Supporting Information for the paper:

Molybdenum dinitrogen complexes facially coordinated by linear tridentate PEP ligands (E = N or P): Impact of the central E donor in *trans*-position to N_2

Svea Hinrichsen[a], Ann-Christin Schnoor[a], Katharina Grund[a], Benedikt Flöser[a], Alexander Schlimm[a], Christian Näther[a], Jan Krahmer[a] and Felix Tuczek*[a]

* Prof. Dr. Felix Tuczek
Fax: +49 (0)431 880-1520
E-Mail: ftuczek@ac.uni-kiel.de

[a] Institut für Anorganische Chemie
Christian-Albrechts-Universität zu Kiel
Max-Eyth-Straße 2
D-24118 Kiel

Content

1 Syntheses:

Synthesis of *N*,*N*-Bis[2-(*p*-toluenesulfonyl)ethyl]benzamine.
p-Toluenesulfonyl chloride (10.5 g, 55.2 mmol) was added to a ice-cooled mixture of *N*-phenyldiethanolamine (5.00 g, 27.6 mmol) in 1,4-dioxane (40 mL). The reaction mixture was stirred for 1 h at 0 °C. Sodium hydroxide (30 %, 30 mL) and water (50 mL) were added and the aqueous layer was extracted three times with CH_2Cl_2 (80 mL). After the removal of the solvent methanol (10 mL) was added and the mixture was placed for 30 min in the freezer. The resulting suspension was filtered and the white product was washed with cold methanol and dried in vacuo to yield 8.55 g (63 %) of a white solid.

Synthesis of *N*,*N*-Bis[2-(diphenylphosphino)ethyl]benzamine (PN(Ph)P).
n-BuLi (2.5 M solution in *n*-hexan, 5.30 mL, 13.0 mmol) was added to a ice-cooled solution of diphenylphosphine (2.40 g, 12.9 mmol) in THF (40 mL). The red solution was added dropwise to a solution of *N*,*N*-bis[2-(*p*-toluenesulfonyl)ethyl]benzamine (3.00 g, 6.13 mmol) in THF (20 mL) and stirred for 18 h at room temperature. Water (10 mL) was added to the reaction mixture and stirred for 30 min. The aqueous layer was removed and the solution was evaporated. The residue was purified via column chromatography (petroleum ether/THF 3:2) to yield 2.95 g (93 %) of a white solid.

Synthesis of *N*,*N*-Bis[3-(methanesulfonyl)propyl]benzamine.
Triethylamine (2.18 g, 21.5 mmol) and methanesulfonylchloride (2.13 g, 18.6 mmol) were added to a ice-cooled mixture of 3-[(3-hydroxypropyl)anilino]-1-propanol (1.50 g, 7.15 mmol) in CH_2Cl_2 (100 mL). The reaction mixture was stirred for 20 min at 0 °C and for 3 d at room temperature. Water (40 mL) was added and the aqueous layer was extracted three times with CH_2Cl_2 (40 mL). The combined organic phases were evaporated to yield 2.44 g (93 %) of a brown oil.

2 Crystal Structure:

2.1 [Mo(N_2)(prPP(Ph)P)(dmpm)] (2)

Table S1. Crystal data and structure refinement for $Mo(N_2)(C_5H_{14}P_2)(C_{36}H_{37}P_3)$.

Empirical formula	$C_{41}H_{51}MoN_2P_5$	
Formula weight	822.62	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.2404(3) Å	α= 90°.
	b = 17.7665(4) Å	β= 98.553(2)°.
	c = 20.0607(6) Å	γ = 90°.
Volume	3961.62(18) $Å^3$	

Z	4
Density (calculated)	1.379 Mg/m^3
Absorption coefficient	0.565 mm^{-1}
F(000)	1712
Crystal size	0.09 x 0.15 x 0-22 mm^3
Theta range for data collection	1.539 to 26.005°.
Index ranges	-13<=h<=13, -19<=k<=21, -24<=l<=24
Reflections collected	30028
Independent reflections	7759 [R(int) = 0.0264]
Completeness to theta = 25.242°	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7759 / 0 / 447
Goodness-of-fit on F^2	1.059
Final R indices [I>2sigma(I)]	R1 = 0.0344, wR2 = 0.0812
R indices (all data)	R1 = 0.0406, wR2 = 0.0841
Extinction coefficient	0.0021(4)
Largest diff. peak and hole	0.444 and -0.481 $e.Å^{-3}$

Comments:
A numerical absorption correction was performed (Tmin/max: 0.8624/0.9414). All non-hydrogen atoms were refined anisotropic. The C-H hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and refined isotropic with $U_{iso}(H) = 1.2\ U_{eq}(C)$ (1.5 for methyl H atoms) using a riding model.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	5864(1)	7222(1)	3520(1)	23(1)
N(1)	5278(2)	8286(1)	3323(1)	29(1)
N(2)	4956(2)	8877(1)	3221(1)	38(1)
P(1)	6744(1)	7735(1)	4609(1)	27(1)
C(1)	7197(2)	7114(1)	5348(1)	32(1)
C(2)	7715(2)	6353(2)	5197(1)	37(1)
C(3)	6815(2)	5801(2)	4814(1)	33(1)
P(2)	6496(1)	5954(1)	3894(1)	27(1)
C(4)	5460(2)	5146(1)	3672(1)	35(1)
C(5)	4165(2)	5256(2)	3797(1)	35(1)
C(6)	3460(2)	5837(1)	3337(1)	33(1)
P(3)	3831(1)	6817(1)	3612(1)	26(1)
C(11)	5952(2)	8448(1)	5063(1)	32(1)
C(12)	4737(2)	8581(2)	4880(1)	36(1)
C(13)	4128(3)	9082(2)	5239(2)	48(1)
C(14)	4734(3)	9462(2)	5784(2)	55(1)
C(15)	5951(3)	9351(2)	5970(2)	53(1)
C(16)	6561(3)	8848(2)	5614(1)	44(1)
C(21)	8133(2)	8288(2)	4595(1)	36(1)
C(22)	8035(3)	9013(2)	4330(2)	49(1)
C(23)	9055(4)	9441(2)	4280(2)	64(1)
C(24)	10187(3)	9149(2)	4492(2)	67(1)
C(25)	10303(3)	8437(2)	4757(2)	62(1)
C(26)	9290(2)	8011(2)	4811(2)	46(1)
C(31)	7837(2)	5498(1)	3628(1)	30(1)
C(32)	8890(2)	5316(1)	4057(1)	34(1)

C(33)	9890(2)	5045(2)	3809(2)	40(1)
C(34)	9869(2)	4932(2)	3126(2)	42(1)
C(35)	8813(2)	5081(2)	2694(1)	40(1)
C(36)	7818(2)	5360(2)	2945(1)	34(1)
C(41)	2661(2)	7352(2)	3061(1)	32(1)
C(42)	2095(2)	7076(2)	2442(1)	38(1)
C(43)	1333(2)	7531(2)	2005(1)	45(1)
C(44)	1125(2)	8260(2)	2176(2)	48(1)
C(45)	1643(3)	8538(2)	2793(2)	53(1)
C(46)	2402(2)	8082(2)	3235(2)	43(1)
C(51)	3109(2)	6764(1)	4389(1)	29(1)
C(52)	1905(2)	6568(2)	4373(1)	34(1)
C(53)	1437(2)	6456(2)	4965(1)	39(1)
C(54)	2143(2)	6553(2)	5585(1)	37(1)
C(55)	3333(2)	6764(2)	5608(1)	36(1)
C(56)	3807(2)	6858(2)	5014(1)	33(1)
C(61)	7930(2)	8443(2)	2689(1)	39(1)
C(62)	9195(2)	7163(2)	3196(1)	37(1)
P(4)	7642(1)	7489(1)	2972(1)	28(1)
C(63)	7082(2)	7036(2)	2156(1)	32(1)
P(5)	5508(1)	6984(1)	2310(1)	28(1)
C(64)	4876(2)	6186(2)	1785(1)	39(1)
C(65)	4803(2)	7750(2)	1780(1)	38(1)

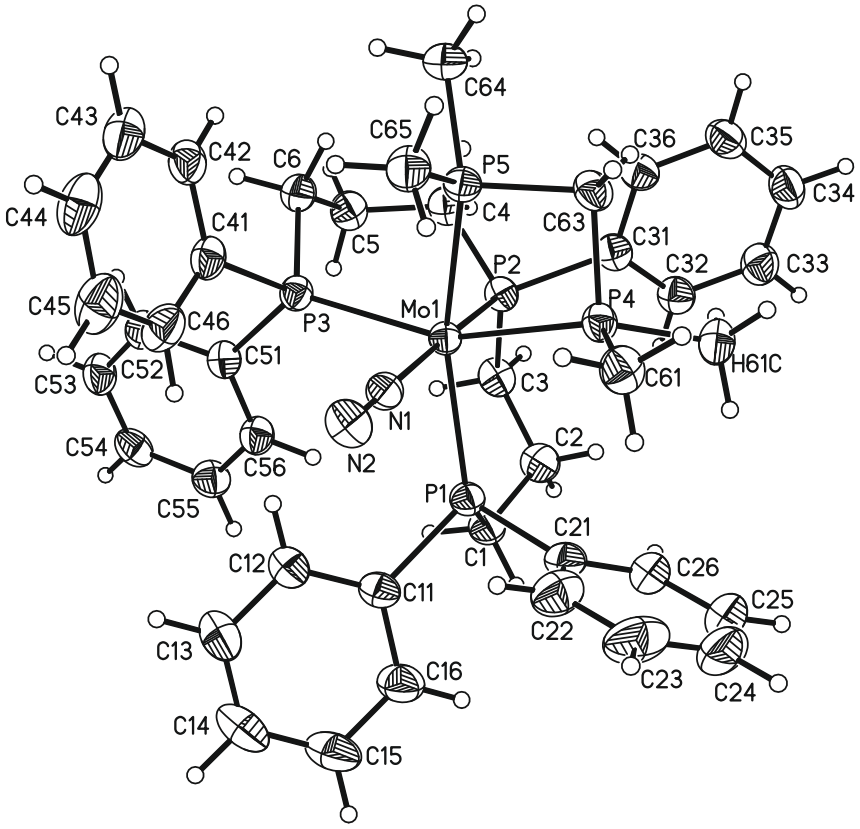

Fig. S1 Crystal structure of [Mo(N_2)(prPP(Ph)P)(dmpm)] (**2**).

Table S3. Bond lengths [Å] and angles [°].

Mo(1)-N(1)	2.021(2)	Mo(1)-P(5)	2.4390(6)
Mo(1)-P(3)	2.4285(6)	Mo(1)-P(2)	2.4460(6)
Mo(1)-P(1)	2.4363(6)	Mo(1)-P(4)	2.4656(6)
N(1)-Mo(1)-P(3)	90.52(6)	P(1)-Mo(1)-P(2)	90.53(2)
N(1)-Mo(1)-P(1)	84.44(6)	P(5)-Mo(1)-P(2)	98.19(2)
P(3)-Mo(1)-P(1)	107.69(2)	N(1)-Mo(1)-P(4)	89.71(6)
N(1)-Mo(1)-P(5)	88.08(6)	P(3)-Mo(1)-P(4)	157.64(2)

P(3)-Mo(1)-P(5)	90.42(2)	P(1)-Mo(1)-P(4)	94.58(2)
P(1)-Mo(1)-P(5)	160.41(2)	P(5)-Mo(1)-P(4)	67.25(2)
N(1)-Mo(1)-P(2)	173.04(6)	P(2)-Mo(1)-P(4)	95.50(2)
P(3)-Mo(1)-P(2)	86.41(2)		
N(1)-N(2)	1.120(3)	N(2)-N(1)-Mo(1)	179.2(2)
P(1)-C(21)	1.848(3)	C(23)-C(24)	1.381(6)
P(1)-C(1)	1.859(2)	C(24)-C(25)	1.370(6)
P(1)-C(11)	1.862(3)	C(25)-C(26)	1.386(4)
C(1)-C(2)	1.520(4)	C(31)-C(36)	1.390(4)
C(2)-C(3)	1.531(4)	C(31)-C(32)	1.394(3)
C(3)-P(2)	1.848(2)	C(32)-C(33)	1.383(4)
P(2)-C(31)	1.858(2)	C(33)-C(34)	1.382(4)
P(2)-C(4)	1.861(3)	C(34)-C(35)	1.386(4)
C(4)-C(5)	1.526(3)	C(35)-C(36)	1.384(4)
C(5)-C(6)	1.525(3)	C(41)-C(46)	1.385(4)
C(6)-P(3)	1.855(3)	C(41)-C(42)	1.399(4)
P(3)-C(41)	1.849(2)	C(42)-C(43)	1.390(4)
P(3)-C(51)	1.864(2)	C(43)-C(44)	1.369(5)
C(11)-C(12)	1.381(4)	C(44)-C(45)	1.379(5)
C(11)-C(16)	1.403(4)	C(45)-C(46)	1.395(4)
C(12)-C(13)	1.387(4)	C(51)-C(56)	1.386(3)
C(13)-C(14)	1.376(5)	C(51)-C(52)	1.394(3)
C(14)-C(15)	1.378(5)	C(52)-C(53)	1.382(4)
C(15)-C(16)	1.388(4)	C(53)-C(54)	1.382(4)
C(21)-C(22)	1.392(4)	C(54)-C(55)	1.383(4)
C(21)-C(26)	1.398(4)	C(55)-C(56)	1.387(4)
C(22)-C(23)	1.392(4)	C(24)-C(23)-C(22)	120.3(4)
C(21)-P(1)-C(1)	101.29(12)	C(25)-C(24)-C(23)	119.7(3)
C(21)-P(1)-C(11)	96.41(12)	C(24)-C(25)-C(26)	120.2(3)
C(1)-P(1)-C(11)	96.20(11)	C(25)-C(26)-C(21)	121.4(3)
C(2)-C(1)-P(1)	115.90(17)	C(36)-C(31)-C(32)	117.1(2)
C(1)-C(2)-C(3)	115.2(2)	C(36)-C(31)-P(2)	117.75(18)
C(2)-C(3)-P(2)	115.03(18)	C(32)-C(31)-P(2)	125.07(19)
C(3)-P(2)-C(31)	100.20(11)	C(33)-C(32)-C(31)	121.3(2)
C(3)-P(2)-C(4)	98.44(12)	C(34)-C(33)-C(32)	120.8(2)
C(31)-P(2)-C(4)	95.77(11)	C(33)-C(34)-C(35)	118.6(2)
C(5)-C(4)-P(2)	116.12(18)	C(36)-C(35)-C(34)	120.3(3)
C(6)-C(5)-C(4)	114.2(2)	C(35)-C(36)-C(31)	121.8(2)
C(5)-C(6)-P(3)	112.42(17)	C(46)-C(41)-C(42)	117.8(2)
C(41)-P(3)-C(6)	101.32(11)	C(46)-C(41)-P(3)	119.25(19)
C(41)-P(3)-C(51)	99.58(11)	C(42)-C(41)-P(3)	122.7(2)
C(6)-P(3)-C(51)	95.39(11)	C(43)-C(42)-C(41)	120.8(3)
C(12)-C(11)-C(16)	118.0(2)	C(44)-C(43)-C(42)	120.3(3)
C(12)-C(11)-P(1)	120.82(19)	C(43)-C(44)-C(45)	119.9(3)
C(16)-C(11)-P(1)	121.1(2)	C(44)-C(45)-C(46)	120.0(3)
C(11)-C(12)-C(13)	121.1(3)	C(41)-C(46)-C(45)	121.0(3)
C(14)-C(13)-C(12)	120.2(3)	C(56)-C(51)-C(52)	117.9(2)
C(13)-C(14)-C(15)	120.0(3)	C(56)-C(51)-P(3)	119.44(18)
C(14)-C(15)-C(16)	119.9(3)	C(52)-C(51)-P(3)	122.40(18)
C(15)-C(16)-C(11)	120.8(3)	C(53)-C(52)-C(51)	120.5(2)
C(22)-C(21)-C(26)	117.5(3)	C(54)-C(53)-C(52)	121.0(2)
C(22)-C(21)-P(1)	118.6(2)	C(53)-C(54)-C(55)	119.1(2)
C(26)-C(21)-P(1)	123.8(2)	C(54)-C(55)-C(56)	119.8(2)
C(21)-C(22)-C(23)	120.9(3)	C(51)-C(56)-C(55)	121.6(2)
C(61)-P(4)	1.830(3)	C(63)-P(5)	1.843(2)
C(62)-P(4)	1.831(2)	P(5)-C(65)	1.833(3)
P(4)-C(63)	1.850(2)	P(5)-C(64)	1.845(3)
C(61)-P(4)-C(62)	99.37(13)	C(65)-P(5)-C(63)	102.07(12)
C(61)-P(4)-C(63)	100.43(12)	C(65)-P(5)-C(64)	98.25(13)
C(62)-P(4)-C(63)	105.36(12)	C(63)-P(5)-C(64)	103.89(12)
P(5)-C(63)-P(4)	94.68(11)		

