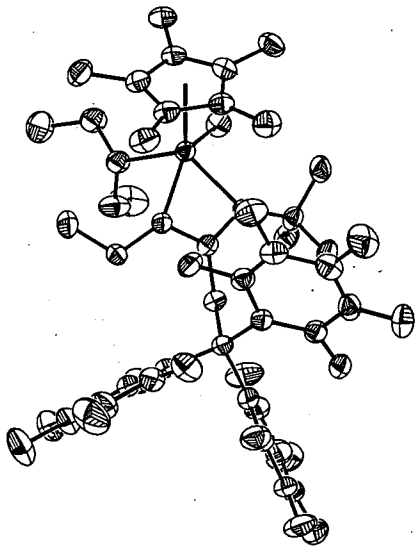
H(18C)	3827	1381	6217	71(14)
H(19A)	7325	4802	6737	45(11)
H(19B)	6431	5240	7250	56(12)
H(20A)	6310	5363	5384	74(16)
H(20B)	6527	6179	6065	100(20)
H(20C)	5299	5709	5834	90(20)
H(19C)	6787	4961	5953	108
H(19D)	5428	5050	5597	108
H(20D)	5201	5767	6808	139
H(20E)	6312	6217	6567	139
H(20F)	6446	5487	7337	139

Crystallographic Analysis of 6.

A colorless block with approximate orthogonal dimensions 0.49 x 0.33 x 0.14mm^3 was placed and optically centered on the Bruker SMART CCD system at –80°C. The initial unit cell was indexed using a least-squares analysis of a random set of reflections collected from three series of 0.3° wide ω-scans, 10 seconds per frame, and 25 frames per series that were well distributed in reciprocal space. Data frames were collected [MoKα] with 0.3° wide ω-scans, 14 seconds per frame and 606 frames per series. Five complete series were collected at varying ϕ angles (ϕ=0°, 72°, 144°, 216°, 288°). Additionally, 200 frames, a repeat of the first series for redundancy and decay purposes, were also collected. The crystal to detector distance was 4.427cm, thus providing a complete sphere of data to $2\theta_{max}$=60.0°. A total of 91343 reflections were collected and corrected for Lorentz and polarization effects and absorption using Blessing's method as incorporated into the program SADABS[1,2] with 13661 unique [R(int)=0.0278]



Structural determination and Refinement:

All crystallographic calculations were performed on a Personal computer (PC) with a Pentium 1.80GHz processor and 512MB of extended memory. The SHELXTL[3] program package was implemented to determine the probable space group and set up the initial files. System symmetry, systematic absences and intensity statistics indicated the unique centric monoclinic space group $P2_1/n$ (no. 14). The structure was determined by direct methods with the successful location of all non-hydrogen atoms using the program XS[4]. The structure was refined with XL[5]. A single difference-Fourier map and least square refinement cycle was required to possibly locate any additional non-hydrogen atoms. Hydrogen atoms were placed in calculated positions but their thermal parameters were allowed to refine during the final convergence stage. A single disordered diethyl ether solvent molecule was modeled and found to be present in a 0.60:0.40 ratio. Hydrogen atoms attached to these carbon atoms were calculated and fixed (xyzU) with thermal parameter(U) dependent upon parent. The final structure was refined to convergence [$\Delta/\sigma \leq 0.003$] with R(F)=5.30%, wR(F^2)=10.55%, GOF=1.103 for all 13661 unique reflections [R(F)=3.58%, wR(F^2)=9.59% for those 10772 data with Fo > 4σ(Fo)]. The final difference-Fourier map was featureless indicating that the structure is both correct and complete.

The function minimized during the full-matrix least-squares refinement was $\Sigma w(Fo^2-Fc^2)$ where $w=1/[\sigma^2(Fo^2)+(0.0536*P)^2+1.4125*P]$ and $P=(\max(Fo^2,0)+2*Fc^2)/3$. An empirical correction for extinction was also attempted but found to be negative and therefore not applied.

Table 21. Crystal data and structure refinement for **6•OEt$_2$**.

Empirical formula	C40 H41 B Cl F15 N2 O Zr	
Formula weight	1062.35	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.7912(4) Å	α= 90°.
	b = 16.2876(5) Å	β= 92.3540(10)°.
	c = 22.7788(6) Å	γ = 90°.
Volume	4741.7(2) Å^3	
Z	4	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	0.385 mm^{-1}	
F(000)	2168	
Crystal size	0.49 x 0.33 x 0.14 mm^3	
Theta range for data collection	2.19 to 30.00°.	
Index ranges	-17<=h<=17, -22<=k<=22, -32<=l<=32	
Reflections collected	91343	
Independent reflections	13661 [R(int) = 0.0278]	
Completeness to theta = 30.00°	98.9 %	
Absorption correction	None	
Max. and min. transmission	0.9462 and 0.8330	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13661 / 17 / 645	
Goodness-of-fit on F^2	1.103	
Final R indices [I>2sigma(I)]	R1 = 0.0358, wR2 = 0.0959 [10772 Data]	
R indices (all data)	R1 = 0.0530, wR2 = 0.1055	
Largest diff. peak and hole	0.599 and -0.373 e.Å^{-3}	

