

THE UTILITY OF DIMOLYBDENUM TETRAKIS(μ -ISOVALERATE) AND TETRAKIS(μ -PIVALATE) IN THE STEREOCHEMICAL STUDIES OF VARIOUS TRANSPARENT COMPOUNDS

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I. General Experimental Methods

The ECD spectra were acquired at room temperature in CHCl_3 , CH_3CN and DMSO (for UV-Spectroscopy, Fluka) on a Jasco J-715 and J-815 spectropolarimeters and were collected at 0.5 nm/step with an integration time of 0.25 s over the range 200–900 nm with 200 nm/min scan speed, 5 scans. For the ECD standard measurements the chiral ligands (*ca.* 0.003 M) was mixed with stock complex $[\text{Mo}_2(\text{COOR})_4]$ (*ca.* 0.002 M) and dissolved in respective solvent (5 mL) so that the molar ratio of the stock complex to ligand was about 1:1.5, in general. In this dimolybdenum methodology the concentration of the chiral complex formed by exchange of achiral carboxylate/s for chiral ligand molecule/s is not known. Thus, the ECD results are reported as the $\Delta\epsilon'$ values which are calculated in the same way as $\Delta\epsilon$ according to equation $\Delta\epsilon' = \Delta A/c \times d$ in which *c* defines the molar concentration of the chiral ligand, *A* - the absorption and *d* - the path length.

UV–Vis spectra were measured on a Varian spectrophotometer UV-Vis Carry 100E or on a Jasco V-670 UV-Vis-NIR spectrophotometer in CHCl_3 , CH_3CN and DMSO.

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II. Spectroscopic Details:

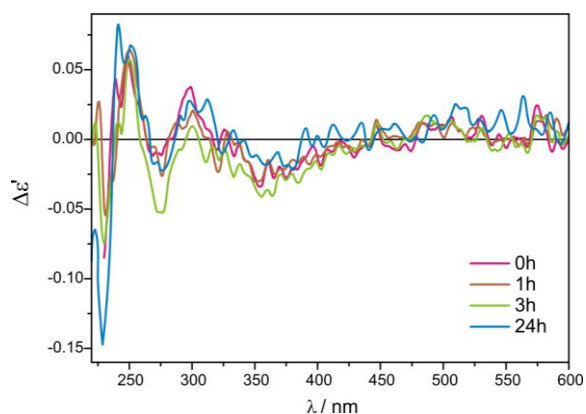


Figure S1. Time-dependent ECD measurements of *in situ* formed Mo_2 -complexes of L-valine (1) with Mo_2 in 1.5:1 ligand-to-complex molar ratio recorded in acetonitrile/water 4:1 ratio.

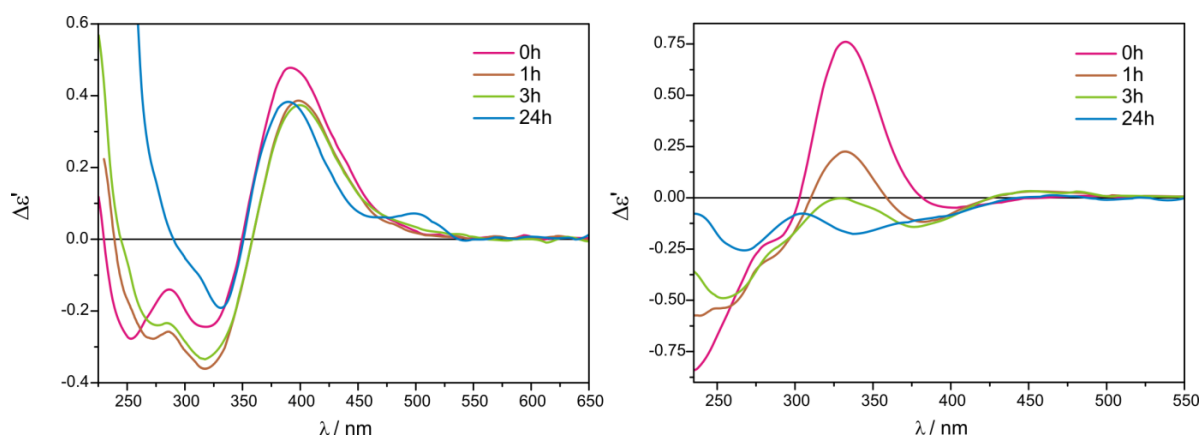


Figure S2. Time-dependent ECD measurements of *in situ* formed Mo_2 -complexes of L-lactic acid (5) with Mo_2 in 1.5:1 ligand-to-complex molar ratio recorded in acetonitrile (right) and in chloroform (left).

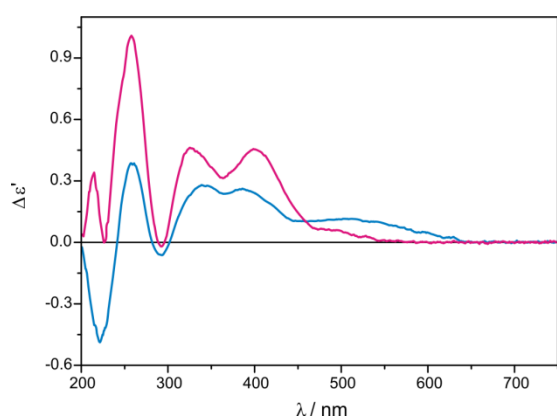


Figure S3. Concentration dependency of D-alaninol (7) with Mo_3 complex recorded in CH_3CN immediately after dissolution; 1.5:1 ligand-to-complex molar ratio (blue), 3:1 ratio (purple).

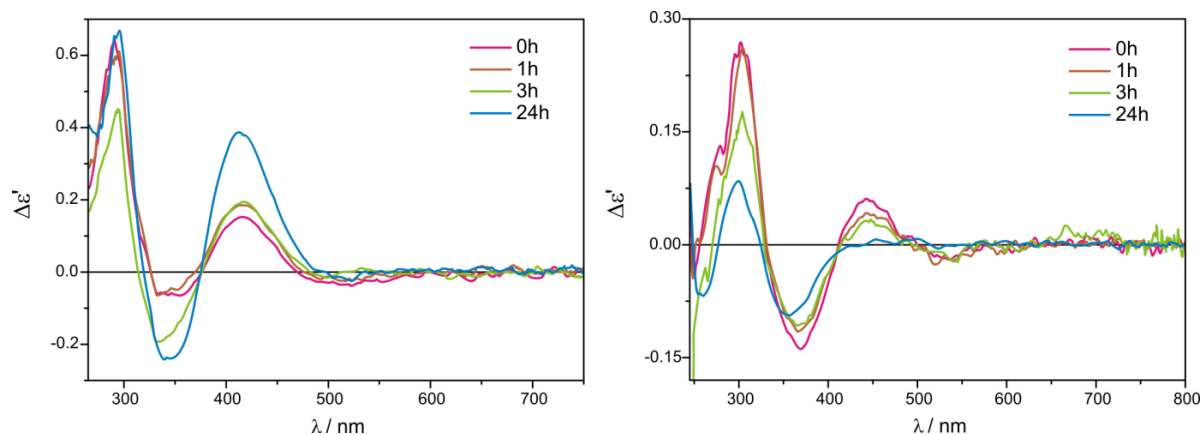


Figure S4. ECD spectra of *in situ* formed Mo_2 -complexes of **Mo2** with (*R*)-propranolol (**10**) in 1.5:1 ligand-to-complex molar ratio, without (left) and with (right) a trace of alkali recorded in CHCl_3 .

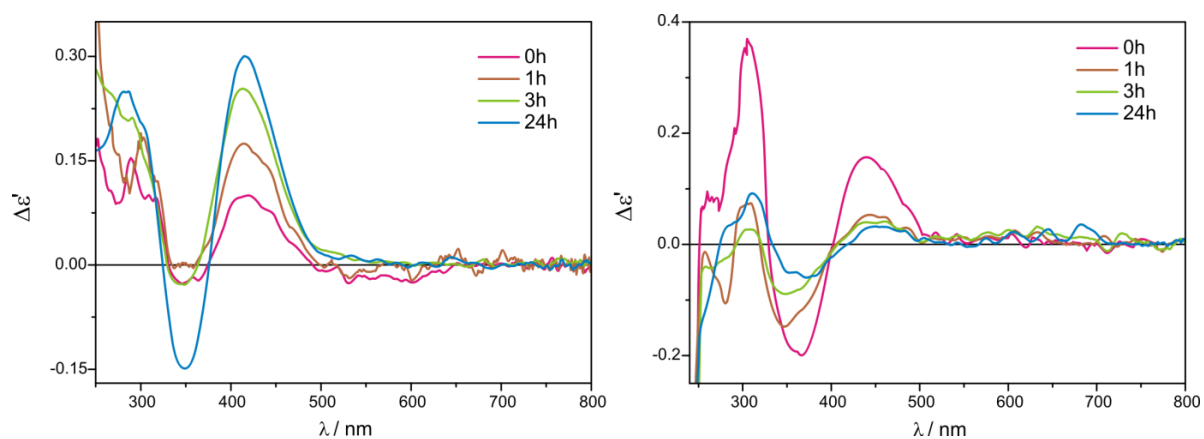


Figure S5. ECD spectra of *in situ* formed Mo_2 -complexes of **Mo3** with (*R*)-propranolol (**10**) in 1.5:1 ligand-to-complex molar ratio, without (left) and with (right) a trace of alkali recorded in CHCl_3 .

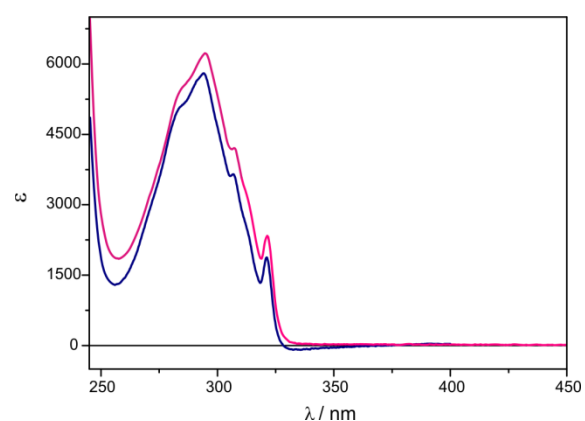


Figure S6. UV-Vis spectra of (*R*)-propranolol (**10**) without (blue line) and with (purple line) a trace of alkali recorded in CHCl_3 .

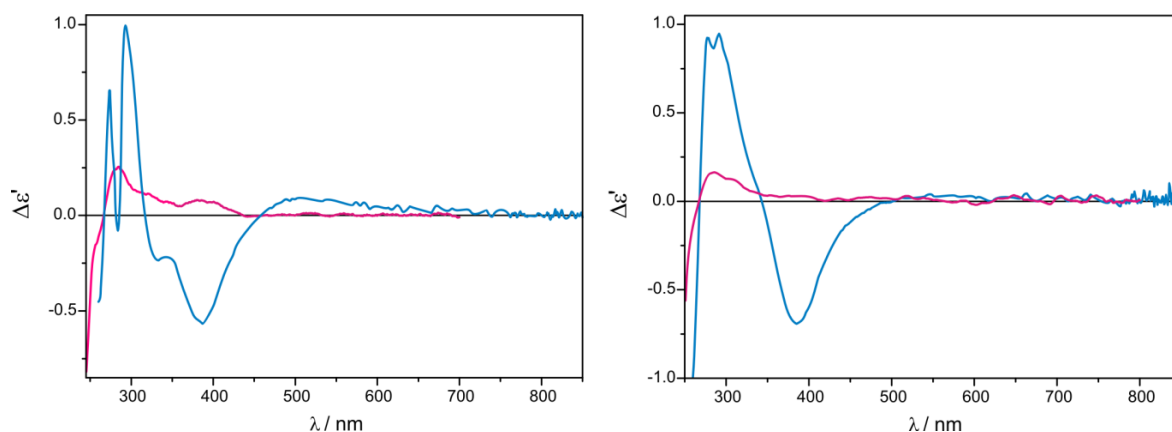


Figure S7. ECD spectra of *in situ* formed Mo₂-complexes of **Mo2** (left) and **Mo3** (right) with *vic*-diamine **15** without (purple line) and with (blue line) a trace of alkali recorded in CHCl₃ immediately after dissolution in 1.5:1 ligand-to-complex molar ratio.

III. Computational Details

As a model for computational study, the stock dimolybdenum *tetrakis*(μ -pivalate) complex [Mo₂{(O₂C₂(CH₃)₃)₄] (**Mo2**) was chosen because of its short side chain compared to the respective μ -isovalerate (**Mo3**) analog. In the calculations *D*- α -alanine (**Ala**, **2**), *L*-mandelic acid (**MA**, **4**), *S*-1-amino-2-propanol (**APol**, **9**), (1*S*,2*S*)-diaminocyclohexane (**DACH**, **11**) and 3-phenyl-propane-1,2-diamine (**PhPDA**, **13**) were selected as chiral ligands. These ligands were chosen due to their size and rigidity to save the computational time and decrease the the number of possible conformers. Formation of bridged and chelated chiral **Mo2**-complexes was considered only (axial arrangements of the chiral ligands were excluded from the consideration because of the very long axial Mo \cdots L distances, where L is a ligand).

Table 1S1. The energies (a.u), relative energies (kcal/mol) and population factors (%) of the mono- and dicoordinated dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes calculated at the (DFT) B3LYP functional combined with LANL2DZ basis set and electron core potential for the molybdenum atoms, and the 6-31+G(d) basis set for C, N, H, O atoms.