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2} U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	23(1)	25(1)	21(1)	1(1)	3(1)	1(1)
N(1)	28(1)	34(1)	24(1)	0(1)	6(1)	-2(1)
N(2)	45(1)	29(1)	40(1)	6(1)	11(1)	4(1)
P(1)	27(1)	30(1)	23(1)	-1(1)	2(1)	2(1)
C(1)	33(1)	40(1)	23(1)	-1(1)	0(1)	5(1)
C(2)	38(1)	40(2)	31(1)	3(1)	-2(1)	10(1)
C(3)	38(1)	32(1)	30(1)	7(1)	8(1)	4(1)
P(2)	28(1)	26(1)	27(1)	2(1)	5(1)	2(1)
C(4)	36(1)	29(1)	40(1)	1(1)	7(1)	0(1)
C(5)	35(1)	30(1)	42(1)	1(1)	10(1)	-4(1)
C(6)	30(1)	36(1)	34(1)	-1(1)	6(1)	-3(1)
P(3)	25(1)	30(1)	25(1)	2(1)	4(1)	0(1)
C(11)	40(1)	31(1)	26(1)	-2(1)	4(1)	2(1)
C(12)	39(1)	36(1)	34(1)	0(1)	8(1)	4(1)
C(13)	47(2)	50(2)	50(2)	-1(1)	15(1)	13(1)
C(14)	74(2)	48(2)	46(2)	-7(1)	21(2)	18(2)
C(15)	74(2)	48(2)	36(2)	-12(1)	3(1)	9(2)
C(16)	50(2)	46(2)	35(1)	-9(1)	-2(1)	7(1)
C(21)	38(1)	42(2)	29(1)	-8(1)	4(1)	-4(1)
C(22)	52(2)	47(2)	46(2)	0(1)	4(1)	-12(1)
C(23)	84(3)	52(2)	56(2)	-6(2)	12(2)	-32(2)
C(24)	55(2)	82(3)	70(2)	-24(2)	21(2)	-36(2)
C(25)	38(2)	77(3)	72(2)	-26(2)	12(2)	-16(2)
C(26)	35(1)	53(2)	51(2)	-13(1)	7(1)	-6(1)
C(31)	33(1)	24(1)	35(1)	2(1)	7(1)	1(1)
C(32)	36(1)	30(1)	36(1)	1(1)	4(1)	4(1)
C(33)	34(1)	38(2)	48(2)	0(1)	4(1)	7(1)
C(34)	37(1)	38(2)	53(2)	-6(1)	16(1)	3(1)
C(35)	44(1)	36(1)	41(1)	-7(1)	13(1)	1(1)
C(36)	37(1)	32(1)	35(1)	-3(1)	6(1)	2(1)
C(41)	25(1)	40(1)	32(1)	5(1)	6(1)	-1(1)
C(42)	32(1)	53(2)	30(1)	3(1)	7(1)	6(1)
C(43)	31(1)	72(2)	31(1)	12(1)	5(1)	2(1)
C(44)	34(1)	60(2)	49(2)	24(2)	0(1)	2(1)
C(45)	41(2)	42(2)	71(2)	14(2)	-4(1)	5(1)
C(46)	35(1)	41(2)	49(2)	4(1)	-6(1)	1(1)
C(51)	28(1)	29(1)	31(1)	3(1)	6(1)	2(1)
C(52)	28(1)	40(1)	34(1)	1(1)	4(1)	2(1)
C(53)	29(1)	44(2)	47(2)	-3(1)	14(1)	-2(1)
C(54)	44(1)	36(1)	35(1)	-1(1)	18(1)	1(1)
C(55)	39(1)	41(2)	28(1)	1(1)	6(1)	2(1)
C(56)	29(1)	36(1)	34(1)	2(1)	6(1)	-1(1)
C(61)	40(1)	35(1)	42(1)	4(1)	12(1)	-3(1)
C(62)	28(1)	44(2)	39(1)	4(1)	7(1)	1(1)
P(4)	26(1)	31(1)	27(1)	2(1)	6(1)	0(1)
C(63)	34(1)	37(1)	26(1)	2(1)	9(1)	2(1)
P(5)	29(1)	34(1)	22(1)	0(1)	3(1)	0(1)
C(64)	40(1)	44(2)	31(1)	-7(1)	3(1)	-2(1)
C(65)	36(1)	47(2)	30(1)	5(1)	4(1)	2(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3).

	x	y	z	U(eq)
H(1A)	7802	7383	5671	39
H(1B)	6484	7028	5575	39
H(2A)	8067	6117	5629	45
H(2B)	8377	6435	4931	45
H(3A)	6049	5836	5000	40
H(3B)	7128	5284	4898	40
H(4A)	5447	5030	3188	42
H(4B)	5796	4702	3932	42
H(5A)	3741	4767	3736	42
H(5B)	4174	5413	4271	42
H(6A)	2588	5751	3331	39
H(6B)	3638	5769	2872	39
H(12)	4311	8326	4502	44
H(13)	3291	9163	5108	58
H(14)	4313	9800	6032	66
H(15)	6373	9619	6342	64
H(16)	7400	8773	5745	53
H(22)	7261	9218	4180	59
H(23)	8973	9935	4099	76
H(24)	10883	9441	4455	81
H(25)	11081	8236	4904	74
H(26)	9383	7519	4999	56
H(32)	8921	5380	4530	41
H(33)	10602	4934	4112	49
H(34)	10563	4757	2955	50
H(35)	8773	4992	2224	48
H(36)	7103	5459	2641	41
H(42)	2234	6571	2317	46
H(43)	955	7335	1586	53
H(44)	625	8574	1870	58
H(45)	1483	9040	2917	63
H(46)	2746	8275	3662	51
H(52)	1401	6510	3952	41
H(53)	619	6312	4946	47
H(54)	1815	6475	5990	44
H(55)	3823	6845	6030	43
H(56)	4631	6989	5035	39
H(61A)	8318	8740	3073	58
H(61B)	7167	8680	2500	58
H(61C)	8460	8419	2344	58
H(62A)	9621	7220	2806	55
H(62B)	9196	6631	3327	55
H(62C)	9600	7462	3573	55
H(63A)	7183	7357	1764	38
H(63B)	7442	6534	2108	38
H(64A)	5087	6237	1330	58
H(64B)	3999	6182	1760	58
H(64C)	5208	5713	1985	58
H(65A)	5195	8227	1925	57
H(65B)	3947	7779	1823	57
H(65C)	4889	7654	1308	57

2.2 [Mo(N_2)(prPPHP)(dmpm)] (3)

Table S6. Crystal data and structure refinement for Mo(N_2)($C_5H_{14}P_2$)($C_{30}H_{53}P_3$).

Empirical formula	$C_{35}H_{47}MoN_2P_5$	
Formula weight	746.53	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.4524(2) Å	α= 90°.
	b = 18.9236(3) Å	β= 93.240(2)°.
	c = 20.0445(4) Å	γ = 90°.
Volume	3579.70(12) $Å^3$	
Z	4	
Density (calculated)	1.385 Mg/m^3	
Absorption coefficient	0.617 mm^{-1}	
F(000)	1552	
Crystal size	0.11 x 0.20 x 0.28 mm^3	
Theta range for data collection	1.481 to 26.004°.	
Index ranges	-11<=h<=11, -23<=k<=23, -23<=l<=24	
Reflections collected	46604	
Independent reflections	7030 [R(int) = 0.0532]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7030 / 0 / 397	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0323, wR2 = 0.0868	
R indices (all data)	R1 = 0.0358, wR2 = 0.0891	
Extinction coefficient	0.0013(3)	
Largest diff. peak and hole	0.622 and -0.716 $e.Å^{-3}$	

Comments:
A numerical absorption correction was performed (Tmin/max: 0.7655/0.9339). All non-hydrogen atoms were refined anisotropic. The C-H hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and refined isotropic with $U_{iso}(H) = 1.2\ U_{eq}(C)$ (1.5 for methyl H atoms) using a riding model. The P-H H atom was located in difference map and was refined isotropic.

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	5232(1)	7008(1)	2733(1)	29(1)
N(1)	3153(2)	7109(1)	2431(1)	35(1)
N(2)	2020(2)	7173(1)	2252(1)	47(1)
P(1)	4494(1)	6783(1)	3854(1)	34(1)
C(1)	5830(2)	6576(1)	4545(1)	44(1)
C(2)	7329(3)	6865(2)	4474(1)	51(1)
C(3)	8141(3)	6501(2)	3931(1)	50(1)
P(2)	7681(1)	6854(1)	3089(1)	38(1)
C(4)	8896(2)	6337(1)	2586(1)	46(1)
C(5)	8318(2)	5624(1)	2341(1)	45(1)
C(6)	7081(2)	5673(1)	1818(1)	40(1)
P(3)	5371(1)	5872(1)	2192(1)	32(1)
C(11)	3523(2)	7537(1)	4202(1)	39(1)
C(12)	4157(3)	8042(1)	4624(1)	44(1)
C(13)	3411(3)	8647(1)	4799(1)	51(1)
C(14)	2028(3)	8742(1)	4564(1)	51(1)
C(15)	1365(3)	8234(1)	4171(1)	48(1)
C(16)	2106(3)	7639(1)	3985(1)	43(1)
C(21)	3173(2)	6095(1)	4041(1)	36(1)
C(22)	2884(3)	5920(1)	4697(1)	49(1)
C(23)	1980(3)	5370(2)	4829(2)	60(1)
C(24)	1324(3)	4997(2)	4311(2)	59(1)
C(25)	1548(3)	5180(1)	3660(2)	54(1)
C(26)	2473(2)	5726(1)	3529(1)	43(1)
C(31)	5163(2)	5001(1)	2602(1)	35(1)
C(32)	5341(2)	4960(1)	3293(1)	42(1)
C(33)	5151(3)	4326(1)	3624(1)	50(1)
C(34)	4794(2)	3721(1)	3269(1)	49(1)
C(35)	4658(2)	3748(1)	2581(1)	46(1)
C(36)	4836(2)	4382(1)	2248(1)	40(1)
C(41)	4116(2)	5756(1)	1461(1)	35(1)
C(42)	2698(2)	5604(1)	1556(1)	43(1)
C(43)	1708(3)	5557(2)	1021(1)	49(1)
C(44)	2104(3)	5665(1)	377(1)	48(1)
C(45)	3500(3)	5823(2)	275(1)	53(1)
C(46)	4485(3)	5865(1)	809(1)	48(1)
P(4)	5484(1)	8275(1)	2914(1)	33(1)
P(5)	5812(1)	7634(1)	1718(1)	35(1)
C(51)	6651(3)	8729(1)	3540(1)	46(1)
C(52)	3960(2)	8864(1)	2901(1)	44(1)
C(53)	6302(2)	8479(1)	2120(1)	38(1)
C(54)	4355(3)	7877(2)	1124(1)	55(1)
C(55)	7206(3)	7512(2)	1124(1)	52(1)

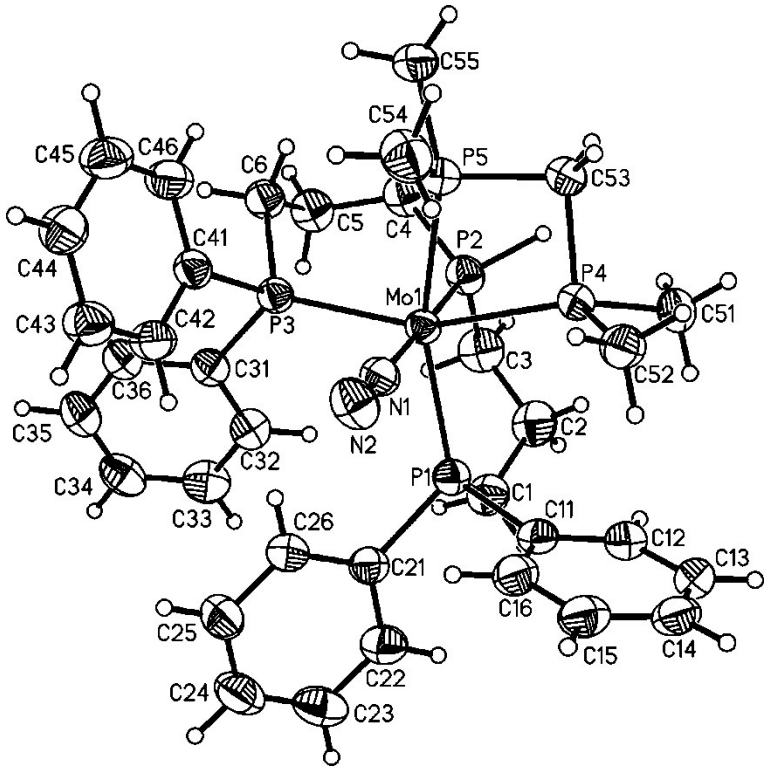

Fig. S2 ORTEP-Plot of [MoN_2(prPPHP)(dmpm)] (**3**).

Table S8. Bond lengths [Å] and angles [°].

Mo(1)-N(1)	2.0323(19)	Mo(1)-P(1)	2.4287(6)
Mo(1)-P(2)	2.4015(6)	Mo(1)-P(4)	2.4338(6)
Mo(1)-P(3)	2.4146(6)	Mo(1)-P(5)	2.4414(6)
N(1)-Mo(1)-P(2)	178.39(5)	P(3)-Mo(1)-P(4)	159.428(19)
N(1)-Mo(1)-P(3)	91.49(5)	P(1)-Mo(1)-P(4)	93.762(19)
P(2)-Mo(1)-P(3)	87.10(2)	N(1)-Mo(1)-P(5)	88.05(5)
N(1)-Mo(1)-P(1)	88.21(5)	P(2)-Mo(1)-P(5)	92.77(2)
P(2)-Mo(1)-P(1)	91.46(2)	P(3)-Mo(1)-P(5)	92.120(19)
P(3)-Mo(1)-P(1)	106.59(2)	P(1)-Mo(1)-P(5)	161.01(2)
N(1)-Mo(1)-P(4)	92.13(5)	P(4)-Mo(1)-P(5)	67.785(19)
P(2)-Mo(1)-P(4)	89.45(2)	N(2)-N(1)-Mo(1)	178.32(19)
N(1)-N(2)	1.116(3)		
P(1)-C(11)	1.853(2)	C(21)-C(26)	1.379(3)
P(1)-C(21)	1.857(2)	C(21)-C(22)	1.398(3)
P(1)-C(1)	1.861(2)	C(22)-C(23)	1.381(4)
C(1)-C(2)	1.533(4)	C(23)-C(24)	1.374(4)
C(2)-C(3)	1.530(4)	C(24)-C(25)	1.379(4)
C(3)-P(2)	1.844(3)	C(25)-C(26)	1.388(3)
P(2)-C(4)	1.851(2)	C(31)-C(32)	1.388(3)
C(4)-C(5)	1.527(3)	C(31)-C(36)	1.394(3)
C(5)-C(6)	1.528(3)	C(32)-C(33)	1.388(3)
C(6)-P(3)	1.858(2)	C(33)-C(34)	1.380(4)
P(3)-C(41)	1.844(2)	C(34)-C(35)	1.379(4)
P(3)-C(31)	1.858(2)	C(35)-C(36)	1.390(3)
C(11)-C(12)	1.390(3)	C(41)-C(46)	1.388(3)
C(11)-C(16)	1.399(3)	C(41)-C(42)	1.395(3)
C(12)-C(13)	1.399(3)	C(42)-C(43)	1.386(3)
C(13)-C(14)	1.376(4)	C(43)-C(44)	1.379(3)
C(14)-C(15)	1.373(4)	C(44)-C(45)	1.379(4)
C(15)-C(16)	1.387(3)	C(45)-C(46)	1.380(4)
C(11)-P(1)-C(21)	96.35(10)	C(24)-C(23)-C(22)	120.0(3)
C(11)-P(1)-C(1)	102.22(11)	C(23)-C(24)-C(25)	120.0(2)
C(21)-P(1)-C(1)	97.93(11)	C(24)-C(25)-C(26)	119.9(3)
C(2)-C(1)-P(1)	116.58(17)	C(21)-C(26)-C(25)	121.1(2)
C(3)-C(2)-C(1)	114.1(2)	C(32)-C(31)-C(36)	118.1(2)
C(2)-C(3)-P(2)	112.70(18)	C(32)-C(31)-P(3)	118.79(17)

C(3)-P(2)-C(4)	100.71(12)	C(36)-C(31)-P(3)	123.08(17)
C(5)-C(4)-P(2)	114.85(16)	C(33)-C(32)-C(31)	121.0(2)
C(4)-C(5)-C(6)	114.4(2)	C(34)-C(33)-C(32)	120.3(2)
C(5)-C(6)-P(3)	112.66(16)	C(35)-C(34)-C(33)	119.4(2)
C(41)-P(3)-C(31)	99.55(10)	C(34)-C(35)-C(36)	120.4(2)
C(41)-P(3)-C(6)	101.02(10)	C(35)-C(36)-C(31)	120.7(2)
C(31)-P(3)-C(6)	96.59(10)	C(46)-C(41)-C(42)	117.0(2)
C(12)-C(11)-C(16)	117.8(2)	C(46)-C(41)-P(3)	123.08(17)
C(12)-C(11)-P(1)	123.57(19)	C(42)-C(41)-P(3)	119.76(16)
C(16)-C(11)-P(1)	118.41(18)	C(43)-C(42)-C(41)	121.3(2)
C(11)-C(12)-C(13)	120.6(2)	C(44)-C(43)-C(42)	120.5(2)
C(14)-C(13)-C(12)	120.3(2)	C(45)-C(44)-C(43)	118.9(2)
C(15)-C(14)-C(13)	119.9(2)	C(44)-C(45)-C(46)	120.5(2)
C(14)-C(15)-C(16)	120.1(2)	C(45)-C(46)-C(41)	121.8(2)
C(15)-C(16)-C(11)	121.2(2)	C(22)-C(21)-P(1)	121.68(18)
C(26)-C(21)-C(22)	117.9(2)	C(23)-C(22)-C(21)	121.0(2)
C(26)-C(21)-P(1)	120.35(17)	P(5)-C(54)	1.829(3)
P(4)-C(52)	1.821(2)	P(5)-C(53)	1.838(2)
P(4)-C(51)	1.837(2)	P(5)-C(55)	1.840(2)
P(4)-C(53)	1.848(2)	C(54)-P(5)-C(55)	98.62(14)
C(52)-P(4)-C(51)	99.61(12)	C(53)-P(5)-C(55)	102.76(11)
C(52)-P(4)-C(53)	103.24(11)	P(5)-C(53)-P(4)	95.02(10)
C(51)-P(4)-C(53)	103.08(11)		
C(54)-P(5)-C(53)	103.13(12)		

