Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information:

Molybdenum dinitrogen complex supported by a cyclohexane-based triphosphine ligand and dmpm

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Crystal Structure of 1,3,5-*cis,cis*-Tris(diphenylphosphino)cyclohexane (tdppcy)

Single crystals suitable for X-ray crystal structure determination were obtained by slow evaporation of a benzene solution of tdppcy over a period of several days.

Table S1 Crystal data and structure refinement for $C_{42}H_{39}P_3$.

Empirical formula	$C_{42}H_{39}P_3$	
Formula weight	636.64	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 10.7012(2) Å	α= 90°.
	b = 23.6772(6) Å	β= 90°.
	c = 13.8942(4) Å	γ = 90°.
Volume	3520.44(15) Å^3	
Z	4	
Density (calculated)	1.201 Mg/m^3	
Absorption coefficient	0.197 mm^{-1}	
F(000)	1344	
Crystal size	0.10 x 0.16 x 0.24 mm^3	
Theta range for data collection	1.699 to 27.005°.	
Index ranges	-13<=h<=11, -30<=k<=30, -17<=l<=17	
Reflections collected	23836	
Reflections [I>2sigma(I)]	7081	
Independent reflections	7671 [R(int) = 0.0606]	
Completeness to theta = 25.242°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7671 / 1 / 406	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0900	
R indices (all data)	R1 = 0.0421, wR2 = 0.0922	
Absolute structure parameter	-0.01(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.178 and -0.208 e.Å^{-3}	

Comments: A numerical absorption correction was performed (Tmin/max: 0.9120/0.9735). All non-hydrogen atoms were refined anisotropic. The C-H hydrogen atoms were positioned with idealized geometry and refined isotropic with $U_{iso}(H) = 1.2\ U_{eq}(C)$ using a riding model.

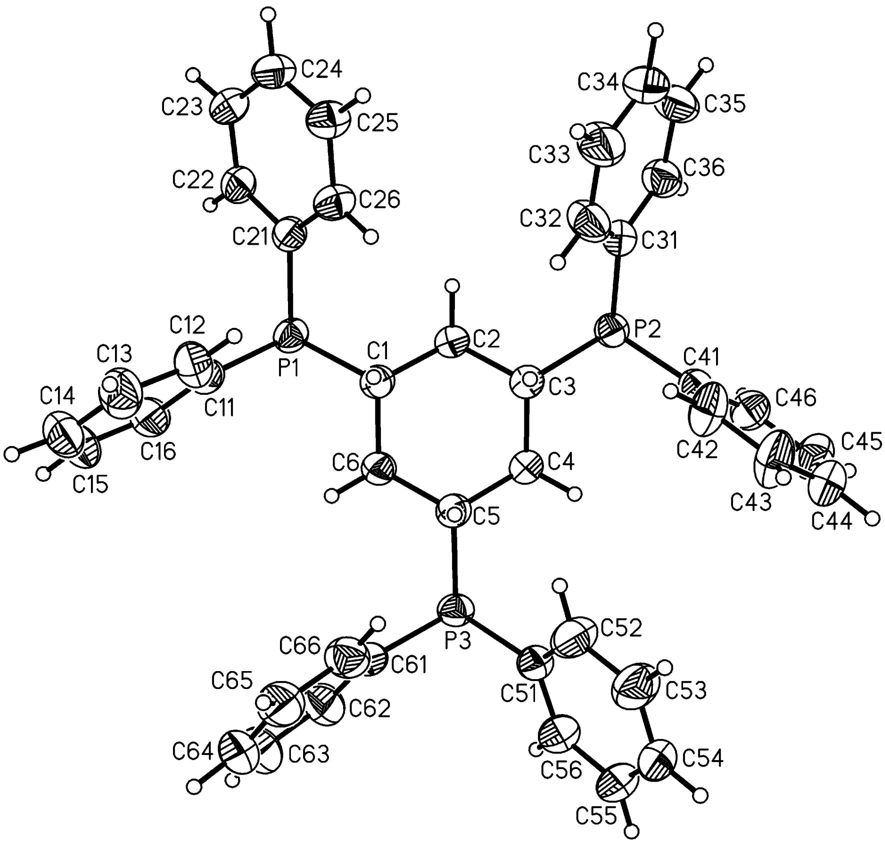

Fig. S1 ORTEP-plot of the ligand tdppcy.

Table S2 Bond lengths [Å] and angles [°].

