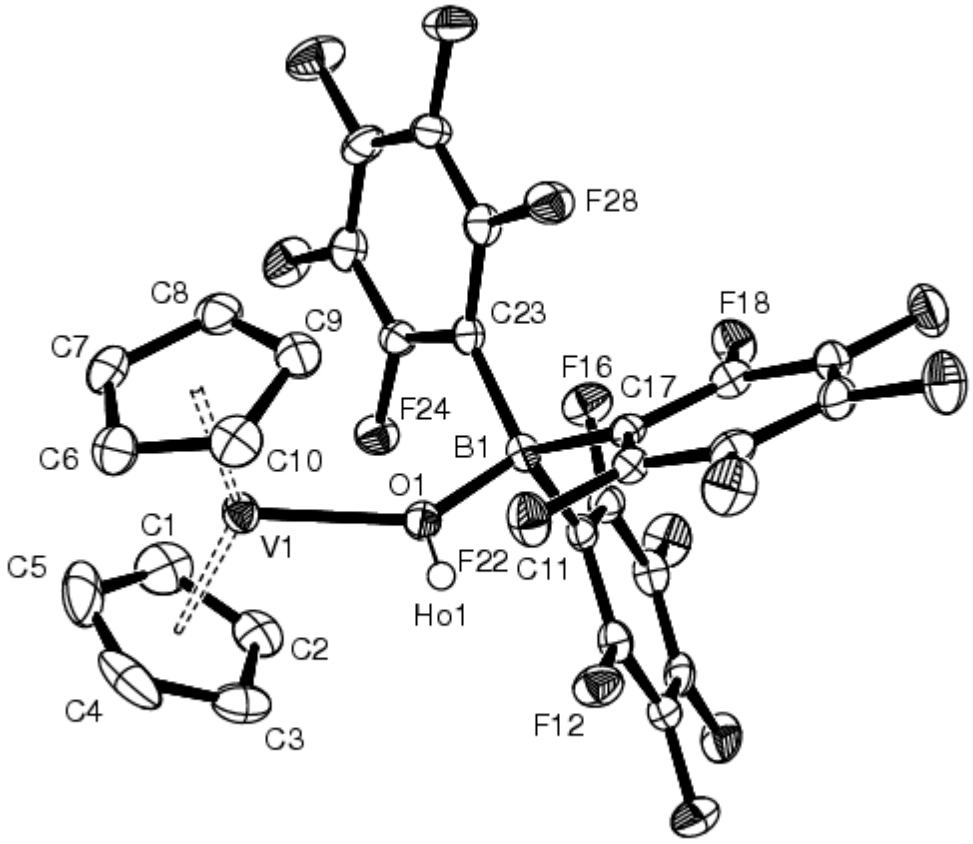
F28
C8
C9
C23
F18
C7
F16
C17
F24
C6
C10
B1
O1
C1
V1
F22
C11
C5
Ho1
C2
C4
C3
F12

Table 6. Crystal data and structure refinement for **2**.

Identification code	rc195d
Empirical formula	C28 H11 B F15 O V
Formula weight	710.12
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/n 1
Unit cell dimensions	a = 11.9753(9) A alpha = 90 deg. b = 17.2725(13) A beta = 103.225(6) deg. c = 12.4722(9) A gamma = 90 deg.
Volume	2511.4(3) A^3
Z, Calculated density	4, 1.878 Mg/m^3
Absorption coefficient	0.532 mm^-1
F(000)	1400
Crystal size	0.3 x 0.2 x 0.12 mm
Theta range for data collection	3.17 to 26.31 deg.
Limiting indices	-14<=h<=14, -21<=k<=21, -15<=l<=10
Reflections collected / unique	18345 / 5126 [R(int) = 0.0342]
Completeness to theta = 26.31	99.8 %
Absorption correction	Empirical (DIFABS)
Max. and min. transmission	0.933 and 0.857
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5126 / 0 / 419
Goodness-of-fit on F^2	0.907
Final R indices [I>2sigma(I)]	R1 = 0.0318, wR2 = 0.0582
R indices (all data)	R1 = 0.0575, wR2 = 0.0637
Largest diff. peak and hole	0.254 and -0.231 e.A^-3

