Supporting Information for

Dipyrrolyl Precursors to Bisalkoxide Molybdenum Olefin Metathesis Catalysts

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1. Experimental Details

For {Mo(NAr)(*syn*-$CHCMe_2Ph$)(η^5-NC_4H_4)(η^1-NC_4H_4)}-{Mo(NAr)(*syn*-$CHCMe_2Ph$)(η^1-NC_4H_4)$_2$} (**06172**)

2. Partially labeled ORTEP drawing

3. Crystal data and structure refinement

4. Atomic coordinates

5. Bond lengths and angles

6. Anisotropic thermal parameters

7. Hydrogen atom coordinates and isotropic displacement parameters

Experimental

All complexes were handled using standard Schlenk techniques or in a Vacuum Atmospheres glove box under an argon or dinitrogen atmosphere. All solvents were dried, degassed, and stored over activated molecular sieves in a dinitrogen-filled glovebox. Pyrrole was distilled from CaH_2 in an inert atmosphere and lithium pyrrolide was prepared using published procedures.[1] Mo(N-2,6-*i*-$Pr_2C_6H_3$)(CHCMe$_2$Ph)(OTf)$_2$DME,[2] Mo(NAd)(CHR)(OTf)$_2$(DME),[2] and Mo(N-2,6-Br_2-4-MeC_6H_2)(CHCMe$_3$)(OTf)$_2$(DME)[3] were synthesized by published procedures. Elemental analyses were performed by Desert Analytics, Tucson, Arizona.

Mo(N-2,6-*i*-$Pr_2C_6H_3$)(CHCMe$_3$)(NC_4H_4)$_2$. To a -35 ºC solution of 0.193 g (0. 27 mmol) Mo(NAr)(CHCMe$_3$)(OTf)$_2$(DME) in 4 mL diethyl ether was added 38.6 mg (0.53 mmol) of $LiNC_4H_4$ as a solid in one portion. The mixture was stirred at room temperature for 1 hour, then all volatiles were removed *in vacuo*. The resulting brown powder was extracted with 5 mL of toluene and the solution was filtered through celite. The celite was washed with toluene (1 mL) and the resulting solution was taken to dryness *in vacuo*. The product may be recrystallized from mixtures of pentane/toluene or pure toluene at-35 ºC as a toluene solvate; 110 mg (74%): ^{1}H NMR (300 MHz, 293K, toluene-d_8) δ 13.5 (br s, 1H, MoC*H*R), 7-6.2 (v br s, overlapping, 11 H, Ar- *H* and NC_4H_4), 3.8-2.9 (br s, 2H, *i*-Pr), 1.3 (br s, 9H, CMe_3), 1.1 (br s, 12H, *i*-Pr).

Mo(N-2,6-*i*-$Pr_2C_6H_3$)(CHCMe$_2$Ph)(NC_4H_4)$_2$. $LiNC_4H_4$ (410 mg, 5.62 mmol) was added as a solid in several small portions a -40 ºC solution of 2.223 g (2.81 mmol) Mo(NAr)(CHCMe$_2$Ph)(OTf)$_2$(DME) in 60 mL of diethyl ether. The mixture was stirred

[1] Deiter, T. *Z. Anorg. Allgem. Chem.* **1971**, *384*, 136-146.
[2] Oskam, J. H.; Fox, H. H.; Yap, K. B.; McConville, D. H.; O'Dell, R.; Lichtenstein, B. J.; Schrock, R. R. *J. Organomet. Chem.* **1993**, *459*, 185-198.
[3] J. Y. Jamieson, Ph.D. thesis, Massachusetts Institute of Technology, 2002.

at room temperature for 1 hour. All volatiles were removed *in vacuo* and the resulting powder was extracted with 65 mL of a 1:1 mixture of toluene and pentane and the solution was filtered through celite. The celite was washed with toluene (3x15 mL) and the resulting solution was reduced to dryness *in vacuo*. The solid was recrystallized from pentane -35 ºC; yield 1.2 g (80%): ^{1}H NMR (toluene-d_8, 500 MHz) (223 K) δ 13.55 (s, 1H, MoC*H*R), 13.16 (s, 1H, MoC*H*R), 7.4-6.7 (m, Ar-H, NC_4H_4), 5.85 (s, 1H, NC_4H_4), 5.10 (s, 1H, NC_4H_4), 4.91 (s, 1H, NC_4H_4), 4.83 (s, 1H, NC_4H_4), 3.85 (sept, 2H, *i*-Pr methine), 2.85 (sept, 2H, *i*-Pr methine), 1.75 (s, 6H, MoCHC*Me*$_2$Ph), 1.71 (s, 3H, MoCHC*Me*$_2$Ph), 1.68 (s, 3H, MoCHC*Me*$_2$Ph), 1.19 (br d, 12H, Ar-*i*-Pr), 1.12 (d, 3H, Ar-*i*-Pr), 1.03 (overlapping d, 6H, Ar-*i*-Pr), 0.55 (d, 3H, Ar-*i*-Pr); (323 K): δ 13.18 (s, 1H, MoC*H*R), 7.33 (d, 2H, MoCHCMe$_2$*Ar*), 7.18 (t, 2H, MoCHCMe$_2$*Ar*), 7.05 (t, 1H, MoCHCMe$_2$*Ar*), 6.86 (m, 3H, MoN*Ar*), 6.44 (s, 4H, NC_4H_4), 6.14, (s, 4H, NC_4H_4), 3.22 (sept, 2H, *i*-Pr methine), 1.56 (s, 6H, MoCHC*Me*$_2$Ar), 0.96 (d, 12H, *i*-Pr methyl). ^{13}C NMR (CD_2Cl_2, 126 MHz, 223 K): 313.9 (J_{CH} 122.8 Hz), 293.9 (J_{CH} 121.3 Hz). Analysis calcd. For $C_{30}H_{37}MoN_3$ (found): C 67.28 (67.38), H 6.96 (7.20), Mo 17.91, N 7.85 (7.70).

