JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1997, 119(49), 11876-11893, DOI:10.1021/ja970697x

Supporting Information for

The Synthesis and Decomposition of Alkyl Complexes of Molybdenum(IV) that Contain a $[(Me_3SiNCH_2CH_2)_3N]^{3-}$ Ligand. Direct Detection of α Elimination Processes that are more than Six Orders of Magnitude Faster than β Elimination Processes.

Richard R. Schrock,* Scott W. Seidel, Nadia C. Zanetti,

Keng-Yu Shih, Myra B. O'Donoghue, William M. Davis, and William M. Reiff

$[N_3N]MoCl$		$[N_3N]MoMe$		$[N_3N]Mo(CH_2SiMe_3)$	
5.0000	0.041050	5.0000	0.039588	5.0000	0.034400
6.0100	0.040657	5.9900	0.039405	5.9900	0.034065
6.9800	0.040370	7.0000	0.039260	6.9900	0.033830
7.9800	0.040124	7.9800	0.039078	7.9900	0.033640
8.9600	0.039904	8.9900	0.038820	8.9900	0.033485
9.9600	0.039667	9.9900	0.038452	9.9900	0.033304
11.980	0.039045	12.000	0.037394	12.000	0.032891
13.980	0.038187	14.010	0.035964	14.010	0.032298
16.000	0.037087	16.010	0.034321	16.010	0.031500
18.030	0.035807	18.010	0.032579	18.010	0.030549
20.020	0.034437	20.010	0.030841	20.010	0.029493
23.090	0.032260	22.930	0.028405	22.980	0.027800
26.050	0.030192	26.020	0.026097	26.030	0.026078
29.020	0.028228	28.960	0.024117	29.130	0.024468
32.020	0.026394	32.120	0.022338	32.130	0.022949
35.010	0.024716	35.110	0.020777	35.110	0.021551
38.010	0.023177	38.120	0.019380	38.120	0.020258
40.980	0.021858	41.010	0.018225	41.000	0.019172
43.970	0.020571	44.000	0.017100	44.000	0.018087
46.970	0.019425	47.010	0.016100	47.000	0.017105
49.960	0.018385	50.000	0.015203	50.000	0.016195
54.960	0.016865	55.030	0.013887	55.030	0.014867
59.910	0.015558	60.030	0.012721	60.030	0.013674
65.030	0.014425	65.030	0.011773	65.040	0.012674
70.100	0.013416	70.050	0.010986	70.050	0.011858
75.170	0.012548	75.080	0.010300	75.080	0.011135
80.060	0.011793	80.070	0.0096973	80.070	0.010483
85.070	0.011142	85.080	0.0091238	85.080	0.0098825
90.320	0.010535	90.080	0.0086253	90.080	0.0093267
95.100	0.0099711	95.080	0.0081692	95.080	0.0088362
100.12	0.0094898	100.09	0.0077508	100.09	0.0084091
110.17	0.0086156	110.08	0.0070341	110.08	0.0076416
120.20	0.0078870	120.01	0.0064317	120.06	0.0069808
130.21	0.0072685	130.08	0.0059310	130.05	0.0064403
140.21	0.0067299	138.87	0.0054310	138.87	0.0058936
150.21	0.0062796	150.22	0.0051755	150.22	0.0056044
160.21	0.0058710	158.84	0.0047557	158.84	0.0051476
170.20	0.0055162	170.25	0.0045441	170.25	0.0049156
180.20	0.0052138	180.17	0.0042512	180.18	0.0045931
190.14	0.0049220	190.16	0.0040113	190.16	0.0043281
200.20	0.0046552	200.16	0.0037937	200.16	0.0040949
220.17	0.0041837	220.11	0.0034180	220.12	0.0036951
240.13	0.0038148	240.13	0.0031084	240.10	0.0033603
260.11	0.0034925	260.13	0.0028509	260.14	0.0030718
280.08	0.0032070	280.15	0.0026024	280.15	0.0027973
300.00	0.0029212	300.15	0.0023374	300.14	0.0025260

[N_3N]MoD		[bitN_3N]Mo		[N_3N]Mo(cyclopentyl)	
5.0000	0.068958	5.0000	0.036816	5.0100	0.063204
5.9900	0.068753	5.9900	0.037120	5.9900	0.062375
6.9800	0.068301	6.9900	0.037310	7.0000	0.061133
7.9800	0.067635	8.0000	0.037574	8.0000	0.059533
8.9900	0.066684	8.9800	0.037423	8.9900	0.057645
9.9900	0.065456	10.000	0.037353	9.9700	0.055621
12.000	0.062381	12.000	0.036479	11.980	0.051206
14.000	0.058773	13.990	0.035285	13.980	0.046900
16.010	0.054943	16.070	0.033724	16.000	0.042918
18.000	0.051183	18.020	0.032120	18.010	0.039389
20.010	0.047601	20.020	0.030464	20.030	0.036259
23.000	0.042771	23.000	0.028068	23.080	0.032245
26.010	0.038565	26.030	0.025800	26.060	0.029020
29.040	0.034945	29.130	0.023764	29.040	0.026334
32.130	0.031941	32.090	0.021949	32.030	0.024055
35.130	0.029328	35.090	0.020346	35.010	0.022114
38.130	0.027025	38.140	0.018882	38.010	0.020442
41.000	0.025194	41.000	0.017702	41.000	0.019053
43.990	0.023409	43.990	0.016568	43.980	0.017755
47.000	0.021869	47.000	0.015540	46.970	0.016634
50.000	0.020484	50.000	0.014620	49.960	0.015615
55.030	0.018531	54.960	0.013292	54.930	0.014198
60.040	0.016835	60.040	0.012117	59.930	0.012984
65.040	0.015463	65.040	0.011168	64.950	0.011949
70.050	0.014349	70.060	0.010397	69.990	0.011055
75.070	0.013382	75.050	0.0097108	75.030	0.010299
80.050	0.012535	80.070	0.0091070	80.070	0.0096569
85.080	0.011761	85.080	0.0085447	85.090	0.0090671
90.080	0.011070	90.090	0.0080547	90.100	0.0085471
95.080	0.010463	95.080	0.0075995	95.120	0.0080770
100.08	0.0099085	100.09	0.0072132	100.13	0.0076538
110.07	0.0089659	110.07	0.0065288	110.16	0.0069094
120.06	0.0081896	120.06	0.0059482	120.19	0.0063035
130.08	0.0075372	130.09	0.0054662	130.21	0.0057869
138.87	0.0068970	138.87	0.0049914	140.23	0.0053472
150.22	0.0065663	150.23	0.0047399	150.25	0.0049662
158.84	0.0060307	158.84	0.0043386	160.24	0.0046273
170.24	0.0057732	170.26	0.0041529	170.26	0.0043414
180.18	0.0054093	180.18	0.0038751	180.25	0.0040895
190.16	0.0050976	190.16	0.0036454	190.22	0.0038508
200.16	0.0048344	200.16	0.0034477	200.19	0.0036343
220.12	0.0043658	220.13	0.0031042	220.24	0.0032567
240.11	0.0039916	240.11	0.0028268	240.22	0.0029517
260.13	0.0036822	260.14	0.0026111	260.22	0.0026711
280.14	0.0034081	280.15	0.0024147	280.28	0.0023717
300.15	0.0031506	300.14	0.0022093	300.14	0.0019236