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6•OEt$_2$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zr(1)	10756(1)	2560(1)	7452(1)	28(1)
Cl(1)	11952(1)	1399(1)	7573(1)	45(1)
N(1)	9399(1)	1825(1)	7165(1)	32(1)
N(2)	9695(1)	3041(1)	6762(1)	32(1)
CNT1	10646(1)	3193(1)	8310(1)	0
C(1)	10029(1)	3669(1)	8084(1)	36(1)
C(2)	9780(1)	2908(1)	8350(1)	36(1)
C(3)	10729(1)	2541(1)	8560(1)	36(1)
C(4)	11564(1)	3072(1)	8424(1)	36(1)
C(5)	11129(1)	3775(1)	8133(1)	36(1)
C(6)	9236(2)	4307(1)	7899(1)	46(1)
C(7)	8683(2)	2623(1)	8457(1)	47(1)
C(8)	10850(2)	1784(1)	8934(1)	49(1)
C(9)	12686(1)	2941(1)	8635(1)	46(1)
C(10)	11699(2)	4550(1)	7981(1)	49(1)
C(11)	9160(1)	2327(1)	6702(1)	30(1)
C(12)	8512(1)	2109(1)	6159(1)	33(1)
B(1)	7271(1)	2426(1)	5992(1)	31(1)
C(13)	6605(1)	2404(1)	6600(1)	31(1)
C(14)	5875(1)	1818(1)	6756(1)	33(1)
F(14)	5631(1)	1174(1)	6401(1)	43(1)
C(15)	5357(1)	1825(1)	7278(1)	38(1)
F(15)	4655(1)	1240(1)	7395(1)	52(1)
C(16)	5564(1)	2436(1)	7683(1)	40(1)
F(16)	5060(1)	2457(1)	8189(1)	57(1)
C(17)	6293(1)	3024(1)	7559(1)	37(1)
F(17)	6508(1)	3629(1)	7949(1)	50(1)
C(18)	6786(1)	2992(1)	7033(1)	33(1)
F(18)	7471(1)	3606(1)	6940(1)	41(1)
C(19)	6718(1)	1807(1)	5480(1)	36(1)

C(20)	5667(2)	1916(1)	5319(1)	42(1)
F(20)	5123(1)	2514(1)	5578(1)	52(1)
C(21)	5108(2)	1442(1)	4913(1)	51(1)
F(21)	4084(1)	1583(1)	4799(1)	75(1)
C(22)	5599(2)	818(1)	4633(1)	56(1)
F(22)	5071(1)	337(1)	4245(1)	77(1)
C(23)	6641(2)	686(1)	4755(1)	56(1)
F(23)	7150(2)	94(1)	4476(1)	84(1)
C(24)	7175(2)	1179(1)	5171(1)	46(1)
F(24)	8204(1)	996(1)	5245(1)	69(1)
C(25)	7191(1)	3334(1)	5654(1)	34(1)
C(26)	7776(1)	3480(1)	5162(1)	40(1)
F(26)	8449(1)	2900(1)	4981(1)	50(1)
C(27)	7710(2)	4183(1)	4821(1)	52(1)
F(27)	8311(1)	4258(1)	4350(1)	74(1)
C(28)	7015(2)	4782(1)	4952(1)	58(1)
F(28)	6926(2)	5465(1)	4619(1)	89(1)
C(29)	6395(2)	4677(1)	5421(1)	53(1)
F(29)	5695(1)	5254(1)	5554(1)	77(1)
C(30)	6490(2)	3966(1)	5754(1)	41(1)
F(30)	5810(1)	3922(1)	6194(1)	51(1)
C(31)	9129(1)	930(1)	7202(1)	38(1)
C(32)	9442(2)	646(1)	7827(1)	48(1)
C(33)	9740(2)	429(1)	6761(1)	50(1)
C(34)	7946(1)	770(1)	7132(1)	48(1)
C(35)	9592(1)	3673(1)	6309(1)	39(1)
C(36)	10262(2)	4417(1)	6434(1)	59(1)
O(37)	12006(1)	2997(1)	6864(1)	41(1)
C(37)	13057(1)	3207(2)	7091(1)	53(1)
C(38)	13529(2)	3908(2)	6770(1)	82(1)
C(39)	11977(2)	2697(2)	6251(1)	58(1)
C(40)	12729(3)	2016(2)	6140(1)	89(1)
O(51)	992(3)	2469(2)	4944(2)	82(1)
C(51)	653(7)	1835(5)	4614(4)	112(2)
C(52)	710(7)	1110(5)	4940(4)	132(3)
C(53)	1534(16)	3030(12)	4467(9)	271(10)

C(54)	1059(8)	3688(6)	4638(4)	145(3)
O(61)	1272(14)	2496(10)	4506(8)	213(6)
C(61)	1050(30)	1792(17)	4815(15)	296(18)
C(62)	1171(10)	1106(8)	4550(6)	129(4)
C(63)	864(9)	3230(7)	4564(5)	103(3)
C(64)	1691(7)	3675(6)	4192(4)	91(2)

Table 23. Bond lengths [Å] and angles [°] for **6•OEt$_2$**.