Mo(NAd)(CHCMe$_2$Ph)(NC$_4$H$_4$)$_2$. $LiNC_4H_4$ (169 mg, 2.32 mmol) was added as a solid in small portions to a -35 ºC solution of 0.890 g (1.16 mmol) Mo(NAd)(CHCMe$_2$Ph)(OTf)$_2$(DME) in 50 mL of diethyl ether. The mixture was stirred at room temperature for 1.5 h, then all volatiles were removed *in vacuo*. The resulting brown powder was extracted with toluene and the solution was filtered through celite. The celite was washed with toluene and the combined filtrates were taken to dryness *in vacuo*. The off-white solid may be recrystallized from toluene at -35 ºC; yield 420 mg (2 crops, 71%): ^{1}H NMR (C_6D_6, 500 MHz, 293 K) δ 13.6 (br s, 1H, MoC*H*R), 12.8 (br s, 1H, MoC*H*R), 7.5, (br s, 4 H, MoCHCMe$_2$*Ph*), 7.0-4.7 (2 overlapping br s, MoCHCMe$_2$*Ph* and NC_4H_4), 1.8-1.6 (br multiplet, 15H, MoN*Ad*), 1.3 (br s, 6H, MoCHC*Me*$_2$Ph). ^{13}C (CD_2Cl_2 126 MHz, 223K): 316.1 (J_{CH} 118.2 Hz), 295.5 (J_{CH} 111.3

Hz). Analysis calcd. For $C_{28}H_{35}MoN_3$ (found): C 66.00 (65.10), H 6.92 (6.60), Mo 18.83, N 8.25 (7.04).

Mo(N-2,6-Br_2-4-MeC_6H_2)(CHCMe_3)(NC_4H_4)$_2$. $LiNC_4H_4$ (35.4 mg, 0.485 mmol) in diethyl ether (~2 mL) was added to a -40 ºC solution of 0.198 g (0.243 mmol) Mo(NAr)(CHCMe_3)(OTf)$_2$(DME) in 3 mL of dichloromethane. The mixture was stirred at room temperature for 1 hour and all volatiles were removed *in vacuo*. The resulting red-brown powder was extracted with benzene and the solution was filtered through celite. The celite was washed with benzene and the combined filtrates were taken to dryness *in vacuo*. The product was recrystallized from pentane containing a few drops of benzene at -35 ºC; yield 94 mg (62%): ^{1}H NMR (300 MHz, C_6D_6, 293 K) δ 13.4 (br s, 1H MoC*H*R), 6.8-6.4 (br overlapping s, 10H, MoN*Ar* and NC_4*H*$_4$), 3.1 (s, 3H, MoNAr methyl), 1.4 (br s, 9H, MoCHC*Me*$_3$). Analysis calcd. For $C_{20}H_{23}MoBr_2N_3$ (found): C 42.81 (42.52), H 4.13 (4.12), Mo 17.10, Br 28.48, N 7.49 (6.83).

Mo(NAd)(CHCMe_2Ph)(NC_4H_4)$_2$(PMe_3). Excess trimethylphosphine (50 μL) was added to 150 mg of Mo(NAd)(CHCMe_2Ph)(NC_4H_4)$_2$ in diethyl ether. The mixture was stirred at room temperature for 30 minutes and the solvent was removed *in vacuo*. Mo(NAd)(CHCMe_2Ph)(NC_4H_4)$_2$(PMe_3) was crystallized from pentane as orange blocks; yield 100 mg (58%): NMR (^{1}H, 300 MHz, C_6D_6) δ 12.49 (d, 1H, $J_{H\text{-}P}$ 4.8Hz, C*H*CMe_2Ph), 8.41 (m, 2H, Ar), 7.05 (m, 6H, Ar), 6.80 (s, 4H, NC_4*H*$_4$), 6.40 (s, 4H, NC_4*H*$_4$), 2.43 (s, 6H), 1.82 (s, 6H), 1.73 (s, 3H, *Ad*), 1.35 (s, 6H), 0.46 (d, 9H, J_{HP} 9.2 Hz, P*Me*$_3$); ^{13}C NMR (C_6D_6) δ 301.73 (d, MoC*H*CMe_2Ph, $^2J_{C\text{-}P}$ 19.5 Hz), 148, 132.19, 129.13, 126.37, 125.96, 109.16, 108.62, 42.22, 36.21, 30.03, 16.50 (d, P*Me*$_3$, $J_{C\text{-}P}$ 25 Hz). Analysis calcd. For $C_{31}H_{44}MoN_3P$ (found): C 63.58 (63.37), H 7.57 (7.45), Mo 16.38, N 7.18 (6.04), P 5.29.

Representative procedure for the *in situ* catalyst generation. The molybdenum precursor (ca. 0.02 mmol) is dissolved in 0.2 mL of C_6D_6. An equimolar amount of diol or two equivalents of alcohol in 0.3 mL of C_6D_6 and the solutions are combined in a Teflon-sealed NMR tube. The ^{1}H NMR spectrum was recorded within 15 minutes. All diols and alcohols thus far examined have proceeded to completion by the time the ^{1}H NMR spectrum was recorded.

Observation of Mo(N-2,6-*i*-$Pr_2C_6H_3$)(CHCMe$_2$Ph)(η^1-NC_4H_4)(η^5-$C_4H_4NB(C_6F_5)_3$). To 23.0 mg (0.021 mmol) of {Mo(N-2,6-*i*-$Pr_2C_6H_3$)(CHCMe$_2$Ph)(NC_4H_4)$_2$}$_2$ in ~0.25 mL of C_6D_6 was added $B(C_6F_5)_3$ (22 mg, 0.043 mmol) in ca. 0.25 mL C_6D_6. The solution was transferred to a Teflon-sealed NMR tube and the ^{1}H NMR spectrum was recorded (500 MHz, 293 K) δ 13.89 (s, 1H, MoC*H*R minor isomer), 13.08 (s, 1H, MoC*H*R major isomer), 7.72 (br s, 1H, η^5-$C_4H_4NB(C_6F_5)_3$), 7.28 (br s, 1H, η^5-$C_4H_4NB(C_6F_5)_3$), 7.08 (m, 4H, MoCHCMe$_2$*Ph*), 7.02 (d, J_{HH}7.6 Hz, 2H, η^1-NC_4H_4), 6.87 (m, 1H, MoCHCMe$_2$*Ph*), 6.78 (d, J_{HH}7.6 Hz, 2H, η^1-NC_4H_4), 5.78 (br s, 1H, η^5-$C_4H_4NB(C_6F_5)_3$), 5.41, (br s, 1H, η^5-$C_4H_4NB(C_6F_5)_3$), 2.82 (br s, 2H, *i*-Pr methine), 1.51 (s, 3H, MoCHC*Me*$_2$Ph), 1.25 (s, 3H, MoCHC*Me*$_2$Ph), 0.92 (br mult, 12H, *i*-Pr methyls).