System	E	E ₀	G	ΔE	ΔE_0	ΔG	X(G.%)
Monocoordinated complexes							
Ala-bridge-1	-1497.791666	-1497.281681	-1497.351646	0.00	0.00	0.00	100
Ala-chel-1	-1497.754040	-1497.244863	-1497.316616	23.61	23.10	21.98	0
Ala-chel-1a	-1497.754560	-1497.245406	-1497.314202	23.28	22.76	23.50	0
MA-bridge-1	-1709.397963	-1708.847753	-1708.921449	0.00	0.00	0.00	100
MA-chel-1b	-1709.360333	-1708.811235	-1708.887197	23.61	22.92	21.49	0
APol-bridge-1	-1423.719037	-1423.189075	-1423.256341	0.00	0.00	0.00	100
APol-chel-1b	-1423.662246	-1423.135596	-1423.205188	35.64	33.56	32.10	0
DACH-bridge-1	-1520.567022	-1519.959795	-1520.028420	0.00	0.00	0.00	100

DACH-chel-1b	-1520.551119	-1519.944528	-1520.014510	9.98	9.58	8.73	0
PhPDA-bridge-1	-1634.882369	-1634.259079	-1634.333209	0.00	0.00	0.00	100
PhPDA-chel-1	-1634.864150	-1634.241735	-1634.319094	11.43	10.88	8.86	0
Dicoordinated complexes							
Ala-bridge-2 <i>cis</i> -b	-1474.514965	-1474.043384	-1474.111214	0.17	0.00	1.65	6
Ala-bridge-2 <i>trans</i>	-1474.514502	-1474.043388	-1474.113838	0.47	0.00	0.00	93
Ala-bridge-2 <i>trans</i> -b	-1474.515243	-1474.043281	-1474.109840	0.00	0.07	2.51	1
Ala-chel-2	-1474.476671	-1474.006464	-1474.075952	24.20	23.17	23.77	0
MA-bridge-2 <i>trans</i>	-1897.725935	-1897.174786	-1897.252700	0.00	0.00	0.00	100
MA-chel-2a	-1897.688653	-1897.138364	-1897.218681	23.39	22.86	21.35	0
APol-bridge-2 <i>cis</i> -b	-1326.380065	-1325.869291	-1325.932478	0.00	0.00	0.00	100
APol-bridge-2 <i>cis</i> -a	-1326.363260	-1325.852144	-1325.915119	10.55	10.76	10.89	0
APol-bridge-2 <i>trans</i> -b	-1326.299511	-1325.793686	-1325.857654	50.55	47.44	46.95	0
APol-bridge-2 <i>trans</i> -a	-1326.363336	-1325.852125	-1325.915070	10.50	10.77	10.92	0
APol-chel-2	-1326.294570	-1325.789927	-1325.857848	53.65	49.80	46.83	0
DACH-bridge-2- <i>trans</i>	-1520.063025	-1519.398085	-1519.467205	10.90	10.62	9.34	0
DACH-bridge-2- <i>cis</i> -b	-1520.066787	-1519.402074	-1519.470708	8.54	8.12	7.14	0
DACH-bridge-2- <i>cis</i> -a	-1520.068139	-1519.403018	-1519.470791	7.69	7.52	7.09	0
DACH-chel-2	-1520.080395	-1519.415009	-1519.482085	0.00	0.00	0.00	100
PhPDA-bridge-2- <i>cis</i> -b	-1748.698153	-1748.001007	-1748.079263	8.50	8.58	7.77	0
PhPDA-bridge-2- <i>cis</i> -a	-1748.697479	-1748.001039	-1748.080206	8.92	8.56	7.17	0
PhPDA-bridge-2- <i>trans</i> -b	-1748.696934	-1748.000159	-1748.078969	9.27	9.12	7.95	0
PhPDA-bridge-2- <i>trans</i> -a	-1748.693280	-1747.996354	-1748.073888	11.56	11.50	11.14	0
PhPDA-chel-2	-1748.711699	-1748.014685	-1748.091639	0.00	0.00	0.00	100

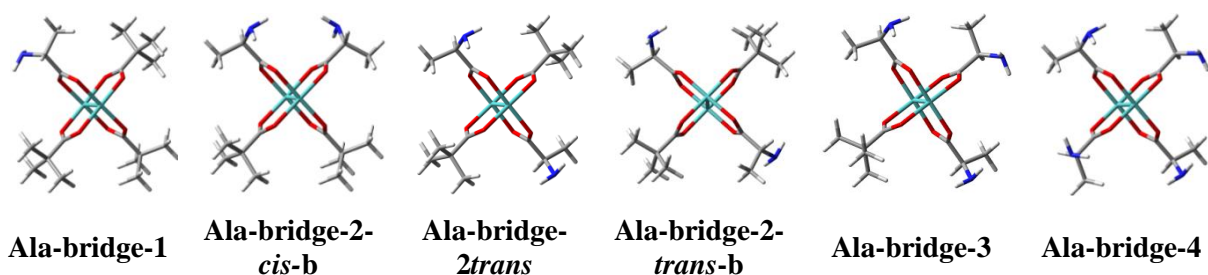


Figure S8. Optimized structures of bridged D- α -alanine (**Ala**, **2**) dimolybdenum *tetrakis*(μ -pivalate) **Mo**₂ complexes.

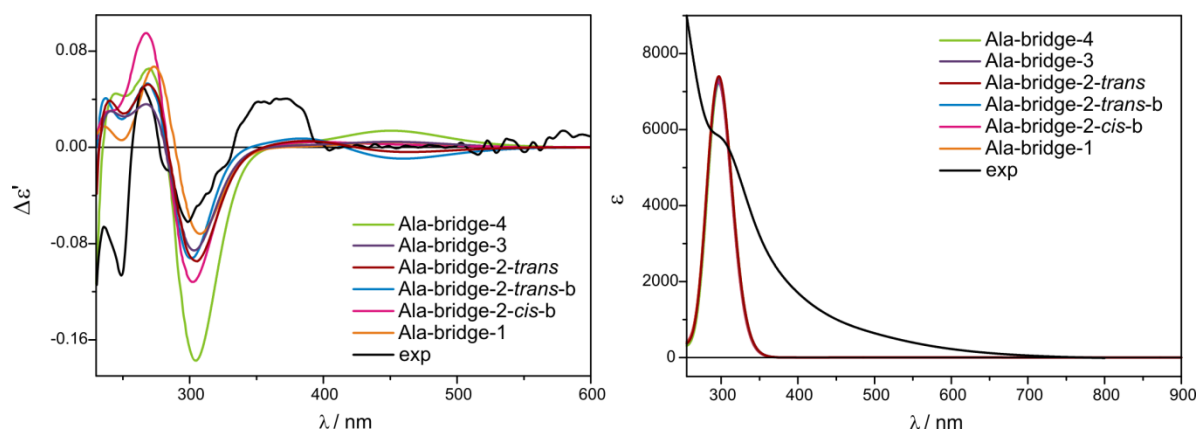


Figure S9. Comparison of the B3LYP calculated ECD (left) and UV-Vis (right) spectra of bridged D- α -alanine (**Ala**, **2**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**2**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in a mixture of acetonitrile-water 4:1 ratio immediately after dissolving).

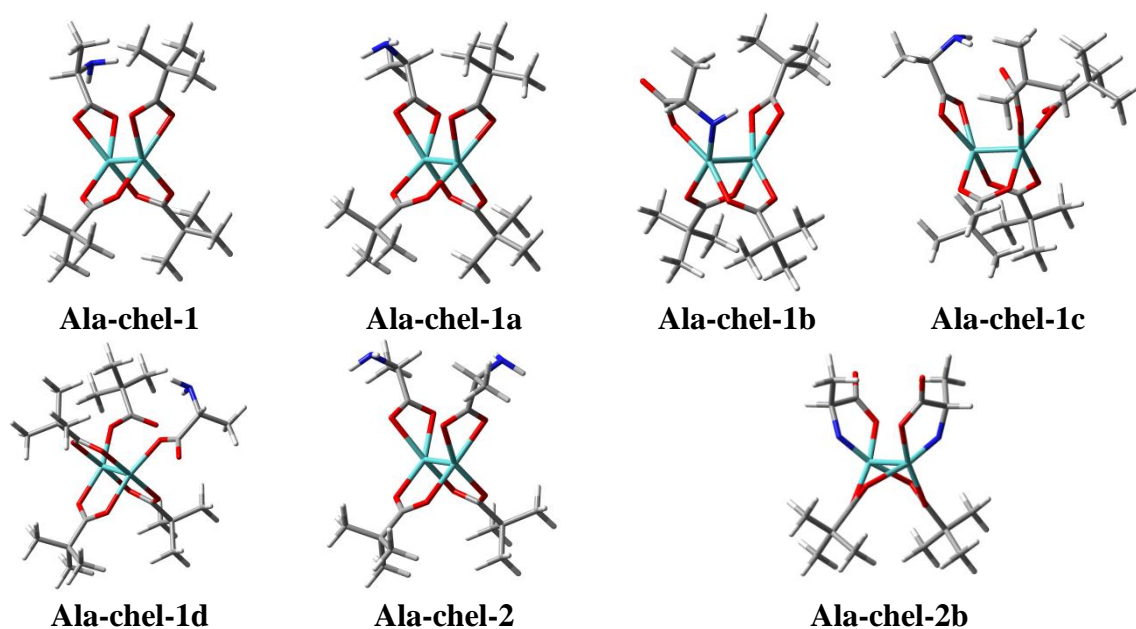


Figure S10. Optimized structures of chelated (chel) D- α -alanine (**Ala**, **2**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes

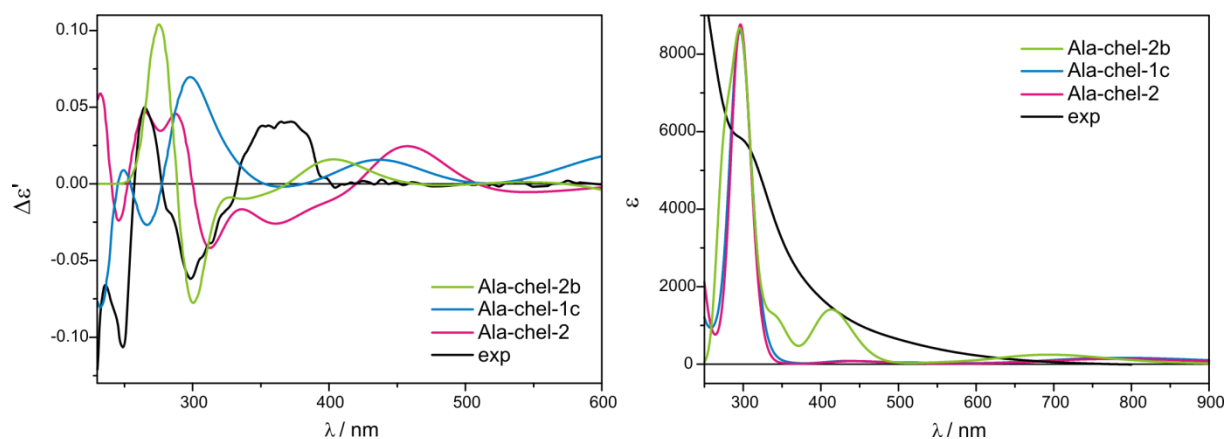


Figure S11. Comparison of the CAM-B3LYP calculated ECD (left) and UV-Vis (right) spectra of chelated (chel) D- α -alanine (**Ala**, **2**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**2+Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in a mixture of acetonitrile-water 4:1 ratio immediately after dissolving).

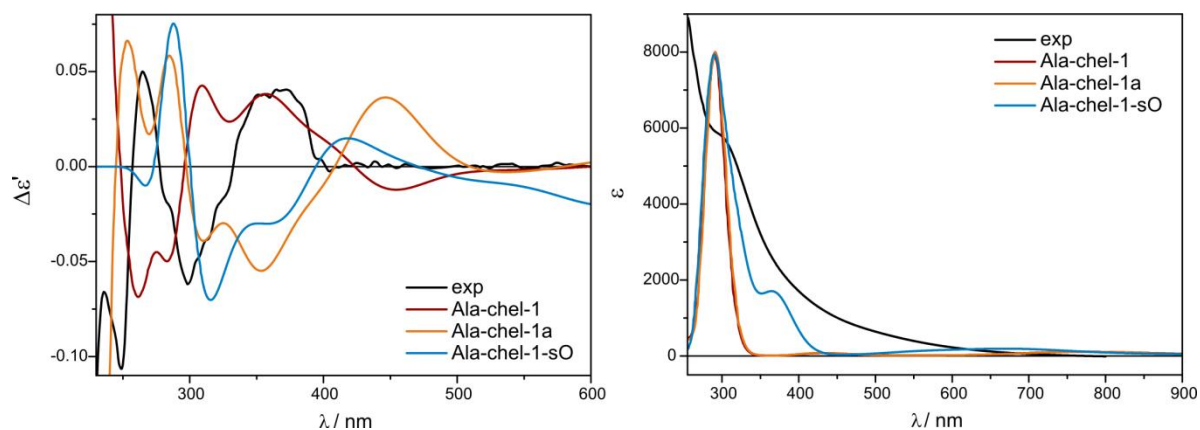


Figure S12. Comparison of the CAM-B3LYP calculated ECD (left) and UV-Vis (right) spectra of chelated (chel) D- α -alanine (**Ala**, **2**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**2+Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in a mixture of acetonitrile-water 4:1 ratio immediately after dissolving).

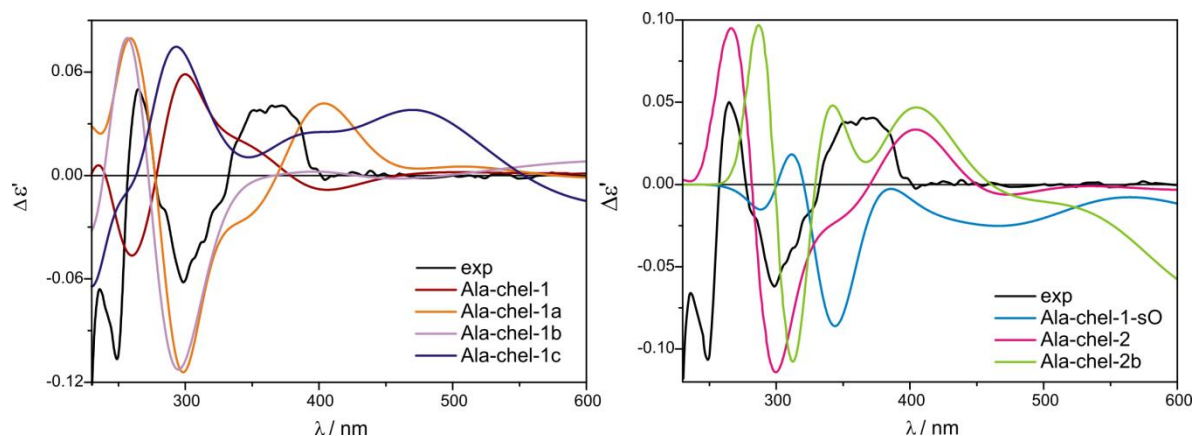


Figure S13. Comparison of the B3LYP calculated ECD spectra of chelated (chel) D- α -alanine (**Ala**, **2**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**2+Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in a mixture of acetonitrile-water 4:1 ratio immediately after dissolving).