Zr(1)-N(2)	2.1802(13)	C(9)-H(9B)	0.9600
Zr(1)-N(1)	2.1862(13)	C(9)-H(9C)	0.9600
Zr(1)-CNT1	2.2193(9)	C(10)-H(10A)	0.9600
Zr(1)-O(37)	2.2437(12)	C(10)-H(10B)	0.9600
Zr(1)-Cl(1)	2.4412(4)	C(10)-H(10C)	0.9600
Zr(1)-C(2)	2.5046(17)	C(11)-C(12)	1.504(2)
Zr(1)-C(1)	2.5116(16)	C(12)-B(1)	1.697(2)
Zr(1)-C(3)	2.5250(17)	C(12)-H(12A)	0.9700
Zr(1)-C(4)	2.5450(16)	C(12)-H(12B)	0.9700
Zr(1)-C(5)	2.5473(16)	B(1)-C(13)	1.657(2)
N(1)-C(11)	1.359(2)	B(1)-C(25)	1.668(2)
N(1)-C(31)	1.502(2)	B(1)-C(19)	1.676(2)
N(2)-C(11)	1.353(2)	C(13)-C(18)	1.388(2)
N(2)-C(35)	1.460(2)	C(13)-C(14)	1.390(2)
C(1)-C(5)	1.418(2)	C(14)-F(14)	1.3523(19)
C(1)-C(2)	1.421(2)	C(14)-C(15)	1.384(2)
C(1)-C(6)	1.501(2)	C(15)-F(15)	1.343(2)
C(2)-C(3)	1.418(2)	C(15)-C(16)	1.376(3)
C(2)-C(7)	1.507(3)	C(16)-F(16)	1.343(2)
C(3)-C(4)	1.418(2)	C(16)-C(17)	1.375(3)
C(3)-C(8)	1.502(2)	C(17)-F(17)	1.3461(19)
C(4)-C(5)	1.426(2)	C(17)-C(18)	1.377(2)
C(4)-C(9)	1.509(2)	C(18)-F(18)	1.3520(18)
C(5)-C(10)	1.505(3)	C(19)-C(24)	1.385(3)
C(6)-H(6A)	0.9600	C(19)-C(20)	1.389(2)
C(6)-H(6B)	0.9600	C(20)-F(20)	1.347(2)
C(6)-H(6C)	0.9600	C(20)-C(21)	1.383(3)
C(7)-H(7A)	0.9600	C(21)-F(21)	1.344(2)
C(7)-H(7B)	0.9600	C(21)-C(22)	1.367(3)
C(7)-H(7C)	0.9600	C(22)-F(22)	1.342(2)
C(8)-H(8A)	0.9600	C(22)-C(23)	1.367(3)
C(8)-H(8B)	0.9600	C(23)-F(23)	1.339(3)
C(8)-H(8C)	0.9600	C(23)-C(24)	1.398(3)
C(9)-H(9A)	0.9600	C(24)-F(24)	1.354(2)

C(25)-C(30)	1.391(3)	C(38)-H(39C)	0.9600
C(25)-C(26)	1.394(2)	C(39)-C(40)	1.496(4)
C(26)-F(26)	1.352(2)	C(39)-H(40A)	0.9700
C(26)-C(27)	1.385(3)	C(39)-H(40B)	0.9700
C(27)-F(27)	1.352(2)	C(40)-H(41A)	0.9600
C(27)-C(28)	1.361(3)	C(40)-H(41B)	0.9600
C(28)-F(28)	1.348(2)	C(40)-H(41C)	0.9600
C(28)-C(29)	1.368(3)	O(51)-C(51)	1.339(9)
C(29)-F(29)	1.341(3)	O(51)-C(53)	1.599(19)
C(29)-C(30)	1.387(3)	C(51)-C(52)	1.396(11)
C(30)-F(30)	1.357(2)	C(51)-H(51A)	0.9700
C(31)-C(33)	1.533(3)	C(51)-H(51B)	0.9700
C(31)-C(32)	1.534(3)	C(52)-H(52A)	0.9600
C(31)-C(34)	1.537(2)	C(52)-H(52B)	0.9600
C(32)-H(32A)	0.9600	C(52)-H(52C)	0.9600
C(32)-H(32B)	0.9600	C(53)-C(54)	1.300(19)
C(32)-H(32C)	0.9600	C(53)-H(53A)	0.9700
C(33)-H(33A)	0.9600	C(53)-H(53B)	0.9700
C(33)-H(33B)	0.9600	C(54)-H(54A)	0.9600
C(33)-H(33C)	0.9600	C(54)-H(54B)	0.9600
C(34)-H(34A)	0.9600	C(54)-H(54C)	0.9600
C(34)-H(34B)	0.9600	O(61)-C(63)	1.313(18)
C(34)-H(34C)	0.9600	O(61)-C(61)	1.38(3)
C(35)-C(36)	1.505(3)	C(61)-C(62)	1.28(3)
C(35)-H(35A)	0.9700	C(61)-H(61A)	0.9700
C(35)-H(35B)	0.9700	C(61)-H(61B)	0.9700
C(36)-H(36A)	0.9600	C(62)-H(62A)	0.9600
C(36)-H(36B)	0.9600	C(62)-H(62B)	0.9600
C(36)-H(36C)	0.9600	C(62)-H(62C)	0.9600
O(37)-C(37)	1.462(2)	C(63)-C(64)	1.561(14)
O(37)-C(39)	1.480(2)	C(63)-H(63A)	0.9700
C(37)-C(38)	1.496(3)	C(63)-H(63B)	0.9700
C(37)-H(38A)	0.9700	C(64)-H(64A)	0.9600
C(37)-H(38B)	0.9700	C(64)-H(64B)	0.9600
C(38)-H(39A)	0.9600	C(64)-H(64C)	0.9600
C(38)-H(39B)	0.9600		