X-Ray Structural Studies

Low temperature diffraction data were collected on a Siemens Platform three-circle diffractometer coupled to a Bruker-AXS SMART Apex CCD detector with graphite-monochromated MoKα radiation (λ = 0.71073 Å), performing φ and ω-scans. The structures were solved by direct methods using SHELXS[4] and refined against F^2 on all data by full-matrix least squares with SHELXL-97.[5] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at

[4] Sheldrick, G. M. *Acta Cryst*. **1990**, *A46*, 467.
[5] Sheldrick, G. M. (**1997**). SHELXL 97, University of Göttingen, Germany.

geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Crystal and structural refinement data for the structure is listed below.

Crystals of {Mo(NAr)(*syn*-$CHCMe_2Ph$)(η^5-NC_4H_4)(η^1-NC_4H_4)}{Mo(NAr)(*syn*-$CHCMe_2Ph$)(η^1-NC_4H_4)$_2$} (**06172**) grown at -40 ºC from a mixture of pentane and toluene were coated with Paratone-N oil (an Exxon-Mobile (TM) product) in a dinitrogen-filled glovebox and examined under a microscope. A suitable crystal measuring 0.10 x 0.08 x 0.03 mm^3 was selected and mounted in a nylon loop. Initial examination of the data indicated that the space group was P21/c. However, no reasonable solution could be obtained *via* direct methods or from the Patterson map. The program CELL_NOW[6] was used to re-determine the unit cell from 999 reflections sampled from several regions in the hemisphere of data. The resulting, slightly different, unit cell was used to integrate the data in the SAINT software package in the triclinic setting. A solution in the space group P1 (#1) was refined isotropically and the routines ADDSYM and NEWSYM in Platon[7] were used to confirm that the correct space group was indeed P21/c. Re-integration in the primitive, monoclinic setting followed by absorption correction with the SADABS[8] package yielded the data set from which the correct initial solution was obtained. Confirmation of the space group/setting was substantiated by the successful refinement of the structure and use of the ADDSYM and NEWSYM functions in the Platon software package.

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[6] Sheldrick, G. M. (2006c). CELL_NOW, Bruker AXS, Inc., Madison, Wisconsin, USA.
[7] Spek, A. L. Acta Cryst. 1990, A46, C34.
[8] Sheldrick, G. M. (2006a). SADABS, Bruker AXS, Inc., Madison, Wisconsin, USA.

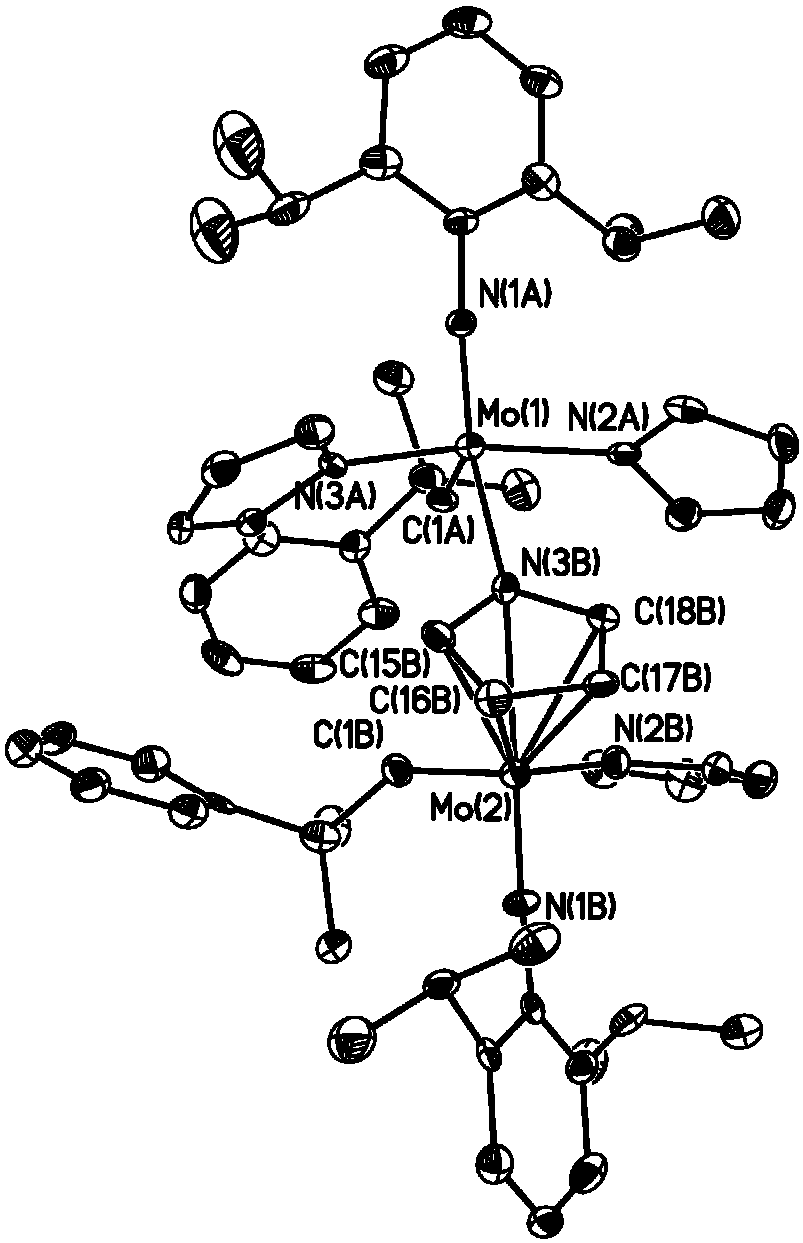

Figure 1. Thermal Ellipsoid Plot (50% probability level) of the structure of **06172**. Hydrogen atoms and co-crystallized solvent molecules have been omitted for clarity. The full labeling scheme may be seen on http://reciprocal.lms.mit.edu/recipnet/index.jsp by searching the code 06172.