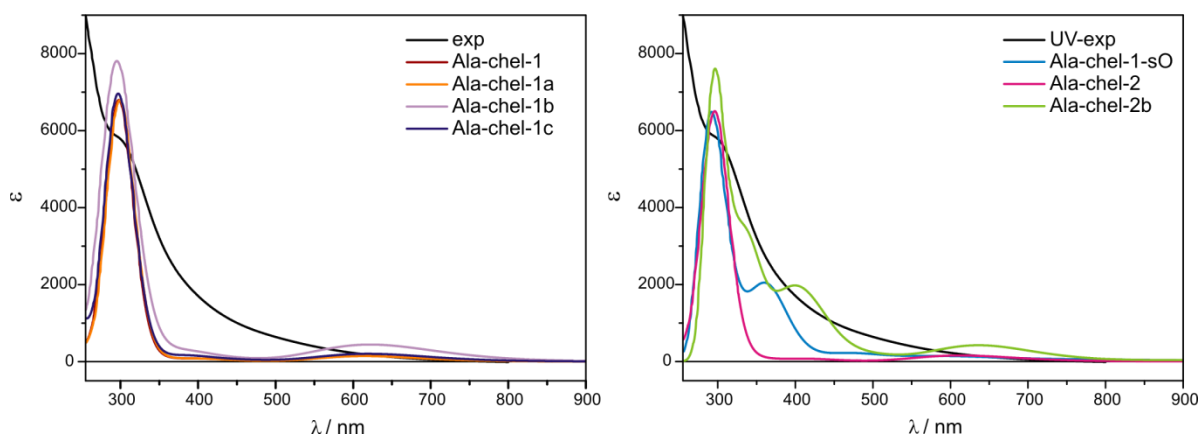


Figure S13B. Comparison of the B3LYP calculated UV-Vis spectra of chelated (chel) D- α -alanine (**Ala**, **2**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**2+Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in a mixture of acetonitrile-water 4:1 ratio immediately after dissolving).

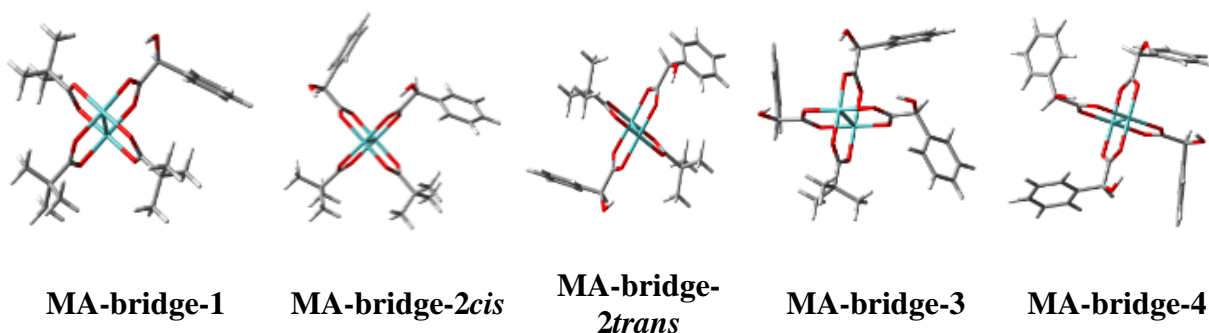


Figure S14. Optimized structures of bridged D- α -mandelic acid (**MA**, **4**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes.

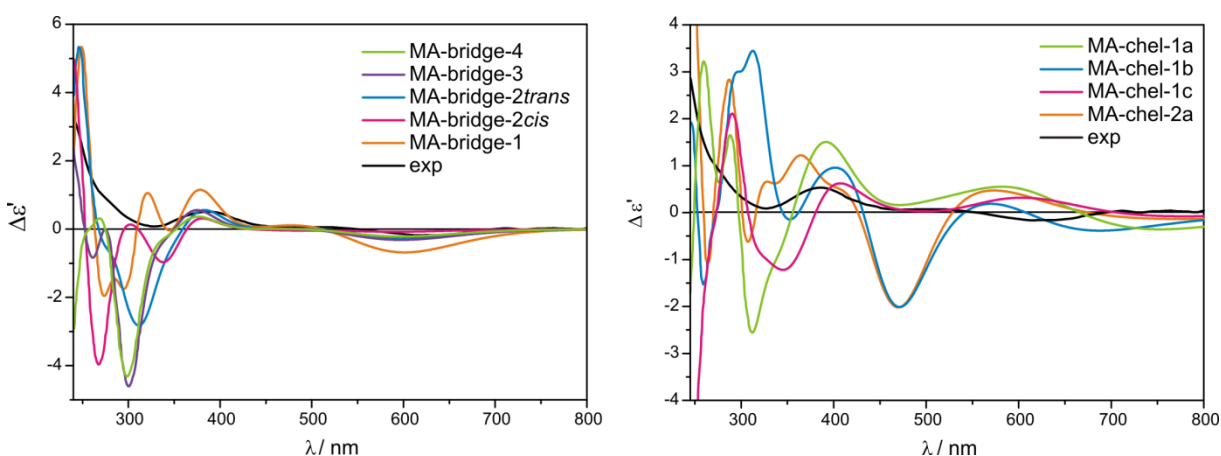


Figure S15. Comparison of the CAM-B3LYP calculated ECD spectra of bridged (left) and chelated (right) D- α -mandelic acid (**MA**, **4**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**4+Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in acetonitrile immediately after dissolving).

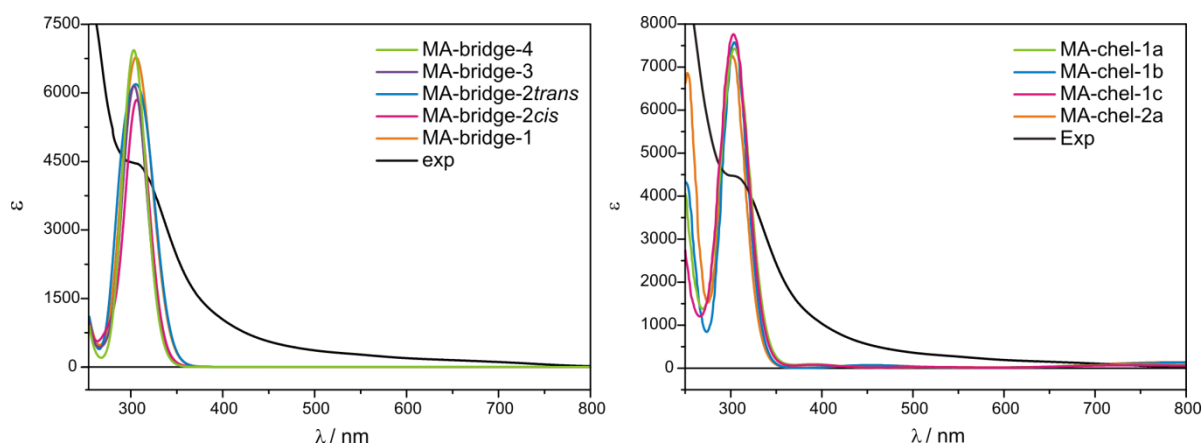


Figure S15B. Comparison of the CAM-B3LYP calculated UV-Vis spectra of bridged (left) and chelated (right) D- α -mandelic acid (**MA**, **4**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**4**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in acetonitrile immediately after dissolving).

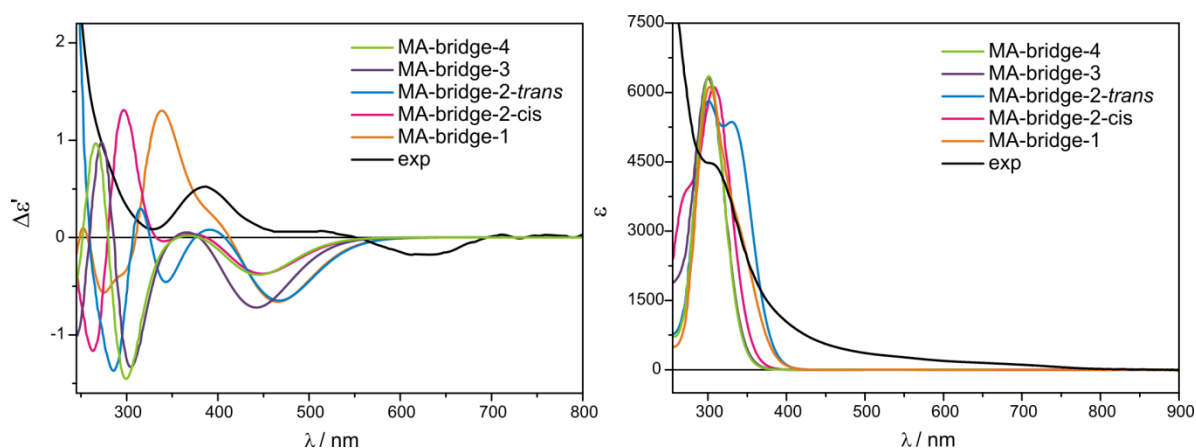


Figure S16. Comparison of the B3LYP calculated ECD (left) and UV-Vis (right) spectra of bridged D- α -mandelic acid (**MA**, **4**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**4** +**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in acetonitrile immediately after dissolving).

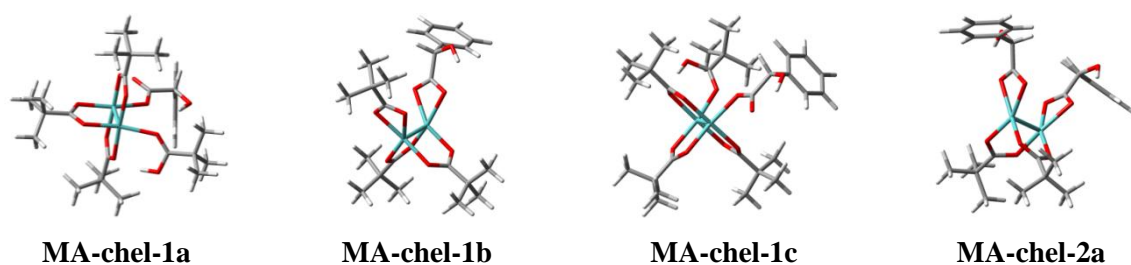


Figure S17. Optimized structures of chelated (chel) D- α -mandelic acid (**MA**, **4**) D- α -mandelic acid (**4**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes.

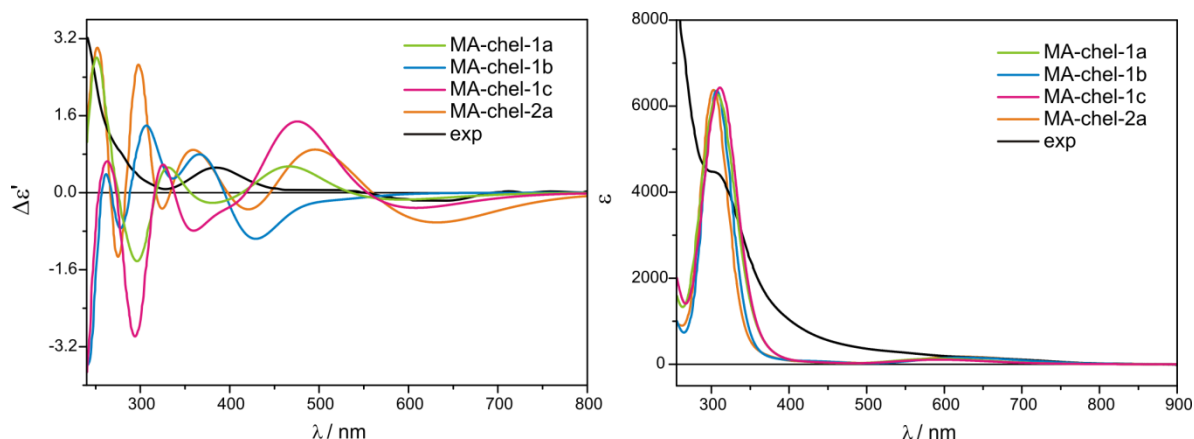


Figure S18. Comparison of the B3LYP calculated ECD (left) and UV-Vis (right) spectra of chelated (chel) *D*- α -mandelic acid (**MA**, **4**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**4**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in acetonitrile immediately after dissolving).

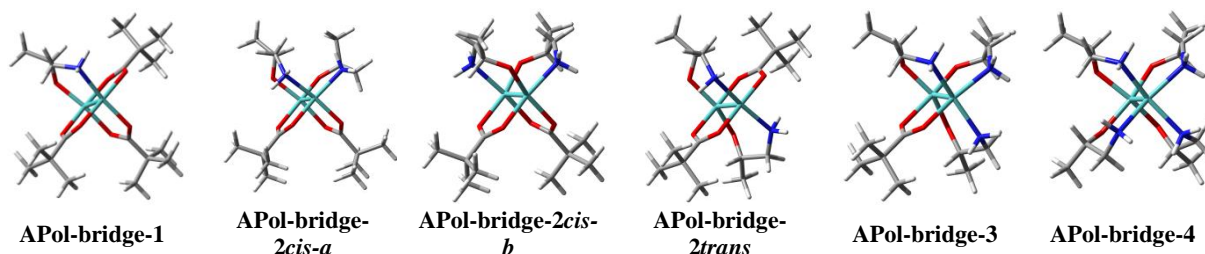


Figure S19. Optimized structures of bridged *S*-1-amino-2-propanol (**APol**, **9**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes.