N(2)-Zr(1)-N(1)	61.17(5)	N(2)-Zr(1)-C(5)	104.76(5)
N(2)-Zr(1)-CNT1	114.08(4)	N(1)-Zr(1)-C(5)	137.24(5)
N(1)-Zr(1)-CNT1	116.11(4)	CNT1-Zr(1)-C(5)	28.36(4)
N(2)-Zr(1)-O(37)	83.84(5)	O(37)-Zr(1)-C(5)	89.79(5)
N(1)-Zr(1)-O(37)	124.84(5)	Cl(1)-Zr(1)-C(5)	115.62(4)
CNT1-Zr(1)-O(37)	116.78(4)	C(2)-Zr(1)-C(5)	54.13(6)
N(2)-Zr(1)-Cl(1)	136.78(4)	C(1)-Zr(1)-C(5)	32.54(5)
N(1)-Zr(1)-Cl(1)	95.52(4)	C(3)-Zr(1)-C(5)	53.93(6)
CNT1-Zr(1)-Cl(1)	108.81(2)	C(4)-Zr(1)-C(5)	32.52(5)
O(37)-Zr(1)-Cl(1)	81.64(4)	C(11)-N(1)-C(31)	125.69(14)
N(2)-Zr(1)-C(2)	101.03(5)	C(11)-N(1)-Zr(1)	93.05(9)
N(1)-Zr(1)-C(2)	87.29(5)	C(31)-N(1)-Zr(1)	134.11(10)
CNT1-Zr(1)-C(2)	28.82(4)	C(11)-N(2)-C(35)	120.25(13)
O(37)-Zr(1)-C(2)	143.78(5)	C(11)-N(2)-Zr(1)	93.48(9)
Cl(1)-Zr(1)-C(2)	114.48(4)	C(35)-N(2)-Zr(1)	143.04(10)
N(2)-Zr(1)-C(1)	85.44(5)	C(5)-C(1)-C(2)	108.19(14)
N(1)-Zr(1)-C(1)	104.90(5)	C(5)-C(1)-C(6)	126.46(16)
CNT1-Zr(1)-C(1)	28.71(4)	C(2)-C(1)-C(6)	124.30(16)
O(37)-Zr(1)-C(1)	113.80(5)	C(5)-C(1)-Zr(1)	75.12(9)
Cl(1)-Zr(1)-C(1)	137.52(4)	C(2)-C(1)-Zr(1)	73.28(9)
C(2)-Zr(1)-C(1)	32.90(6)	C(6)-C(1)-Zr(1)	126.75(12)
N(2)-Zr(1)-C(3)	133.76(5)	C(3)-C(2)-C(1)	107.94(15)
N(1)-Zr(1)-C(3)	104.46(5)	C(3)-C(2)-C(7)	127.25(17)
CNT1-Zr(1)-C(3)	28.56(4)	C(1)-C(2)-C(7)	124.30(16)
O(37)-Zr(1)-C(3)	129.76(5)	C(3)-C(2)-Zr(1)	74.41(10)
Cl(1)-Zr(1)-C(3)	84.94(4)	C(1)-C(2)-Zr(1)	73.82(9)
C(2)-Zr(1)-C(3)	32.76(5)	C(7)-C(2)-Zr(1)	124.10(12)
C(1)-Zr(1)-C(3)	54.24(5)	C(4)-C(3)-C(2)	108.13(15)
N(2)-Zr(1)-C(4)	136.73(5)	C(4)-C(3)-C(8)	124.26(16)
N(1)-Zr(1)-C(4)	136.80(5)	C(2)-C(3)-C(8)	127.13(17)
CNT1-Zr(1)-C(4)	28.34(4)	C(4)-C(3)-Zr(1)	74.54(9)
O(37)-Zr(1)-C(4)	98.13(5)	C(2)-C(3)-Zr(1)	72.83(9)
Cl(1)-Zr(1)-C(4)	85.71(4)	C(8)-C(3)-Zr(1)	124.82(12)
C(2)-Zr(1)-C(4)	54.09(6)	C(3)-C(4)-C(5)	107.96(14)
C(1)-Zr(1)-C(4)	54.03(5)	C(3)-C(4)-C(9)	124.01(16)
C(3)-Zr(1)-C(4)	32.47(6)	C(5)-C(4)-C(9)	127.53(16)