Table 1. Crystal data and structure refinement for {Mo(NAr)(CHR)(NC_4H_4)$_2$}$_2$.

Identification code	06172	
Empirical formula	C67 H82 Mo2 N6	
Formula weight	1163.27	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 24.903(12) Å	α= 90^o
	b = 12.723(5) Å	β= 106.001(12)^o
	c = 19.434(9) Å	γ = 90^o
Volume	5919(4) Å^3	
Z	4	
Density (calculated)	1.305 Mg/m^3	
Absorption coefficient	0.469 mm^{-1}	
F(000)	2440	
Crystal size	0.10 x 0.08 x 0.03 mm^3	
Theta range for data collection	1.70 to 21.97°.	
Index ranges	-26<=h<=25, 0<=k<=13, 0<=l<=20	
Reflections collected	7216	
Independent reflections	7216 [R(int) = 0.1879]	
Completeness to theta = 21.97^o	99.6 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9861 and 0.9546	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7216 / 0 / 670	
Goodness-of-fit on F^2	1.013	
Final R indices [I>2sigma(I)]	R1 = 0.0412, wR2 = 0.0775	
R indices (all data)	R1 = 0.0753, wR2 = 0.0901	
Largest diff. peak and hole	0.590 and -0.534 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for {Mo(NAr)(CHR)(NC_4H_4)$_2$}$_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	3042(1)	8833(1)	4794(1)	15(1)
Mo(2)	1260(1)	9284(1)	3435(1)	16(1)
N(1A)	3711(2)	8566(3)	5307(2)	15(1)
N(2A)	2949(2)	7481(3)	4169(2)	18(1)
N(3A)	2778(2)	9826(3)	5499(2)	16(1)
N(1B)	573(2)	9542(3)	2975(2)	16(1)
N(2B)	1584(2)	8780(3)	2624(2)	18(1)
N(3B)	2048(2)	8621(3)	4418(2)	17(1)
C(1A)	3201(2)	9782(4)	4150(3)	17(1)
C(2A)	3661(2)	10288(4)	3889(3)	21(1)
C(3A)	3722(2)	9622(4)	3256(3)	29(2)
C(4A)	4217(2)	10277(4)	4472(3)	26(1)
C(5A)	3493(2)	11426(4)	3668(3)	17(1)
C(6A)	3495(2)	12174(4)	4195(3)	23(1)
C(7A)	3377(2)	13223(4)	4019(3)	26(1)
C(8A)	3246(2)	13539(4)	3313(3)	28(2)
C(9A)	3221(2)	12800(4)	2784(3)	26(1)
C(10A)	3351(2)	11751(4)	2960(3)	24(1)
C(11A)	2805(2)	7348(4)	3437(3)	21(1)
C(12A)	2658(2)	6321(4)	3270(3)	25(1)
C(13A)	2708(2)	5785(4)	3908(3)	25(1)
C(14A)	2886(2)	6507(4)	4449(3)	22(1)
C(15A)	2631(2)	10869(4)	5439(3)	17(1)
C(16A)	2388(2)	11154(4)	5966(3)	21(1)
C(17A)	2380(2)	10237(4)	6378(3)	23(1)
C(18A)	2621(2)	9459(4)	6080(3)	21(1)
C(19A)	4235(2)	8243(4)	5738(3)	16(1)
C(20A)	4556(2)	7535(4)	5453(3)	22(1)
C(21A)	5056(2)	7183(4)	5908(3)	25(1)
C(22A)	5231(2)	7515(4)	6605(3)	29(2)

C(23A)	4922(2)	8235(4)	6870(3)	29(1)
C(24A)	4421(2)	8623(4)	6443(3)	23(1)
C(25A)	4377(2)	7171(4)	4677(3)	24(1)
C(26A)	4814(2)	7493(4)	4293(3)	31(2)
C(27A)	4279(2)	5983(4)	4617(3)	34(2)
C(28A)	4093(2)	9443(5)	6726(3)	33(2)
C(29A)	4306(3)	10534(5)	6630(3)	58(2)
C(30A)	4091(3)	9295(5)	7494(3)	58(2)
C(1B)	1561(2)	10676(4)	3538(3)	20(1)
C(2B)	1398(2)	11805(4)	3341(3)	21(1)
C(3B)	1753(2)	12191(4)	2857(3)	30(2)
C(4B)	779(2)	11925(4)	2919(3)	25(1)
C(5B)	1506(2)	12448(4)	4032(3)	18(1)
C(6B)	1904(2)	13232(4)	4213(3)	24(1)
C(7B)	1966(2)	13822(4)	4826(3)	29(1)
C(8B)	1646(2)	13645(4)	5281(3)	26(1)
C(9B)	1259(2)	12844(4)	5127(3)	26(1)
C(10B)	1194(2)	12252(4)	4514(3)	22(1)
C(11B)	1845(2)	9337(4)	2197(3)	24(1)
C(12B)	1867(2)	8742(4)	1624(3)	28(1)
C(13B)	1622(2)	7766(4)	1694(3)	26(1)
C(14B)	1454(2)	7811(4)	2298(3)	20(1)
C(15B)	1666(2)	9114(4)	4704(3)	20(1)
C(16B)	1160(2)	8570(4)	4521(3)	18(1)
C(17B)	1234(2)	7679(4)	4127(3)	18(1)
C(18B)	1773(2)	7743(4)	4063(3)	18(1)
C(19B)	16(2)	9695(4)	2584(3)	17(1)
C(20B)	-395(2)	9841(4)	2951(3)	18(1)
C(21B)	-932(2)	10069(4)	2548(3)	22(1)
C(22B)	-1069(2)	10113(4)	1815(3)	22(1)
C(23B)	-669(2)	9943(4)	1458(3)	26(1)
C(24B)	-115(2)	9740(4)	1835(3)	18(1)
C(25B)	-252(2)	9681(4)	3752(3)	22(1)
C(26B)	-623(2)	10295(5)	4123(3)	38(2)
C(27B)	-281(2)	8497(4)	3899(3)	29(2)
C(28B)	320(2)	9543(4)	1433(3)	22(1)

C(29B)	362(2)	10463(4)	951(3)	31(2)
C(30B)	190(2)	8524(4)	995(3)	26(1)
C(1T)	6467(2)	4402(4)	3582(3)	26(1)
C(2T)	5918(2)	4583(5)	3559(3)	31(2)
C(3T)	5741(2)	5558(5)	3710(3)	36(2)
C(4T)	6107(3)	6385(5)	3884(3)	33(2)
C(5T)	6661(2)	6216(5)	3907(3)	30(1)
C(6T)	6837(2)	5230(4)	3765(3)	25(1)
C(7T)	6658(3)	3336(4)	3424(3)	37(2)

Table 3. Bond lengths [Å] and angles [°] for {Mo(NAr)(CHR)(NC_4H_4)$_2$}$_2$.