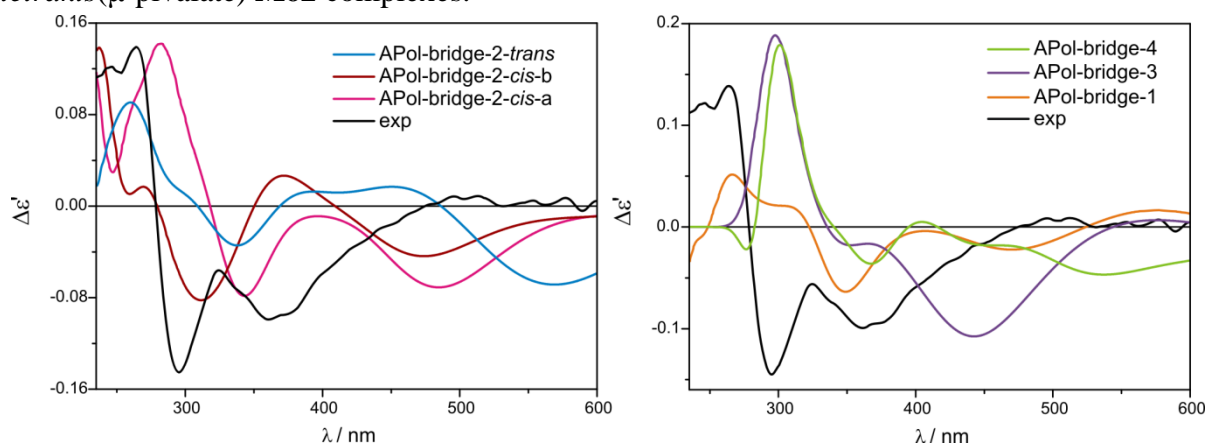


Figure S20. Comparison of the CAM-B3LYP calculated ECD spectra of bridged *S*-1-amino-2-propanol (**APol**, **9**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**9**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

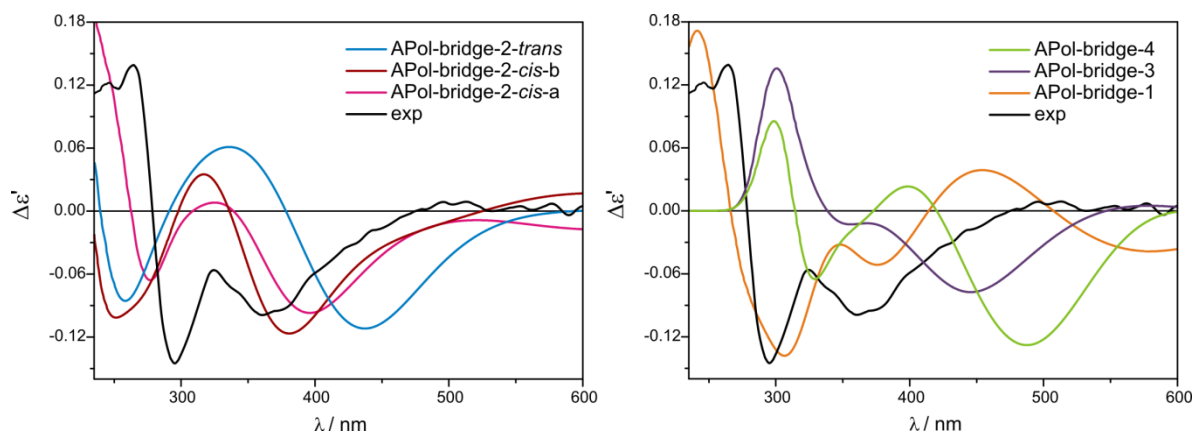


Figure S21. Comparison of the B3LYP calculated ECD spectra of bridged *S*-1-amino-2-propanol (APol, **9**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**9**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

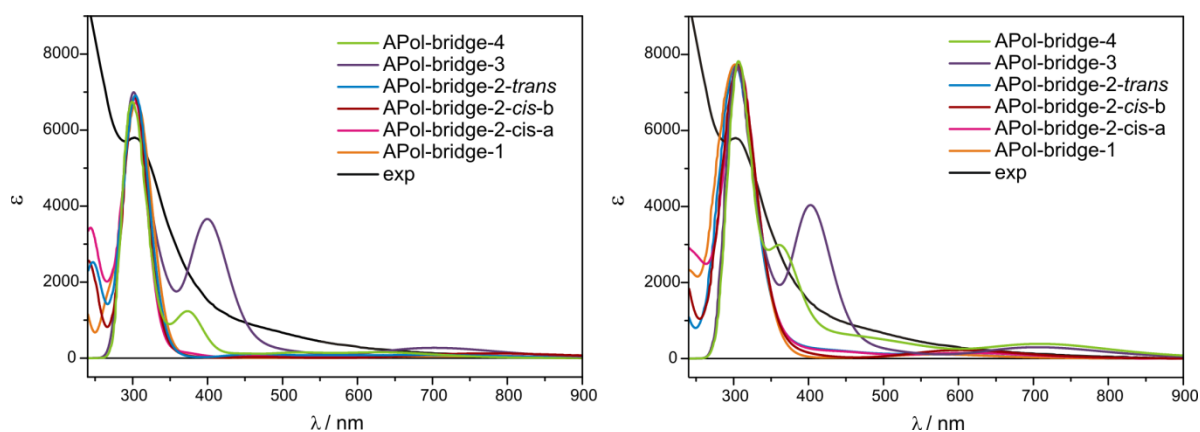


Figure S22. Comparison of UV-Vis spectra of the CAM-B3LYP (left) and B3LYP (right) of bridge *S*-1-amino-2-propanol (APol, **9**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**9**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

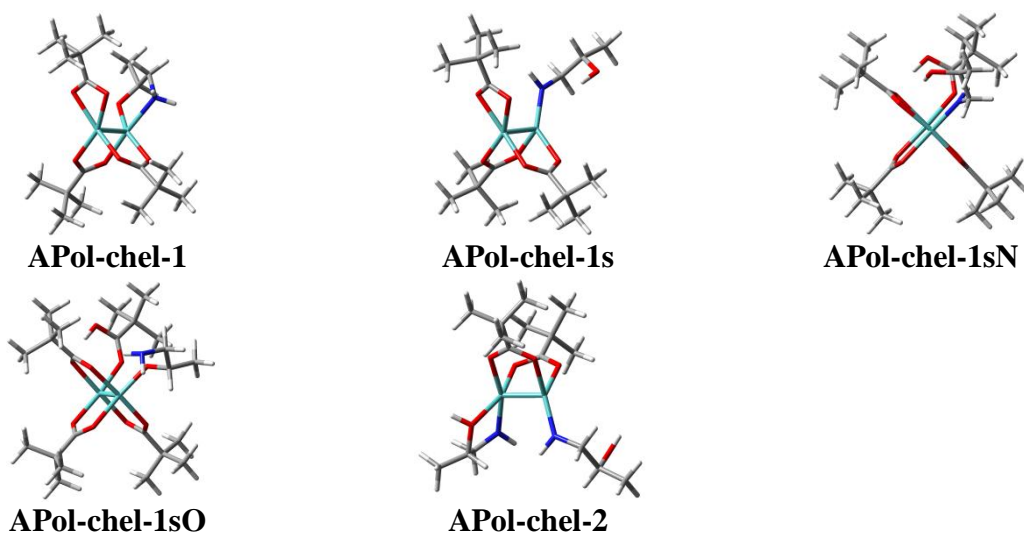


Figure S23. Optimized structures of selected mono- and disubstituted chelated (chel) *S*-1-amino-2-propanol (**APol**, **9**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes.

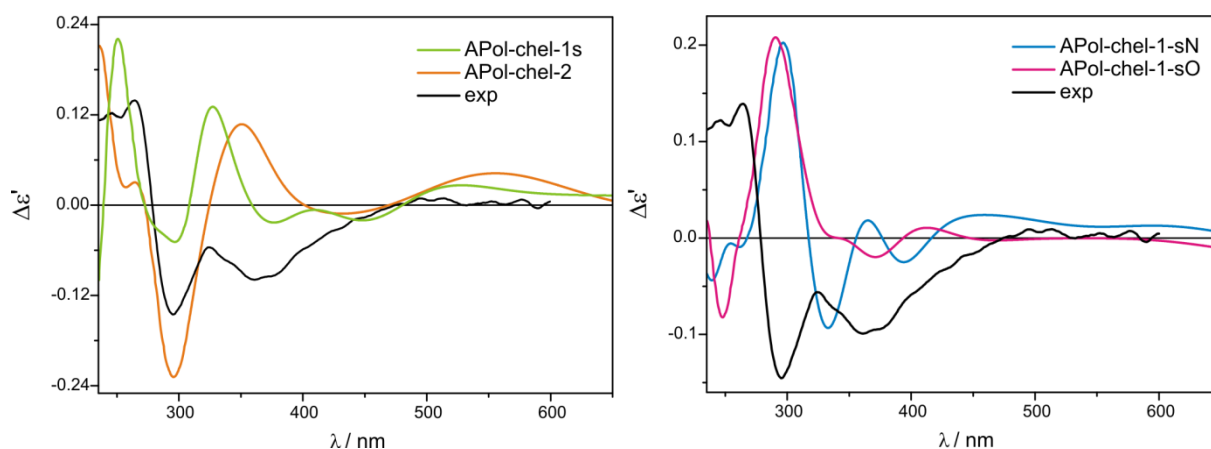


Figure S24. Comparison of the CAM-B3LYP calculated ECD spectra of chelated (chel) *S*-1-amino-2-propanol (**APol**, **9**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**9**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

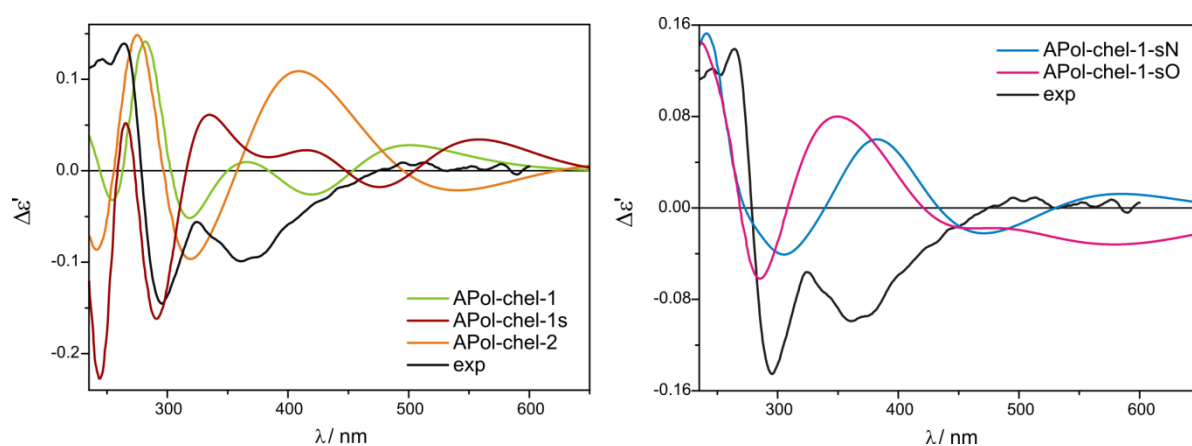


Figure S25. Comparison of the B3LYP calculated ECD spectra of chelated (chel) *S*-1-amino-2-propanol (**APol**, **9**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**9**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

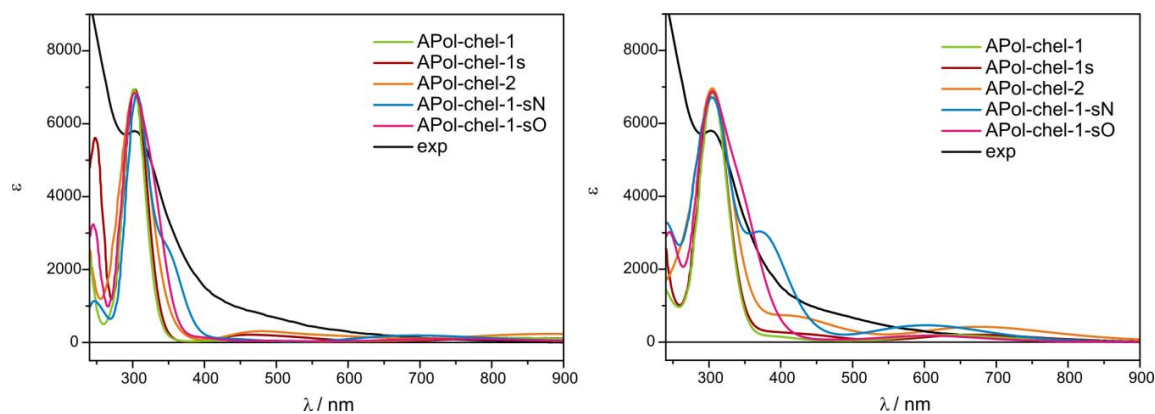


Figure S26. Comparison of UV-Vis spectra of the CAM-B3LYP (left) and B3LYP (right) of chelated *S*-1-amino-2-propanol (**APol**, **9**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**9+Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

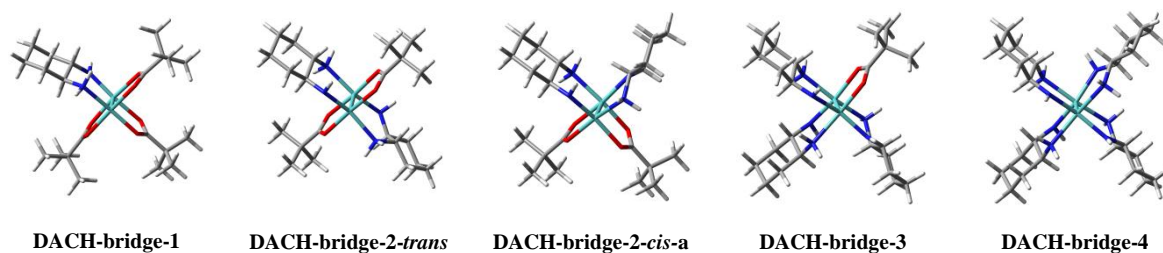


Figure S27. Optimized structures of bridged (*1S,2S*)-diaminocyclohexane (**DACH**, **11**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes.