C(1)-C(2)	1.530(4)	C(31)-C(36)	1.391(4)
C(1)-C(6)	1.539(4)	C(32)-C(33)	1.372(5)
C(1)-P(1)	1.857(3)	C(33)-C(34)	1.380(5)
C(2)-C(3)	1.531(4)	C(34)-C(35)	1.367(6)
C(3)-C(4)	1.522(4)	C(35)-C(36)	1.388(5)
C(3)-P(2)	1.859(3)	C(41)-C(46)	1.380(4)
C(4)-C(5)	1.530(4)	C(41)-C(42)	1.385(4)
C(5)-C(6)	1.533(4)	C(42)-C(43)	1.380(5)
C(5)-P(3)	1.857(3)	C(43)-C(44)	1.378(5)
P(1)-C(21)	1.840(3)	C(44)-C(45)	1.365(6)
P(1)-C(11)	1.843(3)	C(45)-C(46)	1.377(5)
C(11)-C(16)	1.387(4)	P(3)-C(61)	1.836(3)
C(11)-C(12)	1.395(5)	P(3)-C(51)	1.846(3)
C(12)-C(13)	1.387(5)	C(51)-C(56)	1.383(4)
C(13)-C(14)	1.372(6)	C(51)-C(52)	1.389(4)
C(14)-C(15)	1.369(7)	C(52)-C(53)	1.385(5)
C(15)-C(16)	1.393(6)	C(53)-C(54)	1.365(6)

Table S2 Bond lengths [Å] and angles [°].

C(21)-C(26)	1.387(4)	C(54)-C(55)	1.379(6)
C(21)-C(22)	1.388(4)	C(55)-C(56)	1.382(5)
C(22)-C(23)	1.378(4)	C(61)-C(62)	1.387(4)
C(23)-C(24)	1.380(5)	C(61)-C(66)	1.392(5)
C(24)-C(25)	1.381(5)	C(62)-C(63)	1.388(6)
C(25)-C(26)	1.387(4)	C(63)-C(64)	1.376(7)
P(2)-C(31)	1.836(3)	C(64)-C(65)	1.366(7)
P(2)-C(41)	1.836(3)	C(65)-C(66)	1.382(5)
C(31)-C(32)	1.387(4)	C(32)-C(31)-P(2)	127.3(2)
C(2)-C(1)-C(6)	109.9(2)	C(36)-C(31)-P(2)	115.7(2)
C(2)-C(1)-P(1)	110.16(18)	C(33)-C(32)-C(31)	121.6(3)
C(6)-C(1)-P(1)	108.65(18)	C(32)-C(33)-C(34)	120.2(4)
C(1)-C(2)-C(3)	111.5(2)	C(35)-C(34)-C(33)	120.0(3)
C(4)-C(3)-C(2)	110.0(2)	C(34)-C(35)-C(36)	119.4(3)
C(4)-C(3)-P(2)	110.83(18)	C(35)-C(36)-C(31)	121.8(3)
C(2)-C(3)-P(2)	108.77(18)	C(46)-C(41)-C(42)	118.1(3)
C(3)-C(4)-C(5)	110.9(2)	C(46)-C(41)-P(2)	118.1(2)
C(4)-C(5)-C(6)	110.9(2)	C(42)-C(41)-P(2)	123.8(2)
C(4)-C(5)-P(3)	108.10(18)	C(43)-C(42)-C(41)	120.5(3)
C(6)-C(5)-P(3)	109.96(18)	C(44)-C(43)-C(42)	120.5(3)
C(5)-C(6)-C(1)	111.5(2)	C(45)-C(44)-C(43)	119.3(3)
C(21)-P(1)-C(11)	99.05(13)	C(44)-C(45)-C(46)	120.4(3)
C(21)-P(1)-C(1)	103.96(12)	C(45)-C(46)-C(41)	121.2(3)
C(11)-P(1)-C(1)	102.31(13)	C(61)-P(3)-C(51)	99.08(13)
C(16)-C(11)-C(12)	118.2(3)	C(61)-P(3)-C(5)	102.60(13)
C(16)-C(11)-P(1)	119.2(3)	C(51)-P(3)-C(5)	103.63(12)
C(12)-C(11)-P(1)	122.5(2)	C(56)-C(51)-C(52)	117.4(3)
C(13)-C(12)-C(11)	121.0(3)	C(56)-C(51)-P(3)	116.9(2)
C(14)-C(13)-C(12)	119.9(4)	C(52)-C(51)-P(3)	125.6(2)
C(15)-C(14)-C(13)	119.8(4)	C(53)-C(52)-C(51)	120.7(3)
C(14)-C(15)-C(16)	120.8(4)	C(54)-C(53)-C(52)	121.2(4)
C(11)-C(16)-C(15)	120.2(4)	C(53)-C(54)-C(55)	118.8(3)
C(26)-C(21)-C(22)	118.3(3)	C(54)-C(55)-C(56)	120.3(3)
C(26)-C(21)-P(1)	126.5(2)	C(55)-C(56)-C(51)	121.5(3)
C(22)-C(21)-P(1)	115.3(2)	C(62)-C(61)-C(66)	117.7(3)
C(23)-C(22)-C(21)	121.0(3)	C(62)-C(61)-P(3)	118.5(3)
C(22)-C(23)-C(24)	120.5(3)	C(66)-C(61)-P(3)	123.6(2)
C(23)-C(24)-C(25)	119.1(3)	C(61)-C(62)-C(63)	121.1(4)
C(24)-C(25)-C(26)	120.4(3)	C(64)-C(63)-C(62)	119.7(4)
C(25)-C(26)-C(21)	120.6(3)	C(65)-C(64)-C(63)	120.1(4)
C(31)-P(2)-C(41)	101.10(13)	C(64)-C(65)-C(66)	120.2(4)
C(31)-P(2)-C(3)	102.78(13)	C(65)-C(66)-C(61)	121.1(4)
C(41)-P(2)-C(3)	101.65(12)		
C(32)-C(31)-C(36)	117.0(3)		