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	-1648(2)	-3089(1)	-4065(2)	41(1)
C(2)	-2364(2)	-3199(1)	-3358(2)	30(1)
C(3)	-3405(2)	-3508(1)	-3954(2)	34(1)
C(4)	-3318(3)	-3598(1)	-5037(2)	48(1)
C(5)	-2234(3)	-3337(2)	-5111(2)	53(1)
C(6)	-3862(2)	-2104(1)	-6471(2)	28(1)
C(7)	-2751(2)	-1777(1)	-6145(2)	29(1)
C(8)	-2798(2)	-1173(1)	-5410(2)	28(1)
C(9)	-3931(2)	-1122(1)	-5291(2)	26(1)
C(10)	-4588(2)	-1696(1)	-5938(2)	28(1)
C(11)	-3141(2)	-1657(1)	-1179(2)	18(1)
C(12)	-3894(2)	-2198(1)	-922(2)	20(1)
C(13)	-3755(2)	-2580(1)	68(2)	23(1)
C(14)	-2795(2)	-2430(1)	874(2)	23(1)
C(15)	-2022(2)	-1895(1)	683(2)	24(1)
C(16)	-2211(2)	-1514(1)	-311(2)	22(1)
C(17)	-4630(2)	-736(1)	-2422(2)	17(1)
C(18)	-4603(2)	-166(1)	-1630(2)	20(1)
C(19)	-5536(2)	257(1)	-1515(2)	22(1)
C(20)	-6585(2)	121(1)	-2215(2)	23(1)
C(21)	-6663(2)	-420(1)	-3031(2)	21(1)
C(22)	-5702(2)	-833(1)	-3110(2)	19(1)
C(23)	-2431(2)	-731(1)	-2711(2)	18(1)
C(24)	-1339(2)	-1030(1)	-2599(2)	19(1)
C(25)	-439(2)	-646(1)	-2876(2)	24(1)
C(26)	-601(2)	83(1)	-3310(2)	26(1)
C(27)	-1668(2)	414(1)	-3448(2)	23(1)
C(28)	-2542(2)	10(1)	-3154(2)	21(1)
F(12)	-4861(1)	-2382(1)	-1696(1)	29(1)
F(13)	-4541(1)	-3091(1)	240(1)	34(1)
F(14)	-2610(1)	-2804(1)	1845(1)	34(1)
F(15)	-1081(1)	-1740(1)	1482(1)	37(1)
F(16)	-1426(1)	-966(1)	-391(1)	31(1)
F(18)	-3591(1)	-4(1)	-927(1)	27(1)
F(19)	-5443(1)	803(1)	-728(1)	32(1)
F(20)	-7509(1)	523(1)	-2104(1)	35(1)
F(21)	-7668(1)	-537(1)	-3756(1)	31(1)
F(22)	-5870(1)	-1363(1)	-3942(1)	27(1)
F(24)	-1101(1)	-1754(1)	-2182(1)	27(1)
F(25)	599(1)	-985(1)	-2717(1)	34(1)
F(26)	250(1)	471(1)	-3600(1)	41(1)
F(27)	-1855(1)	1131(1)	-3867(1)	34(1)
F(28)	-3565(1)	380(1)	-3371(1)	29(1)
V(1)	-3213(1)	-2313(1)	-4651(1)	20(1)
O(1)	-3709(1)	-1884(1)	-3266(1)	21(1)
B(1)	-3466(2)	-1242(1)	-2412(2)	18(1)

Table 8. Bond lengths [A] and angles [deg] for **2**.