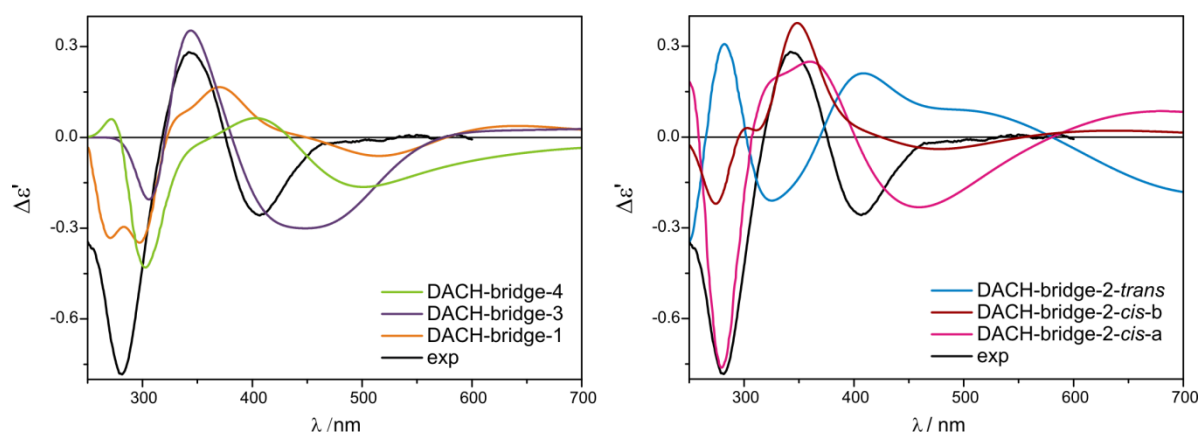


Figure S28. Comparison of the B3LYP calculated ECD spectra of bridged (*1S,2S*)-diaminocyclohexane (**DACH**, **11**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**11+Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

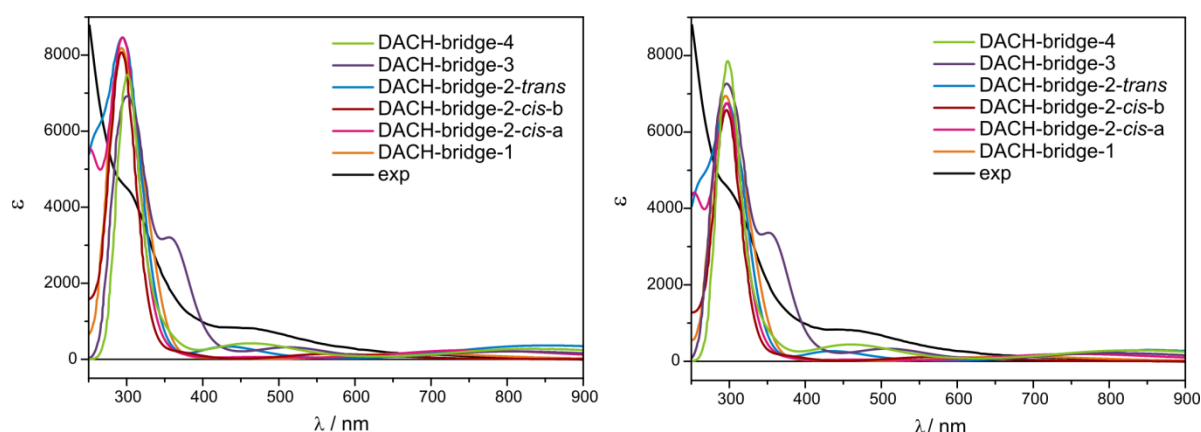


Figure S29. Comparison of UV-Vis spectra of the CAM-B3LYP (left) and B3LYP (right) of bridge (*1S,2S*)-diaminocyclohexane (**DACH**, **11**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**11+Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

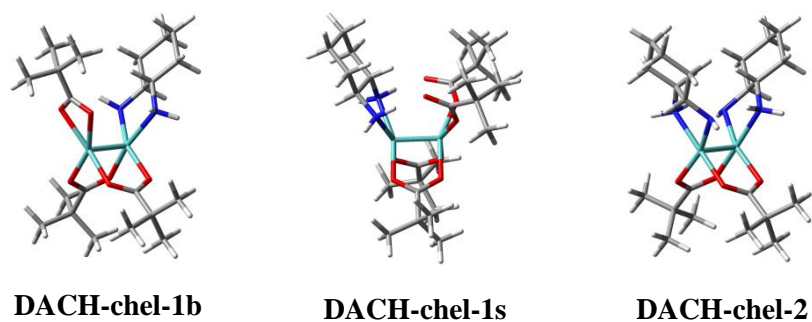


Figure S30. Optimized structures of chelated (chel) (1*S*,2*S*)-diaminocyclohexane (**DACH**, **11**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes.

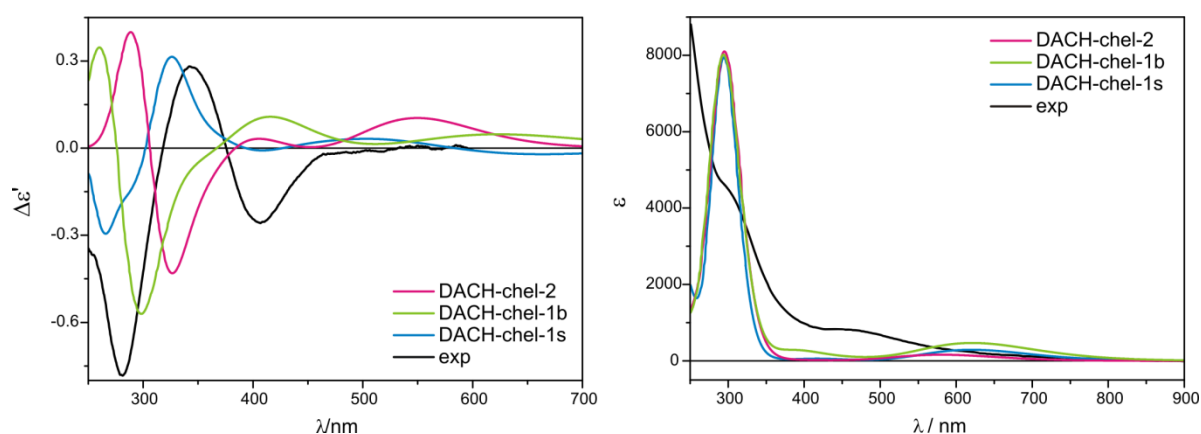


Figure S31. Comparison of the B3LYP calculated ECD (left) and UV-Vis (right) spectra of chelated (chel) (1*S*,2*S*)-diaminocyclohexane (**DACH**, **11**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**11**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

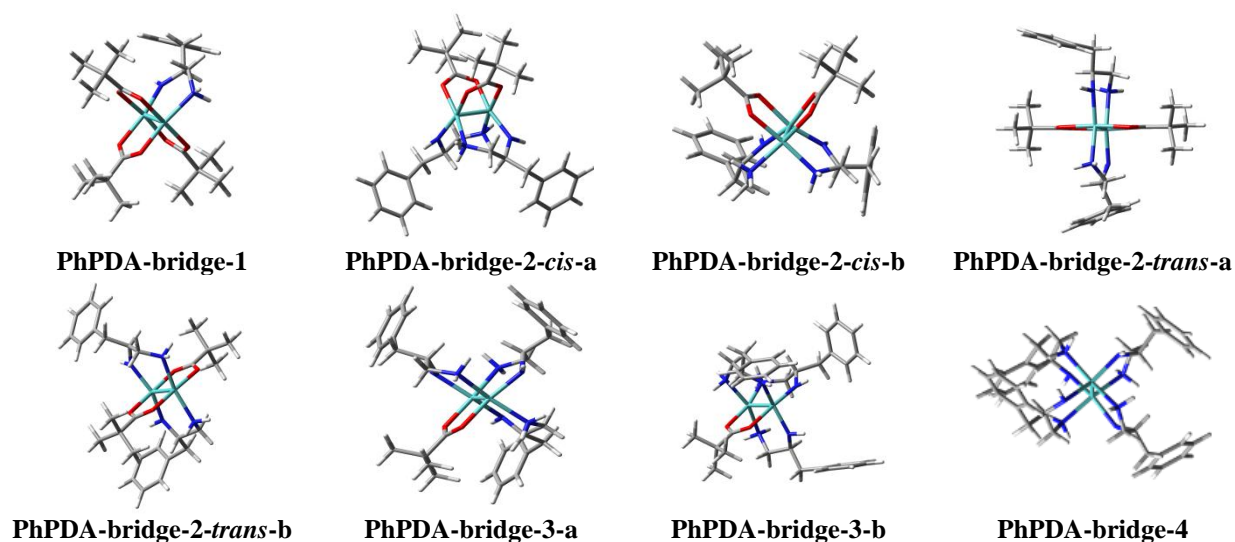


Figure S32. Optimized structures of bridged 3-phenyl-propane-1,2-diamine (**PhPDA**, **13**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes.

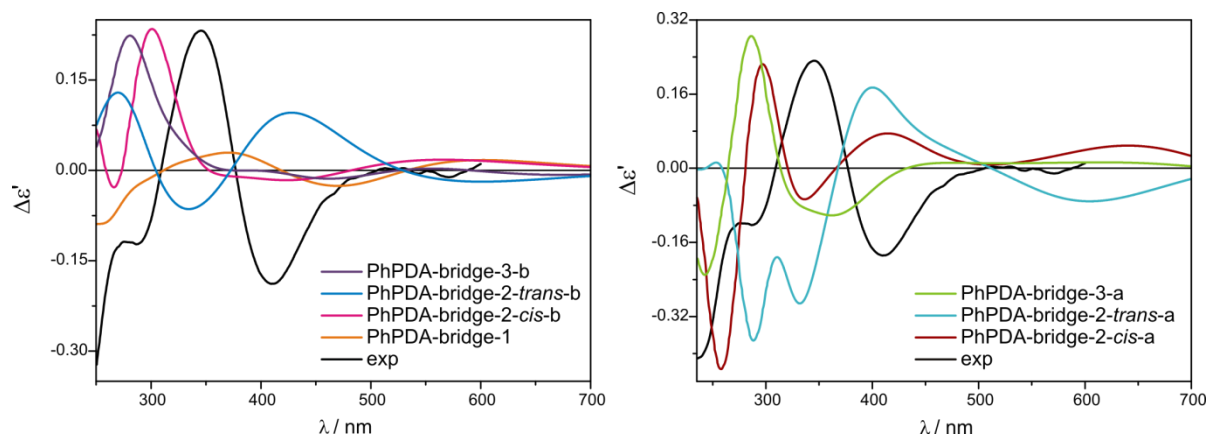


Figure S33. Comparison of the CAM-B3LYP calculated ECD spectra of bridge 3-phenyl-propane-1,2-diamine (**PhPDA**, **13**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**13**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

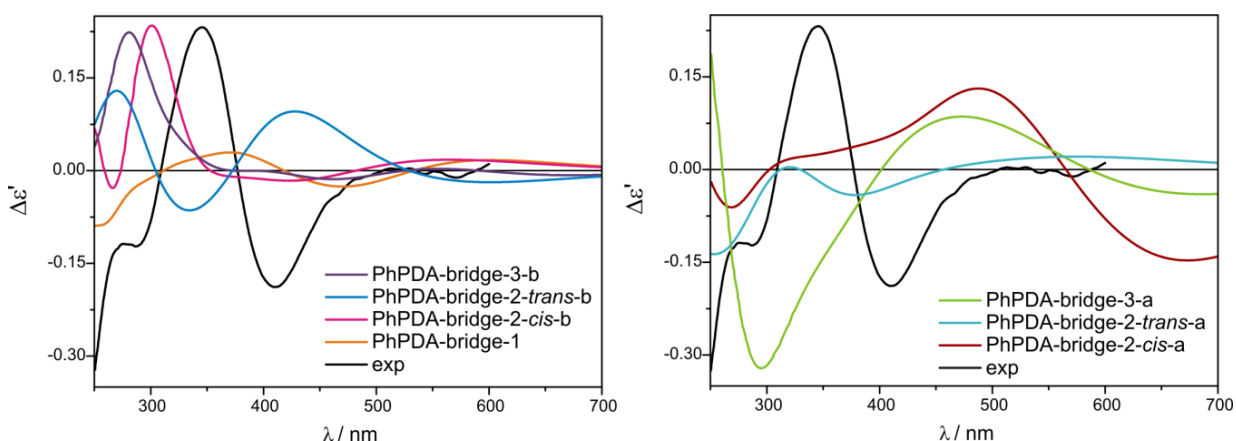


Figure S34 Comparison of the B3LYP calculated ECD spectra of bridged 3-phenyl-propane-1,2-diamine (**PhPDA**, **13**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**13**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

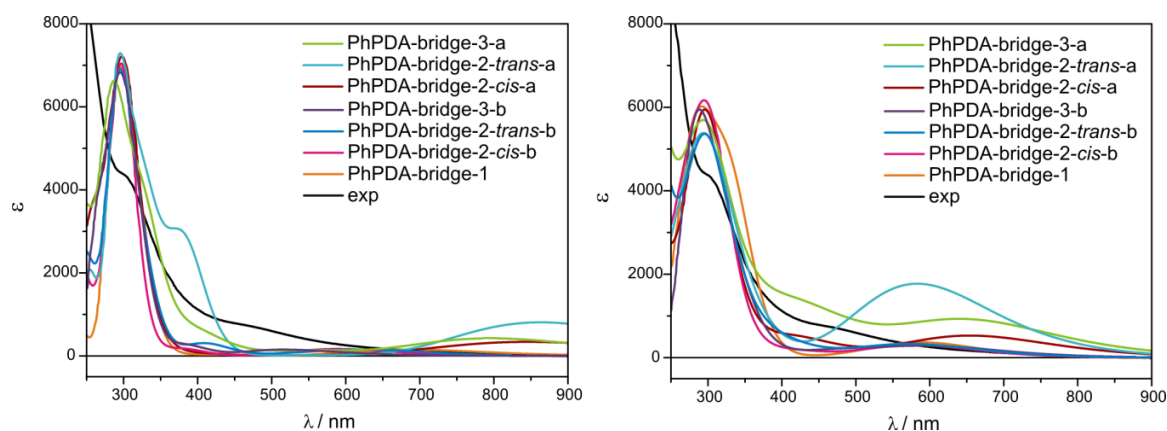


Figure S35. Comparison of UV-Vis spectra of the CAM-B3LYP (left) and B3LYP (right) of bridge 3-phenyl-propane-1,2-diamine (**PhPDA**, **13**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**13**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

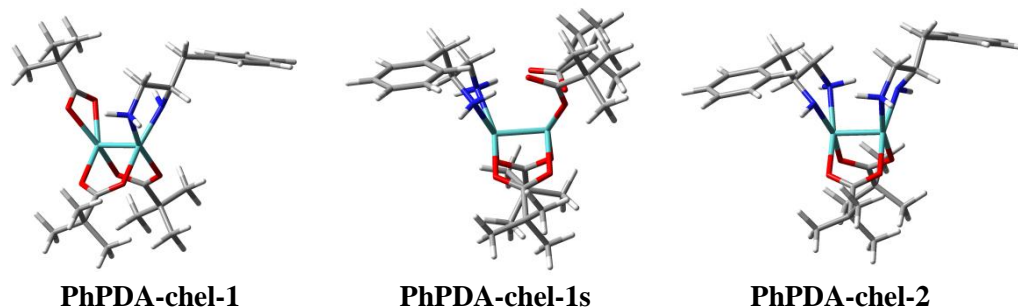


Figure S36. Optimized structures of selected mono- and disubstituted chelated (chel) 3-phenyl-propane-1,2-diamine (**PhPDA**, **13**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes.