Crystal Structure of [Mo(N_2)(tdppcy)(dmpm)]

Single crystals suitable for X-ray crystal structure determination were obtained by slow evaporation of a benzene solution of [Mo(N_2)(tdppcy)(dmpm)] over a period of several days.

Table S3 Crystal data and structure refinement for [Mo(N_2)(tdppcy)(dmpm)].

Empirical formula	$C_{59}H_{48}MoN_2P_5$	
Formula weight	1035.78	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.9372(4) Å	α= 90°.
	b = 22.1222(5) Å	β= 108.947(3)°.
	c = 19.5024(7) Å	γ = 90°.
Volume	5279.2(3) $Å^3$	
Z	4	
Density (calculated)	1.303 Mg/m^3	
Absorption coefficient	0.439 mm^{-1}	
F(000)	2132	
Crystal size	0.08 x 0.10 x 0.12 mm^3	
Theta range for data collection	1.902 to 25.299°.	
Index ranges	-15<=h<=15, -25<=k<=26, -19<=l<=23	
Reflections collected	25674	
Reflections [I>2sigma(I)]	7003	
Independent reflections	9552 [R(int) = 0.0494]	
Completeness to theta = 25.242°	99.2 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9552 / 192 / 659	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0598, wR2 = 0.1440	
R indices (all data)	R1 = 0.0862, wR2 = 0.1587	
Extinction coefficient	0.0025(4)	
Largest diff. peak and hole	0.631 and -0.672 e.$Å^{-3}$	

Comments: A numerical absorption correction was performed (Tmin/max: 0.9063/0.9540). All non-hydrogen atoms were refined anisotropic. The C-H H atoms were positioned with idealized geometry and were refined isotropic with $U_{iso}(H) = 1.2\ U_{eq}(C)$ using a riding model. The asymmetric unit contains two benzene solvate molecules of which one is disordered in two orientations in ratio 50:50. This molecule was refined with a split model using restraints for the geometrical parameters and for the anisotropic displacement parameters (SAME and SADI).