C(3)-C(4)-Zr(1)	72.99(9)	C(5)-C(10)-H(10C)	109.5
C(5)-C(4)-Zr(1)	73.83(9)	H(10A)-C(10)-H(10C)	109.5
C(9)-C(4)-Zr(1)	125.29(12)	H(10B)-C(10)-H(10C)	109.5
C(1)-C(5)-C(4)	107.77(15)	N(2)-C(11)-N(1)	110.01(13)
C(1)-C(5)-C(10)	125.03(15)	N(2)-C(11)-C(12)	123.10(14)
C(4)-C(5)-C(10)	126.65(15)	N(1)-C(11)-C(12)	126.48(14)
C(1)-C(5)-Zr(1)	72.35(9)	C(11)-C(12)-B(1)	126.27(13)
C(4)-C(5)-Zr(1)	73.65(9)	C(11)-C(12)-H(12A)	105.7
C(10)-C(5)-Zr(1)	126.28(13)	B(1)-C(12)-H(12A)	105.7
C(1)-C(6)-H(6A)	109.5	C(11)-C(12)-H(12B)	105.7
C(1)-C(6)-H(6B)	109.5	B(1)-C(12)-H(12B)	105.7
H(6A)-C(6)-H(6B)	109.5	H(12A)-C(12)-H(12B)	106.2
C(1)-C(6)-H(6C)	109.5	C(13)-B(1)-C(25)	112.44(13)
H(6A)-C(6)-H(6C)	109.5	C(13)-B(1)-C(19)	110.59(13)
H(6B)-C(6)-H(6C)	109.5	C(25)-B(1)-C(19)	101.28(12)
C(2)-C(7)-H(7A)	109.5	C(13)-B(1)-C(12)	108.30(12)
C(2)-C(7)-H(7B)	109.5	C(25)-B(1)-C(12)	114.37(13)
H(7A)-C(7)-H(7B)	109.5	C(19)-B(1)-C(12)	109.70(13)
C(2)-C(7)-H(7C)	109.5	C(18)-C(13)-C(14)	112.79(15)
H(7A)-C(7)-H(7C)	109.5	C(18)-C(13)-B(1)	120.18(14)
H(7B)-C(7)-H(7C)	109.5	C(14)-C(13)-B(1)	126.98(14)
C(3)-C(8)-H(8A)	109.5	F(14)-C(14)-C(15)	114.40(14)
C(3)-C(8)-H(8B)	109.5	F(14)-C(14)-C(13)	121.36(14)
H(8A)-C(8)-H(8B)	109.5	C(15)-C(14)-C(13)	124.22(16)
C(3)-C(8)-H(8C)	109.5	F(15)-C(15)-C(16)	119.40(16)
H(8A)-C(8)-H(8C)	109.5	F(15)-C(15)-C(14)	120.78(16)
H(8B)-C(8)-H(8C)	109.5	C(16)-C(15)-C(14)	119.82(16)
C(4)-C(9)-H(9A)	109.5	F(16)-C(16)-C(17)	120.74(17)
C(4)-C(9)-H(9B)	109.5	F(16)-C(16)-C(15)	120.59(17)
H(9A)-C(9)-H(9B)	109.5	C(17)-C(16)-C(15)	118.66(16)
C(4)-C(9)-H(9C)	109.5	F(17)-C(17)-C(16)	119.78(16)
H(9A)-C(9)-H(9C)	109.5	F(17)-C(17)-C(18)	120.85(16)
H(9B)-C(9)-H(9C)	109.5	C(16)-C(17)-C(18)	119.36(16)
C(5)-C(10)-H(10A)	109.5	F(18)-C(18)-C(17)	115.56(14)
C(5)-C(10)-H(10B)	109.5	F(18)-C(18)-C(13)	119.28(14)
H(10A)-C(10)-H(10B)	109.5	C(17)-C(18)-C(13)	125.12(15)