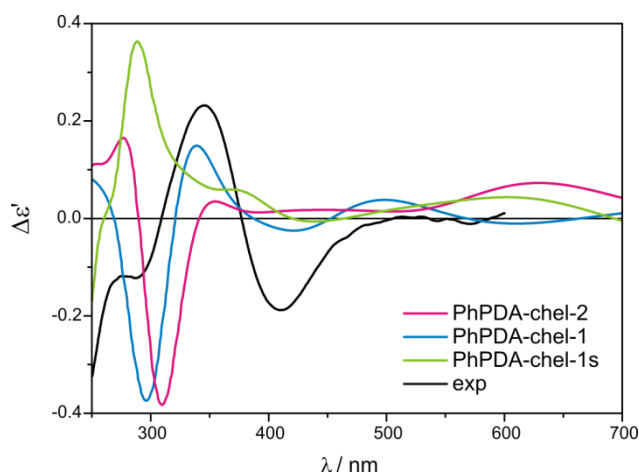


Figure S37. Comparison of the CAM-B3LYP calculated ECD spectra of chelated 3-phenyl-propane-1,2-diamine (**PhPDA**, **13**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**13**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

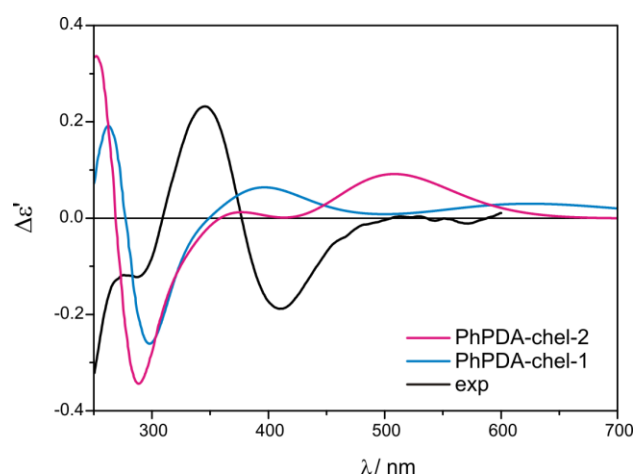


Figure S38. Comparison of the B3LYP calculated ECD spectra of chelated (chel) 3-phenyl-propane-1,2-diamine (**PhPDA**, **13**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**13**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

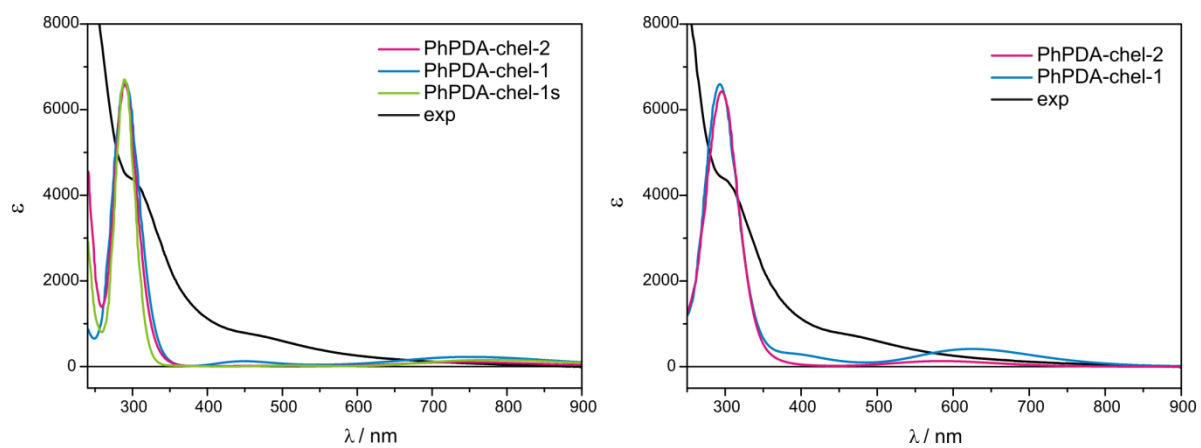


Figure S39. Comparison of UV-Vis spectra of the CAM-B3LYP (left) and B3LYP (right) of chelated 3-phenyl-propane-1,2-diamine (**PhPDA**, **13**) dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes with experimental data (**13**+**Mo2**, 1.5:1 ligand-to-complex molar ratio, recorded in chloroform immediately after dissolving).

Table 2SI. The Cartesian Coordinates of Alanine (Ala) substituted dimolybdenum *tetrakis*(μ -pivalate) **Mo₂** complexes.

Ala-bridge-1				Ala-bridge-2cis-b			
Mo	-0.01411800	-0.09330200	-1.09089600	Mo	-0.03762700	-0.22533900	-1.05475600
O	-2.13263000	-0.36807700	-1.14069200	O	-1.54350400	1.28337300	-1.03855500
O	2.10671700	0.17661100	-1.13977500	O	1.47100500	1.28384200	-1.14565900
O	-0.28837700	2.02445800	-1.06127900	C	-1.95406400	1.72692000	0.09062600
C	-2.75480700	-0.50084400	-0.02921300	C	-3.02946000	2.81597200	0.10827200
C	-4.26064000	-0.77562900	-0.05003700	Mo	0.03730600	-0.23993800	1.07233500
Mo	-0.00469500	-0.16605100	1.03325000	C	1.95424700	1.72810900	-0.04611800
C	2.73766400	0.23130700	-0.02849000	O	-1.47058200	1.27115200	1.18291500
C	-0.37649200	2.61081500	0.07364700	O	1.54392800	1.27155600	1.07517200
O	-2.12451000	-0.44233600	1.08221100	C	3.03413000	2.81180200	-0.09625000
O	2.11499800	0.10239300	1.08312800	C	4.25217300	2.24638500	-0.86469000
O	-0.27953700	1.94292800	1.16027900	H	5.03512900	3.01158600	-0.92494400
C	4.24635800	0.49047200	-0.00666800	H	4.67255500	1.37148200	-0.35448400
C	-0.61420300	4.12256100	0.10717100	H	3.97763300	1.95332400	-1.88285500
C	4.46500600	1.92086400	0.54672700	C	2.46539900	4.03331400	-0.85568700
H	4.06358300	2.01943000	1.56060300	H	1.59109100	4.44939800	-0.34080400
H	5.53874200	2.14101800	0.57859400	H	3.22938900	4.81765700	-0.91299300
H	3.98394900	2.67205400	-0.09099600	H	2.16986700	3.76482500	-1.87462100
C	4.84253200	0.38477800	-1.42083200	C	3.45953900	3.22979600	1.32153800
H	5.92145400	0.57466300	-1.37612800	H	3.87146400	2.38481100	1.88323000
H	4.69041900	-0.61353400	-1.84586300	H	4.23191400	4.00519900	1.25603300
H	4.39487200	1.11515600	-2.10218200	H	2.61648400	3.63597600	1.89057300
C	4.92486600	-0.53367500	0.92929900	C	-2.46701800	4.06091500	-0.61854300
H	4.77917900	-1.55885700	0.56816300	H	-1.57784700	4.45088700	-0.10875800
H	6.00302500	-0.33806400	0.96672600	H	-2.19716100	3.82770800	-1.65332200
H	4.52682600	-0.46760000	1.94622000	H	-3.22544700	4.85267100	-0.62968400
C	0.51454600	4.81675400	-0.68961400	C	-3.41631400	3.18390000	1.55058900
H	0.34947400	5.90069700	-0.69055500	H	-4.18617100	3.96433800	1.53307800
H	1.49545000	4.62394300	-0.23879600	H	-3.81864100	2.32047200	2.09109500
H	0.53819000	4.47066900	-1.72753600	H	-2.55714100	3.56492500	2.11251400
C	-1.97578100	4.40897200	-0.57087400	C	-4.27015600	2.29131400	-0.65166700
H	-2.79817200	3.92171800	-0.03344900	H	-4.68581300	1.40005300	-0.16643300
H	-2.16479700	5.48904100	-0.57152400	H	-5.04765500	3.06431500	-0.66252800
H	-1.98427500	4.05714500	-1.60727200	H	-4.02285100	2.03672800	-1.68688100
C	-0.63229300	4.64533700	1.55342900	C	4.40920200	-2.57184200	-0.32474700
H	0.32017300	4.45712400	2.06036400	C	3.04839300	-3.26226600	-0.12614900
H	-0.80704300	5.72769600	1.54692900	C	1.94788500	-2.19891700	-0.07126400
H	-1.42762300	4.17496900	2.14092900	O	1.47062600	-1.75043500	-1.16941400
C	-4.94682900	0.20507700	-1.02530700	O	1.54824100	-1.76081500	1.05948600
H	-4.81468600	1.24445500	-0.70153000	N	3.10046600	-4.14328100	1.04211000
H	-4.54357700	0.10697400	-2.03749400	H	5.18787400	-3.33116100	-0.44822800
H	-6.02242600	-0.00457100	-1.05972100	H	4.40030700	-1.92913800	-1.21075200
C	-4.86500800	-0.62703000	1.35691800	H	4.66142400	-1.95551300	0.54684000
H	-5.94142900	-0.83103000	1.31434500	H	2.83991500	-3.88113300	-1.00558500
H	-4.41193200	-1.32721300	2.06564100	H	2.21614800	-4.63893800	1.14948500
H	-4.72655600	0.38764600	1.74670900	H	3.21356100	-3.58480700	1.88800000
C	-4.45859300	-2.22812200	-0.55222500	C	-4.41153400	-2.57187500	0.32699700
H	-3.97518900	-2.94975200	0.11703500	C	-3.05316200	-3.26036100	0.10599800
H	-5.52953100	-2.46138100	-0.58515400	C	-1.95133600	-2.19772800	0.06334900
H	-4.04724900	-2.35944800	-1.55851500	O	-1.47416200	-1.76290900	1.16653200
C	2.11822100	-4.61930300	-0.42529500	O	-1.55003400	-1.74681400	-1.06170000
C	0.61487600	-4.37907500	-0.19869400	N	-3.11425800	-4.12019900	-1.07735500
C	0.35314500	-2.87196000	-0.12764800	H	-5.19063400	-3.33228100	0.44064100
O	0.25707200	-2.21378600	-1.22009600	H	-4.39557000	-1.94695500	1.22554400

O	0.26841500	-2.29669900	1.00871000	H	-4.66855600	-1.93791400	-0.53041200
N	0.15887300	-5.13196600	0.97093100	H	-2.83965900	-3.89533400	0.97272400
H	2.30012600	-5.69048300	-0.55828000	H	-2.23121900	-4.61473200	-1.19936500
H	2.47276800	-4.08865100	-1.31447200	H	-3.23208800	-3.54669800	-1.91246000
H	2.69983100	-4.27392200	0.43826600				
H	0.06799000	-4.74996700	-1.07253300				
H	-0.84447000	-5.00719100	1.10054200				
H	0.59833700	-4.75790600	1.81189600				
Ala-bridge-2trans				Ala-bridge-2trans-b			
Mo	0.00798300	-0.00158500	1.11959400	Mo	-0.05204200	-0.06827400	1.06391000
O	2.12124900	-0.31205200	1.15362200	O	2.08141100	-0.01379700	1.09752200
O	-2.10510200	0.30730400	1.18373400	O	-2.18706700	-0.13177400	1.12847000
C	2.73821900	-0.41937000	0.03638400	C	2.70606600	0.07275400	-0.01747800
C	4.23897200	-0.72047400	0.04675700	C	4.23663800	0.09366900	-0.00572700
Mo	-0.00619000	0.00517100	-1.00585400	Mo	-0.07164300	0.06749900	-1.05751800
C	-2.73674800	0.42046000	0.07725000	C	-2.82964500	-0.07668400	0.02388800
O	2.10676900	-0.30604500	-1.07020500	O	2.06348100	0.12762600	-1.12210000
O	-2.11945800	0.31573300	-1.04005500	O	-2.20520500	0.01376700	-1.09094900
C	-4.23905900	0.71373000	0.06633000	C	-4.36009500	-0.10268600	0.01211400
C	-4.94684000	-0.32619900	-0.83111700	C	-4.82894800	-1.24328500	-0.92023800
H	-4.81679900	-1.34237000	-0.43981500	H	-4.48141100	-2.21904600	-0.55986200
H	-6.02143100	-0.11110200	-0.86405900	H	-5.92470800	-1.26481700	-0.95099300
H	-4.55815400	-0.29847500	-1.85357300	H	-4.45802000	-1.10054000	-1.93977000
C	-4.82064200	0.66171400	1.48924600	C	-4.91790600	-0.32137600	1.42858400
H	-4.34839900	1.40099900	2.14421100	H	-4.60769600	0.47691700	2.11061400
H	-5.89525300	0.87579800	1.45107200	H	-6.01358000	-0.33221600	1.39061400
H	-4.68655900	-0.32692100	1.94156800	H	-4.58258200	-1.27570000	1.84897000
C	-4.43737500	2.12990800	-0.52832400	C	-4.85571300	1.25488300	-0.54251600
H	-4.04528800	2.18991100	-1.54864500	H	-4.48045700	1.42971200	-1.55586600
H	-5.50703100	2.36940300	-0.55543100	H	-5.95171700	1.25957000	-0.57484500
H	-3.93553500	2.89100500	0.08116600	H	-4.53242100	2.08646700	0.09509000
C	4.95023200	0.29107300	0.97281500	C	4.70969700	1.23710000	0.92100400
H	4.55700400	0.24064300	1.99258000	H	4.33816200	1.10067600	1.94119200
H	6.02308500	0.06739600	1.00460900	H	5.80554100	1.25438100	0.95184000
H	4.82912000	1.31768900	0.60679800	H	4.36602200	2.21237700	0.55591000
C	4.82694000	-0.63712800	-1.37210500	C	4.79519200	0.30350900	-1.42325500
H	5.90039400	-0.85704200	-1.33457900	H	5.89089500	0.31099300	-1.38524000
H	4.35414400	-1.35809900	-2.04667100	H	4.48252300	-0.49720300	-2.10132000
H	4.69941000	0.36288600	-1.80089700	H	4.46296600	1.25677600	-1.84841700
C	4.42474300	-2.15287500	0.60622700	C	4.72775500	-1.26265600	0.55588700
H	5.49269500	-2.39992300	0.63313300	H	5.82378100	-1.27133800	0.58668000
H	4.02650200	-2.23632500	1.62257700	H	4.35327100	-1.43009900	1.57076300
H	3.92145800	-2.89484400	-0.02519600	H	4.40007900	-2.09670500	-0.07611600
C	-2.16843000	-4.47702500	0.36379600	C	1.27666700	4.78667800	0.58128200
C	-0.67735100	-4.24229700	0.06225300	C	-0.15084700	4.28420700	0.30211900
C	-0.39768700	-2.73658600	0.04883400	C	-0.13644500	2.75761500	0.18161000
O	-0.28995900	-2.12420500	1.16624300	O	-0.11300500	2.05975100	1.25314800
O	-0.30773300	-2.11682400	-1.06391200	O	-0.12502400	2.20936400	-0.97151600
N	-0.29790700	-4.94422000	-1.16425800	N	-0.71076600	4.98087300	-0.85661700
H	-2.35598500	-5.55132500	0.45744800	H	1.25451000	5.86732100	0.75429200
H	-2.46446900	-3.98473500	1.29524100	H	1.70110600	4.29723500	1.46336100
H	-2.79403600	-4.08610100	-0.44807000	H	1.93265200	4.58642700	-0.27468200
H	-0.08749200	-4.66022100	0.88582300	H	-0.77641600	4.51930800	1.17051500
H	0.69766100	-4.82247600	-1.34576900	H	-1.67130200	4.67990000	-1.01743500
H	-0.77993800	-4.52815600	-1.96101600	H	-0.19243400	4.72272800	-1.69620300
C	2.19517000	4.46641700	0.30000500	C	1.49234600	-4.70328400	-0.71049400
C	0.68813300	4.24388500	0.07931600	C	0.06961400	-4.28403000	-0.30008400
C	0.40153700	2.73981500	0.06157500	C	0.00469200	-2.75860100	-0.17529800