Mo(1)-N(1A)	1.725(4)	C(12A)-C(13A)	1.391(7)
Mo(1)-C(1A)	1.859(5)	C(13A)-C(14A)	1.374(7)
Mo(1)-N(2A)	2.082(4)	C(15A)-C(16A)	1.374(7)
Mo(1)-N(3A)	2.097(4)	C(16A)-C(17A)	1.419(7)
Mo(1)-N(3B)	2.395(4)	C(17A)-C(18A)	1.366(7)
Mo(2)-N(1B)	1.730(4)	C(19A)-C(24A)	1.407(7)
Mo(2)-C(1B)	1.912(5)	C(19A)-C(20A)	1.414(7)
Mo(2)-N(2B)	2.060(4)	C(20A)-C(21A)	1.387(7)
Mo(2)-C(16B)	2.373(5)	C(20A)-C(25A)	1.523(7)
Mo(2)-C(15B)	2.403(5)	C(21A)-C(22A)	1.369(7)
Mo(2)-C(17B)	2.456(5)	C(22A)-C(23A)	1.384(7)
Mo(2)-C(18B)	2.471(5)	C(23A)-C(24A)	1.383(7)
Mo(2)-N(3B)	2.479(4)	C(24A)-C(28A)	1.518(7)
N(1A)-C(19A)	1.404(6)	C(25A)-C(27A)	1.531(7)
N(2A)-C(11A)	1.379(6)	C(25A)-C(26A)	1.535(7)
N(2A)-C(14A)	1.379(6)	C(28A)-C(30A)	1.507(8)
N(3A)-C(15A)	1.373(6)	C(28A)-C(29A)	1.516(8)
N(3A)-C(18A)	1.375(6)	C(1B)-C(2B)	1.513(7)
N(1B)-C(19B)	1.400(6)	C(2B)-C(5B)	1.532(7)
N(2B)-C(14B)	1.383(6)	C(2B)-C(3B)	1.537(7)
N(2B)-C(11B)	1.383(6)	C(2B)-C(4B)	1.542(7)
N(3B)-C(15B)	1.376(6)	C(5B)-C(6B)	1.382(7)
N(3B)-C(18B)	1.390(6)	C(5B)-C(10B)	1.394(7)
C(1A)-C(2A)	1.519(7)	C(6B)-C(7B)	1.380(7)
C(2A)-C(4A)	1.530(7)	C(7B)-C(8B)	1.362(7)
C(2A)-C(3A)	1.534(7)	C(8B)-C(9B)	1.378(7)
C(2A)-C(5A)	1.536(7)	C(9B)-C(10B)	1.381(7)
C(5A)-C(10A)	1.386(7)	C(11B)-C(12B)	1.359(7)
C(5A)-C(6A)	1.396(7)	C(12B)-C(13B)	1.407(7)
C(6A)-C(7A)	1.389(7)	C(13B)-C(14B)	1.352(7)
C(7A)-C(8A)	1.379(7)	C(15B)-C(16B)	1.395(7)
C(8A)-C(9A)	1.382(7)	C(16B)-C(17B)	1.409(7)
C(9A)-C(10A)	1.394(7)	C(17B)-C(18B)	1.383(7)
C(11A)-C(12A)	1.371(7)	C(19B)-C(24B)	1.403(7)

C(19B)-C(20B)	1.411(7)	N(2B)-Mo(2)-C(15B)	127.86(16)
C(20B)-C(21B)	1.381(7)	C(16B)-Mo(2)-C(15B)	33.95(16)
C(20B)-C(25B)	1.513(7)	N(1B)-Mo(2)-C(17B)	105.61(17)
C(21B)-C(22B)	1.373(7)	C(1B)-Mo(2)-C(17B)	141.38(19)
C(22B)-C(23B)	1.378(7)	N(2B)-Mo(2)-C(17B)	103.58(16)
C(23B)-C(24B)	1.395(7)	C(16B)-Mo(2)-C(17B)	33.87(16)
C(24B)-C(28B)	1.519(7)	C(15B)-Mo(2)-C(17B)	55.28(17)
C(25B)-C(26B)	1.532(7)	N(1B)-Mo(2)-C(18B)	135.13(17)
C(25B)-C(27B)	1.539(7)	C(1B)-Mo(2)-C(18B)	123.28(19)
C(28B)-C(29B)	1.522(7)	N(2B)-Mo(2)-C(18B)	82.71(16)
C(28B)-C(30B)	1.536(7)	C(16B)-Mo(2)-C(18B)	54.77(17)
C(1T)-C(2T)	1.376(7)	C(15B)-Mo(2)-C(18B)	53.65(17)
C(1T)-C(6T)	1.381(7)	C(17B)-Mo(2)-C(18B)	32.59(15)
C(1T)-C(7T)	1.496(7)	N(1B)-Mo(2)-N(3B)	157.32(16)
C(2T)-C(3T)	1.374(8)	C(1B)-Mo(2)-N(3B)	91.72(18)
C(3T)-C(4T)	1.372(8)	N(2B)-Mo(2)-N(3B)	95.18(15)
C(4T)-C(5T)	1.385(8)	C(16B)-Mo(2)-N(3B)	55.84(16)
C(5T)-C(6T)	1.381(7)	C(15B)-Mo(2)-N(3B)	32.69(14)
N(1A)-Mo(1)-C(1A)	99.5(2)	C(17B)-Mo(2)-N(3B)	55.21(15)
N(1A)-Mo(1)-N(2A)	96.24(16)	C(18B)-Mo(2)-N(3B)	32.62(14)
C(1A)-Mo(1)-N(2A)	98.82(19)	C(19A)-N(1A)-Mo(1)	173.9(3)
N(1A)-Mo(1)-N(3A)	99.65(17)	C(11A)-N(2A)-C(14A)	105.8(4)
C(1A)-Mo(1)-N(3A)	102.26(18)	C(11A)-N(2A)-Mo(1)	131.2(3)
N(2A)-Mo(1)-N(3A)	150.98(16)	C(14A)-N(2A)-Mo(1)	121.2(3)
N(1A)-Mo(1)-N(3B)	155.16(16)	C(15A)-N(3A)-C(18A)	105.5(4)
C(1A)-Mo(1)-N(3B)	105.19(18)	C(15A)-N(3A)-Mo(1)	130.6(3)
N(2A)-Mo(1)-N(3B)	77.85(14)	C(18A)-N(3A)-Mo(1)	122.9(3)
N(3A)-Mo(1)-N(3B)	77.54(14)	C(19B)-N(1B)-Mo(2)	176.7(4)
N(1B)-Mo(2)-C(1B)	100.5(2)	C(14B)-N(2B)-C(11B)	105.7(4)
N(1B)-Mo(2)-N(2B)	101.80(17)	C(14B)-N(2B)-Mo(2)	122.4(3)
C(1B)-Mo(2)-N(2B)	98.28(19)	C(11B)-N(2B)-Mo(2)	130.4(4)
N(1B)-Mo(2)-C(16B)	101.58(18)	C(15B)-N(3B)-C(18B)	105.4(4)
C(1B)-Mo(2)-C(16B)	113.26(19)	C(15B)-N(3B)-Mo(1)	126.6(3)
N(2B)-Mo(2)-C(16B)	136.06(17)	C(18B)-N(3B)-Mo(1)	124.6(3)
N(1B)-Mo(2)-C(15B)	128.59(18)	C(15B)-N(3B)-Mo(2)	70.6(3)
C(1B)-Mo(2)-C(15B)	86.18(19)	C(18B)-N(3B)-Mo(2)	73.4(3)