C(1)-C(2)	1.376(3)
C(1)-C(5)	1.400(3)
C(1)-V(1)	2.284(2)
C(1)-H(1)	0.9800
C(2)-C(3)	1.403(3)
C(2)-V(1)	2.288(2)
C(2)-H(2)	0.9800
C(3)-C(4)	1.388(3)
C(3)-V(1)	2.273(2)
C(3)-H(3)	0.9800
C(4)-C(5)	1.396(4)
C(4)-V(1)	2.269(2)
C(4)-H(4)	0.9800
C(5)-V(1)	2.267(2)
C(5)-H(5)	0.9800
C(6)-C(10)	1.399(3)
C(6)-C(7)	1.417(3)
C(6)-V(1)	2.254(2)
C(6)-H(6)	0.9800
C(7)-C(8)	1.398(3)
C(7)-V(1)	2.260(2)
C(7)-H(7)	0.9800
C(8)-C(9)	1.401(3)
C(8)-V(1)	2.288(2)
C(8)-H(8)	0.9800
C(9)-C(10)	1.401(3)
C(9)-V(1)	2.302(2)
C(9)-H(9)	0.9800
C(10)-V(1)	2.284(2)
C(10)-H(10)	0.9800
C(11)-C(16)	1.386(3)
C(11)-C(12)	1.386(3)
C(11)-B(1)	1.660(3)
C(12)-F(12)	1.365(2)
C(12)-C(13)	1.376(3)
C(13)-F(13)	1.343(2)
C(13)-C(14)	1.367(3)
C(14)-F(14)	1.346(2)
C(14)-C(15)	1.368(3)
C(15)-F(15)	1.349(2)
C(15)-C(16)	1.375(3)
C(16)-F(16)	1.354(2)
C(17)-C(22)	1.381(3)
C(17)-C(18)	1.390(3)
C(17)-B(1)	1.643(3)
C(18)-F(18)	1.352(2)
C(18)-C(19)	1.370(3)
C(19)-F(19)	1.346(2)
C(19)-C(20)	1.376(3)
C(20)-F(20)	1.340(2)
C(20)-C(21)	1.369(3)
C(21)-F(21)	1.345(2)
C(21)-C(22)	1.377(3)
C(22)-F(22)	1.363(2)
C(23)-C(24)	1.384(3)
C(23)-C(28)	1.389(3)
C(23)-B(1)	1.633(3)
C(24)-F(24)	1.360(2)

C(24)-C(25)	1.375(3)
C(25)-F(25)	1.347(2)
C(25)-C(26)	1.368(3)
C(26)-F(26)	1.337(2)
C(26)-C(27)	1.374(3)
C(27)-F(27)	1.343(2)
C(27)-C(28)	1.375(3)
C(28)-F(28)	1.353(2)
V(1)-O(1)	2.0875(14)
O(1)-B(1)	1.518(3)
O(1)-HO1	0.75(2)

C(2)-C(1)-C(5)	107.6(2)
C(2)-C(1)-V(1)	72.63(12)
C(5)-C(1)-V(1)	71.42(13)
C(2)-C(1)-H(1)	126.1
C(5)-C(1)-H(1)	126.1
V(1)-C(1)-H(1)	126.1
C(1)-C(2)-C(3)	108.8(2)
C(1)-C(2)-V(1)	72.34(13)
C(3)-C(2)-V(1)	71.52(12)
C(1)-C(2)-H(2)	125.5
C(3)-C(2)-H(2)	125.5
V(1)-C(2)-H(2)	125.5
C(4)-C(3)-C(2)	107.6(2)
C(4)-C(3)-V(1)	72.03(14)
C(2)-C(3)-V(1)	72.66(12)
C(4)-C(3)-H(3)	126.0
C(2)-C(3)-H(3)	126.0
V(1)-C(3)-H(3)	126.0
C(3)-C(4)-C(5)	107.8(2)
C(3)-C(4)-V(1)	72.39(13)
C(5)-C(4)-V(1)	72.01(14)
C(3)-C(4)-H(4)	125.9
C(5)-C(4)-H(4)	125.9
V(1)-C(4)-H(4)	125.9
C(4)-C(5)-C(1)	108.2(2)
C(4)-C(5)-V(1)	72.14(14)
C(1)-C(5)-V(1)	72.75(13)
C(4)-C(5)-H(5)	125.8
C(1)-C(5)-H(5)	125.8
V(1)-C(5)-H(5)	125.8
C(10)-C(6)-C(7)	107.9(2)
C(10)-C(6)-V(1)	73.20(12)
C(7)-C(6)-V(1)	71.91(11)
C(10)-C(6)-H(6)	125.9
C(7)-C(6)-H(6)	125.9
V(1)-C(6)-H(6)	125.9
C(8)-C(7)-C(6)	108.02(19)
C(8)-C(7)-V(1)	73.20(12)
C(6)-C(7)-V(1)	71.51(12)
C(8)-C(7)-H(7)	125.8
C(6)-C(7)-H(7)	125.8
V(1)-C(7)-H(7)	125.8
C(7)-C(8)-C(9)	107.60(19)
C(7)-C(8)-V(1)	71.00(12)
C(9)-C(8)-V(1)	72.77(12)
C(7)-C(8)-H(8)	126.1
C(9)-C(8)-H(8)	126.1
V(1)-C(8)-H(8)	126.1
C(10)-C(9)-C(8)	108.84(19)
C(10)-C(9)-V(1)	71.50(12)