C(24)-C(19)-C(20)	112.59(16)	N(1)-C(31)-C(33)	110.83(15)
C(24)-C(19)-B(1)	128.52(16)	N(1)-C(31)-C(32)	107.08(14)
C(20)-C(19)-B(1)	118.89(15)	C(33)-C(31)-C(32)	109.04(15)
F(20)-C(20)-C(21)	115.70(18)	N(1)-C(31)-C(34)	112.72(13)
F(20)-C(20)-C(19)	119.26(15)	C(33)-C(31)-C(34)	111.54(16)
C(21)-C(20)-C(19)	125.0(2)	C(32)-C(31)-C(34)	105.32(16)
F(21)-C(21)-C(22)	120.06(18)	C(31)-C(32)-H(32A)	109.5
F(21)-C(21)-C(20)	120.4(2)	C(31)-C(32)-H(32B)	109.5
C(22)-C(21)-C(20)	119.5(2)	H(32A)-C(32)-H(32B)	109.5
F(22)-C(22)-C(23)	120.2(2)	C(31)-C(32)-H(32C)	109.5
F(22)-C(22)-C(21)	120.8(2)	H(32A)-C(32)-H(32C)	109.5
C(23)-C(22)-C(21)	118.97(17)	H(32B)-C(32)-H(32C)	109.5
F(23)-C(23)-C(22)	120.31(18)	C(31)-C(33)-H(33A)	109.5
F(23)-C(23)-C(24)	120.1(2)	C(31)-C(33)-H(33B)	109.5
C(22)-C(23)-C(24)	119.6(2)	H(33A)-C(33)-H(33B)	109.5
F(24)-C(24)-C(19)	121.84(16)	C(31)-C(33)-H(33C)	109.5
F(24)-C(24)-C(23)	113.87(18)	H(33A)-C(33)-H(33C)	109.5
C(19)-C(24)-C(23)	124.3(2)	H(33B)-C(33)-H(33C)	109.5
C(30)-C(25)-C(26)	112.15(16)	C(31)-C(34)-H(34A)	109.5
C(30)-C(25)-B(1)	127.49(15)	C(31)-C(34)-H(34B)	109.5
C(26)-C(25)-B(1)	119.84(15)	H(34A)-C(34)-H(34B)	109.5
F(26)-C(26)-C(27)	115.61(17)	C(31)-C(34)-H(34C)	109.5
F(26)-C(26)-C(25)	119.68(16)	H(34A)-C(34)-H(34C)	109.5
C(27)-C(26)-C(25)	124.69(19)	H(34B)-C(34)-H(34C)	109.5
F(27)-C(27)-C(28)	120.48(19)	N(2)-C(35)-C(36)	113.57(14)
F(27)-C(27)-C(26)	119.8(2)	N(2)-C(35)-H(35A)	108.9
C(28)-C(27)-C(26)	119.73(19)	C(36)-C(35)-H(35A)	108.9
F(28)-C(28)-C(27)	120.6(2)	N(2)-C(35)-H(35B)	108.9
F(28)-C(28)-C(29)	120.3(2)	C(36)-C(35)-H(35B)	108.9
C(27)-C(28)-C(29)	119.13(18)	H(35A)-C(35)-H(35B)	107.7
F(29)-C(29)-C(28)	120.21(19)	C(35)-C(36)-H(36A)	109.5
F(29)-C(29)-C(30)	120.4(2)	C(35)-C(36)-H(36B)	109.5
C(28)-C(29)-C(30)	119.4(2)	H(36A)-C(36)-H(36B)	109.5
F(30)-C(30)-C(29)	113.84(17)	C(35)-C(36)-H(36C)	109.5
F(30)-C(30)-C(25)	121.29(15)	H(36A)-C(36)-H(36C)	109.5
C(29)-C(30)-C(25)	124.86(18)	H(36B)-C(36)-H(36C)	109.5

C(37)-O(37)-C(39)	113.42(15)	H(52A)-C(52)-H(52B)	109.5
C(37)-O(37)-Zr(1)	122.10(11)	C(51)-C(52)-H(52C)	109.5
C(39)-O(37)-Zr(1)	117.92(12)	H(52A)-C(52)-H(52C)	109.5
O(37)-C(37)-C(38)	112.94(19)	H(52B)-C(52)-H(52C)	109.5
O(37)-C(37)-H(38A)	109.0	C(54)-C(53)-O(51)	92.7(13)
C(38)-C(37)-H(38A)	109.0	C(54)-C(53)-H(53A)	113.2
O(37)-C(37)-H(38B)	109.0	O(51)-C(53)-H(53A)	113.2
C(38)-C(37)-H(38B)	109.0	C(54)-C(53)-H(53B)	113.2
H(38A)-C(37)-H(38B)	107.8	O(51)-C(53)-H(53B)	113.2
C(37)-C(38)-H(39A)	109.5	H(53A)-C(53)-H(53B)	110.5
C(37)-C(38)-H(39B)	109.5	C(53)-C(54)-H(54A)	109.5
H(39A)-C(38)-H(39B)	109.5	C(53)-C(54)-H(54B)	109.5
C(37)-C(38)-H(39C)	109.5	H(54A)-C(54)-H(54B)	109.5
H(39A)-C(38)-H(39C)	109.5	C(53)-C(54)-H(54C)	109.5
H(39B)-C(38)-H(39C)	109.5	H(54A)-C(54)-H(54C)	109.5
O(37)-C(39)-C(40)	114.4(2)	H(54B)-C(54)-H(54C)	109.5
O(37)-C(39)-H(40A)	108.6	C(63)-O(61)-C(61)	128(2)
C(40)-C(39)-H(40A)	108.6	C(62)-C(61)-O(61)	117(3)
O(37)-C(39)-H(40B)	108.6	C(62)-C(61)-H(61A)	108.0
C(40)-C(39)-H(40B)	108.6	O(61)-C(61)-H(61A)	108.0
H(40A)-C(39)-H(40B)	107.6	C(62)-C(61)-H(61B)	108.0
C(39)-C(40)-H(41A)	109.5	O(61)-C(61)-H(61B)	108.0
C(39)-C(40)-H(41B)	109.5	H(61A)-C(61)-H(61B)	107.3
H(41A)-C(40)-H(41B)	109.5	C(61)-C(62)-H(62A)	109.5
C(39)-C(40)-H(41C)	109.5	C(61)-C(62)-H(62B)	109.5
H(41A)-C(40)-H(41C)	109.5	H(62A)-C(62)-H(62B)	109.5
H(41B)-C(40)-H(41C)	109.5	C(61)-C(62)-H(62C)	109.5
C(51)-O(51)-C(53)	101.4(9)	H(62A)-C(62)-H(62C)	109.5
O(51)-C(51)-C(52)	110.1(7)	H(62B)-C(62)-H(62C)	109.5
O(51)-C(51)-H(51A)	109.6	O(61)-C(63)-C(64)	95.0(12)
C(52)-C(51)-H(51A)	109.6	O(61)-C(63)-H(63A)	112.7
O(51)-C(51)-H(51B)	109.6	C(64)-C(63)-H(63A)	112.7
C(52)-C(51)-H(51B)	109.6	O(61)-C(63)-H(63B)	112.7
H(51A)-C(51)-H(51B)	108.1	C(64)-C(63)-H(63B)	112.7
C(51)-C(52)-H(52A)	109.5	H(63A)-C(63)-H(63B)	110.2
C(51)-C(52)-H(52B)	109.5	C(63)-C(64)-H(64A)	109.5