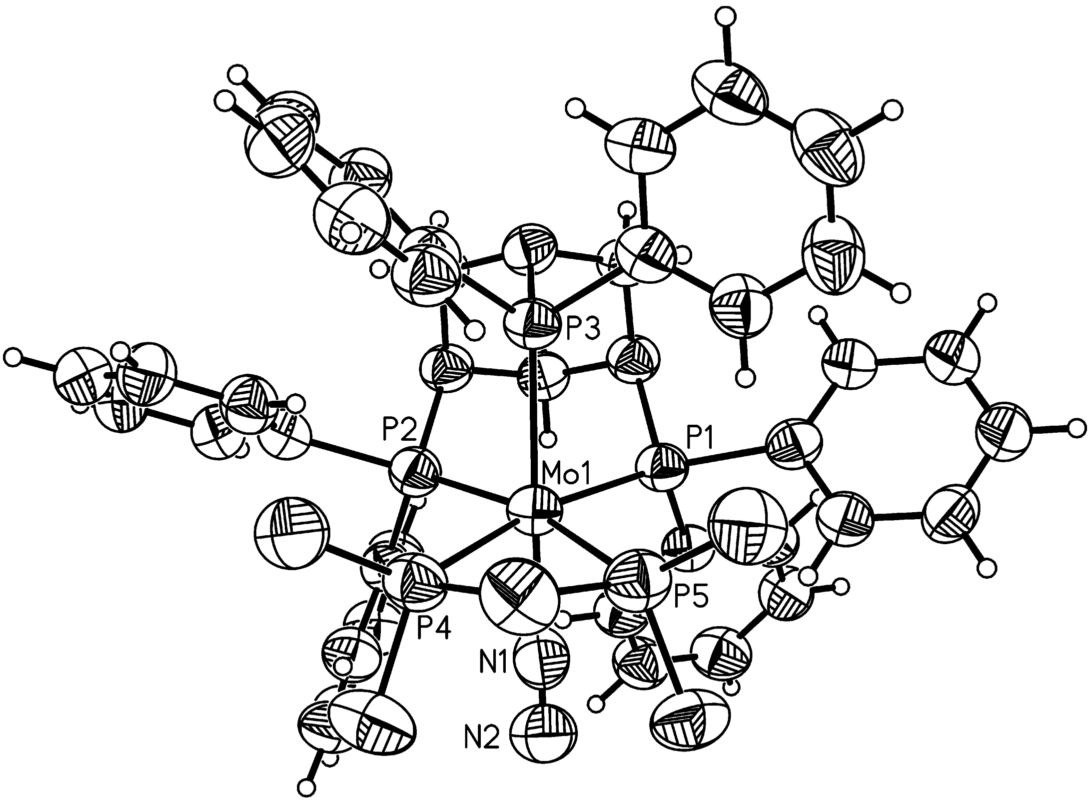

Fig. S2 ORTEP-plot of [Mo(N_2)(tdppcy)(dmpm)].

Table S4 Bond lengths [Å] and angles [°].

Mo(1)-N(1)	2.058(5)	Mo(1)-P(3)	2.4607(11)
Mo(1)-P(2)	2.4070(13)	Mo(1)-P(4)	2.4964(14)
Mo(1)-P(1)	2.4361(12)	Mo(1)-P(5)	2.5077(15)
N(1)-Mo(1)-P(2)	91.38(13)	P(1)-Mo(1)-P(4)	169.92(5)
N(1)-Mo(1)-P(1)	89.83(12)	P(3)-Mo(1)-P(4)	101.19(4)
P(2)-Mo(1)-P(1)	87.77(4)	N(1)-Mo(1)-P(5)	83.38(13)
N(1)-Mo(1)-P(3)	174.16(13)	P(2)-Mo(1)-P(5)	166.87(5)
P(2)-Mo(1)-P(3)	85.76(4)	P(1)-Mo(1)-P(5)	104.19(5)
P(1)-Mo(1)-P(3)	84.98(4)	P(3)-Mo(1)-P(5)	100.46(4)
N(1)-Mo(1)-P(4)	84.33(13)	P(4)-Mo(1)-P(5)	67.03(5)
P(2)-Mo(1)-P(4)	100.55(5)	N(2)-N(1)-Mo(1)	179.0(5)
N(1)-N(2)	1.067(6)	C(31)-C(32)	1.396(7)

Table S4 Bond lengths [Å] and angles [°].

C(1)-C(2)	1.536(6)	C(32)-C(33)	1.399(6)
C(1)-C(6)	1.540(6)	C(33)-C(34)	1.372(8)
C(1)-P(1)	1.867(5)	C(34)-C(35)	1.377(8)
C(2)-C(3)	1.539(6)	C(35)-C(36)	1.387(6)
C(3)-C(4)	1.537(6)	C(41)-C(46)	1.381(7)
C(3)-P(2)	1.865(5)	C(41)-C(42)	1.391(7)
C(4)-C(5)	1.554(6)	C(42)-C(43)	1.387(7)
C(5)-C(6)	1.521(6)	C(43)-C(44)	1.364(8)
C(5)-P(3)	1.858(5)	C(44)-C(45)	1.376(8)
P(1)-C(11)	1.849(5)	C(45)-C(46)	1.390(7)
P(1)-C(21)	1.864(4)	P(3)-C(51)	1.851(5)
C(11)-C(16)	1.394(7)	P(3)-C(61)	1.867(5)
C(11)-C(12)	1.404(6)	C(51)-C(52)	1.389(7)
C(12)-C(13)	1.387(7)	C(51)-C(56)	1.391(7)
C(13)-C(14)	1.376(8)	C(52)-C(53)	1.396(7)
C(14)-C(15)	1.379(8)	C(53)-C(54)	1.369(9)
C(15)-C(16)	1.386(7)	C(54)-C(55)	1.373(9)
C(21)-C(26)	1.388(6)	C(55)-C(56)	1.390(7)
C(21)-C(22)	1.393(7)	C(61)-C(66)	1.367(7)
C(22)-C(23)	1.381(6)	C(61)-C(62)	1.405(6)
C(23)-C(24)	1.382(7)	C(62)-C(63)	1.387(8)
C(24)-C(25)	1.371(8)	C(63)-C(64)	1.375(9)
C(25)-C(26)	1.394(6)	C(64)-C(65)	1.368(8)
P(2)-C(31)	1.850(4)	C(65)-C(66)	1.406(7)
P(2)-C(41)	1.857(5)		
C(31)-C(36)	1.393(7)	C(16)-C(11)-P(1)	116.3(3)
C(2)-C(1)-C(6)	109.8(4)	C(12)-C(11)-P(1)	126.0(4)
C(2)-C(1)-P(1)	111.0(3)	C(13)-C(12)-C(11)	120.5(5)
C(6)-C(1)-P(1)	113.6(3)	C(14)-C(13)-C(12)	120.8(5)
C(1)-C(2)-C(3)	116.2(4)	C(13)-C(14)-C(15)	119.6(5)
C(4)-C(3)-C(2)	109.1(4)	C(14)-C(15)-C(16)	120.0(5)
C(4)-C(3)-P(2)	109.6(3)	C(15)-C(16)-C(11)	121.5(5)
C(2)-C(3)-P(2)	114.9(3)	C(26)-C(21)-C(22)	117.4(4)
C(3)-C(4)-C(5)	115.3(4)	C(26)-C(21)-P(1)	121.0(4)
C(6)-C(5)-C(4)	109.1(4)	C(22)-C(21)-P(1)	121.6(3)
C(6)-C(5)-P(3)	111.6(3)	C(23)-C(22)-C(21)	121.8(4)
C(4)-C(5)-P(3)	115.3(3)	C(22)-C(23)-C(24)	120.2(5)
C(5)-C(6)-C(1)	115.4(4)	C(25)-C(24)-C(23)	118.9(5)
C(11)-P(1)-C(21)	95.3(2)	C(24)-C(25)-C(26)	121.1(5)
C(11)-P(1)-C(1)	101.3(2)	C(21)-C(26)-C(25)	120.6(5)
C(21)-P(1)-C(1)	96.56(19)	C(31)-P(2)-C(41)	95.4(2)
C(16)-C(11)-C(12)	117.6(5)		