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2} U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	26(1)	31(1)	31(1)	0(1)	3(1)	-1(1)
N(1)	34(1)	32(1)	38(1)	0(1)	6(1)	-1(1)
N(2)	29(1)	47(1)	64(1)	2(1)	-2(1)	1(1)
P(1)	35(1)	35(1)	32(1)	1(1)	3(1)	-1(1)
C(1)	47(1)	50(1)	36(1)	2(1)	-2(1)	1(1)
C(2)	45(1)	67(2)	41(1)	-2(1)	-10(1)	-3(1)
C(3)	36(1)	62(2)	52(1)	3(1)	-5(1)	4(1)
P(2)	28(1)	41(1)	45(1)	-1(1)	0(1)	-1(1)
C(4)	30(1)	50(1)	57(2)	-1(1)	3(1)	2(1)
C(5)	31(1)	46(1)	60(2)	-2(1)	5(1)	8(1)
C(6)	34(1)	39(1)	49(1)	-4(1)	10(1)	2(1)
P(3)	29(1)	32(1)	35(1)	-1(1)	5(1)	0(1)
C(11)	46(1)	38(1)	34(1)	2(1)	12(1)	-3(1)
C(12)	48(1)	47(1)	39(1)	-2(1)	10(1)	-6(1)
C(13)	65(2)	41(1)	48(1)	-8(1)	21(1)	-9(1)
C(14)	60(2)	44(1)	52(1)	1(1)	27(1)	5(1)
C(15)	48(1)	49(1)	48(1)	5(1)	15(1)	7(1)
C(16)	45(1)	43(1)	41(1)	0(1)	9(1)	3(1)
C(21)	37(1)	35(1)	38(1)	2(1)	7(1)	2(1)
C(22)	51(1)	54(2)	41(1)	6(1)	8(1)	-2(1)
C(23)	61(2)	62(2)	57(2)	20(1)	18(1)	-5(1)
C(24)	54(2)	47(2)	79(2)	9(1)	22(1)	-8(1)
C(25)	46(1)	50(2)	68(2)	-8(1)	13(1)	-10(1)
C(26)	39(1)	47(1)	45(1)	-3(1)	11(1)	-5(1)
C(31)	30(1)	36(1)	40(1)	2(1)	2(1)	2(1)
C(32)	40(1)	41(1)	44(1)	2(1)	0(1)	2(1)
C(33)	51(1)	51(2)	48(1)	13(1)	1(1)	6(1)
C(34)	40(1)	42(1)	66(2)	16(1)	3(1)	1(1)
C(35)	39(1)	36(1)	64(2)	3(1)	1(1)	-1(1)
C(36)	38(1)	37(1)	46(1)	2(1)	3(1)	-1(1)
C(41)	36(1)	30(1)	39(1)	-1(1)	5(1)	-1(1)
C(42)	38(1)	54(1)	36(1)	2(1)	5(1)	-3(1)
C(43)	37(1)	66(2)	43(1)	3(1)	1(1)	-5(1)
C(44)	48(1)	55(2)	39(1)	4(1)	-5(1)	-2(1)
C(45)	54(1)	71(2)	35(1)	7(1)	5(1)	-9(1)
C(46)	43(1)	63(2)	40(1)	2(1)	8(1)	-10(1)
P(4)	33(1)	32(1)	35(1)	-1(1)	5(1)	-3(1)
P(5)	37(1)	37(1)	33(1)	1(1)	6(1)	-3(1)
C(51)	50(1)	44(1)	44(1)	-5(1)	2(1)	-12(1)
C(52)	46(1)	38(1)	49(1)	2(1)	11(1)	4(1)
C(53)	40(1)	36(1)	40(1)	1(1)	9(1)	-3(1)
C(54)	63(2)	52(2)	49(2)	11(1)	-8(1)	-7(1)
C(55)	63(2)	47(1)	49(1)	-3(1)	26(1)	-6(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3).

	x	y	z	U(eq)
H(1A)	5475	6761	4966	53
H(1B)	5894	6056	4589	53
H(2A)	7264	7377	4372	62
H(2B)	7874	6812	4907	62
H(3A)	7933	5989	3936	60
H(3B)	9171	6562	4034	60
H(2)	8630(20)	7441(11)	3169(10)	24(5)
H(4A)	9130	6623	2193	55
H(4B)	9789	6256	2858	55
H(5A)	8005	5354	2729	55
H(5B)	9095	5355	2148	55
H(6A)	6995	5219	1573	48
H(6B)	7285	6047	1492	48
H(12)	5106	7976	4796	53
H(13)	3861	8993	5081	61
H(14)	1533	9159	4674	61
H(15)	397	8289	4025	57
H(16)	1642	7295	3706	52
H(22)	3316	6183	5057	58
H(23)	1812	5250	5278	72
H(24)	715	4614	4402	71
H(25)	1072	4932	3301	65
H(26)	2626	5848	3079	52
H(32)	5597	5371	3543	50
H(33)	5267	4309	4098	60
H(34)	4643	3289	3497	59
H(35)	4441	3329	2334	56
H(36)	4734	4395	1774	48
H(42)	2404	5530	1997	51
H(43)	749	5450	1098	58
H(44)	1427	5631	10	57
H(45)	3785	5904	-165	64
H(46)	5442	5972	727	58
H(51A)	6724	9229	3421	69
H(51B)	7595	8513	3553	69
H(51C)	6257	8687	3980	69
H(52A)	3490	8820	3323	66
H(52B)	3293	8736	2528	66
H(52C)	4276	9353	2845	66
H(53A)	5857	8890	1885	46
H(53B)	7340	8547	2177	46
H(54A)	3582	8083	1366	83
H(54B)	4013	7455	882	83
H(54C)	4691	8224	806	83
H(55A)	7304	7945	863	79
H(55B)	6950	7119	822	79
H(55C)	8107	7406	1370	79

3 Spectroscopic Data of $^{15}N_2$-2, 3 and $^{15}N_2$-3

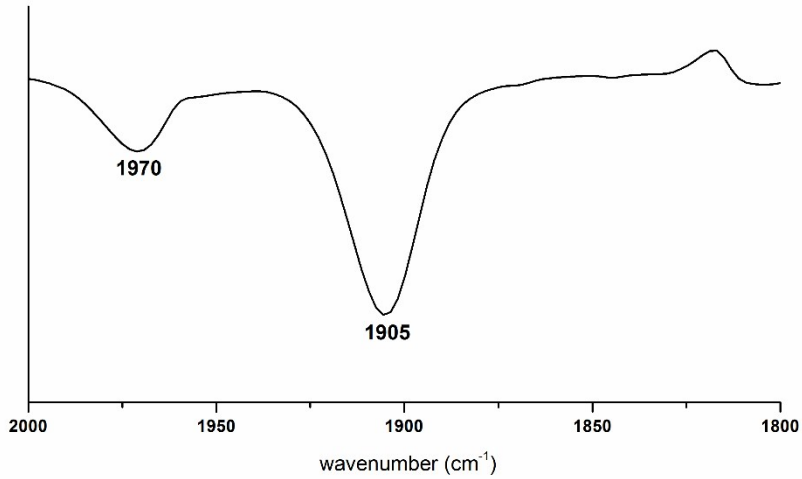

Fig. S3 Liquid IR spectrum of a benzene solution of [Mo($^{15}N_2$)(prPP(Ph)P)(dmpm)] ($^{15}N_2$-**2**). The band at 1970 cm^{-1} derives from the $^{14}N_2$-complex.

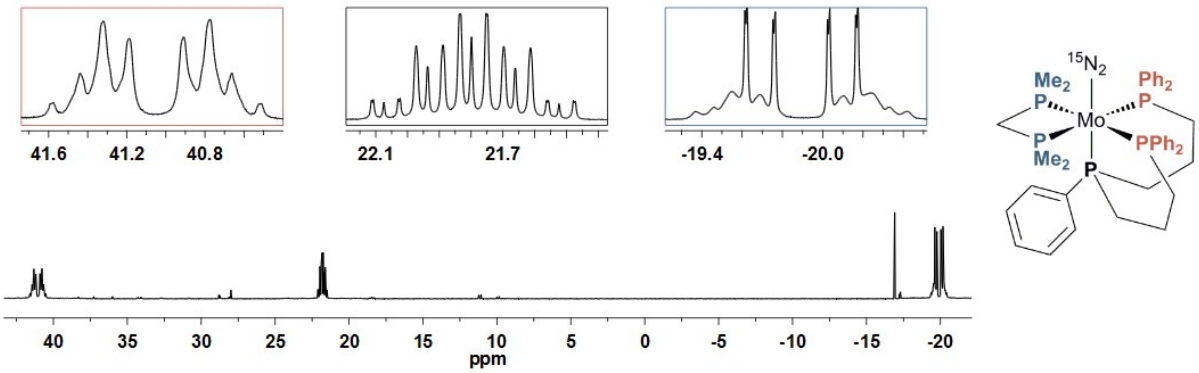

Fig. S4 ^{31}P-NMR spectrum of [Mo($^{15}N_2$)(prPP(Ph)P)(dmpm)] ($^{15}N_2$-**2**) at room temperature in benzene-d_6 with enlargement of the AA'XX'M-pattern. The M signal shows an additional splitting due to the ^{15}N nuclei.

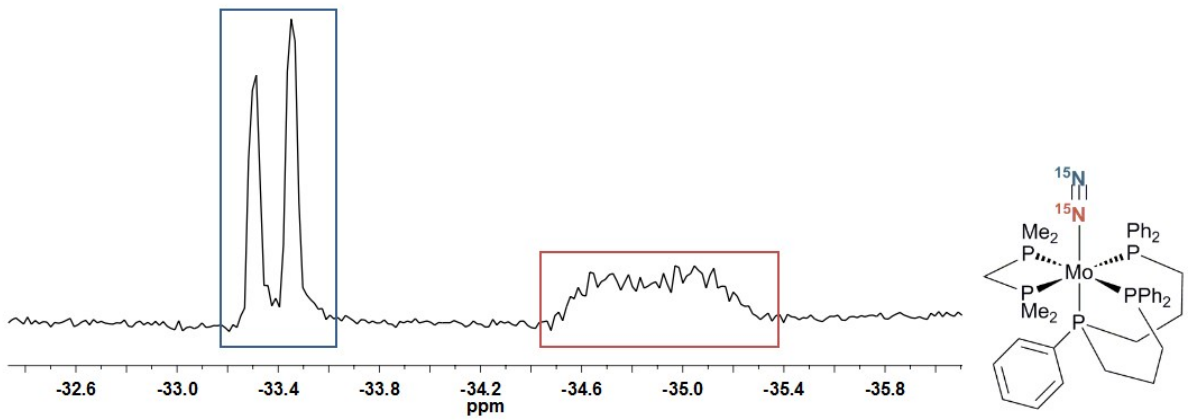

Fig. S5 ^{15}N-NMR spectrum of [Mo($^{15}N_2$)(prPP(Ph)P)(dmpm)] ($^{15}N_2$-**2**) at room temperature in benzene-d_6.

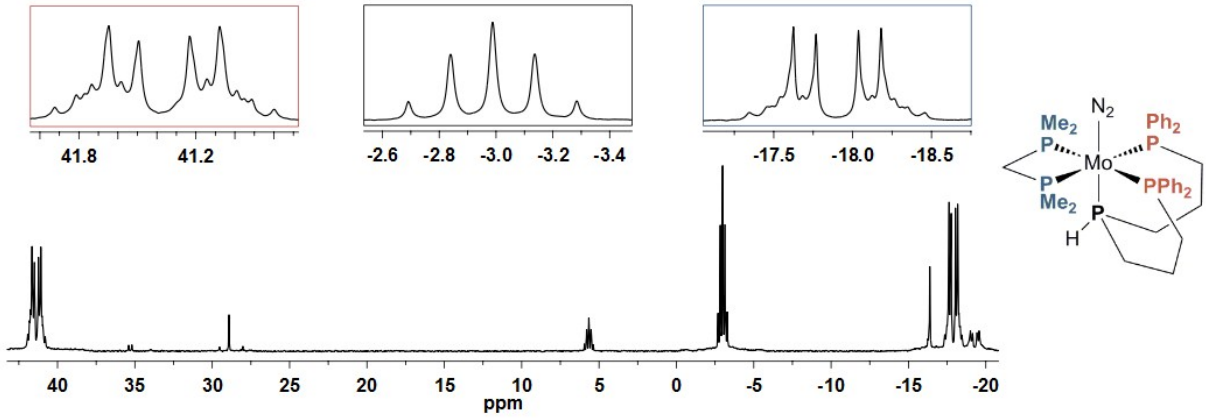

Fig. S6 ^{31}P-NMR spectrum of **3** at room temperature in thf-d_8 with enlargement of the AA'XX'M-pattern.

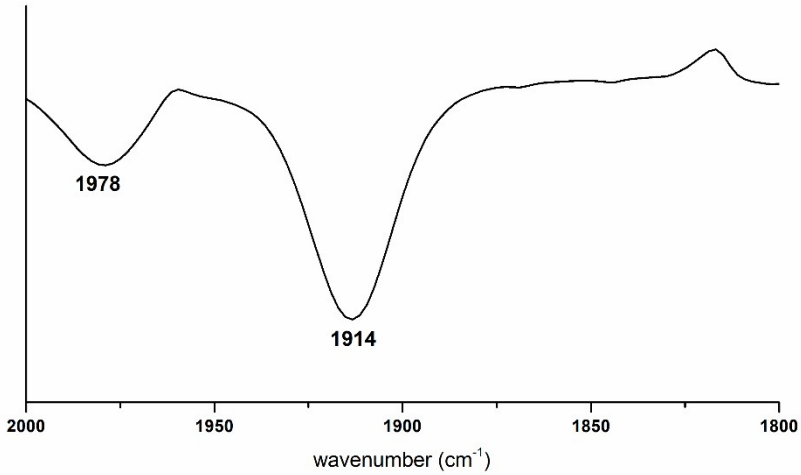

Fig. S7 Liquid IR spectrum of a benzene solution of [Mo($^{15}N_2$)(prPPHP)(dmpm)] ($^{15}N_2$-**3**). The band at 1978 cm^{-1} derives from the $^{14}N_2$-complex.

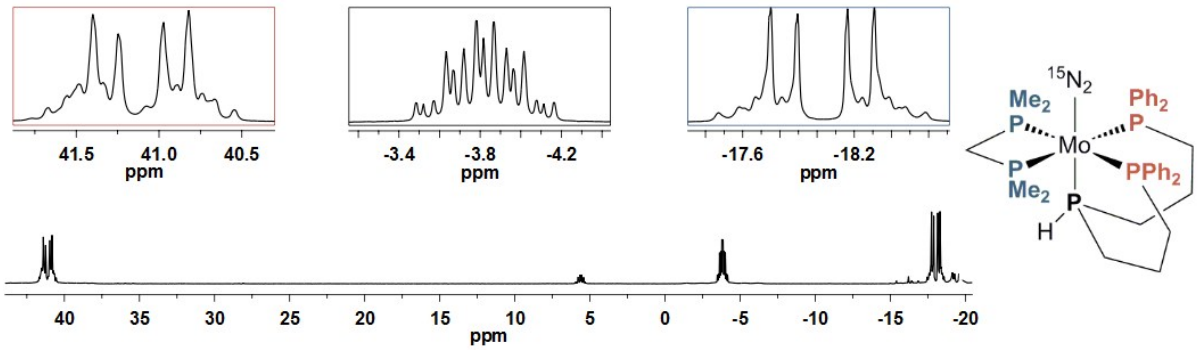

Fig. S8 ^{31}P-NMR spectrum of [Mo($^{15}N_2$)(prPPHP)(dmpm)] ($^{15}N_2$-**3**) at room temperature in benzene-d_6 with enlargement of the AA'XX'M-pattern. The M signal shows an additional splitting due to the ^{15}N nuclei.