C(63)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(63)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5

Table 24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6•OEt$_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	26(1)	28(1)	30(1)	0(1)	-2(1)	0(1)
Cl(1)	38(1)	39(1)	58(1)	0(1)	0(1)	10(1)
N(1)	31(1)	28(1)	37(1)	2(1)	-3(1)	-2(1)
N(2)	29(1)	32(1)	35(1)	5(1)	-4(1)	-3(1)
C(1)	35(1)	34(1)	38(1)	-7(1)	-5(1)	5(1)
C(2)	34(1)	42(1)	34(1)	-5(1)	0(1)	3(1)
C(3)	38(1)	40(1)	29(1)	1(1)	-1(1)	5(1)
C(4)	34(1)	39(1)	33(1)	-4(1)	-6(1)	5(1)
C(5)	36(1)	34(1)	38(1)	-6(1)	-7(1)	2(1)
C(6)	44(1)	38(1)	55(1)	-9(1)	-13(1)	12(1)
C(7)	35(1)	60(1)	47(1)	-4(1)	5(1)	1(1)
C(8)	55(1)	52(1)	40(1)	12(1)	-5(1)	4(1)
C(9)	37(1)	55(1)	44(1)	-1(1)	-11(1)	5(1)
C(10)	49(1)	36(1)	61(1)	-2(1)	-13(1)	-6(1)
C(11)	26(1)	30(1)	34(1)	-1(1)	1(1)	1(1)
C(12)	31(1)	34(1)	34(1)	-3(1)	-2(1)	-1(1)
B(1)	29(1)	34(1)	30(1)	-1(1)	-2(1)	-3(1)
C(13)	28(1)	32(1)	32(1)	2(1)	-3(1)	0(1)
C(14)	32(1)	32(1)	36(1)	2(1)	-1(1)	0(1)
F(14)	50(1)	35(1)	43(1)	-1(1)	1(1)	-11(1)
C(15)	31(1)	39(1)	44(1)	9(1)	3(1)	1(1)
F(15)	47(1)	50(1)	61(1)	8(1)	14(1)	-12(1)
C(16)	34(1)	49(1)	36(1)	2(1)	7(1)	8(1)
F(16)	54(1)	73(1)	46(1)	-2(1)	21(1)	3(1)
C(17)	36(1)	39(1)	36(1)	-5(1)	-2(1)	7(1)
F(17)	54(1)	51(1)	45(1)	-16(1)	4(1)	4(1)
C(18)	30(1)	33(1)	36(1)	-1(1)	-3(1)	0(1)
F(18)	39(1)	41(1)	44(1)	-7(1)	0(1)	-11(1)
C(19)	40(1)	38(1)	30(1)	1(1)	-2(1)	-9(1)
C(20)	42(1)	48(1)	34(1)	5(1)	-6(1)	-12(1)