C(8)-C(9)-V(1)	71.67(12)
C(10)-C(9)-H(9)	125.5
C(8)-C(9)-H(9)	125.5
V(1)-C(9)-H(9)	125.5
C(6)-C(10)-C(9)	107.6(2)
C(6)-C(10)-V(1)	70.90(12)
C(9)-C(10)-V(1)	72.91(11)
C(6)-C(10)-H(10)	126.1
C(9)-C(10)-H(10)	126.1
V(1)-C(10)-H(10)	126.1
C(16)-C(11)-C(12)	112.78(17)
C(16)-C(11)-B(1)	128.58(18)
C(12)-C(11)-B(1)	118.57(17)
F(12)-C(12)-C(13)	115.60(17)
F(12)-C(12)-C(11)	118.98(17)
C(13)-C(12)-C(11)	125.42(18)
F(13)-C(13)-C(14)	120.60(18)
F(13)-C(13)-C(12)	120.87(18)
C(14)-C(13)-C(12)	118.53(19)
F(14)-C(14)-C(13)	120.57(19)
F(14)-C(14)-C(15)	120.20(18)
C(13)-C(14)-C(15)	119.23(18)
F(15)-C(15)-C(14)	119.28(18)
F(15)-C(15)-C(16)	120.61(19)
C(14)-C(15)-C(16)	120.11(19)
F(16)-C(16)-C(15)	115.26(17)
F(16)-C(16)-C(11)	120.88(17)
C(15)-C(16)-C(11)	123.85(19)
C(22)-C(17)-C(18)	113.24(17)
C(22)-C(17)-B(1)	127.32(17)
C(18)-C(17)-B(1)	119.33(16)
F(18)-C(18)-C(19)	116.99(17)
F(18)-C(18)-C(17)	118.55(17)
C(19)-C(18)-C(17)	124.45(18)
F(19)-C(19)-C(18)	121.07(18)
F(19)-C(19)-C(20)	119.54(18)
C(18)-C(19)-C(20)	119.38(18)
F(20)-C(20)-C(21)	120.83(18)
F(20)-C(20)-C(19)	120.14(18)
C(21)-C(20)-C(19)	119.02(18)
F(21)-C(21)-C(20)	120.03(18)
F(21)-C(21)-C(22)	120.56(18)
C(20)-C(21)-C(22)	119.41(18)
F(22)-C(22)-C(21)	114.96(17)
F(22)-C(22)-C(17)	120.58(17)
C(21)-C(22)-C(17)	124.46(18)
C(24)-C(23)-C(28)	112.71(17)
C(24)-C(23)-B(1)	121.61(18)
C(28)-C(23)-B(1)	125.57(17)
F(24)-C(24)-C(25)	115.56(17)
F(24)-C(24)-C(23)	119.53(17)
C(25)-C(24)-C(23)	124.91(19)
F(25)-C(25)-C(26)	120.15(18)
F(25)-C(25)-C(24)	120.21(19)
C(26)-C(25)-C(24)	119.64(19)
F(26)-C(26)-C(25)	121.37(19)
F(26)-C(26)-C(27)	120.17(19)
C(25)-C(26)-C(27)	118.46(18)
F(27)-C(27)-C(26)	119.99(18)
F(27)-C(27)-C(28)	120.10(18)
C(26)-C(27)-C(28)	119.91(19)
F(28)-C(28)-C(27)	114.65(18)