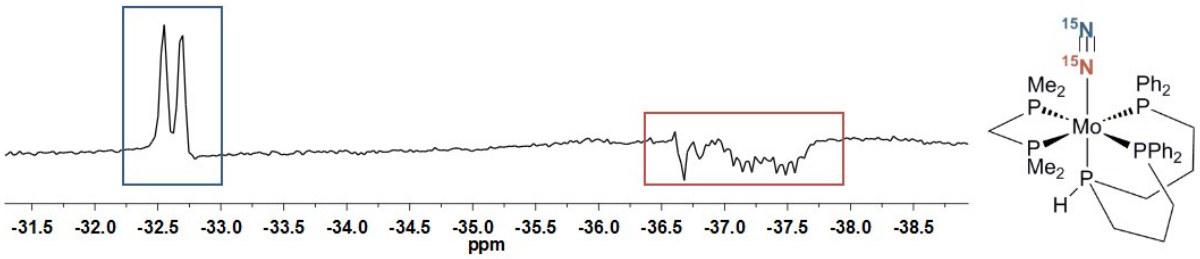

Fig. S9 ^{15}N-NMR spectrum of [Mo($^{15}N_2$)(prPPHP)(dmpm)] ($^{15}N_2$-**3**) at room temperature in benzene-d_6.

4 Spectroscopic and Theoretical Data of 4, 6, $^{15}N_2$-4, 5, 7, $^{15}N_2$-5 and $^{15}N_2$-7

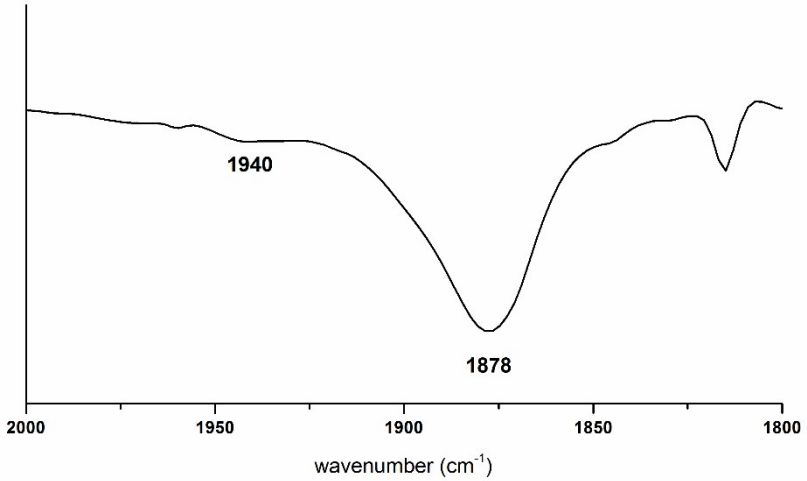

Fig. S10 Liquid IR spectrum of a benzene solution of [Mo($^{15}N_2$)(PN(Ph)P)(dmpm)] ($^{15}N_2$-**4**). The low-intensity band at 1940 cm^{-1} derives from the $^{14}N_2$-complex.

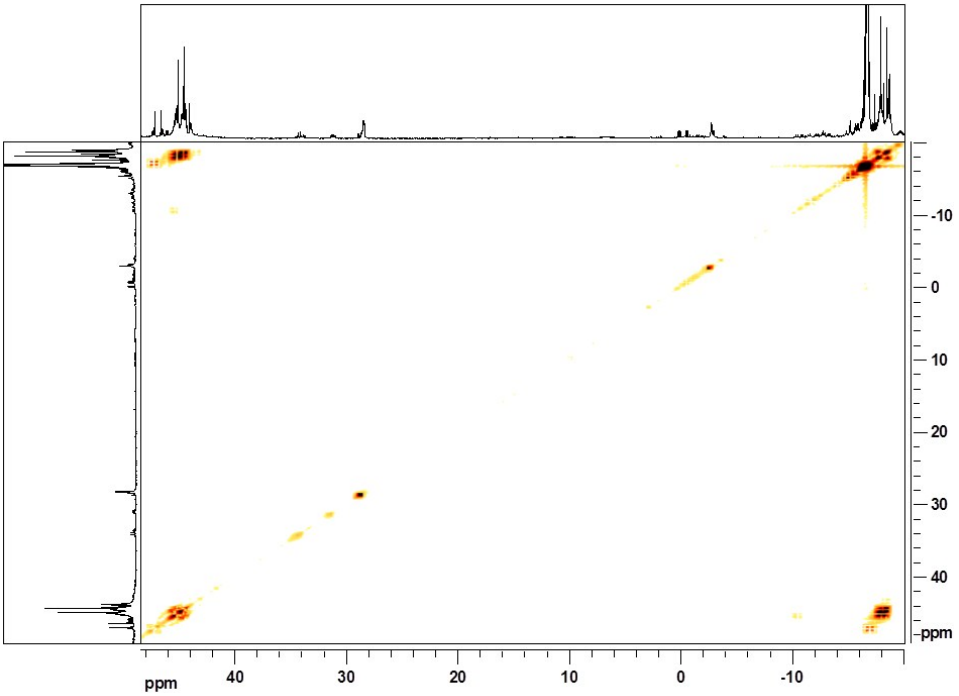

Fig. S11 ^{31}P-COSY-NMR spectrum of [Mo(N_2)(prPN(Ph)P)(dmpm)] (**5**) and [Mo(N_2)$_2$(prPN(Ph)P)(dmpm)] (**7**). The assignment of the half spectra to each other can be seen.

Table S11. Comparison of the chemical shifts and coupling constants of **4** and **6**.

	4	**6**
	δ / ppm	
$\mathbf{P_{AA'}}$	45.67	42.33
$\mathbf{P_{XX'}}$	-17.70	-17.23
	|J| / Hz	
$J_{AA'}$	-10.70	-10.30
$J_{XX'}$	-10.70	-14.10
$J_{A'X/AX'}$	111.12	108.90
$\lvert J_{AX/A'X'}\rvert$	24.40	23.20

Table S12. Comparison of the chemical shifts and coupling constants of **5** and **7**.

	5	**7**	**7**
	δ / ppm		
$\mathbf{P_{AA'}}$	47.00	45.55	44.86
$\mathbf{P_{XX'}}$	-17.22	-18.06	-18.27
	|J| / Hz		
$J_{AA'}$	-6.80	-10.30	-11.60
$J_{XX'}$	-16.50	-15.10	-14.10
$J_{A'X/AX'}$	109.30	108.60	108.80
$\lvert J_{AX/A'X'}\rvert$	25.40	23.80	23.00

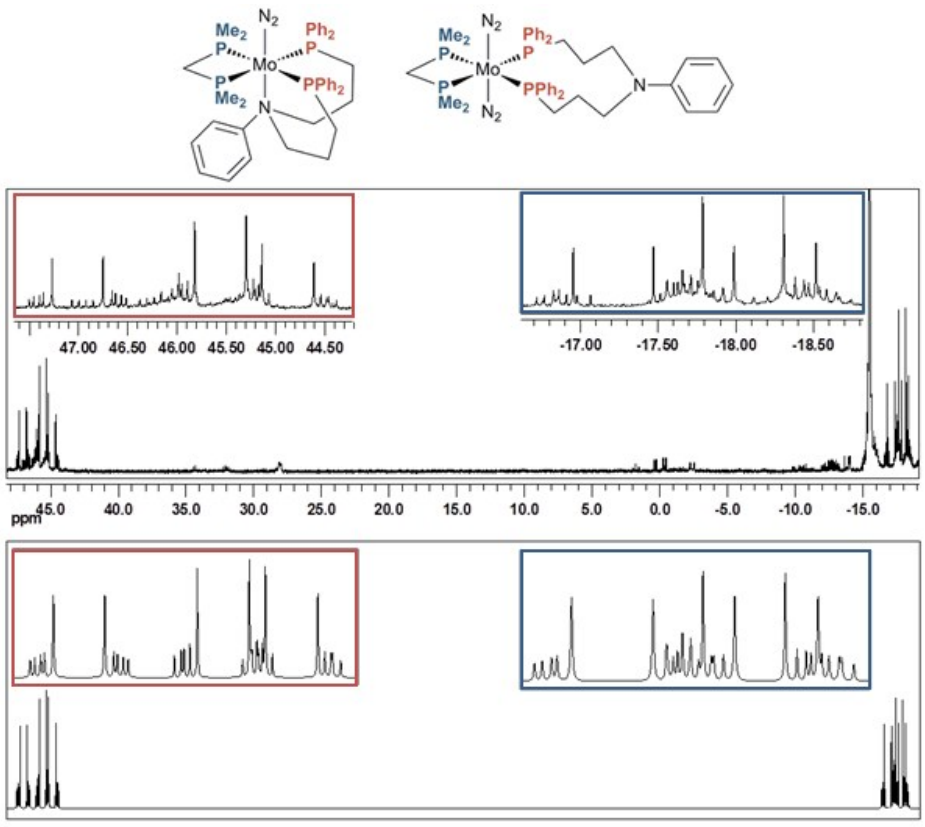

Fig. S12 $^{31}P\{^{1}H\}$-NMR spectrum of [Mo(N_2)(prPN(Ph)P)(dmpm)] (**5**) and [Mo(N_2)$_2$(prPN(Ph)P)(dmpm)] (**7**) (top: measured; bottom: simulated).

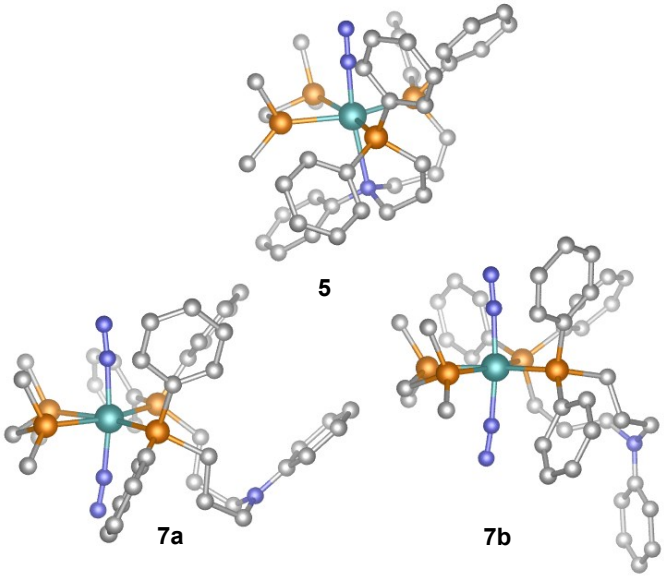

Fig. S13 Optimized structures of [Mo(N_2)(prPN(Ph)P)(dmpm)] (**5**) (top) and the isomers of [Mo(N_2)$_2$(prPN(Ph)P)(dmpm)] (**7**) (bottom : *syn*-**7a** (left) and *anti*-**7b** (right)).

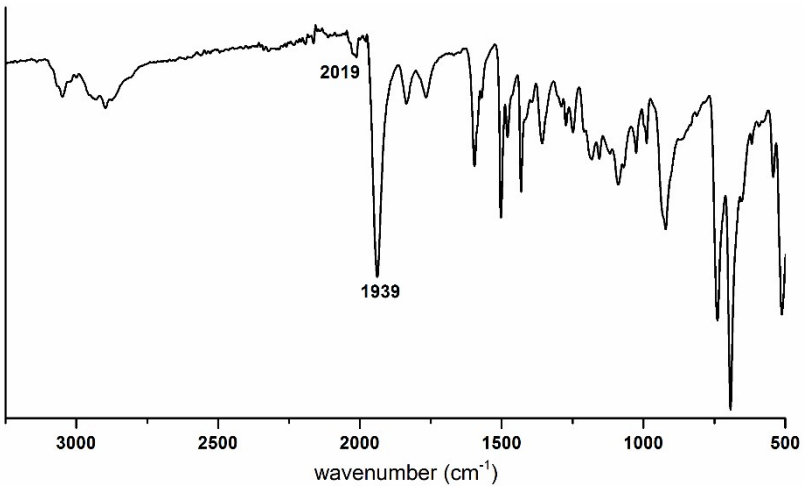

Fig. S14 IR spectrum of [Mo(N_2)(prPN(Ph)P)(dmpm)] (**5**) and [Mo(N_2)$_2$(prPN(Ph)P)(dmpm)] (**7**).

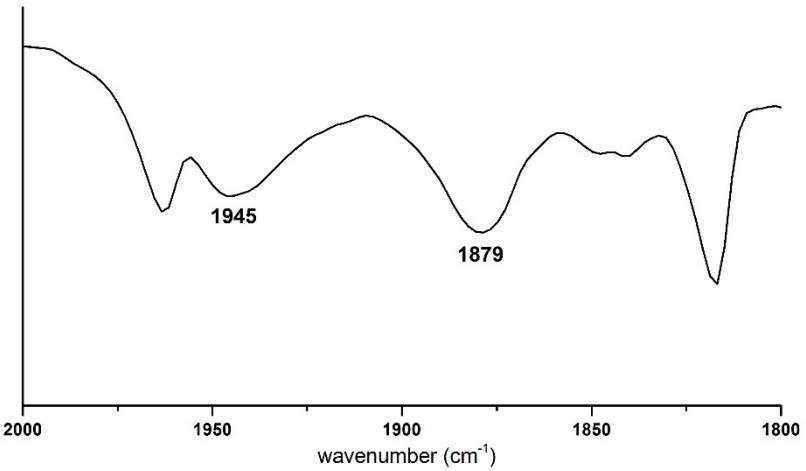

Fig. S15 Liquid IR spectrum of a benzene solution of [Mo($^{15}N_2$)(prPN(Ph)P)(dmpm)] ($^{15}N_2$-**5**) and [Mo($^{15}N_2$)$_2$(prPN(Ph)P)(dmpm)] ($^{15}N_2$-**7**)). The band at 1945 cm^{-1} derives from the $^{14}N_2$-complex.

5 Spectroscopic Investigation of the Reactivity of $^{15}N_2$-2, 4 and $^{15}N_2$-4 with $AlMe_3$

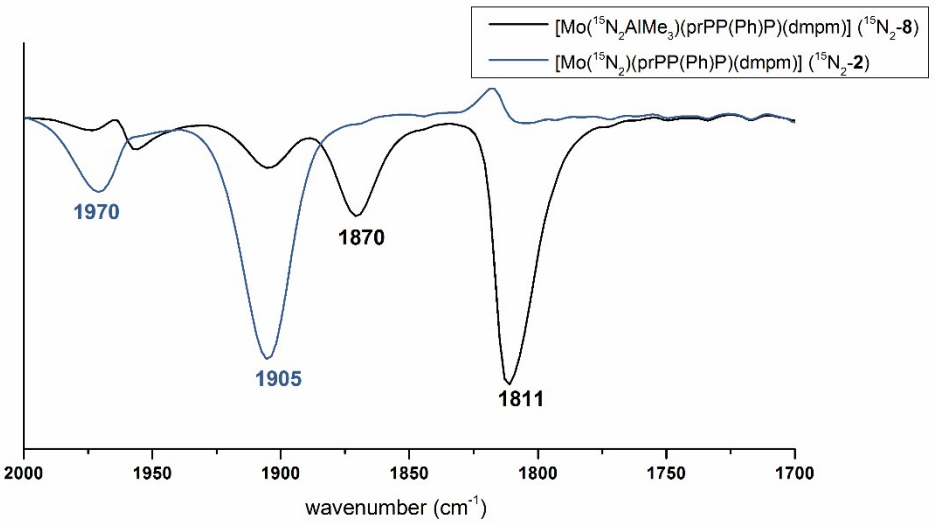

Fig. S16 Liquid IR spectra of benzene solutions of [Mo($^{15}N_2$)(prPP(Ph)P)(dmpm)] ($^{15}N_2$-**2**) (blue) and [Mo($^{15}N_2AlMe_3$)(prPP(Ph)P)(dmpm)] ($^{15}N_2$-**8**) (black). The bands at 1970 cm^{-1} and 1870 cm^{-1}, respectively, derive from the $^{14}N_2$-complexes.

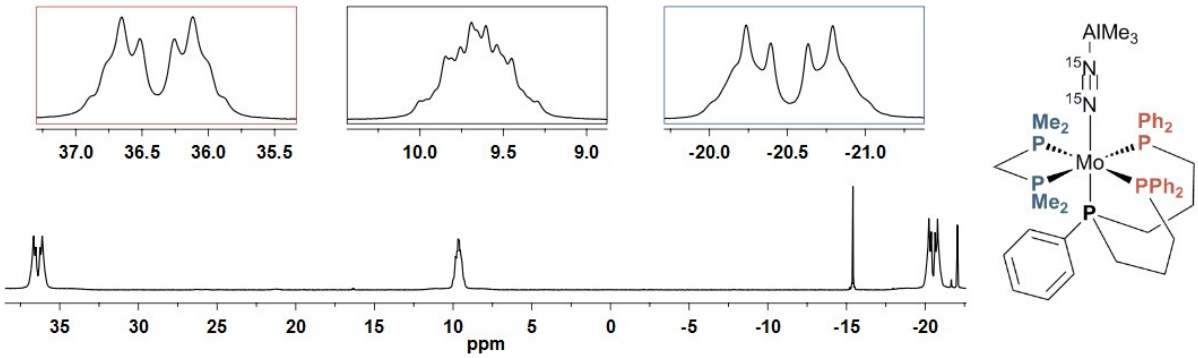

Fig. S17 ^{31}P-NMR spectrum of [Mo($^{15}N_2AlMe_3$)(prPP(Ph)P)(dmpm)] ($^{15}N_2$-**8**) in benzene-d_6.