Mo(1)-N(3B)-Mo(2)	136.74(17)	C(20A)-C(25A)-C(27A)	111.9(4)
C(2A)-C(1A)-Mo(1)	145.1(4)	C(20A)-C(25A)-C(26A)	110.2(4)
C(1A)-C(2A)-C(4A)	111.2(4)	C(27A)-C(25A)-C(26A)	110.3(4)
C(1A)-C(2A)-C(3A)	106.5(4)	C(30A)-C(28A)-C(29A)	109.5(5)
C(4A)-C(2A)-C(3A)	108.6(4)	C(30A)-C(28A)-C(24A)	114.9(5)
C(1A)-C(2A)-C(5A)	108.6(4)	C(29A)-C(28A)-C(24A)	110.1(5)
C(4A)-C(2A)-C(5A)	109.7(4)	C(2B)-C(1B)-Mo(2)	141.5(4)
C(3A)-C(2A)-C(5A)	112.1(4)	C(1B)-C(2B)-C(5B)	108.3(4)
C(10A)-C(5A)-C(6A)	118.3(5)	C(1B)-C(2B)-C(3B)	107.4(4)
C(10A)-C(5A)-C(2A)	122.2(5)	C(5B)-C(2B)-C(3B)	112.0(4)
C(6A)-C(5A)-C(2A)	119.5(5)	C(1B)-C(2B)-C(4B)	112.8(4)
C(7A)-C(6A)-C(5A)	121.1(5)	C(5B)-C(2B)-C(4B)	108.7(4)
C(8A)-C(7A)-C(6A)	120.0(5)	C(3B)-C(2B)-C(4B)	107.6(4)
C(7A)-C(8A)-C(9A)	119.5(5)	C(6B)-C(5B)-C(10B)	116.8(5)
C(8A)-C(9A)-C(10A)	120.6(5)	C(6B)-C(5B)-C(2B)	123.3(5)
C(5A)-C(10A)-C(9A)	120.4(5)	C(10B)-C(5B)-C(2B)	119.9(5)
C(12A)-C(11A)-N(2A)	109.8(5)	C(7B)-C(6B)-C(5B)	120.9(5)
C(11A)-C(12A)-C(13A)	107.7(5)	C(8B)-C(7B)-C(6B)	121.6(5)
C(14A)-C(13A)-C(12A)	106.6(5)	C(7B)-C(8B)-C(9B)	118.7(5)
C(13A)-C(14A)-N(2A)	110.2(5)	C(8B)-C(9B)-C(10B)	120.0(5)
N(3A)-C(15A)-C(16A)	110.7(5)	C(9B)-C(10B)-C(5B)	121.8(5)
C(15A)-C(16A)-C(17A)	106.3(5)	C(12B)-C(11B)-N(2B)	109.8(5)
C(18A)-C(17A)-C(16A)	106.2(5)	C(11B)-C(12B)-C(13B)	107.2(5)
C(17A)-C(18A)-N(3A)	111.2(5)	C(14B)-C(13B)-C(12B)	107.0(5)
N(1A)-C(19A)-C(24A)	118.9(4)	C(13B)-C(14B)-N(2B)	110.3(5)
N(1A)-C(19A)-C(20A)	119.1(4)	N(3B)-C(15B)-C(16B)	110.3(4)
C(24A)-C(19A)-C(20A)	122.0(5)	N(3B)-C(15B)-Mo(2)	76.7(3)
C(21A)-C(20A)-C(19A)	117.5(5)	C(16B)-C(15B)-Mo(2)	71.8(3)
C(21A)-C(20A)-C(25A)	120.0(5)	C(15B)-C(16B)-C(17B)	107.1(5)
C(19A)-C(20A)-C(25A)	122.5(5)	C(15B)-C(16B)-Mo(2)	74.2(3)
C(22A)-C(21A)-C(20A)	121.0(5)	C(17B)-C(16B)-Mo(2)	76.3(3)
C(21A)-C(22A)-C(23A)	120.9(5)	C(18B)-C(17B)-C(16B)	106.0(5)
C(24A)-C(23A)-C(22A)	121.0(5)	C(18B)-C(17B)-Mo(2)	74.3(3)
C(23A)-C(24A)-C(19A)	117.5(5)	C(16B)-C(17B)-Mo(2)	69.8(3)
C(23A)-C(24A)-C(28A)	121.0(5)	C(17B)-C(18B)-N(3B)	111.1(4)
C(19A)-C(24A)-C(28A)	121.5(5)	C(17B)-C(18B)-Mo(2)	73.1(3)