F(28)-C(28)-C(23)	120.93(17)
C(27)-C(28)-C(23)	124.37(18)
O(1)-V(1)-C(6)	132.73(7)
O(1)-V(1)-C(7)	135.00(7)
C(6)-V(1)-C(7)	36.58(7)
O(1)-V(1)-C(5)	138.39(8)
C(6)-V(1)-C(5)	87.12(9)
C(7)-V(1)-C(5)	82.72(9)
O(1)-V(1)-C(4)	120.66(8)
C(6)-V(1)-C(4)	87.35(9)
C(7)-V(1)-C(4)	103.78(9)
C(5)-V(1)-C(4)	35.85(9)
O(1)-V(1)-C(3)	86.11(7)
C(6)-V(1)-C(3)	119.31(8)
C(7)-V(1)-C(3)	138.88(8)
C(5)-V(1)-C(3)	59.41(9)
C(4)-V(1)-C(3)	35.58(8)
O(1)-V(1)-C(10)	96.90(7)
C(6)-V(1)-C(10)	35.90(7)
C(7)-V(1)-C(10)	60.14(8)
C(5)-V(1)-C(10)	121.18(9)
C(4)-V(1)-C(10)	108.15(9)
C(3)-V(1)-C(10)	124.98(8)
O(1)-V(1)-C(1)	108.14(8)
C(6)-V(1)-C(1)	119.06(9)
C(7)-V(1)-C(1)	99.64(9)
C(5)-V(1)-C(1)	35.83(9)
C(4)-V(1)-C(1)	59.67(9)
C(3)-V(1)-C(1)	59.42(8)
C(10)-V(1)-C(1)	154.95(9)
O(1)-V(1)-C(8)	99.64(7)
C(6)-V(1)-C(8)	60.18(8)
C(7)-V(1)-C(8)	35.80(7)
C(5)-V(1)-C(8)	113.17(9)
C(4)-V(1)-C(8)	139.55(9)
C(3)-V(1)-C(8)	172.25(8)
C(10)-V(1)-C(8)	59.81(8)
C(1)-V(1)-C(8)	113.47(9)
O(1)-V(1)-C(2)	79.55(7)
C(6)-V(1)-C(2)	144.39(8)
C(7)-V(1)-C(2)	134.66(8)
C(5)-V(1)-C(2)	58.91(8)
C(4)-V(1)-C(2)	59.23(8)
C(3)-V(1)-C(2)	35.81(7)
C(10)-V(1)-C(2)	160.22(8)
C(1)-V(1)-C(2)	35.03(8)
C(8)-V(1)-C(2)	139.88(8)
O(1)-V(1)-C(9)	79.35(7)
C(6)-V(1)-C(9)	59.46(8)
C(7)-V(1)-C(9)	59.36(8)
C(5)-V(1)-C(9)	141.63(9)
C(4)-V(1)-C(9)	143.42(8)
C(3)-V(1)-C(9)	151.94(8)
C(10)-V(1)-C(9)	35.58(7)
C(1)-V(1)-C(9)	148.24(9)
C(8)-V(1)-C(9)	35.55(7)
C(2)-V(1)-C(9)	156.05(8)
B(1)-O(1)-V(1)	142.57(13)
B(1)-O(1)-HO1	112.4(18)
V(1)-O(1)-HO1	104.7(18)
O(1)-B(1)-C(23)	105.57(15)
O(1)-B(1)-C(17)	110.89(16)

C(23)-B(1)-C(17)	113.36(16)
O(1)-B(1)-C(11)	107.55(16)
C(23)-B(1)-C(11)	114.57(16)
C(17)-B(1)-C(11)	104.85(15)