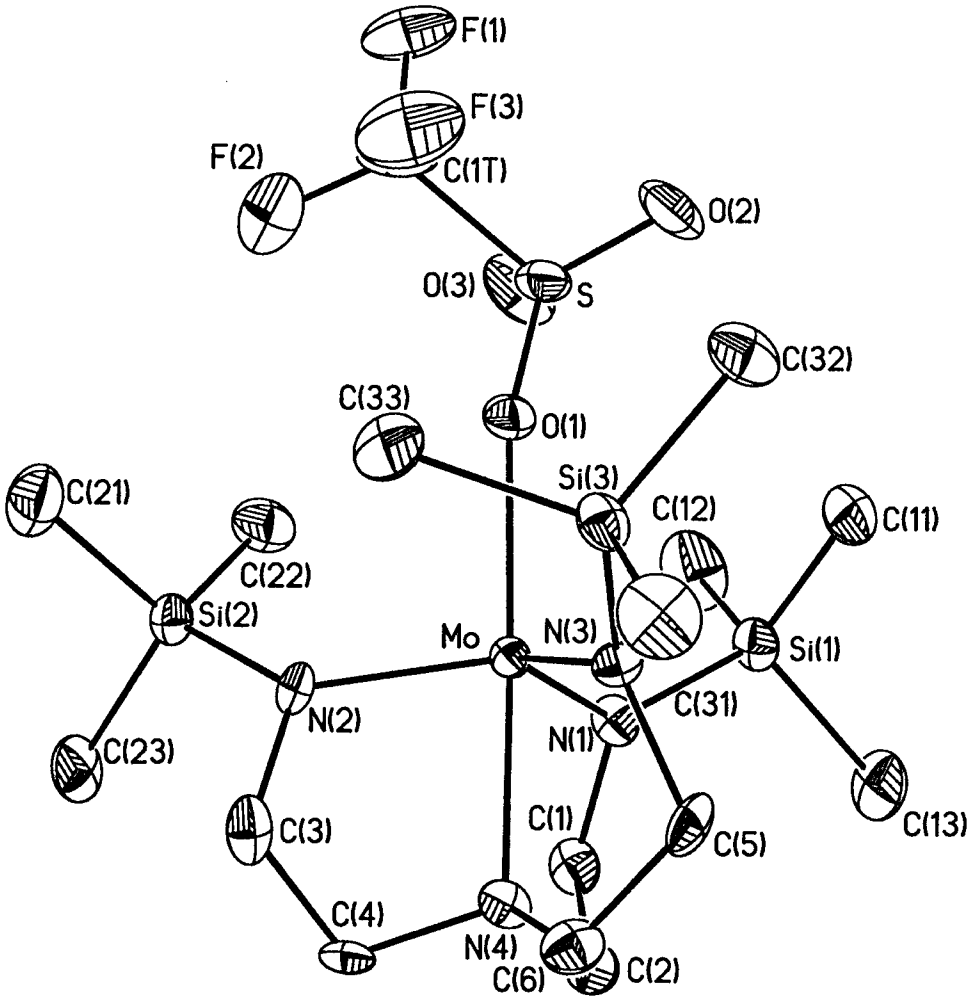
F(1)
F(3)
F(2)
C(1T)
O(2)
O(3)
S
C(32)
C(33)
O(1)
Si(3)
C(21)
C(12)
C(11)
C(22)
Si(2)
Mo
N(3)
Si(1)
C(31)
N(2)
N(1)
C(23)
C(3)
C(1)
C(5)
C(13)
C(4)
N(4)
C(6)
C(2)

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

A. Crystal Data

Identification code	95066
Empirical formula	$C_{16}H_{39}F_3MoN_4O_3SSi_3$
Formula weight	604.78
Temperature	188(2) K
Wavelength	0.71073 Å
Crystal morphology	
Crystal size	0.32 x 0.29 x 0.23 mm
Crystal system	Orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	a = 20.951(4) Å alpha = 90° b = 10.999(2) Å beta = 90° c = 12.050(2) Å gamma = 90°
Volume, Z	2776.7(10) $Å^3$, 4
Density (calculated)	1.447 Mg/m^3
Absorption coefficient	0.720 mm^{-1}
F(000)	1256

B. Data Collection and Reduction

Diffractometer	Siemens SMART/CCD
Scan Type	ω Scans
Scan angle	0.30°
θ range for data collection	1.94 to 19.99°
Limiting indices	$-13 \le h \le 23$, $-12 \le k \le 6$, $-13 \le l \le 13$

Reflections collected	7745
Independent reflections	2595 (R_{int} = 0.0866)
Absorption correction	None

C. Solution and Refinement

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2559 / 1 / 282
Goodness-of-fit on F^2	0.996
Final R indices [I>2σ(I)]	R1 = 0.0486, wR2 = 0.1068
R indices (all data)	R1 = 0.0644, wR2 = 0.1542
Absolute structure parameter	0.61(10)
Extinction coefficient	0.0034(5)
Largest diff. peak and hole	0.458 and -0.725 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1b. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo	1517(1)	2516(1)	6351(1)	21(1)
S	1606(2)	1605(3)	3521(3)	42(1)
Si(1)	907(1)	-328(2)	6319(4)	34(1)
Si(2)	542(2)	4726(3)	5398(3)	32(1)
Si(3)	3077(2)	2839(3)	5995(2)	32(1)
F(1)	1742(5)	2463(9)	1521(9)	103(3)
F(2)	1427(5)	3775(8)	2689(9)	111(3)
F(3)	2399(5)	3191(8)	2708(8)	99(3)
O(1)	1670(4)	2217(7)	4594(7)	34(2)
O(2)	2090(4)	739(8)	3298(7)	57(2)
O(3)	970(4)	1281(8)	3247(8)	62(3)
N(1)	931(4)	1189(8)	6774(7)	27(2)
N(2)	1144(3)	4163(6)	6245(9)	24(2)
N(3)	2427(4)	2377(7)	6780(7)	26(2)
N(4)	1427(4)	2912(10)	8109(7)	22(2)
C(1T)	1810(10)	2837(14)	2555(13)	69(4)
C(1)	561(5)	1521(9)	7764(9)	33(3)
C(2)	1030(5)	1935(10)	8635(10)	32(3)
C(3)	1293(5)	4875(10)	7257(10)	35(3)
C(4)	1107(5)	4118(9)	8245(9)	33(3)
C(5)	2488(5)	2104(10)	7983(9)	36(3)
C(6)	2083(5)	2937(11)	8622(10)	37(3)
C(11)	1653(6)	-751(10)	5642(11)	51(4)
C(12)	208(7)	-554(12)	5411(13)	72(5)
C(13)	815(6)	-1336(10)	7558(12)	54(4)
C(21)	872(6)	5913(11)	4489(11)	52(4)
C(22)	174(6)	3492(12)	4603(10)	46(4)
C(23)	-95(5)	5421(9)	6250(13)	50(3)
C(31)	3777(6)	3178(12)	6907(11)	55(4)
C(32)	3318(5)	1599(11)	5042(10)	44(3)
C(33)	2867(6)	4257(10)	5232(10)	47(3)

Table 3. Bond lengths [Å] and angles [°] for 1b.

Mo-N(3)	1.980(8)	Mo-N(2)	1.977(7)
Mo-N(1)	1.974(8)	Mo-O(1)	2.166(8)
Mo-N(4)	2.171(9)	S-O(2)	1.417(8)
S-O(3)	1.417(8)	S-O(1)	1.465(9)
S-C(1T)	1.84(2)	Si(1)-N(1)	1.757(9)
Si(1)-C(11)	1.824(13)	Si(1)-C(12)	1.845(13)
Si(1)-C(13)	1.869(13)	Si(2)-N(2)	1.736(9)
Si(2)-C(22)	1.832(12)	Si(2)-C(23)	1.849(13)
Si(2)-C(21)	1.839(12)	Si(3)-N(3)	1.735(9)
Si(3)-C(32)	1.853(12)	Si(3)-C(33)	1.864(12)
Si(3)-C(31)	1.870(12)	F(1)-C(1T)	1.32(2)
F(2)-C(1T)	1.32(2)	F(3)-C(1T)	1.31(2)
N(1)-C(1)	1.469(13)	N(2)-C(3)	1.48(2)
N(3)-C(5)	1.486(13)	N(4)-C(2)	1.499(14)
N(4)-C(4)	1.495(14)	N(4)-C(6)	1.508(13)
C(1)-C(2)	1.507(14)	C(3)-C(4)	1.50(2)
C(5)-C(6)	1.47(2)		