N(3B)-C(18B)-Mo(2)	74.0(3)
N(1B)-C(19B)-C(24B)	118.7(5)
N(1B)-C(19B)-C(20B)	119.5(5)
C(24B)-C(19B)-C(20B)	121.7(5)
C(21B)-C(20B)-C(19B)	117.7(5)
C(21B)-C(20B)-C(25B)	121.9(5)
C(19B)-C(20B)-C(25B)	120.3(4)
C(22B)-C(21B)-C(20B)	121.4(5)
C(21B)-C(22B)-C(23B)	120.6(5)
C(22B)-C(23B)-C(24B)	120.8(5)
C(23B)-C(24B)-C(19B)	117.7(5)
C(23B)-C(24B)-C(28B)	120.2(5)
C(19B)-C(24B)-C(28B)	122.1(5)
C(20B)-C(25B)-C(26B)	114.4(4)
C(20B)-C(25B)-C(27B)	108.3(4)
C(26B)-C(25B)-C(27B)	110.3(5)
C(24B)-C(28B)-C(29B)	111.7(4)
C(24B)-C(28B)-C(30B)	110.7(4)
C(29B)-C(28B)-C(30B)	110.4(4)
C(2T)-C(1T)-C(6T)	117.9(5)
C(2T)-C(1T)-C(7T)	120.9(5)
C(6T)-C(1T)-C(7T)	121.2(5)
C(3T)-C(2T)-C(1T)	121.3(6)
C(4T)-C(3T)-C(2T)	120.9(6)
C(3T)-C(4T)-C(5T)	118.5(6)
C(6T)-C(5T)-C(4T)	120.3(5)
C(1T)-C(6T)-C(5T)	121.2(5)

Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3) for {Mo(NAr)(CHR)(NC_4H_4)$_2$}$_2$. 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)	15(1)	15(1)	15(1)	0(1)	1(1)	1(1)
Mo(2)	14(1)	15(1)	18(1)	-1(1)	2(1)	0(1)
N(1A)	15(2)	14(3)	13(2)	2(2)	2(2)	0(2)
N(2A)	13(2)	17(3)	18(3)	3(2)	-2(2)	2(2)
N(3A)	14(2)	12(3)	18(3)	-1(2)	0(2)	4(2)
N(1B)	15(3)	20(3)	11(2)	5(2)	0(2)	0(2)
N(2B)	18(2)	16(3)	19(3)	-3(2)	6(2)	0(2)
N(3B)	19(3)	12(3)	18(3)	-3(2)	1(2)	-1(2)
C(1A)	17(3)	19(3)	13(3)	2(2)	1(2)	6(2)
C(2A)	21(3)	20(3)	21(3)	5(3)	3(3)	1(3)
C(3A)	38(4)	25(3)	28(3)	5(3)	17(3)	1(3)
C(4A)	21(3)	25(3)	32(4)	5(3)	6(3)	-1(3)
C(5A)	9(3)	20(3)	24(3)	-3(3)	7(2)	-6(2)
C(6A)	22(3)	26(4)	25(3)	2(3)	11(3)	-2(3)
C(7A)	28(4)	23(4)	29(4)	-6(3)	9(3)	-1(3)
C(8A)	22(3)	17(3)	47(4)	11(3)	14(3)	3(3)
C(9A)	22(3)	34(4)	21(3)	17(3)	5(3)	2(3)
C(10A)	23(3)	31(4)	17(3)	9(3)	6(3)	2(3)
C(11A)	15(3)	24(4)	24(4)	0(3)	4(3)	-2(3)
C(12A)	25(3)	25(4)	24(4)	-9(3)	5(3)	-4(3)
C(13A)	23(3)	14(3)	37(4)	-4(3)	4(3)	-2(3)
C(14A)	16(3)	27(4)	22(3)	7(3)	3(3)	8(3)
C(15A)	14(3)	16(3)	18(3)	-2(2)	-1(2)	-1(2)
C(16A)	24(3)	16(3)	19(3)	-8(3)	-2(3)	5(3)
C(17A)	20(3)	37(4)	15(3)	-5(3)	5(3)	3(3)
C(18A)	21(3)	24(3)	19(3)	3(3)	5(3)	0(3)
C(19A)	12(3)	18(3)	17(3)	4(3)	1(3)	-1(2)
C(20A)	18(3)	21(3)	30(4)	2(3)	11(3)	-3(3)
C(21A)	17(3)	25(3)	32(4)	6(3)	6(3)	4(3)
C(22A)	12(3)	34(4)	35(4)	9(3)	-1(3)	-2(3)
C(23A)	20(3)	35(4)	25(3)	2(3)	-3(3)	-3(3)