Table 9. Anisotropic displacement parameters (A^2 x 10^3) for **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	30(1)	34(2)	60(2)	14(1)	14(1)	18(1)
C(2)	36(1)	22(1)	29(1)	7(1)	-1(1)	11(1)
C(3)	35(1)	21(1)	45(2)	9(1)	6(1)	1(1)
C(4)	73(2)	19(1)	41(2)	-8(1)	-10(2)	10(1)
C(5)	90(2)	34(2)	46(2)	8(1)	37(2)	35(2)
C(6)	36(1)	32(1)	14(1)	0(1)	2(1)	-2(1)
C(7)	36(1)	34(1)	19(1)	4(1)	11(1)	-1(1)
C(8)	37(1)	25(1)	20(1)	3(1)	6(1)	-5(1)
C(9)	38(1)	22(1)	18(1)	6(1)	4(1)	8(1)
C(10)	26(1)	31(1)	24(1)	5(1)	0(1)	4(1)
C(11)	18(1)	17(1)	19(1)	-1(1)	7(1)	4(1)
C(12)	18(1)	23(1)	17(1)	-3(1)	1(1)	2(1)
C(13)	29(1)	17(1)	27(1)	0(1)	14(1)	2(1)
C(14)	33(1)	25(1)	14(1)	4(1)	9(1)	11(1)
C(15)	22(1)	29(1)	19(1)	-3(1)	0(1)	7(1)
C(16)	20(1)	23(1)	23(1)	1(1)	7(1)	1(1)
C(17)	18(1)	17(1)	16(1)	3(1)	5(1)	-1(1)
C(18)	16(1)	23(1)	18(1)	3(1)	2(1)	-2(1)
C(19)	29(1)	20(1)	20(1)	-2(1)	9(1)	-1(1)
C(20)	19(1)	22(1)	31(1)	4(1)	13(1)	6(1)
C(21)	15(1)	25(1)	23(1)	4(1)	4(1)	-2(1)
C(22)	23(1)	18(1)	17(1)	0(1)	8(1)	-1(1)
C(23)	19(1)	20(1)	15(1)	-2(1)	4(1)	1(1)
C(24)	22(1)	19(1)	16(1)	1(1)	3(1)	0(1)
C(25)	17(1)	31(1)	25(1)	-1(1)	5(1)	3(1)
C(26)	22(1)	31(1)	27(1)	1(1)	9(1)	-9(1)
C(27)	31(1)	16(1)	22(1)	0(1)	7(1)	-3(1)
C(28)	18(1)	23(1)	21(1)	0(1)	3(1)	4(1)
F(12)	28(1)	32(1)	25(1)	0(1)	4(1)	-9(1)
F(13)	42(1)	32(1)	34(1)	5(1)	18(1)	-8(1)
F(14)	49(1)	37(1)	19(1)	8(1)	12(1)	11(1)
F(15)	30(1)	52(1)	23(1)	2(1)	-4(1)	3(1)
F(16)	26(1)	37(1)	27(1)	1(1)	1(1)	-10(1)
F(18)	22(1)	28(1)	28(1)	-7(1)	1(1)	-1(1)
F(19)	36(1)	29(1)	34(1)	-11(1)	12(1)	2(1)
F(20)	26(1)	38(1)	44(1)	-2(1)	13(1)	12(1)
F(21)	15(1)	39(1)	35(1)	0(1)	2(1)	2(1)
F(22)	22(1)	32(1)	26(1)	-9(1)	3(1)	0(1)
F(24)	24(1)	23(1)	35(1)	6(1)	7(1)	6(1)
F(25)	18(1)	45(1)	42(1)	7(1)	10(1)	5(1)
F(26)	29(1)	45(1)	53(1)	12(1)	16(1)	-9(1)
F(27)	42(1)	21(1)	43(1)	9(1)	15(1)	-1(1)
F(28)	25(1)	23(1)	40(1)	9(1)	10(1)	7(1)
V(1)	23(1)	19(1)	18(1)	0(1)	4(1)	3(1)
O(1)	21(1)	21(1)	21(1)	-2(1)	7(1)	-2(1)
B(1)	20(1)	18(1)	18(1)	-2(1)	5(1)	1(1)

2. Theoretical studies

Computational details

The crystallographic structure of two vanadium complexes was extracted from this work or from the Cambridge Data Base and their electronic structure was investigated at the B3PW91/6-31G* level in the singlet or triplet spin state using Gaussian03[1]. The geometries of Cp_2VH and $Cp_4V_2H_2$ were optimized at the same level of calculation at the singlet, triplet and also in the quintet spin state for the latter.