O	0.30578800	2.12044200	1.17631000	O	-0.02212000	-2.06050900	-1.24671100
O	0.29727900	2.12742400	-1.05402700	O	-0.00012900	-2.21043000	0.97766300
N	0.24591900	4.96264900	-1.11642800	N	-0.34257300	-5.01360900	0.89898100
H	2.39459400	5.53823400	0.39768900	H	1.51689100	-5.78353700	-0.88532200
H	2.54003200	3.95978600	1.20677800	H	1.80522200	-4.19044600	-1.62502400
H	2.77167700	4.08313100	-0.55086600	H	2.21105400	-4.46481500	0.08314600
H	0.14685600	4.65416100	0.93898100	H	-0.61678600	-4.55519200	-1.11063400
H	-0.75923000	4.85038100	-1.24323100	H	-1.29783200	-4.76388300	1.15190200
H	0.68003000	4.55257400	-1.94325400	H	0.23766700	-4.73245800	1.68920900
Ala-bridge-3				Ala-bridge-4			
Mo	-0.01411800	-0.09330200	-1.09089600	Mo	0.00002700	-0.00002500	1.19195100
O	-2.13263000	-0.36807700	-1.14069200	Mo	-0.00001500	-0.00000500	-0.93408500
O	2.10671700	0.17661100	-1.13977500	C	-2.83768200	4.09567600	0.31012400
O	-0.28837700	2.02445800	-1.06127900	C	-3.36750200	2.66080200	0.13983400
C	-2.75480700	-0.50084400	-0.02921300	C	-2.18626800	1.68730500	0.12741900
C	-4.26064000	-0.77562900	-0.05003700	O	-1.69494200	1.30049500	1.24329300
Mo	-0.00469500	-0.16605100	1.03325000	O	-1.69379000	1.30251200	-0.98679300
C	2.73766400	0.23130700	-0.02849000	N	-4.23119800	2.58244100	-1.03912400
C	-0.37649200	2.61081500	0.07364700	H	-3.68203500	4.78628300	0.40100900
O	-2.12451000	-0.44233600	1.08221100	H	-2.21379900	4.18237600	1.20534800
O	2.11499800	0.10239300	1.08312800	H	-2.23877100	4.39314000	-0.55934200
O	-0.27953700	1.94292800	1.16027900	H	-3.97126500	2.40627100	1.01768100
C	4.24635800	0.49047200	-0.00666800	H	-4.61979900	1.64450800	-1.12969200
C	-0.61420300	4.12256100	0.10717100	H	-3.67873000	2.74060100	-1.88165400
C	4.46500600	1.92086400	0.54672700	C	2.83779300	-4.09568000	0.30986300
H	4.06358300	2.01943000	1.56060300	C	3.36753500	-2.66077700	0.13957600
H	5.53874200	2.14101800	0.57859400	C	2.18626700	-1.68734000	0.12729900
H	3.98394900	2.67205400	-0.09099600	O	1.69500500	-1.30055000	1.24320900
C	4.84253200	0.38477800	-1.42083200	O	1.69375400	-1.30251500	-0.98688000
H	5.92145400	0.57466300	-1.37612800	N	4.23111100	-2.58233000	-1.03946400
H	4.69041900	-0.61353400	-1.84586300	H	3.68219200	-4.78624800	0.40064600
H	4.39487200	1.11515600	-2.10218200	H	2.21399400	-4.18244600	1.20513800
C	4.92486600	-0.53367500	0.92929900	H	2.23881600	-4.39313700	-0.55956700
H	4.77917900	-1.55885700	0.56816300	H	3.97137300	-2.40625200	1.01737300
H	6.00302500	-0.33806400	0.96672600	H	4.61965700	-1.64437800	-1.13002500
H	4.52682600	-0.46760000	1.94622000	H	3.67855800	-2.74047700	-1.88193500
C	0.51454600	4.81675400	-0.68961400	C	-4.09571600	-2.83740900	0.31013800
H	0.34947400	5.90069700	-0.69055500	C	-2.66091000	-3.36743000	0.13984400
H	1.49545000	4.62394300	-0.23879600	C	-1.68729200	-2.18629500	0.12737200
H	0.53819000	4.47066900	-1.72753600	O	-1.30050900	-1.69498700	1.24325200
C	-1.97578100	4.40897200	-0.57087400	O	-1.30254000	-1.69377300	-0.98682400
H	-2.79817200	3.92171800	-0.03344900	N	-2.58263500	-4.23120000	-1.03906600
H	-2.16479700	5.48904100	-0.57152400	H	-4.78644200	-3.68165400	0.40107300
H	-1.98427500	4.05714500	-1.60727200	H	-4.18230400	-2.21347600	1.20533600
C	-0.63229300	4.64533700	1.55342900	H	-4.39311800	-2.23848800	-0.55934400
H	0.32017300	4.45712400	2.06036400	H	-2.40643500	-3.97118800	1.01771900
H	-0.80704300	5.72769600	1.54692900	H	-1.64474200	-4.61991700	-1.12963000
H	-1.42762300	4.17496900	2.14092900	H	-2.74073800	-3.67877900	-1.88163900
C	-4.94682900	0.20507700	-1.02530700	C	4.09572000	2.83754700	0.30996800
H	-4.81468600	1.24445500	-0.70153000	C	2.66087300	3.36746100	0.13974300
H	-4.54357700	0.10697400	-2.03749400	C	1.68731900	2.18626700	0.12734900
H	-6.02242600	-0.00457100	-1.05972100	O	1.30055600	1.69493900	1.24324000
C	-4.86500800	-0.62703000	1.35691800	O	1.30250700	1.69376700	-0.98684300
H	-5.94142900	-0.83103000	1.31434500	N	2.58249900	4.23119000	-1.03919300
H	-4.41193200	-1.32721300	2.06564100	H	4.78638300	3.68185300	0.40084300
H	-4.72655600	0.38764600	1.74670900	H	4.18241000	2.21364300	1.20517700
C	-4.45859300	-2.22812200	-0.55222500	H	4.39311600	2.23863100	-0.55951800
H	-3.97518900	-2.94975200	0.11703500	H	2.40640900	3.97122500	1.01761400

H	-5.52953100	-2.46138100	-0.58515400	H	1.64458400	4.61985000	-1.12972000
H	-4.04724900	-2.35944800	-1.55851500	H	2.74059200	3.67873600	-1.88174600
C	2.11822100	-4.61930300	-0.42529500				
C	0.61487600	-4.37907500	-0.19869400				
C	0.35314500	-2.87196000	-0.12764800				
O	0.25707200	-2.21378600	-1.22009600				
O	0.26841500	-2.29669900	1.00871000				
N	0.15887300	-5.13196600	0.97093100				
H	2.30012600	-5.69048300	-0.55828000				
H	2.47276800	-4.08865100	-1.31447200				
H	2.69983100	-4.27392200	0.43826600				
H	0.06799000	-4.74996700	-1.07253300				
H	-0.84447000	-5.00719100	1.10054200				
H	0.59833700	-4.75790600	1.81189600				
Ala-chel-1				Ala-chel-1a			
Mo	-0.03714400	-0.22134100	-0.94354200	Mo	0.06946500	-0.19989000	-1.01559200
O	1.82021000	-1.43652800	-1.23057900	O	-1.82680700	0.71591700	-1.76157000
O	-1.56129300	-1.66501000	-0.84973500	O	1.48995700	1.28174700	-1.43579000
C	-2.12944700	-1.90819000	0.27119200	C	2.00510700	1.95070700	-0.47335800
C	-3.14684000	-3.03874200	0.40742400	C	2.97441200	3.09923900	-0.74280600
Mo	-0.28480400	0.21577700	1.13848800	Mo	0.24083300	0.18704800	1.08408000
O	-1.80521300	-1.21959000	1.30378200	O	1.67030100	1.67484000	0.73424500
O	1.84269200	0.70003500	-1.70354500	O	-1.75975100	-1.43177500	-1.34359200
C	2.45174900	-0.42690400	-1.69866300	C	-2.41504700	-0.42019000	-1.77780600
C	3.85174100	-0.56246200	-2.29193700	C	-3.83711100	-0.58885200	-2.30691900
O	-1.45171800	1.23765300	-1.45274500	O	1.59811800	-1.63681000	-0.90270200
O	-1.70749400	1.68246000	0.69667500	O	1.75592400	-1.24556800	1.27018400
C	-2.00596800	1.92485600	-0.52671400	C	2.12104400	-1.90796300	0.23398400
C	-3.00504700	3.03221000	-0.85279600	C	3.13554500	-3.03906300	0.38576600
C	4.57357800	-1.78593900	-1.69841300	C	-4.43508200	0.76789300	-2.71482800
H	4.69767900	-1.68827600	-0.61390600	H	-4.48016200	1.45819000	-1.86569000
H	4.02450400	-2.71140300	-1.89628900	H	-3.84879500	1.24370700	-3.50791500
H	5.56993100	-1.87445600	-2.14718000	H	-5.45534000	0.61876900	-3.08752100
C	4.66358500	0.72020900	-2.02274100	C	-4.69725800	-1.23605300	-1.19682600
H	5.65728900	0.62553200	-2.47600900	H	-5.71786600	-1.38728700	-1.56757100
H	4.17307400	1.60070600	-2.44786100	H	-4.29154300	-2.20656500	-0.89536600
H	4.79689000	0.88901700	-0.94780800	H	-4.75137100	-0.59371400	-0.30984400
C	3.67200600	-0.75135500	-3.82088400	C	-3.78003500	-1.53178500	-3.53306500
H	3.16347000	0.10856100	-4.27052600	H	-3.36756400	-2.50903100	-3.26333700
H	4.65686400	-0.85128600	-4.29219900	H	-4.79278800	-1.68071500	-3.92568000
H	3.09378700	-1.65494000	-4.04550400	H	-3.16559400	-1.10540300	-4.33511200
C	-4.41331700	-2.49699200	1.10731600	C	4.21572600	2.93316500	0.16229900
H	-5.13871400	-3.30972200	1.22987200	H	4.90735500	3.76607700	-0.00967400
H	-4.17910400	-2.09213800	2.09651900	H	3.93863700	2.92797600	1.22076800
H	-4.88726600	-1.70619300	0.51373000	H	4.74693700	1.99999700	-0.06005300
C	-3.51182600	-3.61156000	-0.97305100	C	3.39988000	3.11594600	-2.22125700
H	-2.63379100	-4.01835400	-1.48471800	H	2.54053300	3.24679000	-2.88644800
H	-4.24095400	-4.42059600	-0.84891500	H	4.09343600	3.94782900	-2.38990900
H	-3.95791000	-2.84751000	-1.61915800	H	3.90860900	2.18703600	-2.50174900
C	-2.50336000	-4.14459700	1.28117600	C	2.24731500	4.42078000	-0.38937600
H	-1.59343600	-4.54073100	0.81496200	H	1.35440800	4.56200700	-1.00980500
H	-2.24618000	-3.76529800	2.27544300	H	1.94460900	4.43764500	0.66271000
H	-3.21134900	-4.97305400	1.40088300	H	2.92145300	5.26687700	-0.56729000
C	-4.35654700	2.67429000	-0.18887800	C	4.37922000	-2.50228900	1.12979600
H	-4.25262500	2.57848200	0.89649000	H	4.11391500	-2.10999400	2.11623800
H	-5.08660600	3.46515100	-0.39726200	H	5.10298000	-3.31453500	1.26462800
H	-4.75551600	1.73206400	-0.58301600	H	4.86852200	-1.70311200	0.56036400
C	-3.18949800	3.16924200	-2.37377600	C	3.54292500	-3.59435700	-0.98974900