N(3)-Mo-N(2)	117.9(3)	N(3)-Mo-N(1)	118.3(3)
N(2)-Mo-N(1)	116.6(3)	N(3)-Mo-O(1)	95.8(3)
N(2)-Mo-O(1)	97.7(4)	N(1)-Mo-O(1)	103.4(3)
N(3)-Mo-N(4)	81.1(3)	N(2)-Mo-N(4)	81.1(4)
N(1)-Mo-N(4)	80.9(4)	O(1)-Mo-N(4)	175.6(3)
O(2)-S-O(3)	117.3(5)	O(2)-S-O(1)	114.2(5)
O(3)-S-O(1)	114.1(5)	O(2)-S-C(1T)	102.1(7)
O(3)-S-C(1T)	104.9(8)	O(1)-S-C(1T)	101.5(6)
N(1)-Si(1)-C(11)	111.0(5)	N(1)-Si(1)-C(12)	109.6(5)
C(11)-Si(1)-C(12)	112.3(7)	N(1)-Si(1)-C(13)	108.5(5)
C(11)-Si(1)-C(13)	107.1(6)	C(12)-Si(1)-C(13)	108.2(6)
N(2)-Si(2)-C(22)	110.4(5)	N(2)-Si(2)-C(23)	110.2(5)
C(22)-Si(2)-C(23)	107.0(6)	N(2)-Si(2)-C(21)	109.3(5)
C(22)-Si(2)-C(21)	111.8(6)	C(23)-Si(2)-C(21)	107.9(6)
N(3)-Si(3)-C(32)	109.7(5)	N(3)-Si(3)-C(33)	109.2(5)
C(32)-Si(3)-C(33)	112.0(5)	N(3)-Si(3)-C(31)	110.7(5)
C(32)-Si(3)-C(31)	107.3(6)	C(33)-Si(3)-C(31)	108.0(6)
S-O(1)-Mo	156.9(5)	C(1)-N(1)-Si(1)	118.3(7)
C(1)-N(1)-Mo	110.7(6)	Si(1)-N(1)-Mo	129.8(5)
C(3)-N(2)-Si(2)	116.6(6)	C(3)-N(2)-Mo	110.3(7)
Si(2)-N(2)-Mo	130.7(5)	C(5)-N(3)-Si(3)	121.6(7)
C(5)-N(3)-Mo	110.7(6)	Si(3)-N(3)-Mo	126.2(5)
C(2)-N(4)-C(4)	110.0(8)	C(2)-N(4)-C(6)	110.2(9)
C(4)-N(4)-C(6)	110.3(9)	C(2)-N(4)-Mo	108.5(7)
C(4)-N(4)-Mo	108.9(7)	C(6)-N(4)-Mo	108.9(6)
F(2)-C(1T)-F(1)	107(2)	F(2)-C(1T)-F(3)	108.9(14)
F(1)-C(1T)-F(3)	109.2(13)	F(2)-C(1T)-S	111.0(11)
F(1)-C(1T)-S	110.1(12)	F(3)-C(1T)-S	110.5(12)
N(1)-C(1)-C(2)	107.2(8)	N(4)-C(2)-C(1)	106.4(9)
N(2)-C(3)-C(4)	107.7(8)	N(4)-C(4)-C(3)	106.8(9)
C(6)-C(5)-N(3)	109.6(9)	C(5)-C(6)-N(4)	107.5(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1b.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mo	21(1)	21(1)	20(1)	-1(1)	0(1)	1(1)
S	47(2)	47(2)	31(2)	-4(2)	2(2)	13(2)
Si(1)	38(2)	25(2)	38(2)	-8(2)	-8(2)	-4(1)
Si(2)	32(2)	28(2)	34(2)	0(2)	-3(2)	4(2)
Si(3)	26(2)	34(2)	37(2)	-3(2)	5(1)	2(1)
F(1)	149(8)	128(7)	31(6)	5(6)	12(6)	13(6)
F(2)	168(10)	80(6)	85(7)	42(6)	28(7)	39(7)
F(3)	88(7)	125(8)	85(7)	21(6)	35(6)	-34(6)
O(1)	42(5)	33(5)	26(6)	-6(4)	12(4)	2(4)
O(2)	61(6)	63(6)	47(6)	-21(5)	0(5)	27(5)
O(3)	36(6)	76(7)	74(7)	-26(5)	-12(5)	4(5)
N(1)	20(5)	30(5)	31(6)	-4(4)	6(4)	-2(4)
N(2)	23(4)	24(4)	23(5)	-2(6)	-7(5)	-2(4)
N(3)	28(5)	23(5)	27(7)	2(4)	-2(4)	-7(4)
N(4)	15(5)	40(6)	12(6)	-4(5)	-1(4)	-1(5)
C(1T)	93(13)	68(12)	46(11)	-3(9)	23(9)	22(11)
C(1)	40(7)	26(7)	33(8)	1(6)	7(7)	-7(6)
C(2)	38(7)	31(7)	28(7)	2(6)	0(6)	-6(6)
C(3)	28(7)	27(7)	49(9)	3(7)	-15(6)	-1(5)
C(4)	32(7)	33(7)	34(8)	-17(6)	-2(6)	-3(6)
C(5)	22(7)	51(7)	33(8)	23(6)	-3(6)	4(6)
C(6)	18(6)	57(8)	35(7)	-5(7)	6(6)	7(6)
C(11)	65(9)	41(7)	47(9)	-2(7)	-2(7)	1(7)
C(12)	74(11)	59(9)	83(12)	-17(10)	-22(9)	-4(8)
C(13)	67(9)	26(7)	70(10)	12(7)	3(8)	-11(7)
C(21)	63(9)	41(8)	52(9)	1(7)	-7(7)	-1(7)
C(22)	28(7)	71(9)	40(8)	6(7)	-3(6)	4(7)
C(23)	47(7)	48(7)	56(8)	-1(9)	-23(8)	18(6)
C(31)	28(7)	58(9)	77(10)	-3(7)	-2(7)	-10(7)
C(32)	27(7)	54(8)	51(9)	-1(7)	5(7)	6(6)
C(33)	45(8)	45(8)	51(9)	1(7)	13(7)	-16(6)