F(20)	36(1)	67(1)	52(1)	-1(1)	-7(1)	-1(1)
C(21)	48(1)	67(1)	37(1)	10(1)	-12(1)	-24(1)
F(21)	50(1)	115(1)	58(1)	3(1)	-21(1)	-28(1)
C(22)	79(2)	56(1)	32(1)	3(1)	-11(1)	-33(1)
F(22)	110(1)	76(1)	44(1)	-3(1)	-21(1)	-51(1)
C(23)	82(2)	46(1)	38(1)	-9(1)	-7(1)	-12(1)
F(23)	120(1)	68(1)	64(1)	-35(1)	-14(1)	6(1)
C(24)	54(1)	45(1)	39(1)	-7(1)	-5(1)	-5(1)
F(24)	63(1)	77(1)	66(1)	-36(1)	-11(1)	18(1)
C(25)	34(1)	37(1)	31(1)	1(1)	-5(1)	-7(1)
C(26)	39(1)	46(1)	34(1)	2(1)	-5(1)	-10(1)
F(26)	48(1)	65(1)	37(1)	1(1)	7(1)	-2(1)
C(27)	58(1)	58(1)	38(1)	12(1)	-6(1)	-21(1)
F(27)	81(1)	91(1)	49(1)	24(1)	9(1)	-23(1)
C(28)	78(2)	44(1)	51(1)	17(1)	-14(1)	-12(1)
F(28)	129(1)	59(1)	78(1)	36(1)	-11(1)	-8(1)
C(29)	65(1)	40(1)	52(1)	6(1)	-13(1)	5(1)
F(29)	104(1)	50(1)	76(1)	8(1)	-9(1)	30(1)
C(30)	44(1)	41(1)	39(1)	2(1)	-4(1)	0(1)
F(30)	49(1)	52(1)	51(1)	5(1)	5(1)	15(1)
C(31)	34(1)	26(1)	54(1)	4(1)	-4(1)	-3(1)
C(32)	45(1)	37(1)	61(1)	18(1)	-6(1)	-2(1)
C(33)	47(1)	31(1)	71(1)	-5(1)	-3(1)	3(1)
C(34)	37(1)	33(1)	73(1)	11(1)	-5(1)	-6(1)
C(35)	37(1)	39(1)	39(1)	12(1)	-6(1)	-5(1)
C(36)	61(1)	45(1)	68(1)	23(1)	-16(1)	-18(1)
O(37)	28(1)	54(1)	39(1)	3(1)	0(1)	-4(1)
C(37)	30(1)	77(2)	52(1)	8(1)	-2(1)	-8(1)
C(38)	53(2)	112(2)	82(2)	18(2)	6(1)	-36(2)
C(39)	40(1)	92(2)	40(1)	-8(1)	3(1)	1(1)
C(40)	74(2)	125(3)	69(2)	-22(2)	20(1)	26(2)

Table 25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6•OEt$_2$**.

	x	y	z	U(eq)
H(6A)	8881	4496	8236	84(9)
H(6B)	8737	4072	7620	75(8)
H(6C)	9582	4760	7720	85(9)
H(7A)	8710	2134	8692	69(8)
H(7B)	8324	2509	8088	57(7)
H(7C)	8317	3045	8660	61(7)
H(8A)	11011	1941	9334	70(8)
H(8B)	11407	1452	8793	66(7)
H(8C)	10210	1476	8913	87(9)
H(9A)	13114	3371	8485	48(6)
H(9B)	12926	2420	8498	66(8)
H(9C)	12731	2951	9057	76(8)
H(10A)	11470	4991	8223	69(8)
H(10B)	11553	4682	7575	72(8)
H(10C)	12438	4469	8047	79(8)
H(12A)	8488	1513	6149	39(5)
H(12B)	8921	2275	5830	42(5)
H(32A)	10179	728	7899	49(6)
H(32B)	9281	73	7868	63(7)
H(32C)	9062	957	8105	86(9)
H(33A)	9536	595	6369	64(7)
H(33B)	9589	-144	6809	57(6)
H(33C)	10476	521	6829	61(7)
H(34A)	7580	1141	7378	54(6)
H(34B)	7800	215	7243	57(6)
H(34C)	7719	855	6729	58(7)
H(35A)	8865	3843	6271	46(6)
H(35B)	9779	3439	5936	53(6)
H(36A)	10064	4666	6795	84(9)
H(36B)	10167	4804	6118	82(9)
H(36C)	10984	4255	6468	95(10)

H(38A)	13506	2730	7060	62(7)
H(38B)	13028	3348	7504	62(7)
H(39A)	13694	3735	6382	88(10)
H(39B)	14156	4086	6979	125(13)
H(39C)	13039	4355	6744	90(11)
H(40A)	12128	3152	5993	83(9)
H(40B)	11274	2508	6148	61(7)
H(41A)	13432	2220	6180	130(15)
H(41B)	12602	1807	5749	103(11)
H(41C)	12634	1583	6419	190(20)
H(51A)	1079	1785	4273	135
H(51B)	-64	1932	4477	135
H(52A)	1430	974	5027	198
H(52B)	381	673	4717	198
H(52C)	357	1183	5300	198
H(53A)	2289	3059	4525	325
H(53B)	1343	2876	4066	325
H(54A)	330	3656	4522	218
H(54B)	1363	4161	4461	218
H(54C)	1133	3733	5058	218
H(61A)	1498	1786	5171	356
H(61B)	335	1825	4934	356
H(62A)	1460	1203	4174	193
H(62B)	504	840	4495	193
H(62C)	1635	760	4781	193
H(63A)	876	3415	4969	124
H(63B)	160	3269	4391	124
H(64A)	2377	3583	4366	137
H(64B)	1546	4254	4184	137
H(64C)	1657	3463	3799	137