ELF topological analysis[2] was carried out with TopMoD. [3] Visualization of ELF isosurfaces and basins were done with the freeware SciAn.[4]

Atomic charges were derived from atoms-in-molecules[5] (AIM) analysis using TopMoD[3]

Topological Analysis of ELF [2]

The topological analysis of the ELF gradient field yields a partition of the molecular space into electronic domains: the ELF basins and corresponding attractors (i. e. , the local maxima of ELF). The latter are classified into core, valence bonding and nonbonding basins. A core basin contains a nucleus X (except a proton) and will be referred to as C(X). A valence bonding basin lies between two or more core basins. Valence basins are further distinguished depending on their connectivity to the core basins. Each valence basin is characterized by its synaptic order which is the number of core basins with which it shares a common boundary. The monosynaptic basins therefore correspond to nonbonded pairs (referred to as V(X)) whereas the di - and polysynaptic ones are related to bi or multicentric bonds (referred to as $V(X_1, X_2, X_3, ...)$.

The average populations of the basins may be obtained by integration of the electron density over the basin. They are not expected to have integral values and the bond populations are about twice the topologically defined Lewis bond orders.

This approach has been extensively used for the study of chemical bonding.[6]

Results

Table 1 compares the ELF analysis of several vanadium complexes. Complex **1**, from this work, exhibits a lengthened B-H distance as compared to usual borohydrides suggesting that the hydride interacts both with B and V. To enlarge our investigations, two other reference vanadium complexes were considered : Cp_2VH for the description of a unperturbed V-H bond and $Cp_4V_2H_2$ for the description of a bridged hydride. As these complexes have not yet been isolated their structure was calculated. Finally the free B-H bond of $HB(C_6F_5)_3^-$ anion extracted from the CDBwas also considered.[7]

The monometallic complexes are always more stable in the triplet spin state while $Cp_4V_2H_2$ is more stable in the quintet state. In the triplet and quintet spin state most stable forms of the latter, however, in order to accommodate the proximity of the V centers one Cp ring becomes η2-coordinated instead of the usual η5 form.

According to the ELF analysis of complex **1**, the H atom interacts with both V and B as it is involved in a trisynaptic basin V(V,H,B) (Table 1) . The contribution of V is slightly lower than the one in triplet or quintet $Cp_4V_2H_2$ and the contribution of B is slightly lower than the one in the $HB(C_6F_5)_3^-$ anion suggesting that both bond are weakened as compared to a free V-H or B-H bond.

Table 1 : Comparison of ELF populations, selected distances and relative energies of the various spin state.

		contribution to V(V,H,B)					
	H basin	V (AIM spin density)	H	B	ΔE Kcal/mol	dV-H (Å)	dB-H (Å)
$Cp_2VHB(C_6F_5)_3$ singulet	1.90 V(V,H,B)	0.12	1.50	0.26	+28.13	1.870	1.337
$Cp_2VHB(C_6F_5)_3$ triplet	1.88 V(V,H,B)	0.11 (0.96)	1.50	0.25		1.870	1.337
Cp_2VH singulet	1.67 V(H,V)	0.28	1.36	-	+23.09	1.652	-
Cp_2VH triplet	1.67 V(H,V)	0.28 (0.96)	1.35	-	-	1.649	-
$HB(C_6F_5)_3^-$	2.01 V(H,B)		1.69	0.31	-	-	0.990
$Cp_4V_2H_2$ singulet	1.73,1.74 V(V,H,B)	0.14	1.44	-	+18.28	1.887x4	V-V 3.183
$Cp_4V_2H_2$ Triplet	1.84,1.85 V(V,H,B)	0.20 (1.04,0.0)	1.47	-	η2 : +2.69	1.838x2 1.793x2	V-V 2.915
$Cp_4V_2H_2$ quintet	1.84,1.83 V(V,H,B)	0.20 (1.22,0.79)	1.43	-	η2	1.823, 1.841x2, 1.862	3.120 V-V

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