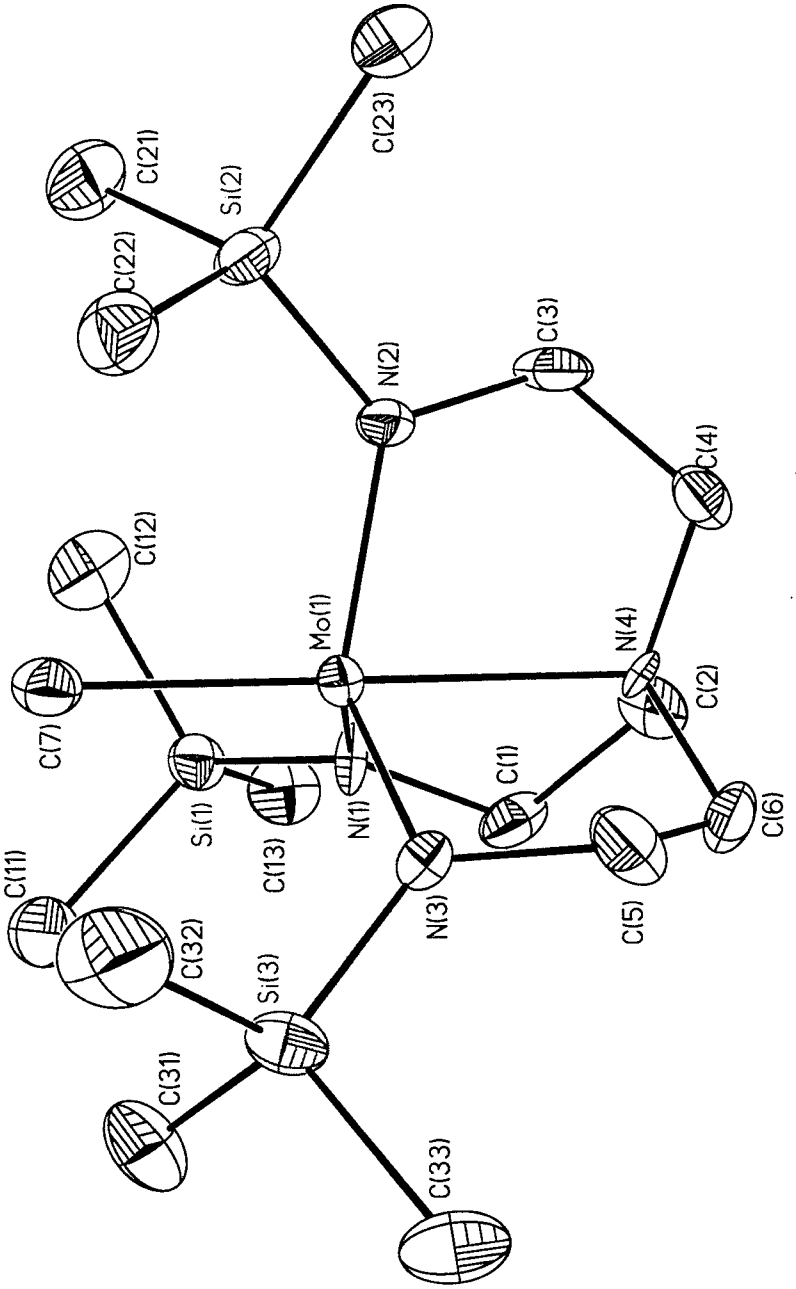
C(23)
C(21)
Si(2)
C(22)
N(2)
C(3)
C(4)
C(12)
Mo(1)
N(4)
C(7)
C(2)
Si(1)
C(13)
N(1)
C(1)
C(6)
C(11)
N(3)
C(5)
C(32)
Si(3)
C(31)
C(33)

Table 1. Crystal data and structure refinement for 2d-d_3.

A. Crystal Data	
Identification code	97001
Empirical formula	$C_{16}H_{39}D_3MoN_4Si_3$
Formula weight	473.77
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal morphology	
Crystal size	0.17 x 0.12 x 0.12 mm
Crystal system	Monoclinic
Space group	Cc
Unit cell dimensions	*a* = 17.35280(10) Å alpha = 90°
	b = 9.6851(2) Å beta = 110.6210(10)°
	c = 15.9445(3) Å gamma = 90°
Volume, Z	2508.00(7) $Å^3$, 4
Density (calculated)	1.255 Mg/m^3
Absorption coefficient	0.673 mm^{-1}
F(000)	1000
B. Data Collection and Reduction	
Diffractometer	Siemens SMART/CCD
Scan Type	ω Scans
Scan angle	0.30°
θ range for data collection	2.45 to 23.28°
Limiting indices	$-19 \le h \le 16$, $-10 \le k \le 10$, $-17 \le l \le 17$
Reflections collected	5023
Independent reflections	2412 (R_{int} = 0.0784)
Absorption correction	None
C. Solution and Refinement	
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	2412 / 2 / 217
Goodness-of-fit on F^2	1.085
Final R indices [I>2σ(I)]	R1 = 0.0660, wR2 = 0.1096
R indices (all data)	R1 = 0.0799, wR2 = 0.1148
Absolute structure parameter	0.08(8)
Extinction coefficient	0.0003(2)
Largest diff. peak and hole	0.720 and -0.800 $eÅ^{-3}$
Weighting Scheme	calc w=1/[\s^2^(Fo^2^)+(0.0159P)^2^+3.1068P] where P=(Fo

Notes Cell constants based upon three sets of fifteen (15) 0.30° ω scans. Refle were harvested using the Siemens XSCANS algorithm.

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 2a-d_3. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	1791(1)	4106(1)	4344(1)	22(1)
Si(1)	3584(2)	5694(4)	4646(3)	34(1)
Si(2)	1842(2)	1898(4)	5982(2)	34(1)
Si(3)	161(2)	6193(4)	3567(3)	37(1)
N(1)	2728(6)	4740(9)	4004(6)	28(2)
N(2)	1907(6)	2283(9)	4960(6)	30(3)
N(3)	682(6)	4651(9)	3537(6)	32(3)
N(4)	1629(6)	2664(9)	3145(6)	25(2)
C(1)	2656(8)	4364(12)	3088(7)	39(3)
C(2)	2367(8)	2875(12)	2891(9)	37(3)
C(3)	2124(8)	1165(11)	4451(8)	41(4)
C(4)	1583(8)	1266(11)	3473(8)	39(4)
C(5)	268(8)	3625(12)	2841(9)	47(4)
C(6)	875(8)	3090(12)	2425(8)	42(4)
C(7)	1942(8)	5467(11)	5487(8)	37(3)
C(11)	3338(9)	7589(13)	4743(9)	59(4)
C(12)	4044(8)	4934(14)	5783(8)	56(4)
C(13)	4378(8)	5650(13)	4120(9)	53(4)
C(21)	2830(10)	2188(14)	6913(9)	65(5)
C(22)	997(9)	2862(13)	6164(9)	49(4)
C(23)	1588(9)	9(13)	6036(8)	55(4)
C(31)	881(9)	7684(13)	3736(10)	56(4)
C(33)	-688(9)	6481(15)	2459(9)	59(4)
C(32)	-304(10)	6171(16)	4460(11)	75(5)

Table 3. Bond lengths [Å] and angles [°] for 22-d_3.

Mo(1)-N(3)	1.973(10)	Mo(1)-N(1)	1.984(9)
Mo(1)-N(2)	1.996(9)	Mo(1)-C(7)	2.188(11)
Mo(1)-N(4)	2.304(9)	Si(1)-N(1)	1.742(9)
Si(1)-C(13)	1.848(14)	Si(1)-C(12)	1.856(13)
Si(1)-C(11)	1.902(13)	Si(2)-N(2)	1.714(9)
Si(2)-C(22)	1.846(14)	Si(2)-C(21)	1.85(2)
Si(2)-C(23)	1.891(13)	Si(3)-N(3)	1.755(10)
Si(3)-C(32)	1.87(2)	Si(3)-C(31)	1.866(14)
Si(3)-C(33)	1.881(13)	N(1)-C(1)	1.468(13)
N(2)-C(3)	1.478(13)	N(3)-C(5)	1.474(14)
N(4)-C(4)	1.464(14)	N(4)-C(6)	1.46(2)
N(4)-C(2)	1.49(2)	C(1)-C(2)	1.52(2)
C(3)-C(4)	1.51(2)	C(5)-C(6)	1.52(2)