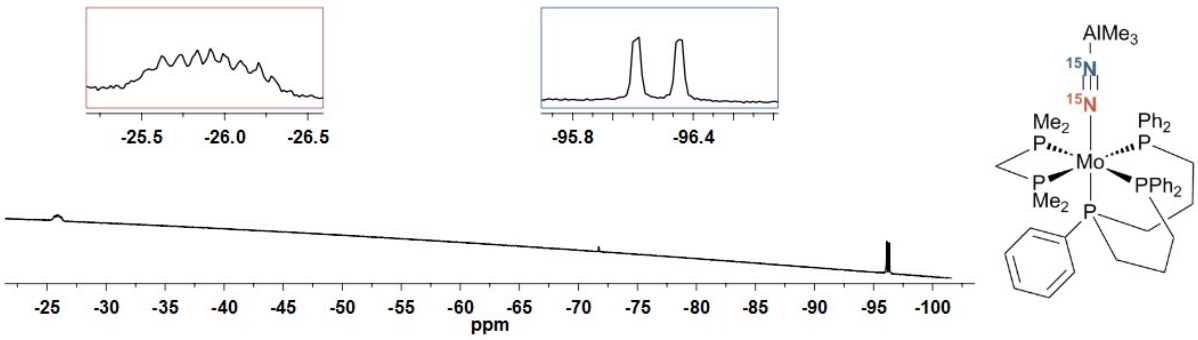

Fig. S18 ^{15}N-NMR spectrum of [Mo($^{15}N_2AlMe_3$)(prPP(Ph)P)(dmpm)] ($^{15}N_2$-**8**) in benzene-d_6.

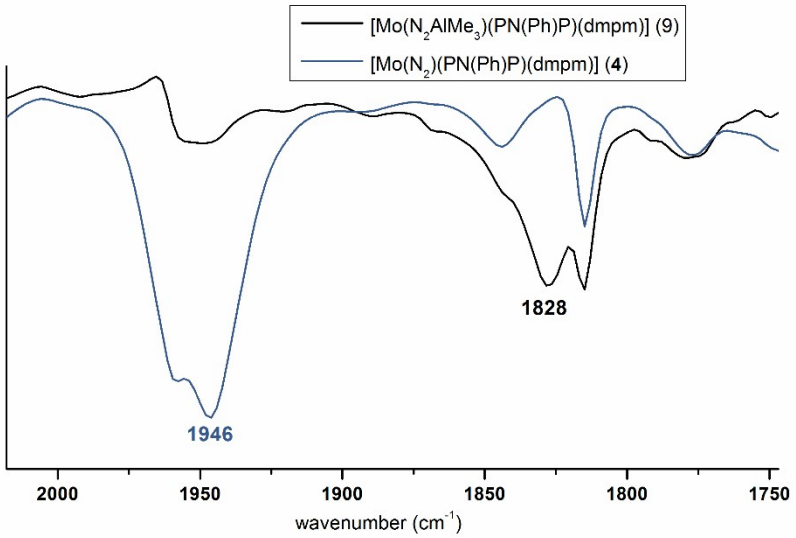

Fig. S19 Liquid IR spectra of benzene solutions of [Mo(N_2)(PN(Ph)P)(dmpm)] (**4**) (black) and [Mo(N_2AlMe$_3$)(PN(Ph)P)(dmpm)] (**9**) (blue).

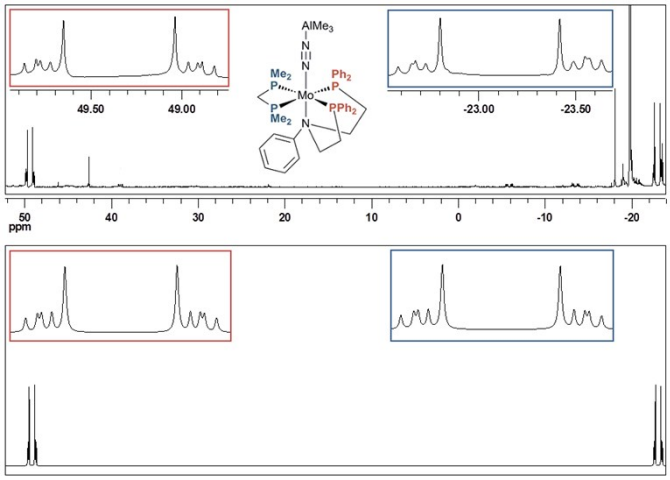

Fig. S20 $^{31}P\{^1H\}$-NMR spectrum of [Mo(N_2AlMe$_3$)(PN(Ph)P)(dmpm)] (**9**) in benzene-d_6 (top: measured; bottom: simulated).

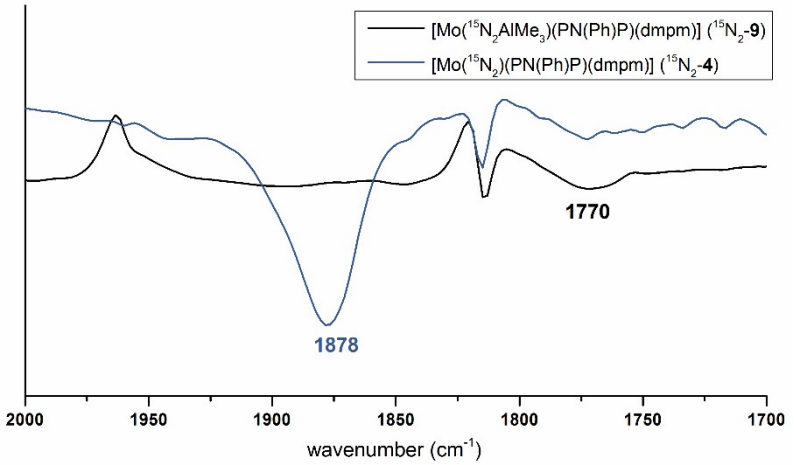

Fig. S21 Liquid IR spectra of benzene solutions of [Mo($^{15}N_2$)(PN(Ph)P)(dmpm)] ($^{15}N_2$-**4**) (blue) and [Mo($^{15}N_2$AlMe$_3$)(PN(Ph)P)(dmpm)] ($^{15}N_2$-**9**) (black).

6 Cartesian coordinates of the optimized structures:

Table S13. Cartesian Coordinates for [Mo(N_2)(prPP(Ph)P)(dmpm)] (**2a**) (coordinates in Angstrom).

C	0.06913381692067	-4.41356152344084	-1.60993283954628
P	2.00410592123479	0.30679975988871	1.90423402850606
P	-0.50345099428683	1.83656159655868	-0.42891227427771
P	-0.87781346625173	-1.71943117162763	-1.38696031044164
P	-1.60413285483894	-0.43995530172401	1.63387373213601
C	-2.64847924032474	-2.01235848465990	1.66393327299736
C	-2.25081360707176	-3.10058412826167	0.67051112096315
C	-2.36644504765063	-2.67804836191760	-0.79780129395185
C	-0.44163748588131	3.24479737175100	0.80719174288171
C	0.82471659084423	3.64769776651305	1.25649022315841
C	0.97808057346789	4.69030924165500	2.16757103381575
C	-0.14474333186435	5.34967574419596	2.67525975481850
C	-1.41176260981247	4.96883817828163	2.23640458632515
C	-1.55565515685244	3.93770247119212	1.30207399344823
C	0.29773614064087	2.78929804297145	-1.80989672138737
C	1.69878982872445	2.79449180961692	-1.88467526229503
C	2.36309507208678	3.50306453028824	-2.88542459428282
C	1.63622410408016	4.21866887565452	-3.83859159365585
C	0.24167734865594	4.22287609432706	-3.77580600648816
C	-0.42138921276475	3.51887789605916	-2.76880044021575
C	-2.97160790059341	0.77751142365450	1.27426999579228
C	-3.22869647389174	0.93268475037132	-0.22888162042159
C	-2.28502584094120	1.89669459103966	-0.96360035744109
C	0.13632682837388	-3.10083257298474	-2.10507714131455
C	1.08197884842233	-2.81919159357931	-3.10460278047690
C	1.94363633116142	-3.80956909185216	-3.57523802018813
C	1.87572815053439	-5.10804767311075	-3.06471117825111
C	-1.51724614614836	-1.01711615826523	-2.98251766475403
C	-0.79890068565204	0.03958412161921	-3.55963742060245
C	-1.20451969321259	0.61000172510350	-4.76689232026634
C	-2.35392035278519	0.14327711768352	-5.40788309648987
C	-3.08133902925607	-0.90619759292545	-4.84165556254940
C	-2.65951976006094	-1.49084259603761	-3.64538704812688
C	0.92868808925333	-5.40705024153909	-2.08360548077256
P	1.57500566561540	-2.28555138495746	1.11656323706544
C	1.89473813877029	1.25697029427719	3.48495512661771
C	3.66301793151208	0.88220951228571	1.32162715227912
C	1.05247096822252	-3.88411345417684	1.90285647672434
C	3.01498327157650	-2.93453890461756	0.16492624746858

H	-0.66227908159435	-4.67718809820187	-0.84560076251450
H	-2.61332596721526	-2.41124624846808	2.68752424500513
H	-3.69297901137977	-1.71258375122368	1.48343286851888
H	-2.89486571068370	-3.97920985700700	0.84440687751110
H	-1.22230254915277	-3.41909864188430	0.88275120747187
H	-2.49731397888978	-3.55526413803014	-1.44797543108160
H	-3.25720917149012	-2.04759319665076	-0.93713894775753
H	1.70836449100249	3.13402889698976	0.87600865073023
H	1.97897848795904	4.98625915223925	2.48829387185288
H	-0.03025903076903	6.15984260995385	3.39695818745824
H	-2.29947941690184	5.48208935681389	2.61137076864581
H	-2.56037068882483	3.69078825463562	0.95913899363520
H	2.27327638615532	2.21848754329844	-1.16124562719339
H	3.45338433601737	3.48146897284006	-2.92757503867224
H	2.15311203701218	4.76723706085943	-4.62771688239323
H	-0.33819098283619	4.78123895960658	-4.51347359534554
H	-1.51030500462360	3.54381189388351	-2.74249080883719
H	-2.69906255912450	1.74577276288692	1.70710406794790
H	-3.87558688536740	0.43772714320133	1.80167500264578
H	-3.17004754991433	-0.04978689473332	-0.71748228466849
H	-4.26254490117825	1.27967205245503	-0.38688833431817
H	-2.26934024224340	1.62632121497385	-2.02865506262508
H	-2.65821935002979	2.92989954513990	-0.90293154612832
H	1.14980345648839	-1.81504755889370	-3.52095241195113
H	2.67412419094832	-3.56159838717165	-4.34725282481947
H	2.55079939730177	-5.88199207997532	-3.43308267721518
H	0.07623107881147	0.43322646472226	-3.04081698319780
H	-0.62730963194837	1.43305175156173	-5.19153149296669
H	-2.68375794335773	0.59564916510405	-6.34474813264570
H	-3.98088362704479	-1.27743396172265	-5.33673765104078
H	-3.23101937394571	-2.32434264310853	-3.23562771070087
H	0.85392523771853	-6.42050228125975	-1.68406967382419
H	1.65647019335216	2.30935817479927	3.29329145281936
H	1.09778499751449	0.83358577509620	4.10575945175200
H	2.84956456742867	1.18926049460954	4.02714476307466
H	4.42499705802569	0.75355846940254	2.10381782168316
H	3.95920926979405	0.32456425761751	0.42433360983424
H	3.61244444365671	1.94696514652991	1.05340769317321
H	0.22010445101382	-3.71747167109410	2.59839560933668
H	0.73275476898985	-4.59538193463400	1.13003378694787
H	1.89749584694455	-4.32179116794380	2.45460665963810
H	3.59077265036397	-2.10257592107409	-0.25757581577370
H	3.66550170128662	-3.54320983864696	0.80933926668714
H	2.65207233080524	-3.54844801778138	-0.66979620263525

Mo	0.35902927201759	-0.36021721352661	0.18849883237559
N	1.81270877927522	-0.26125534818451	-1.17871043866855
N	2.65096530538053	-0.24017097857910	-1.95151511850946
C	2.37574089334884	-1.40061680355754	2.53427099792265
H	1.77253783530074	-1.56128870043356	3.44080522840052
H	3.42808431485889	-1.64529806490460	2.75250661921850
C	-1.38724677629864	-0.15487844386340	3.45075078185022
C	-0.92355463828124	-1.20385601416758	4.26276565304973
C	-1.54193040598794	1.11008177263882	4.04003125709932
C	-1.26045905137413	1.31211586871202	5.39279885449880
C	-0.80715379670010	0.25801707845747	6.18697222593927
C	-0.63675529603144	-1.00474557803397	5.61291017017936
H	-0.77536695167869	-2.19577211562101	3.83138519752172
H	-1.85663493120844	1.96495157463412	3.44229198563513
H	-1.38632938930663	2.30750930831906	5.82270045520099
H	-0.58301815178468	0.41835476994841	7.24248412369174
H	-0.27827046156148	-1.83893262086362	6.21907351973061

Table S14. Cartesian Coordinates for [Mo(N_2)(prPP(Ph)P)(dmpm)] (**2b**) (coordinates in Angstrom).

C	-0.54769807093496	-4.02054197180510	-1.97596845752551
P	2.25754689080342	0.45782847693217	2.38272429415782
P	-0.26739818225615	2.12264116542977	0.06136433218149
P	-0.67251204383970	-1.26808194061344	-1.06593365467395
P	-1.25272831173515	-0.44821663892238	2.12319490318498
C	-2.15739888982142	-2.09753538253053	2.07204468150661
C	-2.08767142822582	-2.85166244574810	0.74231384337805
C	-2.29010543482895	-1.98522296821345	-0.50949860696631
C	0.36908011904574	3.60471592430900	0.99806180739081
C	1.75305766082694	3.67499043592230	1.20689815750440
C	2.33594301968294	4.75661038922415	1.86485904539456
C	1.53268100521950	5.78780536366787	2.35850454478972
C	0.15251660314237	5.73282729701437	2.16178793682804
C	-0.42219814054823	4.65949205519155	1.47484180439397
C	-0.01825890580348	2.83508771690537	-1.63723147061031
C	1.28939973348744	3.10419549152473	-2.07406458346469
C	1.52662732873633	3.66385464246187	-3.32823083167301
C	0.45942997092026	3.97288351285265	-4.17430322528867
C	-0.84269445208842	3.70048643025445	-3.75724816210466
C	-1.07942722128535	3.13268380141374	-2.50442110310914
C	-2.79154475371673	0.61241702625090	1.96216306817697
C	-2.60004346554543	2.09491263879753	1.65623245019011
C	-2.09308847409920	2.36725696224246	0.23859106212978
C	0.11111055025098	-2.79242816884025	-1.80998288727806

C	1.44605060944218	-2.70212419520608	-2.23660804539371
C	2.09216102581788	-3.78955153335251	-2.82469176162651
C	1.42802126237427	-5.00953177619676	-2.96966003802522
C	-1.17765499873532	-0.46565885407879	-2.65991348782831
C	-0.16845045785825	-0.04749051800587	-3.54387182584859
C	-0.48667381851186	0.52516209517230	-4.77174438734820
C	-1.82242790060370	0.71801424810186	-5.13473811699584
C	-2.83321562627638	0.34507372614343	-4.25068745092473
C	-2.51365594326258	-0.24649452268452	-3.02438354579579
C	0.10695522868067	-5.12086952856788	-2.53647971393652
P	1.86278548533941	-2.04343062960106	1.39130799336208
C	2.10727558191330	1.42672965062313	3.94605016944893
C	3.98603580975212	0.93542002452316	1.91693717298416
C	1.28229918336793	-3.73202870590967	1.88089591389150
C	3.42040243837070	-2.56039805799875	0.54101034146420
H	-1.58595547071265	-4.14152408978523	-1.66869739208529
H	-1.75395506642034	-2.73538604069723	2.86916555190484
H	-3.20455046673774	-1.89186441734963	2.34759036113169
H	-2.84386416748211	-3.65348430396040	0.76153714348779
H	-1.11504284646129	-3.35854168963556	0.66927513491682
H	-2.74821212218976	-2.55889729652645	-1.32760927828882
H	-2.97211459015097	-1.14928346021384	-0.30227307866681
H	2.37367117114961	2.85416962576085	0.84587321206945
H	3.41889472789925	4.79114842205430	2.00146439878281
H	1.98004718987445	6.63007487358866	2.88863461763828
H	-0.48546539708539	6.53477110203029	2.53851952399631
H	-1.50043345327032	4.66188529119915	1.31466058047699
H	2.13651098223427	2.87961521682257	-1.42912690580284
H	2.55291631501829	3.86190136402310	-3.64257689981071
H	0.64321091699391	4.41616028399113	-5.15451507758105
H	-1.68673336617832	3.91808595400498	-4.41407828163148
H	-2.10744210614087	2.91207586299062	-2.22166418287030
H	-3.37373532534954	0.47428133025552	2.88685934538026
H	-3.38605794386520	0.16133374588575	1.15352220459227
H	-1.91693467492240	2.56029705804923	2.38326481001815
H	-3.57155065906099	2.60008747433776	1.78884896787672
H	-2.57158426277022	1.67841301251512	-0.47489282082928
H	-2.35647232942984	3.38691102340023	-0.07861036802714
H	1.99448604317176	-1.77161455103629	-2.10140288480622
H	3.12528734583372	-3.68278345569294	-3.16128977787744
H	1.93579098467361	-5.86557029603244	-3.41694187793630
H	0.87922298509552	-0.16710764248486	-3.26865401150819
H	0.31461669391755	0.84030435971077	-5.44159920315482
H	-2.07123409398500	1.17120137727177	-6.09569878312525