C(24A)	16(3)	26(4)	26(4)	5(3)	5(3)	-4(3)
C(25A)	19(3)	25(3)	28(4)	0(3)	9(3)	5(3)
C(26A)	27(3)	38(4)	29(4)	-6(3)	9(3)	4(3)
C(27A)	30(4)	30(4)	41(4)	-7(3)	8(3)	4(3)
C(28A)	23(3)	43(4)	26(4)	-8(3)	-7(3)	5(3)
C(29A)	99(4)	47(3)	44(3)	1(3)	44(3)	13(3)
C(30A)	99(4)	47(3)	44(3)	1(3)	44(3)	13(3)
C(1B)	17(3)	15(3)	26(3)	-2(3)	4(2)	0(2)
C(2B)	16(3)	24(3)	23(3)	6(3)	7(3)	0(3)
C(3B)	37(4)	21(3)	31(4)	2(3)	12(3)	-4(3)
C(4B)	24(3)	24(3)	22(3)	-3(3)	-1(3)	1(3)
C(5B)	13(3)	14(3)	24(3)	8(3)	1(3)	9(3)
C(6B)	21(3)	25(3)	25(3)	1(3)	6(3)	-3(3)
C(7B)	19(3)	23(3)	35(4)	-6(3)	-7(3)	-5(3)
C(8B)	28(4)	26(4)	23(3)	-2(3)	3(3)	2(3)
C(9B)	22(3)	32(4)	20(3)	-1(3)	2(3)	3(3)
C(10B)	14(3)	18(3)	33(4)	2(3)	4(3)	-6(2)
C(11B)	22(3)	23(3)	31(4)	6(3)	13(3)	-2(3)
C(12B)	27(3)	34(4)	28(4)	1(3)	17(3)	-4(3)
C(13B)	28(3)	29(4)	18(3)	-6(3)	4(3)	2(3)
C(14B)	18(3)	17(3)	23(3)	-3(3)	2(3)	-1(2)
C(15B)	22(3)	20(3)	17(3)	0(2)	4(3)	8(3)
C(16B)	19(3)	23(3)	15(3)	0(2)	9(3)	0(3)
C(17B)	13(3)	19(3)	18(3)	2(3)	-1(2)	1(2)
C(18B)	17(3)	17(3)	18(3)	0(2)	0(3)	4(2)
C(19B)	21(3)	6(3)	21(3)	-1(2)	1(3)	2(2)
C(20B)	18(3)	10(3)	25(3)	-6(2)	3(3)	3(2)
C(21B)	21(3)	22(3)	24(4)	-2(3)	8(3)	-3(3)
C(22B)	15(3)	18(3)	30(4)	-2(3)	0(3)	-1(2)
C(23B)	31(4)	25(4)	17(3)	0(3)	0(3)	-6(3)
C(24B)	18(3)	15(3)	20(3)	1(2)	2(3)	-4(2)
C(25B)	12(3)	31(4)	19(3)	-8(3)	0(2)	5(3)
C(26B)	35(4)	53(4)	25(4)	-11(3)	6(3)	8(3)
C(27B)	29(4)	36(4)	18(3)	7(3)	3(3)	-6(3)
C(28B)	19(3)	27(3)	14(3)	1(3)	-3(2)	-7(3)
C(29B)	43(4)	34(4)	19(3)	1(3)	12(3)	-4(3)

C(30B)	23(3)	31(4)	23(3)	2(3)	2(3)	0(3)
C(1T)	25(4)	28(4)	21(3)	6(3)	3(3)	0(3)
C(2T)	26(4)	44(4)	20(3)	2(3)	4(3)	-12(3)
C(3T)	25(4)	52(5)	31(4)	3(3)	7(3)	8(4)
C(4T)	42(4)	37(4)	23(4)	4(3)	11(3)	13(3)
C(5T)	36(4)	30(4)	23(3)	5(3)	8(3)	-5(3)
C(6T)	19(3)	30(4)	28(3)	4(3)	7(3)	3(3)
C(7T)	47(4)	26(4)	38(4)	5(3)	12(3)	-5(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (≈^{2}x 10 ^{3}) for {Mo(NAr)(CHR)(NC_4H_4)$_2$}$_2$.

	x	y	z	U(eq)
H(10B)	2855	10063	3872	20
H(10C)	3369	9623	2878	43
H(10D)	3820	8899	3417	43
H(10E)	4018	9918	3071	43
H(11C)	4184	10700	4880	39
H(11D)	4511	10573	4281	39
H(11E)	4314	9552	4629	39
H(57A)	3579	11962	4681	28
H(25A)	3386	13723	4385	32
H(44A)	3175	14258	3192	34
H(19A)	3113	13009	2296	31
H(39A)	3344	11255	2592	28
H(58A)	2807	7886	3099	25
H(17A)	2543	6029	2802	30
H(9A)	2634	5062	3960	30
H(50A)	2955	6357	4945	27
H(28A)	2690	11330	5083	20
H(15A)	2252	11831	6039	26
H(10L)	2236	10175	6781	28
H(11A)	2672	8757	6252	26
H(10F)	5280	6704	5734	30
H(10A)	5570	7248	6910	34
H(10K)	5055	8465	7352	34
H(27A)	4017	7529	4433	28
H(61A)	4871	8256	4333	47
H(61B)	4683	7296	3787	47
H(61C)	5167	7134	4515	47
H(10H)	3997	5788	4860	50
H(10I)	4629	5616	4841	50
H(10J)	4147	5784	4111	50

H(8A)	3697	9403	6426	40
H(20B)	4091	11058	6811	88
H(20C)	4264	10663	6120	88
H(20D)	4701	10588	6896	88
H(48A)	3868	9852	7630	88
H(48B)	4475	9327	7804	88
H(48C)	3928	8609	7549	88
H(46A)	1943	10649	3805	23
H(12A)	2150	12128	3113	44
H(12B)	1664	12928	2729	44
H(12C)	1671	11763	2421	44
H(65A)	542	11688	3216	37
H(65B)	702	11499	2482	37
H(65C)	699	12665	2790	37
H(22A)	2138	13367	3911	28
H(91A)	2239	14364	4934	35
H(52A)	1689	14067	5696	32
H(81A)	1038	12698	5443	31
H(86A)	929	11697	4417	27
H(24A)	1988	10030	2290	29
H(10G)	2020	8948	1248	34
H(80A)	1582	7186	1376	31
H(54A)	1273	7257	2474	24
H(11F)	1755	9717	5047	24
H(55A)	839	8696	4726	22
H(11G)	970	7075	3981	21
H(11B)	1952	7195	3831	22
H(45A)	-1213	10197	2784	26
H(20A)	-1442	10263	1550	27
H(41A)	-771	9965	950	31
H(26A)	143	9915	3963	26
H(90A)	-598	11048	4028	57
H(90B)	-496	10170	4640	57
H(90C)	-1011	10062	3937	57
H(71A)	-37	8115	3668	43
H(71B)	-666	8251	3707	43

H(71C)	-159	8371	4417	43
H(78A)	690	9456	1795	26
H(83A)	452	11105	1239	47
H(83B)	5	10554	586	47
H(83C)	657	10323	718	47
H(31A)	169	7937	1313	40
H(31B)	486	8388	764	40
H(31C)	-168	8597	629	40
H(2TA)	5656	4024	3438	37
H(3TA)	5359	5660	3693	43
H(4TA)	5983	7059	3986	40
H(5TA)	6920	6779	4021	36
H(6TA)	7220	5121	3794	31
H(7TA)	7060	3354	3471	55
H(7TB)	6456	3131	2935	55
H(7TC)	6582	2826	3764	55