N(3)-Mo(1)-N(1)	116.4(4)	N(3)-Mo(1)-N(2)	117.6(4)
N(1)-Mo(1)-N(2)	117.2(4)	N(3)-Mo(1)-C(7)	100.7(4)
N(1)-Mo(1)-C(7)	99.9(4)	N(2)-Mo(1)-C(7)	99.3(4)
N(3)-Mo(1)-N(4)	79.3(4)	N(1)-Mo(1)-N(4)	80.4(4)
N(2)-Mo(1)-N(4)	80.4(4)	C(7)-Mo(1)-N(4)	179.7(4)
N(1)-Si(1)-C(13)	109.8(5)	N(1)-Si(1)-C(12)	110.3(5)
C(13)-Si(1)-C(12)	107.5(6)	N(1)-Si(1)-C(11)	113.0(6)
C(13)-Si(1)-C(11)	106.5(6)	C(12)-Si(1)-C(11)	109.6(6)
N(2)-Si(2)-C(22)	111.2(5)	N(2)-Si(2)-C(21)	112.1(6)
C(22)-Si(2)-C(21)	111.0(6)	N(2)-Si(2)-C(23)	110.4(5)
C(22)-Si(2)-C(23)	105.8(6)	C(21)-Si(2)-C(23)	105.9(6)
N(3)-Si(3)-C(32)	112.1(6)	N(3)-Si(3)-C(31)	109.8(5)
C(32)-Si(3)-C(31)	110.3(7)	N(3)-Si(3)-C(33)	109.9(6)
C(32)-Si(3)-C(33)	108.1(7)	C(31)-Si(3)-C(33)	106.5(7)
C(1)-N(1)-Si(1)	118.2(7)	C(1)-N(1)-Mo(1)	113.8(7)
Si(1)-N(1)-Mo(1)	128.0(5)	C(3)-N(2)-Si(2)	118.5(7)
C(3)-N(2)-Mo(1)	112.3(6)	Si(2)-N(2)-Mo(1)	129.1(5)
C(5)-N(3)-Si(3)	118.4(8)	C(5)-N(3)-Mo(1)	114.5(7)
Si(3)-N(3)-Mo(1)	127.1(5)	C(4)-N(4)-C(6)	113.2(9)
C(4)-N(4)-C(2)	112.7(9)	C(6)-N(4)-C(2)	111.5(9)
C(4)-N(4)-Mo(1)	105.7(7)	C(6)-N(4)-Mo(1)	107.1(7)
C(2)-N(4)-Mo(1)	106.1(7)	N(1)-C(1)-C(2)	110.3(9)
N(4)-C(2)-C(1)	109.0(9)	N(2)-C(3)-C(4)	109.5(9)
N(4)-C(4)-C(3)	109.6(9)	N(3)-C(5)-C(6)	109.2(11)
N(4)-C(6)-C(5)	108.7(10)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 22-d_3.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Mo(1)	26(1)	21(1)	21(1)	-2(1)	9(1)	1(1)
Si(1)	30(2)	29(2)	36(2)	-1(2)	5(2)	-5(2)
Si(2)	37(2)	39(2)	22(2)	6(2)	7(2)	0(2)
Si(3)	32(2)	33(2)	48(3)	8(2)	18(2)	7(2)
N(1)	27(6)	37(6)	22(6)	-18(5)	10(5)	-10(5)
N(2)	42(7)	23(6)	25(6)	5(5)	12(5)	9(5)
N(3)	44(7)	31(5)	19(6)	1(5)	8(5)	0(5)
N(4)	37(7)	26(6)	6(5)	-1(5)	-2(5)	-1(5)
C(1)	35(8)	48(9)	28(7)	12(6)	5(6)	-10(7)
C(2)	46(9)	34(8)	48	0(7)	37(6)	15(7)
C(3)	61(10)	30(7)	42(9)	18(7)	31(9)	16(7)
C(4)	58(10)	23(8)	40(8)	-5(6)	21(8)	-8(7)
C(5)	44(9)	30(7)	63(10)	-7(7)	13(8)	2(7)
C(6)	56(10)	43(8)	19(7)	-5(6)	5(7)	-14(8)
C(7)	42(9)	31(8)	37(8)	5(6)	12(7)	-1(7)
C(11)	58(11)	48(9)	52(10)	-5(7)	-5(8)	-11(8)
C(12)	26(8)	76(11)	54(10)	1(8)	1(7)	-30(8)
C(13)	40(9)	55(10)	61(10)	3(8)	16(8)	-9(8)
C(21)	71(12)	66(10)	37(9)	2(8)	-10(8)	15(9)
C(22)	58(10)	52(9)	44(10)	-2(7)	24(9)	-7(8)
C(23)	79(12)	52(9)	39(9)	5(7)	29(8)	-4(9)
C(31)	47(10)	43(9)	81(11)	-14(8)	28(9)	3(8)
C(33)	38(9)	66(10)	64(11)	20(9)	7(8)	20(7)
C(32)	70(13)	88(13)	78(13)	10(10)	41(11)	37(11)

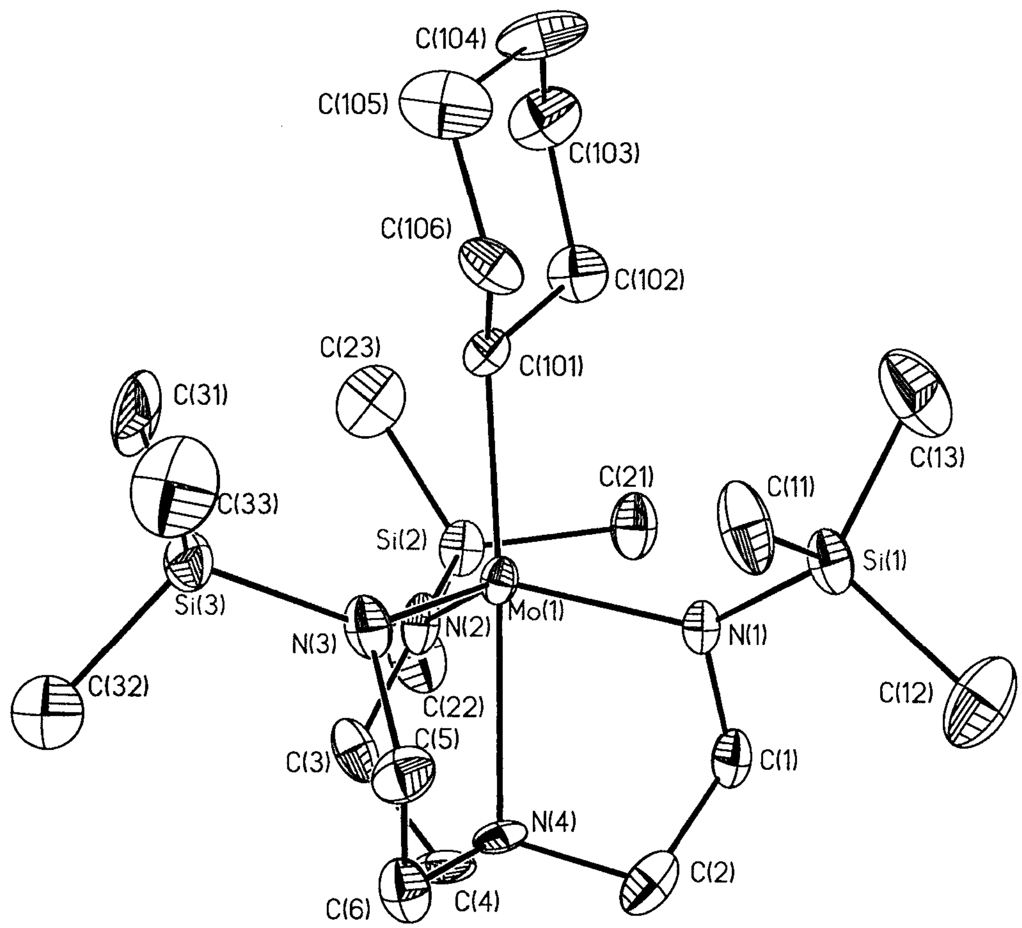

Table 1. Crystal data and structure refinement for 2j.

A. Crystal Data	
Identification code	96208
Empirical formula	$C_{21}H_{50}MoN_4Si_3$
Formula weight	538.86
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal morphology	
Crystal size	0.20 x 0.11 x 0.11 mm
Crystal system	Hexagonal
Space group	$P6_3$
Unit cell dimensions	a = 20.820(6) Å alpha = 90°
	b = 20.820(6) Å beta = 90°
	c = 11.680(5) Å gamma = 120°
Volume, Z	4385(3) $Å^3$, 6
Density (calculated)	1.224 Mg/m^3
Absorption coefficient	0.586 mm^{-1}
F(000)	1728
B. Data Collection and Reduction	
Diffractometer	Siemens SMART/CCD
Scan Type	ω Scans
Scan angle	0.30°
θ range for data collection	1.13 to 20.00°
Limiting indices	$-19 \le h \le 23$, $-23 \le k \le 13$, $-12 \le l \le 12$
Reflections collected	12846
Independent reflections	2728 (R_{int} = 0.1181)
Absorption correction	None
C. Solution and Refinement	
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	2679 / 1 / 259
Goodness-of-fit on F^2	1.113
Final R indices [I>2σ(I)]	R1 = 0.0569, wR2 = 0.1488
R indices (all data)	R1 = 0.0670, wR2 = 0.1702
Absolute structure parameter	0.43(10)
Extinction coefficient	0.0003(2)
Largest diff. peak and hole	0.653 and -0.421 $eÅ^{-3}$
Weighting Scheme	calc w=1/[\s^2^(Fo^2^)+(0.0522P)^2^+13.5431P] where P=(F

Notes Cell constants based upon three sets of fifteen (15) 0.30° ω scans. Refle were harvested using the Siemens XSCANS algorithm.