Table S4 Bond lengths [Å] and angles [°].

C(31)-P(2)-C(3)	103.0(2)	C(51)-P(3)-C(61)	94.3(2)
C(41)-P(2)-C(3)	96.3(2)	C(5)-P(3)-C(61)	97.5(2)
C(36)-C(31)-C(32)	117.4(4)	C(52)-C(51)-C(56)	116.7(5)
C(36)-C(31)-P(2)	116.8(3)	C(52)-C(51)-P(3)	126.9(4)
C(32)-C(31)-P(2)	125.8(4)	C(56)-C(51)-P(3)	116.2(4)
C(31)-C(32)-C(33)	121.0(5)	C(51)-C(52)-C(53)	121.5(5)
C(34)-C(33)-C(32)	120.0(5)	C(54)-C(53)-C(52)	120.1(6)
C(33)-C(34)-C(35)	120.0(4)	C(53)-C(54)-C(55)	120.0(5)
C(34)-C(35)-C(36)	120.1(5)	C(54)-C(55)-C(56)	119.6(6)
C(35)-C(36)-C(31)	121.5(5)	C(55)-C(56)-C(51)	122.1(6)
C(46)-C(41)-C(42)	117.1(5)	C(66)-C(61)-C(62)	117.8(4)
C(46)-C(41)-P(2)	120.3(4)	C(66)-C(61)-P(3)	120.1(3)
C(42)-C(41)-P(2)	122.6(4)	C(62)-C(61)-P(3)	122.1(4)
C(43)-C(42)-C(41)	121.5(5)	C(63)-C(62)-C(61)	120.8(6)
C(44)-C(43)-C(42)	120.3(5)	C(64)-C(63)-C(62)	120.0(5)
C(43)-C(44)-C(45)	119.5(5)	C(65)-C(64)-C(63)	120.4(5)
C(44)-C(45)-C(46)	120.1(5)	C(64)-C(65)-C(66)	119.4(6)
C(41)-C(46)-C(45)	121.5(5)	C(61)-C(66)-C(65)	121.6(5)
C(51)-P(3)-C(5)	101.4(2)	P(5)-C(73)	1.846(7)
P(4)-C(72)	1.838(6)	P(5)-C(75)	1.849(6)
P(4)-C(71)	1.849(6)	P(5)-C(74)	1.849(6)
P(4)-C(73)	1.851(7)	C(73)-P(5)-C(74)	101.6(3)
C(72)-P(4)-C(71)	97.5(3)	C(75)-P(5)-C(74)	97.6(3)
C(72)-P(4)-C(73)	101.4(3)	P(5)-C(73)-P(4)	96.8(3)
C(71)-P(4)-C(73)	102.5(3)	C(83)-C(84)	1.377(9)
C(73)-P(5)-C(75)	103.1(3)	C(84)-C(85)	1.354(10)
C(81)-C(82)	1.362(9)	C(85)-C(86)	1.379(9)
C(81)-C(86)	1.382(9)	C(85)-C(84)-C(83)	120.8(7)
C(82)-C(83)	1.363(9)	C(84)-C(85)-C(86)	119.9(7)
C(82)-C(81)-C(86)	120.0(6)	C(85)-C(86)-C(81)	119.3(7)
C(81)-C(82)-C(83)	120.5(6)	C(91')-C(92')	1.355(19)
C(82)-C(83)-C(84)	119.4(7)	C(91')-C(96')	1.37(2)
C(91)-C(92)	1.357(19)	C(92')-C(93')	1.41(2)
C(91)-C(96)	1.37(2)	C(93')-C(94')	1.37(3)
C(92)-C(93)	1.41(2)	C(94')-C(95')	1.34(3)
C(93)-C(94)	1.37(3)	C(95')-C(96')	1.38(2)
C(94)-C(95)	1.34(3)	C(92')-C(91')-C(96')	120.7(18)
C(95)-C(96)	1.37(3)	C(91')-C(92')-C(93')	119.0(19)
C(92)-C(91)-C(96)	120.6(18)	C(94')-C(93')-C(92')	120(2)
C(91)-C(92)-C(93)	117.9(19)	C(95')-C(94')-C(93')	119(2)
C(94)-C(93)-C(92)	121(2)	C(94')-C(95')-C(96')	122(2)
C(95)-C(94)-C(93)	119(2)	C(91')-C(96')-C(95')	118.6(19)
C(94)-C(95)-C(96)	122(2)		
C(91)-C(96)-C(95)	120(2)		