H	-3.88060733847921	0.50148041315532	-4.51695452992824
H	-3.32563038179013	-0.54933876254846	-2.36266088676557
H	-0.42618817880467	-6.06790712383356	-2.64085932856935
H	1.99576337413618	2.49098425324614	3.69902078418355
H	1.21930053683621	1.10226729757842	4.49925744700015
H	2.99955560406133	1.29047103097284	4.57454692020145
H	4.68656872974359	0.64219914975131	2.71177150375211
H	4.27672006257187	0.45254365144725	0.97621243270222
H	4.05551868072552	2.02176946977712	1.77717652885682
H	0.39023081150776	-3.66295552148825	2.51547336449075
H	1.01882908976037	-4.29093371367332	0.97145071967920
H	2.06953347838425	-4.27944479230493	2.41966111563180
H	3.95768263200408	-1.68360943253146	0.15929709466042
H	4.06980111242172	-3.11526652217639	1.23329810490907
H	3.17002663183404	-3.20322610004839	-0.31190994328097
Mo	0.63431993259878	-0.08042930885047	0.59455272631523
N	2.09858170689838	0.23854642576331	-0.71891528172283
N	2.97357373238409	0.40154454527583	-1.43457641942787
C	2.52715219561552	-1.29107101389995	2.95261928075850
H	1.82888216564884	-1.48715933759552	3.77760945863783
H	3.54701160212788	-1.57370842304659	3.26153571288310
C	-1.02290978923490	-0.33788268312488	3.96559806545314
C	-0.45974654884134	-1.40477640598127	4.68479740973256
C	-1.33147569335648	0.83205404366942	4.67900973402581
C	-1.08107572858909	0.93428577293196	6.04866264077486
C	-0.51182779170321	-0.13361304125163	6.74372307299803
C	-0.20565188417319	-1.30779522893492	6.05367973816723
H	-0.21443546204018	-2.33757590088519	4.17508166441027
H	-1.76222958791922	1.68981776780599	4.16459728228041
H	-1.32907585749414	1.85925989661103	6.57239994170793
H	-0.31240627299564	-0.05365494256708	7.81319036538862
H	0.23188843531469	-2.15684683440424	6.58217608588290

Table S15. Cartesian Coordinates for [Mo(N_2)(prPP(Ph)P)(dmpm)] (**2c**) (coordinates in Angstrom).

C	-0.92569548720561	-3.69072465570166	-0.75304798810459
P	1.78048896222207	1.13010448911794	2.34009706238772
P	-0.30864565107150	2.64018781026280	0.09205781077733
P	-0.40310550162546	-0.94212359236967	-1.43183992935115
P	-1.56998896698086	-0.12715248916982	1.61365583589872
C	-3.04644628966783	-0.73881083749522	0.63960268831730
C	-3.11773492137413	-0.18565650032981	-0.78363866452352
C	-2.25885253885416	-0.95666281787246	-1.78231486904002
C	1.05676186932729	3.89125106744080	0.07455983416674

C	1.90708597643527	3.91441033264893	-1.04349845059955
C	3.01420179599930	4.75820856749405	-1.08690448115942
C	3.29207789774817	5.61056533055326	-0.01403356824649
C	2.44381740719446	5.61624371276129	1.09350329019095
C	1.33602912635080	4.76449826813973	1.13644423194588
C	-1.25128281283196	3.34064876863051	-1.36502399678591
C	-1.55844186722148	4.70773663649987	-1.46094368604510
C	-2.23819838847148	5.20780337064910	-2.57042275540857
C	-2.61326319756501	4.35085969853993	-3.61105552926760
C	-2.29713353066209	2.99490976036682	-3.53503657349702
C	-1.62160308665354	2.50173086506665	-2.41593520622872
C	-2.42551355870224	1.26194123030351	2.52922060190818
C	-2.65683858680917	2.53313230791584	1.70743912657884
C	-1.37560736698336	3.33103296530889	1.45271585979223
C	-0.03564905782943	-2.75727153020138	-1.30046928348056
C	1.24175509062488	-3.20721647311978	-1.67868841229581
C	1.60959177062574	-4.54226107796949	-1.52155108830296
C	0.71021557766055	-5.46230721461841	-0.97243588980728
C	0.16820793956978	-0.69691287587848	-3.18861931015041
C	0.79237863062089	0.49688842906387	-3.56459823002099
C	1.15309396081124	0.72886984642046	-4.89395054208777
C	0.89054930563047	-0.23376036678923	-5.86836613335360
C	0.26447957517995	-1.43052657614698	-5.50661156216261
C	-0.09211729100737	-1.65978665256393	-4.17838697007974
C	-0.55879632182813	-5.02892205227140	-0.58690155714014
P	1.81385462326232	-1.44441262771268	1.44690073200427
C	1.31594022569180	2.12161321880112	3.83799415717813
C	3.43739979978869	1.88431531865429	2.04299469472438
C	1.38000628655527	-3.13895386331220	2.02512228794151
C	3.49169680426182	-1.80657296962535	0.76781636987874
H	-1.92600675344100	-3.37895370652566	-0.44977296437237
H	-3.01339583503685	-1.83474890470543	0.59239612714895
H	-3.94934378574085	-0.48062562693817	1.21369390332868
H	-4.16371869025968	-0.21435877740908	-1.13158011798491
H	-2.81934775438047	0.87184678781729	-0.79478516896964
H	-2.60138898456580	-1.99966542597845	-1.85964302941297
H	-2.37549862559214	-0.52116436484049	-2.78476513977156
H	1.69880493043358	3.25817857229575	-1.88897026681417
H	3.66665806673482	4.74684459474622	-1.96151746871593
H	4.16083525391718	6.26989163065399	-0.04536667942930
H	2.64088068689696	6.28782125897862	1.93153325221224
H	0.68514592295128	4.79485503657367	2.01043489750351
H	-1.24021160760622	5.39548255466573	-0.67433740315671
H	-2.46780185606082	6.27346685019944	-2.63121218369442

H	-3.13882987808995	4.74565523829036	-4.48231442000535
H	-2.56375373164342	2.31838377187079	-4.34939200711235
H	-1.34826089812804	1.44984871413022	-2.35664846488459
H	-1.80827962066246	1.51955578196534	3.40252534429691
H	-3.37777458648758	0.86675637979489	2.91643999385640
H	-3.35743649168371	3.17421922761347	2.26747477036803
H	-3.16278558541912	2.30503457972916	0.75557931728081
H	-1.61741240075682	4.37699485176130	1.21517980998039
H	-0.77082060031485	3.33348243116484	2.37111771779439
H	1.94867527658098	-2.49874142233977	-2.11545867852624
H	2.60382069195597	-4.86896600833367	-1.83259549172840
H	0.99782919871967	-6.50712944914066	-0.84724811318700
H	0.98635683251534	1.25121224989709	-2.80503495556742
H	1.64317906349737	1.66575363470896	-5.16449563900697
H	1.17343085338756	-0.05577754992238	-6.90736280436249
H	0.05447725231899	-2.18919824046139	-6.26311040847242
H	-0.57150357434370	-2.60184077223374	-3.90533953980094
H	-1.27116482618835	-5.73487825981972	-0.15551644180728
H	1.30502154850716	3.18805993976364	3.57608081697856
H	0.31863605332473	1.84042099476657	4.19768006875184
H	2.04761037760780	1.96731399568371	4.64454629923419
H	4.03184514890698	1.89779553505563	2.96788757602234
H	3.97320887659276	1.31816306654833	1.27210386879378
H	3.30868364151240	2.91095989766550	1.67608248023046
H	0.48189816482392	-3.10308202331730	2.65023914039644
H	1.18126672710892	-3.78547756731041	1.16166315207454
H	2.21319567611754	-3.55873308650943	2.60773450880511
H	3.98343360851836	-0.88786209820377	0.42823744081348
H	4.11412739071395	-2.30193438052847	1.52659357609881
H	3.38605152010270	-2.47383048739013	-0.09711281861248
Mo	0.49783554809103	0.37042618246896	0.40257622060471
N	2.13288960119077	0.73906848151493	-0.69178781377720
N	3.10149730722131	0.90253017027617	-1.26759043641035
C	2.21022389375848	-0.53924232397528	3.02113941540028
H	1.46196860317470	-0.82514674616573	3.77458405765160
H	3.22091746302906	-0.66976743598216	3.44127622441671
C	-1.58427653890275	-1.36254327060693	3.00513377400218
C	-1.99974441203138	-2.69418652482389	2.84794458548569
C	-1.08036317063063	-0.98972246057737	4.26319994696489
C	-0.99313760092023	-1.90093298717133	5.31563816423170
C	-1.41127757020907	-3.22135956761753	5.13815097429812
C	-1.91700738523320	-3.61120934710431	3.89803448411668
H	-2.37406531983258	-3.04639147304505	1.88823255882610
H	-0.74437525369487	0.03362901599679	4.43046094351958

H	-0.59632225119271	-1.57583896375246	6.27928840183946
H	-1.34334938475851	-3.93769645769206	5.95803999105252
H	-2.24392840862047	-4.64037253766685	3.73842474465201

Table S16. Cartesian Coordinates for [Mo(N_2)(prPPHP)(dmpm)] (**3a**) (coordinates in Angstrom).

90

symmetry c1

C	-0.321354000	0.365921000	-4.555898000
P	0.955705000	2.544602000	1.207234000
P	-0.355647000	-0.812727000	1.761776000
P	-0.843197000	-0.645223000	-1.918435000
P	-2.166124000	1.564314000	0.276462000
C	-3.458200000	1.618260000	-1.093684000
C	-2.991636000	1.144185000	-2.468080000
C	-2.578376000	-0.330960000	-2.511573000
C	-0.075588000	-0.112343000	3.472115000
C	1.249934000	0.165992000	3.846712000
C	1.549556000	0.740103000	5.079812000
C	0.523006000	1.065857000	5.972301000
C	-0.796635000	0.784398000	5.622234000
C	-1.089895000	0.190506000	4.389896000
C	0.653123000	-2.353986000	2.068314000
C	2.017715000	-2.333095000	1.741667000
C	2.830754000	-3.443859000	1.970989000
C	2.292421000	-4.604773000	2.529569000
C	0.937960000	-4.637506000	2.864382000
C	0.128568000	-3.521772000	2.641874000
C	-3.210292000	0.789799000	1.603450000
C	-3.255972000	-0.729878000	1.391660000
C	-2.066690000	-1.541668000	1.930682000
C	0.119919000	-0.436804000	-3.491387000
C	1.403747000	-1.001281000	-3.577436000
C	2.224707000	-0.752841000	-4.676109000
C	1.781780000	0.064786000	-5.719288000
C	-0.854152000	-2.498258000	-1.827225000
C	0.183372000	-3.103936000	-1.106678000
C	0.257874000	-4.490494000	-0.975537000
C	-0.723021000	-5.297103000	-1.555912000
C	-1.762987000	-4.707579000	-2.278551000
C	-1.823710000	-3.319440000	-2.422967000
C	0.501690000	0.617011000	-5.656777000
P	0.571753000	2.642007000	-1.504004000
C	0.210078000	3.361938000	2.685090000

C	2.746532000	2.619571000	1.648062000
C	-0.443766000	3.635486000	-2.693444000
C	2.167492000	2.665274000	-2.424298000
H	-1.319857000	0.803375000	-4.541002000
H	-3.827529000	2.653032000	-1.156664000
H	-4.309336000	1.000123000	-0.765628000
H	-3.812823000	1.305757000	-3.186757000
H	-2.159000000	1.773873000	-2.804719000
H	-2.678625000	-0.729099000	-3.532359000
H	-3.247632000	-0.927624000	-1.872304000
H	2.060921000	-0.081495000	3.160460000
H	2.589904000	0.936479000	5.346729000
H	0.753124000	1.525007000	6.934793000
H	-1.608680000	1.019164000	6.313178000
H	-2.129849000	-0.042372000	4.161712000
H	2.446377000	-1.445482000	1.282065000
H	3.887264000	-3.401670000	1.700201000
H	2.923669000	-5.478105000	2.702082000
H	0.504166000	-5.537708000	3.304125000
H	-0.922170000	-3.577650000	2.923970000
H	-2.774172000	1.056117000	2.575254000
H	-4.221941000	1.222308000	1.567659000
H	-3.350800000	-0.930944000	0.312353000
H	-4.173159000	-1.137898000	1.846008000
H	-2.015948000	-2.487624000	1.371243000
H	-2.234220000	-1.807550000	2.985323000
H	1.770336000	-1.639610000	-2.774315000
H	3.219713000	-1.199715000	-4.714229000
H	2.426323000	0.262830000	-6.577080000
H	0.925207000	-2.470621000	-0.621650000
H	1.072105000	-4.933126000	-0.399209000
H	-0.680655000	-6.381913000	-1.443493000
H	-2.532220000	-5.332143000	-2.737336000
H	-2.635873000	-2.885825000	-3.007157000
H	0.134755000	1.244114000	-6.471954000
H	0.336856000	2.723757000	3.568070000
H	-0.864775000	3.504222000	2.510124000
H	0.677543000	4.339784000	2.871947000
H	3.060861000	3.648518000	1.875134000
H	3.342695000	2.227623000	0.813611000
H	2.928536000	1.987395000	2.526277000
H	-1.436349000	3.833012000	-2.267463000
H	-0.560544000	3.084531000	-3.636256000
H	0.052693000	4.594200000	-2.903922000

H	2.969549000	2.253693000	-1.799597000
H	2.430749000	3.684083000	-2.742617000
H	2.069123000	2.018877000	-3.307805000
Mo	0.044181000	0.704621000	-0.111272000
N	1.902913000	0.055604000	-0.500311000
N	2.977497000	-0.226338000	-0.758223000
C	0.820102000	3.849110000	-0.113367000
H	-0.121567000	4.400942000	0.036465000
H	1.646469000	4.572761000	-0.203306000
H	-2.323053000	2.928019000	0.709008000

Table S17. Cartesian Coordinates for [Mo(N_2)(prPPHP)(dmpm)] (**3b**) (coordinates in Angstrom).

90

symmetry c1

Mo	-0.796180000	-0.404927000	0.612122000
P	-2.992469000	-1.197325000	-0.029956000
P	-1.661434000	1.773469000	1.233246000
P	1.593325000	-0.424202000	1.068514000
P	-0.715212000	-2.664129000	-0.272702000
P	-1.181285000	-1.237609000	2.841585000
N	-0.505322000	0.277819000	-1.251923000
N	-0.383018000	0.618184000	-2.332167000
C	-1.882861000	-0.154967000	4.214082000
C	-1.737704000	1.356940000	4.034158000
C	-2.550245000	1.900544000	2.852183000
C	0.154460000	-2.163231000	3.765988000
C	1.553987000	-1.549397000	3.687393000
C	2.199375000	-1.684523000	2.303697000
C	-2.545117000	-2.995296000	-0.215440000
C	-2.956512000	2.422546000	0.072986000
C	-4.329721000	2.403366000	0.364579000
C	-5.274703000	2.787407000	-0.590737000
C	-4.865400000	3.201637000	-1.858546000
C	-3.500483000	3.242612000	-2.155950000
C	-2.559041000	2.862478000	-1.201307000
C	-0.554584000	3.265105000	1.255835000
C	-0.698413000	4.361851000	2.115746000
C	0.202203000	5.429061000	2.064789000
C	1.243636000	5.428137000	1.135392000
C	1.388111000	4.347321000	0.263562000
C	0.506565000	3.270867000	0.338513000
C	2.596721000	0.997420000	1.724510000
C	3.916848000	1.268126000	1.336567000

C	4.617656000	2.334132000	1.905758000
C	4.018724000	3.131351000	2.883959000
C	2.007549000	1.810386000	2.699893000
C	2.709482000	2.861871000	3.286788000
C	2.579527000	-0.872580000	-0.423164000
C	3.166212000	-2.133029000	-0.614748000
C	3.785692000	-2.460832000	-1.823696000
C	3.835832000	-1.531112000	-2.863096000
C	3.270870000	-0.265848000	-2.679526000
C	2.651739000	0.057859000	-1.474435000
H	-2.156026000	-2.285624000	3.010734000
H	-1.421343000	-0.471740000	5.162076000
H	-2.954529000	-0.400633000	4.287804000
H	-0.676855000	1.631997000	3.930385000
H	-2.083593000	1.846428000	4.959331000
H	-2.874739000	2.936685000	3.026191000
H	-3.464685000	1.297995000	2.748171000
H	0.180173000	-3.178636000	3.339640000
H	-0.166234000	-2.268693000	4.814246000
H	2.197629000	-2.061803000	4.421125000
H	1.534359000	-0.491948000	3.999010000
H	1.975022000	-2.684700000	1.904228000
H	3.293009000	-1.585729000	2.374751000
H	-2.775572000	-3.509820000	0.731289000
H	-2.997254000	-3.558503000	-1.048101000
H	-4.682259000	2.093366000	1.348295000
H	-6.336524000	2.764747000	-0.337362000
H	-5.602578000	3.497049000	-2.606779000
H	-3.163400000	3.570635000	-3.140784000
H	-1.500663000	2.903301000	-1.455077000
H	-1.513303000	4.398023000	2.839926000
H	0.085130000	6.267733000	2.754101000
H	1.946984000	6.261633000	1.098954000
H	2.209279000	4.326979000	-0.454921000
H	0.650606000	2.394648000	-0.296057000
H	4.399900000	0.648591000	0.579488000
H	5.640174000	2.541054000	1.583338000
H	4.567743000	3.966302000	3.322772000
H	0.966355000	1.625358000	2.965676000
H	2.222629000	3.488713000	4.035704000
H	3.152275000	-2.873851000	0.184901000
H	4.234758000	-3.448069000	-1.949286000
H	4.315458000	-1.787919000	-3.808835000
H	3.303790000	0.471420000	-3.483315000

H	2.211962000	1.047273000	-1.346597000
C	-3.711548000	-0.757676000	-1.666853000
H	-4.526748000	-1.441290000	-1.944932000
H	-2.924876000	-0.791003000	-2.431410000
H	-4.094109000	0.270960000	-1.624239000
C	-4.527644000	-1.239665000	0.998227000
H	-4.275002000	-1.565845000	2.016127000
H	-5.275560000	-1.925498000	0.574230000
H	-4.957273000	-0.230526000	1.044130000
C	-0.279569000	-2.902952000	-2.047454000
H	-0.573964000	-3.900456000	-2.404129000
H	0.806018000	-2.776981000	-2.163163000
H	-0.770242000	-2.132943000	-2.655613000
C	0.013203000	-4.221429000	0.416205000
H	-0.240173000	-4.312074000	1.480337000
H	1.106452000	-4.191161000	0.315517000
H	-0.365965000	-5.103794000	-0.120161000

Table S18. Cartesian Coordinates for [Mo(N_2)(prPPHP)(dmpm)] (**3c**) (coordinates in Angstrom).