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 2j. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	-6642(1)	13(1)	-9754(1)	24(1)
Si(1)	-4935(1)	1527(1)	-10007(2)	38(1)
Si(2)	-6920(1)	-1726(1)	-9932(2)	35(1)
Si(3)	-8159(1)	239(2)	-9908(2)	39(1)
N(1)	-5564(4)	649(4)	-9422(6)	34(2)
N(2)	-7105(4)	-1061(4)	-9310(7)	34(2)
N(3)	-7273(4)	457(4)	-9419(6)	35(2)
N(4)	-6603(4)	75(4)	-7683(9)	25(3)
C(1)	-5373(5)	459(6)	-8327(9)	44(3)
C(2)	-5806(5)	537(5)	-7360(9)	41(3)
C(3)	-7452(5)	-1194(5)	-8216(9)	41(3)
C(4)	-6928(6)	-715(6)	-7292(8)	45(3)
C(5)	-7054(6)	880(6)	-8338(8)	40(3)
C(6)	-7062(5)	415(5)	-7366(9)	39(3)
C(11)	-5413(5)	2080(5)	-10278(10)	55(3)
C(12)	-4179(6)	2054(6)	-8960(11)	74(4)
C(13)	-4490(7)	1456(7)	-11337(12)	88(4)
C(21)	-5912(5)	-1327(5)	-10166(10)	51(3)
C(22)	-7210(6)	-2516(5)	-8891(11)	66(3)
C(23)	-7487(7)	-2147(6)	-11233(11)	71(4)
C(31)	-8529(6)	-496(7)	-11038(13)	79(4)
C(32)	-8858(6)	-149(6)	-8731(11)	65(3)
C(33)	-8109(7)	1109(7)	-10489(13)	78(4)
C(101)	-6735(6)	-53(5)	-11604(12)	34(5)
C(102)	-6265(5)	-295(5)	-12307(9)	44(3)
C(103)	-6465(6)	-419(6)	-13599(11)	60(3)
C(104)	-6476(8)	235(8)	-14138(10)	65(4)
C(105)	-6947(7)	470(6)	-13477(11)	65(4)
C(106)	-6696(5)	621(5)	-12235(9)	40(3)

Table 3. Bond lengths [Å] and angles [°] for 2j.

Mo(1)-N(3)	1.987(7)	Mo(1)-N(1)	1.991(7)
Mo(1)-N(2)	2.012(7)	Mo(1)-C(101)	2.167(14)
Mo(1)-N(4)	2.422(10)	Si(1)-N(1)	1.769(8)
Si(1)-C(13)	1.852(13)	Si(1)-C(12)	1.857(11)
Si(1)-C(11)	1.888(9)	Si(2)-N(2)	1.767(8)
Si(2)-C(21)	1.852(9)	Si(2)-C(23)	1.854(12)
Si(2)-C(22)	1.886(11)	Si(3)-N(3)	1.760(8)
Si(3)-C(32)	1.867(12)	Si(3)-C(31)	1.871(12)
Si(3)-C(33)	1.888(11)	N(1)-C(1)	1.452(12)
N(2)-C(3)	1.426(12)	N(3)-C(5)	1.475(12)
N(4)-C(6)	1.491(11)	N(4)-C(2)	1.491(12)
N(4)-C(4)	1.504(13)	C(1)-C(2)	1.504(14)
C(3)-C(4)	1.504(14)	C(5)-C(6)	1.488(14)
C(101)-C(102)	1.542(14)	C(101)-C(106)	1.551(13)
C(102)-C(103)	1.553(14)	C(103)-C(104)	1.51(2)
C(104)-C(105)	1.509(14)	C(105)-C(106)	1.521(14)

N(3)-Mo(1)-N(1)	116.1(3)	N(3)-Mo(1)-N(2)	113.9(3)
N(1)-Mo(1)-N(2)	116.3(3)	N(3)-Mo(1)-C(101)	99.6(3)
N(1)-Mo(1)-C(101)	105.8(3)	N(2)-Mo(1)-C(101)	102.0(3)
N(3)-Mo(1)-N(4)	77.9(3)	N(1)-Mo(1)-N(4)	76.9(3)
N(2)-Mo(1)-N(4)	77.7(3)	C(101)-Mo(1)-N(4)	177.0(3)
N(1)-Si(1)-C(13)	112.5(5)	N(1)-Si(1)-C(12)	109.1(5)
C(13)-Si(1)-C(12)	106.9(6)	N(1)-Si(1)-C(11)	110.5(4)
C(13)-Si(1)-C(11)	110.2(6)	C(12)-Si(1)-C(11)	107.4(5)
N(2)-Si(2)-C(21)	110.6(4)	N(2)-Si(2)-C(23)	111.7(4)
C(21)-Si(2)-C(23)	113.7(6)	N(2)-Si(2)-C(22)	108.6(5)
C(21)-Si(2)-C(22)	106.5(5)	C(23)-Si(2)-C(22)	105.4(5)
N(3)-Si(3)-C(32)	111.2(5)	N(3)-Si(3)-C(31)	112.9(4)
C(32)-Si(3)-C(31)	104.6(5)	N(3)-Si(3)-C(33)	108.8(5)
C(32)-Si(3)-C(33)	109.7(6)	C(31)-Si(3)-C(33)	109.5(7)
C(1)-N(1)-Si(1)	117.3(6)	C(1)-N(1)-Mo(1)	111.2(6)
Si(1)-N(1)-Mo(1)	128.2(4)	C(3)-N(2)-Si(2)	120.3(6)
C(3)-N(2)-Mo(1)	111.2(6)	Si(2)-N(2)-Mo(1)	126.4(4)
C(5)-N(3)-Si(3)	113.7(6)	C(5)-N(3)-Mo(1)	111.6(6)
Si(3)-N(3)-Mo(1)	131.9(4)	C(6)-N(4)-C(2)	113.7(7)
C(6)-N(4)-C(4)	113.6(7)	C(2)-N(4)-C(4)	112.0(7)
C(6)-N(4)-Mo(1)	105.1(6)	C(2)-N(4)-Mo(1)	106.5(6)
C(4)-N(4)-Mo(1)	105.1(6)	N(1)-C(1)-C(2)	111.7(8)
N(4)-C(2)-C(1)	106.0(8)	N(2)-C(3)-C(4)	112.7(8)
C(3)-C(4)-N(4)	106.7(8)	N(3)-C(5)-C(6)	111.4(8)
C(5)-C(6)-N(4)	108.6(8)	C(102)-C(101)-C(106)	106.7(10)
C(102)-C(101)-Mo(1)	120.0(7)	C(106)-C(101)-Mo(1)	116.9(7)
C(101)-C(102)-C(103)	114.2(9)	C(104)-C(103)-C(102)	112.2(9)
C(105)-C(104)-C(103)	112.7(11)	C(104)-C(105)-C(106)	110.0(9)
C(105)-C(106)-C(101)	114.2(9)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 2j.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mo(1)	20(1)	21(1)	32(1)	-3(1)	-3(1)	11(1)
Si(1)	29(1)	28(1)	53(2)	5(2)	9(1)	10(1)
Si(2)	33(1)	22(1)	52(2)	-2(1)	-2(2)	15(1)
Si(3)	32(1)	50(2)	43(2)	-6(2)	-1(2)	26(1)
N(1)	19(4)	39(5)	39(5)	0(4)	0(3)	9(4)
N(2)	21(4)	11(4)	59(6)	-3(3)	-3(4)	0(3)
N(3)	31(4)	32(4)	51(6)	-2(4)	6(4)	22(4)
N(4)	40(7)	18(5)	13(6)	3(3)	-6(3)	12(4)
C(1)	22(6)	59(7)	48(7)	1(5)	-3(5)	17(6)
C(2)	45(7)	18(5)	53(7)	-2(5)	-21(6)	12(5)
C(3)	36(6)	31(6)	58(8)	20(6)	19(6)	18(5)
C(4)	63(7)	66(8)	19(6)	-15(6)	-6(6)	43(7)
C(5)	48(7)	44(7)	37(7)	3(5)	-8(5)	30(6)
C(6)	34(6)	30(6)	55(7)	-6(6)	6(5)	16(5)
C(11)	37(6)	38(6)	96(9)	21(6)	21(6)	23(5)
C(12)	69(8)	39(7)	101(10)	-16(7)	-33(8)	18(6)
C(13)	76(9)	65(9)	98(11)	21(8)	38(8)	17(8)
C(21)	36(6)	44(6)	75(9)	-4(6)	0(6)	22(5)
C(22)	63(7)	34(6)	102(10)	22(7)	21(7)	24(6)
C(23)	81(9)	50(7)	89(9)	-9(7)	-13(8)	39(7)
C(31)	28(6)	87(10)	94(10)	-50(8)	-22(6)	8(6)
C(33)	89(9)	63(8)	108(10)	12(7)	-8(8)	57(8)
C(101)	29(7)	40(8)	32(9)	-1(5)	-6(5)	16(5)
C(102)	53(6)	44(6)	46(7)	-3(5)	0(6)	33(6)
C(103)	77(8)	69(8)	55(8)	-18(7)	-12(7)	51(7)
C(104)	112(10)	66(8)	29(6)	-24(7)	-26(7)	54(7)
C(105)	113(10)	62(8)	57(8)	5(6)	9(7)	72(8)
C(106)	53(7)	34(6)	38(6)	-2(5)	15(6)	26(5)