Mass spectrum of [Mo(N_2)(tdppcy)(dmpm)]

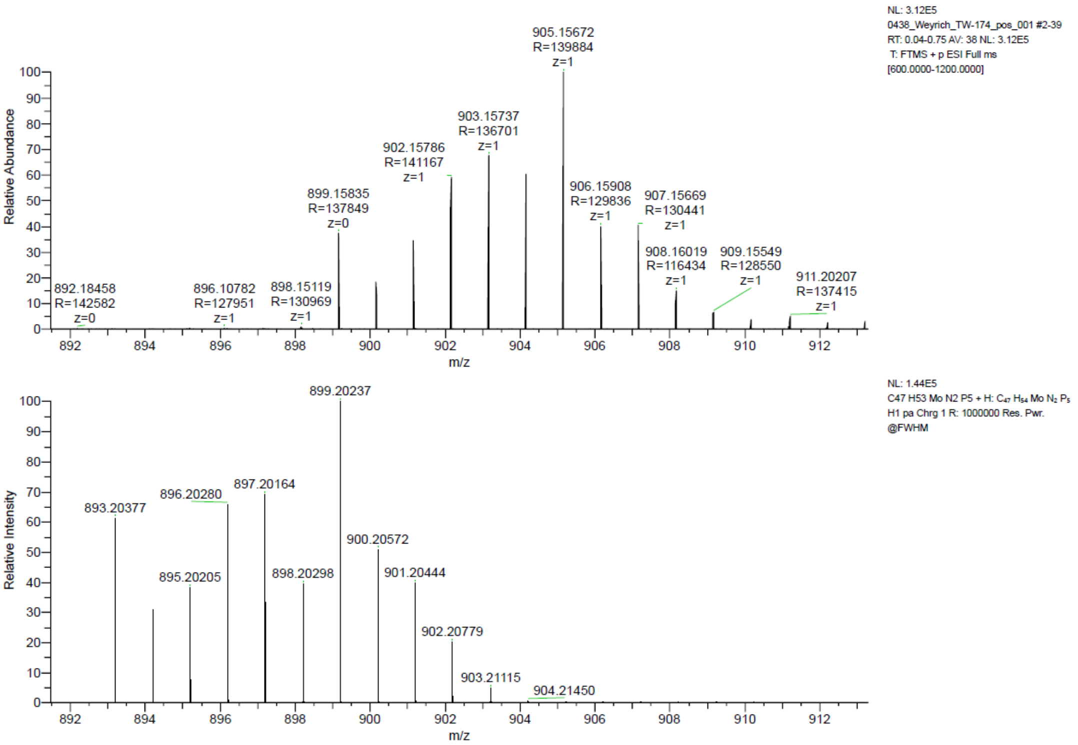

Fig. S3 Mass spectrum of complex **2**.