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symmetry c1

C	-0.436634000	0.226488000	-3.646542000
P	1.562794000	3.262120000	1.524510000
P	-0.419468000	0.337165000	2.796966000
P	-0.678883000	-0.302537000	-0.827813000
P	-1.812328000	2.530834000	0.775322000
C	-3.320156000	1.950103000	-0.160244000
C	-3.004984000	1.254097000	-1.484089000
C	-2.469608000	-0.174555000	-1.309525000
C	0.845443000	-0.309158000	3.990429000
C	2.199024000	-0.049011000	3.755498000
C	3.176297000	-0.462016000	4.665498000
C	2.807244000	-1.140885000	5.826854000
C	1.456167000	-1.405412000	6.073678000
C	0.483787000	-0.992026000	5.163956000
C	-1.571334000	-1.116212000	2.709055000
C	-1.128795000	-2.441374000	2.824866000
C	-2.003328000	-3.510482000	2.624553000
C	-3.340441000	-3.279460000	2.301541000
C	-3.798083000	-1.964681000	2.185495000
C	-2.920563000	-0.900068000	2.387408000
C	-2.647826000	2.957602000	2.400374000
C	-1.718917000	2.832871000	3.605763000

C	-1.406680000	1.398522000	4.021930000
C	0.143412000	-0.329841000	-2.496043000
C	1.436028000	-0.871156000	-2.604307000
C	2.126200000	-0.845061000	-3.814838000
C	1.543797000	-0.272386000	-4.949307000
C	-0.538677000	-2.128518000	-0.503139000
C	0.568399000	-2.586482000	0.224368000
C	0.797759000	-3.951720000	0.398834000
C	-0.101749000	-4.884732000	-0.117915000
C	-1.227140000	-4.440211000	-0.814570000
C	-1.435909000	-3.074964000	-1.017723000
C	0.257635000	0.260495000	-4.859312000
P	0.978768000	2.839655000	-1.106124000
C	1.307074000	4.541494000	2.845692000
C	3.386299000	3.054795000	1.746907000
C	-0.064366000	3.616581000	-2.417490000
C	2.504426000	2.519443000	-2.084972000
H	-1.446035000	0.637105000	-3.611971000
H	-3.981289000	2.815956000	-0.317813000
H	-3.857303000	1.249446000	0.497882000
H	-3.928751000	1.204124000	-2.084153000
H	-2.297352000	1.867611000	-2.063254000
H	-2.625078000	-0.748843000	-2.234697000
H	-3.031918000	-0.685958000	-0.512556000
H	2.478342000	0.481812000	2.847248000
H	4.228621000	-0.255965000	4.460301000
H	3.567932000	-1.466673000	6.538620000
H	1.159854000	-1.936953000	6.980126000
H	-0.567314000	-1.211452000	5.361685000
H	-0.086437000	-2.643231000	3.070057000
H	-1.628503000	-4.531893000	2.706530000
H	-4.020595000	-4.116789000	2.138647000
H	-4.843472000	-1.766368000	1.939569000
H	-3.294604000	0.120674000	2.292683000
H	-3.050638000	3.978179000	2.320977000
H	-3.514228000	2.287384000	2.522122000
H	-0.779092000	3.357619000	3.398738000
H	-2.177980000	3.346955000	4.467495000
H	-2.336274000	0.860944000	4.261869000
H	-0.805401000	1.415311000	4.941741000
H	1.912157000	-1.320461000	-1.733310000
H	3.128383000	-1.274035000	-3.869965000
H	2.085189000	-0.249808000	-5.896240000
H	1.248699000	-1.863120000	0.671409000

H	1.674548000	-4.283388000	0.958439000
H	0.067621000	-5.953127000	0.027515000
H	-1.945098000	-5.160509000	-1.211747000
H	-2.310443000	-2.758231000	-1.586083000
H	-0.217166000	0.699117000	-5.739383000
H	2.069628000	5.329989000	2.763817000
H	1.381520000	4.076743000	3.838886000
H	0.314152000	4.998901000	2.745784000
H	3.900682000	4.024744000	1.694125000
H	3.793864000	2.380719000	0.983985000
H	3.577711000	2.604637000	2.730942000
H	-1.002545000	3.981202000	-1.978997000
H	-0.295756000	2.864629000	-3.183292000
H	0.463101000	4.457888000	-2.890109000
H	3.285910000	2.104593000	-1.436012000
H	2.870055000	3.440724000	-2.560832000
H	2.279979000	1.772446000	-2.857698000
Mo	0.277901000	1.339805000	0.682746000
N	2.035079000	0.393348000	0.494448000
N	3.061468000	-0.079858000	0.334673000
C	1.449579000	4.278520000	-0.027306000
H	0.569280000	4.935244000	0.063609000
H	2.322049000	4.886197000	-0.319243000
H	-1.803202000	3.868426000	0.238577000

Table S19. Cartesian Coordinates for [Mo(N_2)(PN(Ph)P)(dmpm)] (**4**) (coordinates in Angstrom).

Mo	-1.27136153984194	0.14974682389290	-0.18562359648865
N	-2.25899906196482	2.30197366950856	0.76502275533631
P	1.11164238413612	0.71121997725254	-0.24839365858263
P	-1.32106077052976	-0.35155382005149	2.14745534222584
P	-3.57681483576851	-0.05812607366406	-0.75829224146854
C	-2.66405142707801	2.06667648183734	2.18092351173183
C	-1.67313372076601	1.26075908732604	3.00461654080926
C	-3.51171408471718	2.62118709812443	-0.01137603367709
C	-4.47576564269222	1.45024231058552	-0.13343992009181
C	0.21858530140987	-0.91695236966451	2.99320011247584
C	0.97654727698579	-1.92115728066824	2.37013194599138
C	0.65711647083321	-0.41000922995990	4.22564725188020
C	1.83707823523843	-0.87884936234400	4.80927882058158
C	2.57945828396785	-1.88361906421204	4.18444660848003
C	2.13975284358354	-2.41069273441052	2.96717859137011
C	-2.51606378607678	-1.52051559895064	2.95950642818856
C	-2.18166962124528	-2.87428272764048	3.12579003697945
C	-3.81309966485588	-1.11493455244133	3.31336534044979
C	-3.10681023156124	-3.78572081855667	3.63730071858354
C	-4.38934175835448	-3.36482664794837	3.99365917349471

C	-4.73840251882122	-2.02316035254773	3.82798810995722
C	-4.70614610700264	-1.41778137666804	-0.22276814279393
C	-4.13373042145670	-2.63387093457974	0.16982748714860
C	-6.10312277887842	-1.28808312125648	-0.22381457012620
C	-4.94348153218563	-3.70518315029332	0.55145548852804
C	-6.33229941216077	-3.56510444349316	0.56288006672819
C	-6.91197614273781	-2.35209402226387	0.17837571541411
C	-3.98268866286643	-0.08333568847635	-2.56396345225137
C	-3.61261671778504	-1.23663886234959	-3.27835693255077
C	-4.54266437513817	0.98836095139104	-3.27197743422653
C	-3.80155270959800	-1.31551282814481	-4.65701229694703
C	-4.35931745433328	-0.23763408207900	-5.35429660763386
C	-4.72870470989311	0.91304810423397	-4.65644555568397
C	2.38019297908096	-0.62165255087323	-0.41479956975808
C	2.06428579295158	1.89086609337558	0.80686988388588
H	-3.60784896352151	1.51792241740343	2.14093141063124
H	-2.88944140593681	3.03588348987535	2.66204720619464
H	-2.07526617978078	1.11924133990984	4.01979290247905
H	-0.70634253754604	1.77532214595201	3.08851868679947
H	-3.20457533573528	2.93746820498779	-1.01261369803075
H	-4.00994314391157	3.48353010911013	0.47217936315814
H	-5.30964202574248	1.74794328767923	-0.78529437383550
H	-4.92841213133710	1.17647500654876	0.82945393315785
H	0.65281385195052	-2.31571610667400	1.40505619094426
H	0.07805767398656	0.35428370674730	4.74605141610029
H	2.17203027078009	-0.46295408515804	5.76160443710017
H	3.49639135886422	-2.25515313441383	4.64515842944884
H	2.71068479800953	-3.19926924948476	2.47301769843885
H	-1.18323680376645	-3.22386607028830	2.86007156610618
H	-4.11968071677808	-0.07592783262941	3.19106323947838
H	-2.82021549188759	-4.83239466060421	3.75812720294718
H	-5.11430605840403	-4.07752893054627	4.38994772322204
H	-5.74012335136460	-1.68042194976764	4.09394180500078
H	-3.04789804699648	-2.72923349883210	0.18665728532335
H	-6.56843673828012	-0.35451375554111	-0.54793548869538
H	-4.48439963328115	-4.64580112429838	0.85924390348748
H	-6.96502441959121	-4.39844749159867	0.87395854659882
H	-7.99801760529460	-2.23816078393228	0.18395911493052
H	-3.16583273857819	-2.07852817555313	-2.74372699615901
H	-4.83169583489738	1.90542466919551	-2.75589673524037
H	-3.51081427505113	-2.22176059778373	-5.19196673438310
H	-4.50442274775978	-0.29680459189772	-6.43415504192723
H	-5.16205459762817	1.76153707169087	-5.18981171052574
H	3.28339464572811	-0.23072044987409	-0.90508866116676
H	1.97354033021883	-1.45559133877143	-1.00171486914610
H	3.07182250065543	2.06889006011476	0.40266842077114
H	1.52434690364037	2.84296879546612	0.87783981652841
H	2.15142934274232	1.46144453561599	1.81567519177300

H	2.64613221896726	-0.99966264922465	0.57983407678941
C	-1.31061071454696	3.39309208357443	0.63506467034044
C	-0.93105322421150	3.81673975764911	-0.64824409258313
C	-0.77217555686315	4.07868614245240	1.73602139936299
C	-0.03576678229160	4.86503650390919	-0.83114786010533
C	0.52023883110079	5.52429176057502	0.27140392542766
C	0.14325997528220	5.12154631367969	1.54951252258842
H	-1.04017458703882	3.81203362822413	2.75473199506704
H	0.55804383547625	5.62077853008693	2.42687589309541
H	1.23266426217281	6.33790560168170	0.13144956698022
H	0.23656936051194	5.16302886995777	-1.84535919884828
H	-1.32764535549349	3.28925253376774	-1.51204021265622
N	-0.84503658736909	-1.68095276883956	-0.63501492024194
N	-0.59279160408552	-2.78070255280634	-0.86991704151385
P	-0.49729542393199	0.74429427439415	-2.44962485715607
C	1.13854246357201	1.46414202514862	-1.95031282079101
C	-1.11642199816804	1.85338561312787	-3.80553815474342
C	0.00164364232833	-0.66787057599304	-3.52772736401060
H	-1.98108332664344	1.37037770087954	-4.28033719402426
H	-0.33182364112233	2.01067923353475	-4.56033075636522
H	-0.90161625694255	-1.13354065186358	-3.94340560493664
H	0.64382934624499	-0.32254353725285	-4.35068078469427
H	-1.44283098054830	2.82957719104965	-3.42477745677591
H	0.53019070970275	-1.42464570968861	-2.93616161482394
H	2.00696063359804	1.23437717587089	-2.58912243206214
H	1.03916998691593	2.55465358946667	-1.85119278278950

Table S20. Cartesian Coordinates for [Mo(N_2)$_2$(PN(Ph)P)(dmpm)] (**6**) (coordinates in Angstrom).

C	2.78140131503078	3.43868155023121	-1.03611795266385
C	3.63484518688269	3.91349304403079	1.17138245047711
C	3.48951730032847	4.53068913161954	-1.54640565461831
C	4.33531744246263	5.00883461175498	0.66686007692062
C	4.26077825786211	5.32258973772728	-0.69468314417033
H	2.16987301878951	2.82800737573791	-1.69593998163064
H	3.71271090855257	3.66976018455593	2.23270122040612
H	3.42921911347577	4.76564185337242	-2.61042526193174
H	4.94105536042830	5.62146997623856	1.33704367993866
H	4.80579206469485	6.18253802944761	-1.08771675812469
C	2.83819393963000	3.12355560340240	0.32589748280733
Mo	0.46442998834469	0.24800559291138	-0.41360272116883
P	1.85801093703686	1.70154117372751	0.97395820116569
P	2.26629505042699	-1.29159238005529	-1.02817479371100
P	-0.37806543029099	-1.64785817603524	-1.72932845676386
N	0.71576432889237	1.07683639844687	-2.23006011084271
N	0.09511886391508	-0.77219505606321	1.26504160641407
N	0.83211137759044	1.42944541214375	-3.30810159253649
N	-0.14690420596278	-1.38280351907883	2.19734739932897
P	-1.67181669795187	1.34610508187972	0.03502901856505

C	-2.02314232939295	1.93555133934409	1.78826440179093
C	-1.87212212652213	3.44108938588140	2.00957296456152
C	1.16475847863301	2.43854011397635	2.55980434024756
C	0.50795664633569	3.81814479476319	2.50966058969361
N	-0.60868700996373	4.03194585889565	1.58228692964640
C	-0.66406741755076	5.31719168786376	0.99234656254898
C	0.48171227568669	5.83333226690464	0.34990530246119
C	-1.82743825719809	6.11192542459751	0.97291434812667
C	0.45639396367211	7.06485922879923	-0.29544391802607
C	-1.84752084504711	7.34170180290221	0.31207048361759
C	-0.71171183891691	7.83303309559411	-0.32967130296267
C	-2.26507849551537	2.78089353170527	-0.95633111750537
C	-1.31822857757934	3.56738345575972	-1.62305087545729
C	-3.61734910242863	3.15730411322789	-1.00967184056177
C	-1.70949404202429	4.69496653068654	-2.34600000869413
C	-4.01000841502940	4.28474933056983	-1.73228631133978
C	-3.05633922655504	5.05360632244537	-2.40606171820835
C	-3.07261305836808	0.15069490979163	-0.14494082400132
C	-3.74237265895096	-0.00654476759323	-1.36936937285476
C	-3.40525492057308	-0.71785512503957	0.90938506783650
C	-4.72013574167602	-0.98902932830545	-1.53237172209367
C	-4.37829990320829	-1.70605535405259	0.74492156185556
C	-5.04359362249030	-1.84525523696532	-0.47569575458242
C	3.22925064647075	0.72649949687565	1.75864505783104
C	2.97676183315357	-0.09487277008583	2.87076983271759
C	4.51896570314072	0.71483304433168	1.20401404267325
C	3.98133818796152	-0.90290716267506	3.40655683809037
C	5.52363097860304	-0.09486968104246	1.73727972646265
C	5.25966277190285	-0.90909978712616	2.84197387420029
C	1.28854264406769	-2.27436969801844	-2.26810960848600
C	-1.31161469464757	-1.55698596379412	-3.31409181070496
C	3.80406423714208	-0.85580723068630	-1.94329126002448
C	2.87490652002999	-2.55846109893478	0.15337019692452
H	-1.38811517155577	1.34284527686314	2.45848112281987
H	-3.06587755148845	1.68410332635521	2.03441692436898
H	-2.06224167248625	3.66406983982723	3.08176446705732
H	-2.67275590766669	3.91743405202743	1.43686228117447
H	1.98982190280996	2.51365754606561	3.28525103204958
H	0.48009330902160	1.67956690778203	2.96084252110591
H	1.27902658613902	4.55963494753323	2.27485649496775
H	0.15822518489621	4.04984974091335	3.53996482546299
H	1.39289713755638	5.24022151209024	0.31566085196480
H	-2.73605595861776	5.78639923339131	1.47571126176183
H	1.36166173593544	7.41527318514958	-0.79569279091995
H	-2.77152571618603	7.92353857675733	0.31164552315813
H	-0.73386677618394	8.79345536838163	-0.84629144080317
H	-0.26467658520783	3.30292437490253	-1.54372917404635
H	-4.36957071123737	2.56252954960576	-0.48780013009870