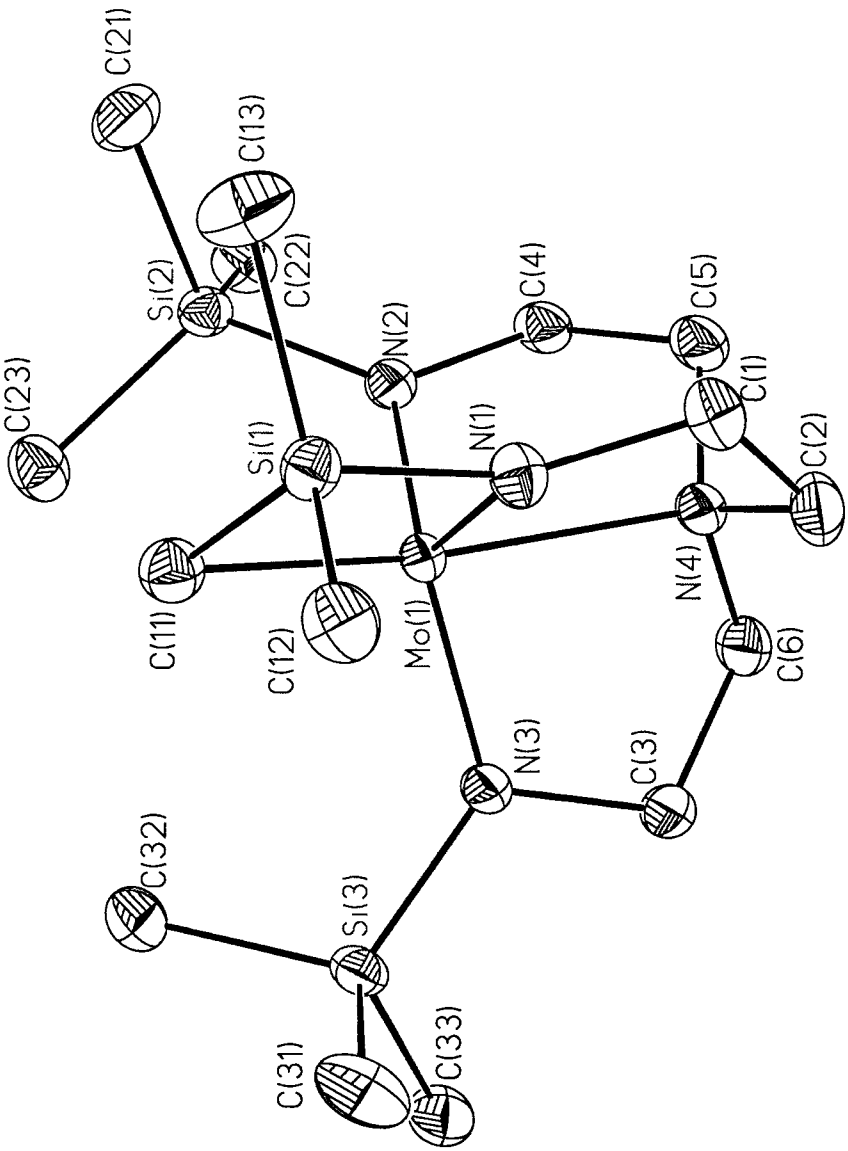
C(21)
C(13)
Si(2)
C(22)
N(2)
C(4)
C(5)
C(23)
Si(1)
N(1)
C(1)
C(2)
C(11)
C(12)
Mo(1)
N(4)
C(6)
N(3)
C(3)
C(32)
Si(3)
C(31)
C(33)

Table 1. Crystal data and structure refinement for [Ln'N$_3$N]Mo.

A. Crystal Data	
Identification code	96150
Empirical formula	$C_{15}H_{38}MoN_4Si_3$
Formula weight	454.70
Temperature	188(2) K
Wavelength	0.71073 Å
Crystal morphology	?
Crystal size	0.60 x 0.43 x 0.34 mm
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 8.972(3) Å alpha = 90°
	b = 17.308(4) Å beta = 100.61(3)°
	c = 15.398(3) Å gamma = 90°
Volume, Z	2350.2(11) Å^3, 4
Density (calculated)	1.285 Mg/m^3
Absorption coefficient	0.716 mm^{-1}
F(000)	960
B. Data Collection and Reduction	
Diffractometer	Siemens SMART/CCD
Scan Type	ω Scans
Scan angle	0.30°
θ range for data collection	1.79 to 23.26°
Limiting indices	$-8 \le h \le 9$, $-16 \le k \le 19$, $-16 \le l \le 16$
Reflections collected	9331
Independent reflections	3337 (R_{int} = 0.0240)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.3072 and 0.2595
C. Solution and Refinement	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3335 / 0 / 204
Goodness-of-fit on F^2	1.125
Final R indices [I>2σ(I)]	R1 = 0.0231, wR2 = 0.0572
R indices (all data)	R1 = 0.0242, wR2 = 0.0583
Extinction coefficient	0.0045(6)
Largest diff. peak and hole	0.293 and -0.248 $e\text{Å}^{-3}$
Weighting Scheme	calc w=1/[\s^2^(Fo^2^)+(0.0177P)^2^+2.2313P]

where P=(Fo

Notes Cell constants based upon three sets of fifteen (15) 0.30° ω scans. Refle were harvested using the Siemens XSCANS algorithm.