Solution-Phase IR Measurement of [Mo($^{15}N_2$)(tdppcy)(dmpm)]

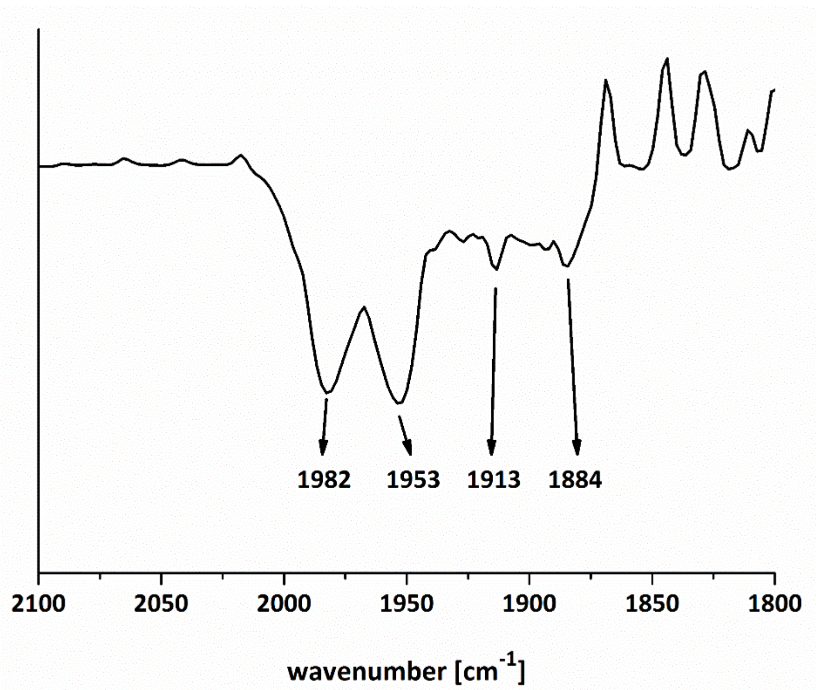

Fig. S4 Solution-phase IR measurement of [Mo($^{15}N_2$)(tdppcy)(dmpm)] (**^{15}N-2**) in THF proves that the prominent double-band feature of the N_2-band also exists in solution. In this case a solid-state effect (i.e. Davydov-splitting) thus can be excluded.

Comparison of the ^{31}P-NMR spectra between [Mo(N_2)(tdppcy)(dmpm)] and [Mo($^{15}N_2$)(tdppcy)(dmpm)]