H	-0.95520530859347	5.30552562091096	-2.84407052263684
H	-5.06408489838695	4.56742884020329	-1.76451869957487
H	-3.36329622698206	5.93921245944038	-2.96502131033133
H	-3.49905462764246	0.65345412237741	-2.20389680029727
H	-2.89042899410192	-0.64050896581196	1.86777758699546
H	-5.23447100158697	-1.08412020487429	-2.49095103631553
H	-4.61558409280852	-2.37129634946157	1.57739827822701
H	-5.80781723858389	-2.61361180061429	-0.60276940761040
H	4.74345386281371	1.35757828301259	0.35108028683871
H	3.76065143704886	-1.53456278310401	4.26916805423812
H	6.51986310425259	-0.08369896566426	1.29046300853932
H	6.04415113832119	-1.54132891869136	3.26083784019728
H	1.49604680818308	-1.87289760723146	-3.27257055656584
H	1.43946979380167	-3.36518861394598	-2.28354710173472
H	-0.91075692822557	-0.73281408758740	-3.91921943891925
H	-2.36913057820087	-1.35912113591787	-3.10329278402389
H	-1.22202575201482	-2.49948209232505	-3.87329486550233
H	4.50856984536446	-0.37177757828909	-1.25557258237480
H	3.55039710368220	-0.14702413217749	-2.74299892361859
H	4.27650352780160	-1.74823149458638	-2.37881540916373
H	2.02126250988882	-2.98715673521905	0.69472117574312
H	3.53718257286438	-2.08006066180406	0.88633016453670
H	3.41955335360307	-3.35833625785538	-0.36855097729417
C	-1.17302047697626	-3.08567581695390	-0.91135908881250
H	-1.19460447264616	-3.96006036411995	-1.57716117710269
H	-2.19887285715283	-2.80930669877627	-0.63240476504679
H	-0.62654767817990	-3.33510427534015	0.00755090093491
H	1.98434554542840	-0.12163537983076	3.32080499700712

Table S21. Cartesian Coordinates for [Mo(N_2)(prPN(Ph)P)(dmpm)] (**5**) (coordinates in Angstrom).

Mo	0.64955636234817	-0.03227079192009	-1.17426134390229
N	1.25702011397006	1.48236026917363	-2.20496226708204
N	1.61877854040917	2.36504672283402	-2.84757485572116
N	0.16999202052008	-2.17453211616076	0.22201984674586
P	2.12479283023842	0.51216042327780	0.67009311623144
P	-1.31912210850070	1.30276107858656	-0.50185759755548
P	-1.18551086021975	-0.10694808886453	-2.85006665959408
P	2.16111761137996	-1.37042179301003	-2.51877983751384
C	-2.49646518537685	0.63012291836426	-1.77077105217788
C	-1.11234191365222	1.14049833939415	-4.20880362129648
C	1.01312093642359	-2.28127994853790	1.47051560013660
C	2.48923688645973	-2.16696985616501	1.27269242823148
C	3.08253940160230	-0.98755572328265	1.00412912392258
C	-1.23871890736978	-2.16704292258166	0.59202094615271
C	0.43132071515339	-3.37065438826184	-0.66899222731196
C	1.87295579521159	-3.66937782601802	-0.95507974248119
C	2.64953838485058	-2.96970785544367	-1.79910505663369

C	-1.24893147541973	3.10527379432452	-0.89656772837532
C	-2.38621656746222	1.38212839440702	1.00589105453679
C	-2.03887123486252	-1.43570157829893	-3.82641779466253
C	3.84105556712465	-0.76139866073788	-3.02119571557269
C	4.35548219797063	0.39970755236563	-2.44000881042567
C	4.63098721083422	-1.46952456008510	-3.94172397462044
C	5.64067755039781	0.84836625623416	-2.75745314804632
C	6.42526055110199	0.13274043026490	-3.66286362719159
C	5.91677641582375	-1.02891481221138	-4.25567635525112
C	1.56045865809304	-1.88536835143513	-4.19472269727165
C	1.52265652296190	-0.92363824384658	-5.21764348707110
C	1.08123734314518	-3.17424879122044	-4.46186751761450
C	1.00806752567763	-1.24290820202229	-6.47404147750376
C	0.52020083226868	-2.52960649388633	-6.72880346202067
C	0.56119492420224	-3.49419545624186	-5.71975846031374
C	3.41184166473935	1.83229763352141	0.55205736820756
C	4.70974710446515	1.68940496257221	1.06501378165320
C	3.05463887753401	3.04810386654911	-0.05109320737082
C	5.63559006572623	2.72825110419227	0.95372024338804
C	5.27425985916624	3.93078110018775	0.34075091207974
C	3.97815422274692	4.08939877774299	-0.15490432746483
C	1.49821520683320	1.01548499468744	2.35564846933080
C	0.72455460297648	2.18153892381661	2.43619588506326
C	1.78031200723935	0.31646509671218	3.53666200356267
C	0.23645506179881	2.63716687614775	3.66021855756061
C	0.50268060632372	1.91904871113824	4.83046905700270
C	1.27604535832668	0.75871497459790	4.76387531843411
C	-2.21734577502626	-2.51357762145344	-0.35767655767391
C	-1.68744655781706	-1.89947311562626	1.90016461209431
C	-3.57029131319580	-2.56304342425631	-0.03307203162399
C	-4.00326236453047	-2.28408693575765	1.26553238208901
C	-3.04649296212532	-1.95540539310286	2.22263568275139
H	-3.07199449875541	-0.17826158152707	-1.29715319050547
H	-3.18855249265744	1.34363207068753	-2.24635810804783
H	-2.11570716861994	1.26987158209694	-4.63875073164114
H	-0.42735142461230	0.79588311165443	-4.99222191834572
H	-0.74438195823271	2.10158365101831	-3.83338084387697
H	0.75488548343329	-3.22316048424336	1.98642416442272
H	0.69707946739191	-1.45129568617309	2.10881962929502
H	3.09036293646358	-3.07461895590433	1.34338353381584
H	4.15450023056223	-0.96399461709716	0.79249689096577
H	-0.03788443785044	-4.25399274013325	-0.20143841189333
H	-0.08090244232090	-3.16978070858532	-1.61627237467550
H	2.28452567384407	-4.56238361120789	-0.47599598987918
H	3.68895332590396	-3.28067204883038	-1.94209579939474
H	-0.68472377957030	3.27040280075725	-1.82236731709611
H	-0.72751395001241	3.63420040817664	-0.08642814686422
H	-2.26048523115855	3.52431302004857	-0.99597346571965

H	-2.74515534150655	0.37639031460318	1.24897844739976
H	-3.24728892561087	2.04191295701106	0.82208186735436
H	-1.81192183724032	1.76078083886857	1.86077668179162
H	-2.96478327060783	-1.04204069491572	-4.27089888364137
H	-2.28432855250917	-2.30879528808410	-3.21125104707543
H	-1.36492284502002	-1.76259285600019	-4.62957071755895
H	3.74166704156821	0.95518075081689	-1.73468400085336
H	4.23577625691823	-2.36789650865724	-4.42109227723376
H	6.02148915634232	1.75982731324663	-2.29270317843910
H	7.42997681084918	0.47861166662323	-3.91304255086008
H	6.52461072743868	-1.59074431135589	-4.96777751924883
H	1.90650532755903	0.08133147759600	-5.02619269217929
H	1.12733064734050	-3.93787948162099	-3.68281192669603
H	0.98971434515895	-0.48565930471709	-7.26043121569361
H	0.11633885115423	-2.77865072841360	-7.71149268308627
H	0.19039668465309	-4.50303460486302	-5.91203922567567
H	5.00672754594254	0.76693464328685	1.56510132694084
H	2.05450608651497	3.17074475997495	-0.46348347246755
H	6.64322626641106	2.59815204074563	1.35321210106465
H	5.99985424560145	4.74109569141846	0.25165256668039
H	3.68493407869312	5.02365814896528	-0.63681402680304
H	0.51055223981946	2.74313335073335	1.52458435221628
H	2.40632595965749	-0.57712456741679	3.49636800854805
H	-0.35651559341788	3.55306115182583	3.70204013038476
H	0.11473329968774	2.26754914745560	5.78905474376563
H	1.49836416218877	0.19647789063787	5.67317022903457
H	-1.92293887126718	-2.74043144837489	-1.37637967341957
H	-1.00021460268923	-1.62451348073042	2.69442976204013
H	-4.28998259413643	-2.82950414454324	-0.80944749764280
H	-5.06166460801994	-2.32792715222777	1.52400530014414
H	-3.34870473576848	-1.73121403329018	3.24714740281994

Table S22. Cartesian Coordinates for *syn*-[Mo(N_2)$_2$(prPN(Ph)P)(dmpm)] (**7a**) (coordinates in Angstrom).

Mo	0.06545058588677	0.96576259514744	-0.45168220558406
N	-1.16364659992441	2.54039211309478	-0.24399589600902
N	-1.61340692824713	-4.08358023802476	1.03313446025428
N	-1.79202608683379	3.48020917955627	-0.13597738399150
P	1.93766891607716	2.41317787394122	0.20241222817461
P	-0.57343193939379	0.29380601153678	1.83117448546240
P	-1.59289635446377	-0.32456190220320	-1.73390067584544
P	1.08145897524517	2.10252273678888	-2.38256967237656
C	2.65380698103881	2.55202177626355	-1.50573980124824
C	1.67206395060813	1.45162583710021	-4.00210110414343
C	1.70020301512954	4.17161964584311	0.68677610957668
C	3.37021527552519	1.93029775498392	1.24923162614977

C	-1.41469134505062	-4.32578739842012	-0.38917423172149
C	-1.11276364856653	-3.07722528706617	-1.23405011015015
C	-2.19232055462151	-1.99899101171935	-1.16738080893136
C	-0.40012422335452	-3.94913644632423	1.82895634552356
C	0.19615283594968	-2.52685571161033	1.86736869195899
C	-0.79718318112463	-1.48287588159277	2.36456929940788
C	-2.88325056102461	-4.01168113968638	1.59418306659931
C	-4.05420941403143	-4.05966504516988	0.79533741130865
C	-3.07774105413797	-3.87016892825265	2.99158654885317
C	-4.35432028174104	-3.79884543804752	3.54276158234260
C	-5.32406071057800	-3.98892575576999	1.36359680641124
C	-5.49704370574719	-3.86009904955143	2.74275116713301
C	0.53439698705549	0.96211522840415	3.14872711161736
C	1.49804460042533	0.18279603596802	3.80278578435674
C	2.37219877682209	0.75542894968370	4.73240797744289
C	2.28849057249521	2.11621741232393	5.03144504199957
C	1.32201037296101	2.90224220952708	4.39302639250498
C	-2.21019908493242	0.85970743740471	2.49631361460265
C	-3.27058838721331	1.06211416155922	1.60757730669657
C	-2.45621952809819	0.96508835234209	3.87465799879707
C	-4.55127943240841	1.36109945609161	2.07569943666681
C	-4.78669259740191	1.46761343634850	3.44699417491369
C	-3.73404717600330	1.26914140414860	4.34565475793399
C	-3.18675590720610	0.56240150524318	-1.98880443875786
C	-3.14774986158335	1.81537745432044	-2.62258564686074
C	-4.30573936944261	2.57039774074664	-2.79527692845927
C	-5.53086748722872	2.09232602306399	-2.32057613015511
C	-5.58318224530926	0.85411810253777	-1.67877884855414
C	-4.42268256713267	0.09150095777776	-1.51899452105368
C	-1.16358449069261	-0.79687565448030	-3.47758646794946
C	0.09391816676131	-1.37427986275321	-3.71671302890931
C	-2.05004202876459	-0.65766524378411	-4.55599540465844
C	0.45233316896954	-1.80916540994899	-4.99288283442631
C	-1.68252217013007	-1.06998268343558	-5.84005177080502
C	-0.43228929094583	-1.65108291219132	-6.06282101382254
C	0.40553853936785	3.72551640746770	-2.93239812784537
H	3.15602841757891	3.49304967308413	-1.78154499865552
H	3.35625595287279	1.71418566897553	-1.64212242233699
H	2.23525276199916	0.52407366577210	-3.84192204964060
H	2.31897419380949	2.19164204190110	-4.49561737510860
H	0.81440079998549	1.22279783011204	-4.64773452676468
H	1.39273300280854	4.21988629124682	1.73843561939923
H	0.90882457437604	4.62318171557428	0.07550663259855
H	2.63285886031291	4.73870592933560	0.55662879474963

H	3.66393678217035	0.90269019801206	0.99661479443141
H	3.07943484346885	1.96017506986267	2.30667459447126
H	4.22169821120235	2.60585086799410	1.08309964913054
H	-2.28889987937779	-4.85458426903223	-0.79127584682240
H	-0.56374018118770	-5.02049884360650	-0.49103673468894
H	-0.97396674165653	-3.40222712790064	-2.27639186527185
H	-0.14613324914463	-2.66032237281335	-0.91819737189297
H	-2.52867927773098	-1.86016328956627	-0.12916207374802
H	-3.06556779730808	-2.29667508524273	-1.76851118687937
H	0.35286710385121	-4.63047947514719	1.40012979358307
H	-0.58920333180141	-4.30753383495946	2.84989599587840
H	0.54357862901899	-2.25403931850974	0.86425736144637
H	1.09705859700903	-2.56092548754836	2.50046915704612
H	-0.90340657647987	-1.50166827984067	3.46068850279138
H	-1.79263511897094	-1.71565654572423	1.95922626224450
H	-3.98158709190059	-4.12674596504739	-0.28772759572539
H	-2.22630978863566	-3.79103606783072	3.66365290173216
H	-4.44973895586923	-3.68396620905187	4.62450621565048
H	-6.19364789728023	-4.02541701406247	0.70380976157441
H	-6.49331271949661	-3.79422111669639	3.18051051840285
H	1.57974506092346	-0.88239539679157	3.58631779240957
H	3.12042474882198	0.13168366003416	5.22522414032175
H	2.96781392877511	2.56311724371172	5.75897575250336
H	1.23999227981413	3.96548158021398	4.62755338044132
H	-3.08828055965937	0.98453277874728	0.53729340135659
H	-1.64451726259183	0.81089910912054	4.58780182938659
H	-5.36146894362957	1.51540495360547	1.36052701997409
H	-5.78560720262689	1.70520683446582	3.81732700372478
H	-3.90961633559713	1.34810459165732	5.42039174104975
H	-2.18955730043944	2.20037855495850	-2.97484931172698
H	-4.25101188659146	3.54101642230185	-3.29138311561818
H	-6.43806331345069	2.68561670142625	-2.44593615094689
H	-6.53317395330181	0.47273914003825	-1.29944644658429
H	-4.49113050741657	-0.86867989214493	-1.00733423062837
H	0.80518929728983	-1.47463285525338	-2.89696471061256
H	-3.03603047095965	-0.22000998738168	-4.39576030001713
H	1.43330521591846	-2.26050037550136	-5.15422314451665
H	-2.38202167170300	-0.94138433509750	-6.66847846650748
H	-0.14811125608833	-1.97768126142809	-7.06465688587162
H	0.03478585298025	4.30122860629560	-2.07590097914784
H	-0.43899752292047	3.54897818243114	-3.61299000039140
H	1.17189580401889	4.30671317810171	-3.46440542549672
C	0.46022620068866	2.33117703489911	3.45833901819296
H	-0.29366799479103	2.94961449512911	2.96602656483977

N	1.47832168609662	-0.44273594349987	-0.64154363112607
N	2.35062847583204	-1.16931846851257	-0.76766972703331

Table S23. Cartesian Coordinates for *anti*-[Mo(N_2)$_2$(prPN(Ph)P)(dmpm)] (**7b**) (coordinates in Angstrom).

Mo	-0.24397844606298	-0.29030698535820	0.26625281015797
N	-0.98878356161765	1.29904367025178	-0.69888766728984
N	-1.48155987185617	2.21237776876148	-1.17396587301710
N	0.35947938561357	-1.85521827128115	1.37350610086248
N	0.64457185379716	-2.74258770208540	2.02408496981754
P	-1.97384715325163	0.24130744247946	1.90760837323168
P	1.44994374032103	1.12710153782210	1.32618360946911
P	-2.34185292634160	-1.47209794767467	-0.19185729875619
P	1.00378852695499	-1.17537223307983	-1.67189803038544
C	-3.39564464360412	-0.38482274433810	0.88537628236036
C	-2.12343467875795	-0.64973131602265	3.50624951886389
C	-2.49198355020698	1.93996956707293	2.38853078266665
C	-2.62163981472488	-3.14233815277037	0.53156611484195
C	-3.29582399664949	-1.61322748675551	-1.76258105531718
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