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for bit. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	1463(1)	5789(1)	2628(1)	22(1)
Si(1)	3860(1)	6381(1)	3957(1)	28(1)
Si(2)	458(1)	4087(1)	3362(1)	28(1)
Si(3)	2695(1)	5717(1)	718(1)	30(1)
N(1)	2066(2)	6655(1)	3422(1)	30(1)
N(2)	42(2)	5028(1)	2991(1)	27(1)
N(3)	1316(2)	5958(1)	1334(1)	28(1)
N(4)	-647(2)	6506(1)	2376(1)	27(1)
C(1)	1000(3)	7269(1)	3523(2)	34(1)
C(2)	-202(3)	7301(2)	2681(2)	38(1)
C(3)	100(3)	6492(2)	920(2)	35(1)
C(4)	-1568(3)	5274(1)	2882(2)	31(1)
C(5)	-1683(3)	6148(2)	2906(2)	34(1)
C(6)	-1222(3)	6466(2)	1413(2)	37(1)
C(11)	3859(3)	5504(2)	3270(2)	34(1)
C(12)	5265(3)	7154(2)	3850(2)	37(1)
C(13)	3907(4)	6219(2)	5158(2)	52(1)
C(21)	1072(4)	4063(2)	4588(2)	47(1)
C(22)	-1285(3)	3478(2)	3059(2)	41(1)
C(23)	1960(3)	3636(2)	2838(2)	40(1)
C(31)	4259(3)	6446(2)	899(2)	54(1)
C(32)	3474(3)	4735(2)	1008(2)	48(1)
C(33)	1871(3)	5714(2)	-489(2)	43(1)

Table 3. Bond lengths [Å] and angles [°] for [HIPTN$_3$N]Mo.

Mo(1)-N(1)	1.948(2)	Mo(1)-N(2)	1.983(2)
Mo(1)-N(3)	1.994(2)	Mo(1)-N(4)	2.237(2)
Mo(1)-C(11)	2.249(3)	Mo(1)-Si(1)	2.8705(11)
Si(1)-N(1)	1.734(2)	Si(1)-C(11)	1.849(3)
Si(1)-C(13)	1.865(3)	Si(1)-C(12)	1.866(3)
Si(2)-N(2)	1.743(2)	Si(2)-C(23)	1.865(3)
Si(2)-C(21)	1.867(3)	Si(2)-C(22)	1.873(3)
Si(3)-N(3)	1.743(2)	Si(3)-C(32)	1.861(3)
Si(3)-C(31)	1.869(3)	Si(3)-C(33)	1.869(3)
N(1)-C(1)	1.456(3)	N(2)-C(4)	1.486(3)
N(3)-C(3)	1.481(3)	N(4)-C(6)	1.479(3)
N(4)-C(5)	1.481(3)	N(4)-C(2)	1.485(3)
C(1)-C(2)	1.527(4)	C(3)-C(6)	1.523(3)
C(4)-C(5)	1.517(4)		

N(1)-Mo(1)-N(2)	116.95(8)	N(1)-Mo(1)-N(3)	118.27(8)
N(2)-Mo(1)-N(3)	116.83(8)	N(1)-Mo(1)-N(4)	79.03(8)
N(2)-Mo(1)-N(4)	81.40(8)	N(3)-Mo(1)-N(4)	81.20(7)
N(1)-Mo(1)-C(11)	76.13(9)	N(2)-Mo(1)-C(11)	110.04(9)
N(3)-Mo(1)-C(11)	110.68(9)	N(4)-Mo(1)-C(11)	155.16(8)
N(1)-Mo(1)-Si(1)	36.16(6)	N(2)-Mo(1)-Si(1)	118.21(6)
N(3)-Mo(1)-Si(1)	124.22(6)	N(4)-Mo(1)-Si(1)	115.11(6)
C(11)-Mo(1)-Si(1)	40.09(7)	N(1)-Si(1)-C(11)	92.93(11)
N(1)-Si(1)-C(13)	111.17(13)	C(11)-Si(1)-C(13)	116.21(13)
N(1)-Si(1)-C(12)	110.19(11)	C(11)-Si(1)-C(12)	117.86(12)
C(13)-Si(1)-C(12)	107.62(13)	N(1)-Si(1)-Mo(1)	41.53(7)
C(11)-Si(1)-Mo(1)	51.56(8)	C(13)-Si(1)-Mo(1)	122.04(10)
C(12)-Si(1)-Mo(1)	128.54(9)	N(2)-Si(2)-C(23)	112.15(11)
N(2)-Si(2)-C(21)	110.98(11)	C(23)-Si(2)-C(21)	109.07(14)
N(2)-Si(2)-C(22)	108.99(11)	C(23)-Si(2)-C(22)	107.03(13)
C(21)-Si(2)-C(22)	108.47(14)	N(3)-Si(3)-C(32)	111.15(11)
N(3)-Si(3)-C(31)	110.24(12)	C(32)-Si(3)-C(31)	110.0(2)
N(3)-Si(3)-C(33)	110.56(12)	C(32)-Si(3)-C(33)	107.36(13)
C(31)-Si(3)-C(33)	107.42(14)	C(1)-N(1)-Si(1)	136.1(2)
C(1)-N(1)-Mo(1)	121.1(2)	Si(1)-N(1)-Mo(1)	102.30(10)
C(4)-N(2)-Si(2)	116.7(2)	C(4)-N(2)-Mo(1)	116.1(2)
Si(2)-N(2)-Mo(1)	127.08(10)	C(3)-N(3)-Si(3)	117.1(2)
C(3)-N(3)-Mo(1)	115.47(14)	Si(3)-N(3)-Mo(1)	125.87(11)
C(6)-N(4)-C(5)	113.2(2)	C(6)-N(4)-C(2)	112.6(2)
C(5)-N(4)-C(2)	111.9(2)	C(6)-N(4)-Mo(1)	106.01(14)
C(5)-N(4)-Mo(1)	105.62(14)	C(2)-N(4)-Mo(1)	106.87(14)
N(1)-C(1)-C(2)	108.2(2)	N(4)-C(2)-C(1)	109.9(2)
N(3)-C(3)-C(6)	110.3(2)	N(2)-C(4)-C(5)	110.6(2)
N(4)-C(5)-C(4)	110.6(2)	N(4)-C(6)-C(3)	109.8(2)
Si(1)-C(11)-Mo(1)	88.35(10)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for [bit N_3N]Mo.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mo(1)	19(1)	24(1)	23(1)	2(1)	5(1)	3(1)
Si(1)	25(1)	29(1)	28(1)	1(1)	2(1)	1(1)
Si(2)	32(1)	26(1)	27(1)	0(1)	7(1)	-1(1)
Si(3)	29(1)	35(1)	27(1)	-2(1)	10(1)	2(1)
N(1)	26(1)	30(1)	32(1)	-1(1)	3(1)	2(1)
N(2)	23(1)	30(1)	27(1)	2(1)	6(1)	1(1)
N(3)	24(1)	36(1)	25(1)	4(1)	7(1)	7(1)
N(4)	22(1)	32(1)	27(1)	3(1)	7(1)	5(1)
C(1)	32(1)	29(1)	40(1)	-5(1)	8(1)	3(1)
C(2)	34(1)	32(1)	48(2)	2(1)	9(1)	10(1)
C(3)	32(1)	47(2)	28(1)	10(1)	7(1)	12(1)
C(4)	24(1)	39(1)	32(1)	1(1)	7(1)	-1(1)
C(5)	25(1)	45(2)	34(1)	2(1)	9(1)	6(1)
C(6)	29(1)	48(2)	34(1)	6(1)	4(1)	12(1)
C(12)	31(1)	38(2)	42(2)	-4(1)	5(1)	-2(1)
C(13)	59(2)	61(2)	34(2)	7(1)	4(1)	-6(2)
C(21)	65(2)	40(2)	33(2)	4(1)	3(1)	8(1)
C(22)	41(2)	35(2)	49(2)	-1(1)	16(1)	-9(1)
C(23)	39(2)	30(1)	53(2)	-3(1)	14(1)	0(1)
C(31)	40(2)	66(2)	61(2)	-16(2)	23(2)	-13(2)
C(32)	54(2)	51(2)	43(2)	1(1)	19(1)	19(1)
C(33)	52(2)	51(2)	30(1)	-4(1)	12(1)	10(1)