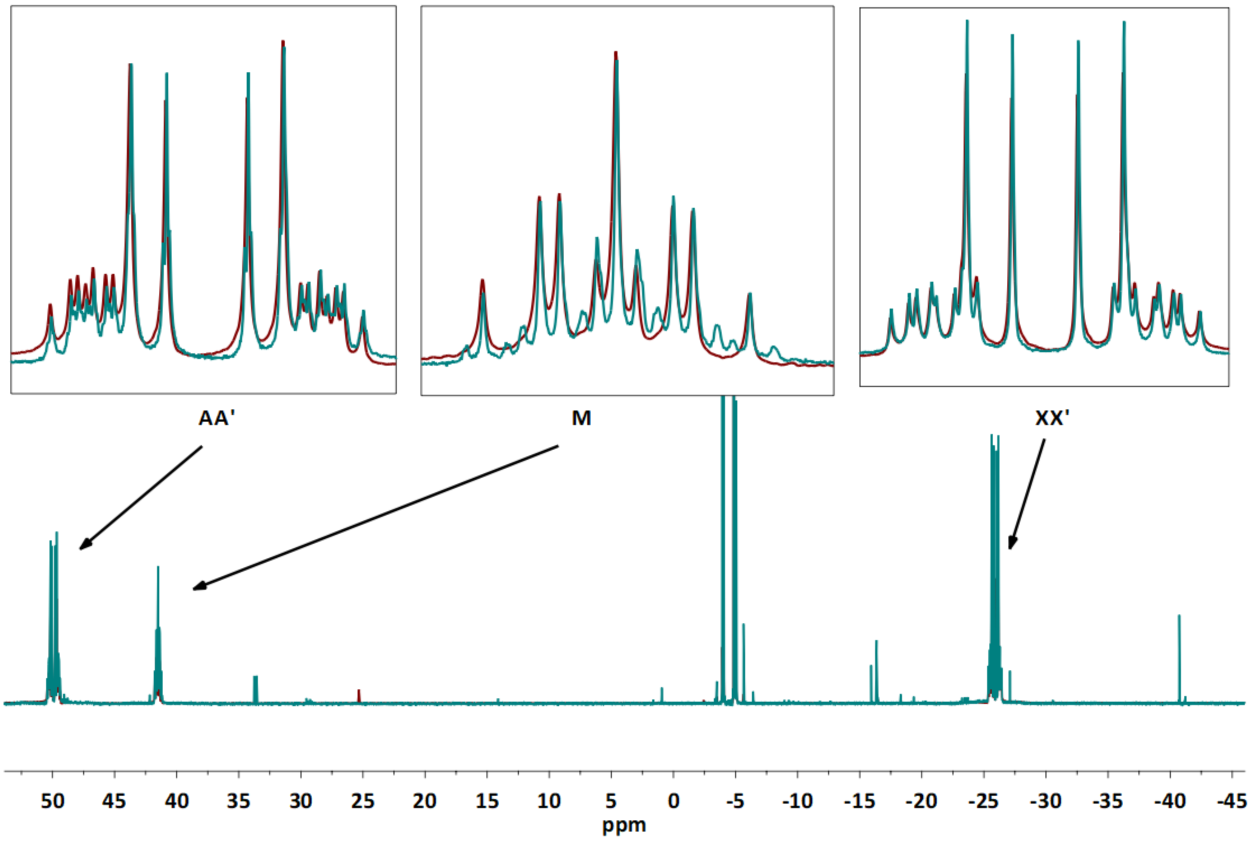

Fig. S5 Depiction of the superimposed ^{31}P-NMR spectrum of [Mo(N_2)(tdppcy)(dmpm)] (**2**, *red*) and [Mo($^{15}N_2$)(tdppcy)(dmpm)] (**^{15}N-2**, *blue*). The magnification for the M-part clearly shows additional signals for the P_{ax} donor atom of ^{15}N-2 (*blue*) due to the coupling with the ^{15}N-atom.

DFT Calculations on the conversion of tdppcy between all-equatorial and all-axial

	SCF [Hartree]	SCF [kJ/mol]	energy [kJ/mol]	entropy [kJ/mol]	chem.pot [kJ/mol]	H [kJ/mol]	G [kJ/mol]	ΔG^0_{solv} (toluol) $\varepsilon = 2.38$ [kJ/mol]	ΔG^0_{solv} (thf) $\varepsilon = 7.58$ [kJ/mol]
tdppcy									
All-axial									
BP86/SV(P)	-2646.63	-6948717.80	1865.12	1.08279	1544.77	-6946852.68	-6947173.03		
B3LYP/SV(P)	-2645.24	-6945084.27	1913.55	1.05833	1600.49	-6943170.72	-6943483.78	-16.87	-40.26
All-equatorial									
BP86/SV(P)	-2646.64	-6948752.03	1867.24	1.09092	1544.46	-6946884.79	-6947207.57		
B3LYP/SV(P)	-2645.26	-6945122.52	1915.37	1.06995	1598.84	-6943207.15	-6943523.68	-18.72	-42.44
1,3,5-Trimethyl-cyclohexane									
All-axial									
BP86/SV(P)	-353.51	-928152.39	674.59	0.39876	558.18	-927477.80	-927594.21		
B3LYP/SV(P)	-353.25	-927463.71	695.32	0.38476	583.08	-926768.39	-926880.63		
All-equatorial									
BP86/SV(P)	-353.53	-928197.85	673.18	0.39960	556.52	-927524.67	-927641.33		
B3LYP/SV(P)	-353.27	-927509.94	693.90	0.38280	582.25	-926816.04	-926927.69		
Methylcyclohexane									
All-axial									
BP86/SV(P)	-274.96	-721919.26	524.06	0.34232	424.48	-721395.20	-721494.78		
All-equatorial									
BP86/SV(P)	-274.97	-721928.31	523.93	0.34256	424.28	-721404.38	-721504.03		

Free Reaction enthalpies of the conformational change: all-equatorial -> all-axial

	$\Delta SCF_{(g)}$ [kJ/mol]	$\Delta H_{(g)}$ [kJ/mol]	$\Delta G_{(g)}$ [kJ/mol]	$\Delta G_{(solv, toluene)}$ [kJ/mol]	$\Delta G_{(solv, thf)}$ [kJ/mol]
tdppcy					
BP86/SV(P)	34.23	32.11	34.54		
B3LYP/SV(P)	38.25	36.43	39.90	41.74	42.08
1,3,5-Trimethylcyclohexane					
BP86/SV(P)	45.46	46.87	47.12		
B3LYP/SV(P)	46.23	47.65	47.06		
Methylcyclohexan					
BP86/SV(P)	9.04	9.17	9.24		
B3LYP/SV(P)	9.26	9.46	9.58		

For validation of the method, 1,3,5-trimethylcyclohexane and methylcyclohexane were calculated. As the energy difference between all-axial and all-equatorial for methylcyclohexan is around 8.1 kJ/mol[a] and the theoretical value is 9.24/9.58 kJ/mol, the method seems to provide reasonable results.

Calculations of the structures and energies were performed on BP86[b]/SV(P)[c] and B3LYP[d]/SV(P) level using TURBOMOLE.[e] For the calculation of the vibrational frequencies and to prove that the optimized structures are minima on the potential energy surface the AOFORCE module was used,[f] which is included in the TURBOMOLE program package. Thermodynamics (enthalpy, entropy, chem. pot.) were taken from the same method as the optimizations. COSMO[g] energies optimized at B3LYP[d]/SV(P) level with $\varepsilon_r = 7.58$ (thf) and 2.38 (toluene).

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