H	-3.91061200	3.96842300	-2.58083500	H	4.26899400	-4.40415700	-0.85329300
H	-2.24758900	3.42221200	-2.87191100	H	2.68130700	-3.99591200	-1.53263200
H	-3.57020700	2.24318900	-2.81728100	H	4.00737600	-2.82217100	-1.61274800
C	-2.47352800	4.35968000	-0.26255000	C	2.47017400	-4.15660400	1.22751100
H	-3.18592800	5.16511100	-0.47585000	H	3.17694600	-4.98437300	1.35855000
H	-2.34770000	4.28908000	0.82232400	H	2.18272900	-3.78941200	2.21798700
H	-1.50884800	4.63383300	-0.70590100	H	1.57551700	-4.54993000	0.73041800
C	4.39750400	-0.13346800	2.61371100	C	-3.14773900	0.30451500	4.49883900
C	3.21242300	0.56943400	3.29712600	C	-3.41553800	0.43029500	2.98853400
C	1.95967300	0.42944200	2.43203900	C	-2.09131200	0.34306900	2.23081900
O	1.39777600	-0.71113300	2.28914400	O	-1.48111200	-0.77629500	2.12357600
O	1.44136200	1.43740800	1.84153600	O	-1.55300400	1.37732500	1.71063000
N	3.56578400	1.94743300	3.63680500	N	-4.19542500	1.63686600	2.71257400
H	5.26503900	-0.11110800	3.28037500	H	-4.10155700	0.28117300	5.03482900
H	4.15610300	-1.17462300	2.38121100	H	-2.59247500	-0.61049400	4.72546900
H	4.66603100	0.37654800	1.68071000	H	-2.56773800	1.16156400	4.86277700
H	2.99212300	0.03868900	4.23169500	H	-4.00781900	-0.43570400	2.66965400
H	2.78919600	2.40262000	4.11459900	H	-4.39371300	1.70852600	1.71545900
H	3.72180000	2.48486600	2.78415700	H	-3.64686100	2.46385800	2.94806800
Ala-chel-1b				Ala-chel-1c			
O	-1.41692800	-1.60157700	-1.10279200	Mo	-0.20994300	0.09490400	-0.66463700
O	-1.77240400	-1.40484600	1.07544300	O	1.03119500	1.80522000	-0.79653300
O	-1.33939200	1.33654000	-1.34383000	O	-1.94517500	1.31327600	-0.81127500
O	-1.69667600	1.57727700	0.83503000	C	-2.72073300	1.42218500	0.19952600
O	1.13430300	1.49817700	1.99992300	C	-4.00529000	2.24556600	0.08307400
O	2.71649400	1.85830400	3.54744300	Mo	-0.71520800	-0.40251600	1.36447400
N	1.24779100	-1.13372400	2.08673200	O	-2.43130300	0.81969700	1.29087800
C	-2.07454600	-1.92351500	-0.05682600	O	0.31375900	3.40941600	0.61510300
C	-3.19521400	-2.96191000	-0.16844200	C	1.00673200	3.02266100	-0.33878300
C	-1.93331100	1.92162600	-0.37462600	C	1.94430900	4.00120300	-1.09718900
C	-2.91524500	3.06728500	-0.64553100	O	-1.38231600	-1.53653200	-1.36513200
C	2.67466100	-0.18678100	-1.54857700	O	-1.89443600	-2.02124700	0.73258400
C	4.13206400	-0.19992800	-2.01521500	C	-1.98299600	-2.28173300	-0.51801800
C	1.99804600	1.09110600	2.88452300	C	-2.77714200	-3.49367200	-1.00850700
C	2.03320900	-0.44375300	3.11029400	O	1.49256900	-1.02300400	-1.28118600
H	1.55513100	-0.57683300	4.09800800	O	3.25416700	-0.67887700	0.08229100
C	3.46893100	-0.97092300	3.22529300	C	2.74341100	-1.13135300	-0.95676600
H	4.01036500	-0.83297700	2.28030400	C	3.60013700	-1.91198700	-1.99125000
H	4.01769600	-0.44737700	4.01437300	C	-4.66430800	2.42968400	1.46136600
H	3.45848500	-2.04202500	3.46020400	H	-3.99974900	2.95531400	2.15595400
C	-4.16588500	-2.53765600	-1.29349400	H	-5.57961000	3.02334500	1.35111600
H	-4.96072900	-3.28616700	-1.39824400	H	-4.93288300	1.46855100	1.91127000
H	-4.63689600	-1.57321500	-1.06775200	C	-3.67466600	3.62437300	-0.52922100
H	-3.64685600	-2.44953300	-2.25284200	H	-3.21224000	3.52029800	-1.51529800
C	-3.96126800	-3.08874800	1.15944000	H	-4.59690700	4.20736200	-0.63957800
H	-4.75773100	-3.83502100	1.05212800	H	-2.99027600	4.19039700	0.11331300
H	-3.30320700	-3.40598400	1.97475900	C	-4.97002300	1.48146600	-0.85756700
H	-4.42268900	-2.13777300	1.44774000	H	-5.22108400	0.49394700	-0.45229800
C	-2.54988400	-4.32193700	-0.53046800	H	-5.90179000	2.04918200	-0.96873100
H	-3.32955900	-5.08752100	-0.62594200	H	-4.52993500	1.34530700	-1.85092500
H	-2.00853100	-4.26261900	-1.48039600	C	-3.83865700	-3.01214500	-2.02410100
H	-1.84828200	-4.64804800	0.24683500	H	-3.37250000	-2.50502100	-2.87464300
C	-3.07002000	3.31982700	-2.15480200	H	-4.40254200	-3.87331600	-2.40211300
H	-3.45410400	2.43433800	-2.67262200	H	-4.54956000	-2.32007400	-1.55701600
H	-3.77630200	4.14301600	-2.31778400	C	-1.79337400	-4.46108900	-1.70984100
H	-2.11519700	3.59346100	-2.61618700	H	-1.30141100	-3.97757500	-2.55966300
C	-2.37365500	4.34218900	0.04370900	H	-1.01943700	-4.81206300	-1.01678700
H	-3.06533900	5.17653700	-0.12534000	H	-2.34000700	-5.33694100	-2.07958900

C	-3.92869500	-0.44168700	-2.66469000	H	4.66073800	-1.57792800	0.60523600
C	5.32811600	0.63633500	0.84584900	C	2.39968000	-4.21867600	0.95991000
H	5.17491900	-0.25191300	1.46769900	H	2.18428600	-4.34626900	-0.10535100
H	6.40569300	0.75735900	0.68282600	H	3.13906400	-4.97215100	1.25521600
H	4.96791300	1.50676000	1.40446700	H	1.47857600	-4.40805700	1.52385900
C	5.15511400	-0.73403300	-1.26740200	C	4.24163800	2.57492900	-0.42179600
H	4.67237100	-0.84309900	-2.24375700	H	4.99736300	3.31787600	-0.70255800
H	6.23492300	-0.62750200	-1.42645000	H	4.04275400	2.67433100	0.65006100
H	4.98613200	-1.65350700	-0.69416900	H	4.66046900	1.57853500	-0.60586300
C	4.86519000	1.77355900	-1.35990600	C	2.39888400	4.21893300	-0.95978800
H	4.48675300	2.66958700	-0.85339500	H	3.13808500	4.97256900	-1.25514100
H	5.94210100	1.90430000	-1.52016800	H	1.47764100	4.40822800	-1.52353700
H	4.37782600	1.69874500	-2.33702500	H	2.18367100	4.34635600	0.10552900
C	1.28689500	4.87376100	0.56190200	C	3.27185800	2.66700400	-2.75316400
H	2.17116800	4.60340300	-0.02811900	H	2.37943000	2.82828500	-3.36733300
H	1.21893000	5.96811500	0.58725200	H	4.02079800	3.41533600	-3.03718900
H	1.43247300	4.51349700	1.58511000	H	3.67280300	1.67594400	-2.98934100
C	-0.18118600	4.82437500	-1.48958200	C	-3.64201200	1.24285600	4.06003800
H	0.66711000	4.55640900	-2.12838200	C	-3.77004300	1.17565900	2.52844700
H	-1.09201800	4.43269500	-1.95447500	C	-2.40051900	0.90113800	1.90636000
H	-0.25532400	5.91820100	-1.46164500	O	-1.80153900	-0.20523800	2.13965300
C	-1.21986100	4.68644100	0.80586000	O	-1.82338100	1.75598900	1.15366700
H	-1.31714800	5.77873000	0.82291900	N	-4.44262300	2.36995900	2.01905600
H	-2.14856800	4.26860500	0.39960700	H	-4.63702700	1.34628000	4.50366900
H	-1.10601000	4.33422400	1.83578600	H	-3.17166500	0.33736100	4.45372800
C	2.06996000	-4.62406900	-1.01997900	H	-3.03732500	2.10680600	4.36242600
H	1.79988700	-4.28495500	-2.02467700	H	-4.39147000	0.30702400	2.27549600
H	3.02920400	-4.16666800	-0.74861900	H	-4.53892200	2.31438700	1.00606300
H	2.20959400	-5.71144900	-1.04779800	H	-3.86833700	3.19343100	2.19890800
C	-0.36558800	-4.92179200	-0.42312100	C	-3.64308900	-1.24226500	-4.05947400
H	-0.25119400	-6.01236300	-0.44605800	C	-3.77034100	-1.17570200	-2.52779800
H	-1.17026000	-4.68044100	0.28176200	C	-2.40050700	-0.90159600	-1.90621000
H	-0.66844500	-4.58648900	-1.42028000	O	-1.80143400	0.20471800	-2.13969600
C	1.37260000	-4.77734100	1.40010700	O	-1.82327800	-1.75647900	-1.15365800
H	0.60552000	-4.55128600	2.14769500	N	-4.44283400	-2.37013100	-2.01858700
H	1.50776500	-5.86511100	1.36629600	H	-4.63834100	-1.34536800	-4.50264800
H	2.31383200	-4.32776500	1.73510500	H	-3.17281800	-0.33666900	-4.45301800
C	-3.48905000	0.89514600	4.22126400	H	-3.03867100	-2.10617000	-4.36253000
C	-2.96575800	-0.49258900	3.81539900	H	-4.39152000	-0.30708800	-2.27416000
C	-1.53030300	-0.34876300	3.26003400	H	-4.53837200	-2.31512000	-1.00549200
O	-1.43552400	-0.24925000	1.97523400	H	-3.86889100	-3.19364500	-2.19934300
O	-0.56865600	-0.30561300	4.05510700				
N	-3.92607400	-1.13669900	2.90855300				
H	-4.46810100	0.79890700	4.70316000				
H	-2.80166600	1.38607400	4.91825500				
H	-3.60203300	1.53874200	3.33972200				
H	-2.89208500	-1.11327700	4.71566100				
H	-3.61129200	-2.08383100	2.69842000				
H	-3.90580400	-0.64522900	2.01428500				
C	-5.26077300	0.32439900	-2.61549700				
H	-5.13629800	1.36463200	-2.93586800				
H	-5.98995100	-0.15352100	-3.28240500				
H	-5.67941000	0.33475000	-1.60337800				
C	-3.38231100	-0.43090200	-4.10977600				
H	-2.44669800	-0.99355900	-4.18419600				
H	-4.11337100	-0.88550600	-4.79092100				
H	-3.19462900	0.59380500	-4.45568300				
C	-4.15710400	-1.90151000	-2.21257500				

H	-4.54056200	-1.94333600	-1.18504900
H	-4.89466000	-2.38586300	-2.86569000
H	-3.22802000	-2.47829800	-2.25428900
Ala-chel-2b			
O	-0.77327600	1.88129700	1.07941500
O	-1.61388000	1.24071900	-0.88726500
O	-1.61331900	-1.24061000	0.88757600
O	-0.77414800	-1.88168400	-1.07955300
O	1.80103200	0.82692300	2.14100900
O	3.80607100	0.40372300	3.09283700
O	1.80030000	-0.82729300	-2.14181600
O	3.80623500	-0.40418000	-3.09176500
N	1.23801100	-1.45899900	1.58423500
N	1.23711500	1.45859200	-1.58490700
C	-1.63889000	1.99679900	0.14526100
C	-2.71344600	3.07655800	0.27032800
C	-1.63916800	-1.99686200	-0.14483300
C	-2.71436900	-3.07606000	-0.26921400
C	2.79650100	0.04211500	2.51049300
C	2.55734600	-1.47505100	2.13156200
H	2.56806800	-2.05297300	3.06663000
C	3.63691400	-2.02429300	1.18699000
H	3.63606200	-1.48743300	0.23455400
H	4.61841600	-1.91733900	1.65839500
C	2.79605800	-0.04259500	-2.51038000
C	2.55659300	1.47467700	-2.13195200
H	2.56730900	2.05229700	-3.06721500
C	3.63581700	2.02448200	-1.18736800
H	3.63482500	1.48800200	-0.23471900
H	4.61744700	1.91749100	-1.65849100
H	3.45464300	3.08585600	-0.99329600
H	3.45595900	-3.08562000	0.99245600
C	-3.47353500	2.85402900	1.59928200
H	-4.23731500	3.63163100	1.71323000
H	-3.97766500	1.88045600	1.61173500
H	-2.79727700	2.90564400	2.45771100
C	-3.69306400	3.02453700	-0.91374300
H	-4.44797900	3.80982500	-0.79231100
H	-3.18110200	3.18814900	-1.86744800
H	-4.21013800	2.06057600	-0.96559700
C	-1.99701800	4.44915000	0.30603600
H	-2.74548200	5.24266600	0.41225300
H	-1.30314800	4.51293500	1.14970000
H	-1.43810500	4.63205300	-0.61922600
C	-3.68965900	-3.02743700	0.91855100
H	-4.20625700	-2.06350700	0.97528800
H	-4.44521300	-3.81215900	0.79744700
H	-3.17425900	-3.19415400	1.86988200
C	-1.99880900	-4.44883400	-0.31220100
H	-2.74805400	-5.24167100	-0.41798400
H	-1.30832800	-4.51021800	-1.15880300
H	-1.43628200	-4.63500500	0.61022300
C	-3.47925500	-2.84867200	-1.59465600
H	-2.80609800	-2.89736600	-2.45570100
H	-4.24353200	-3.62579000	-1.70857700
H	-3.98329700	-1.87500600	-1.60180700
Mo	0.16198300	0.10048600	-1.28727200
Mo	0.16293900	-0.10079300	1.28650800

Table 2SI. The Cartesian Coordinates of Mandelic acid (MA) substituted dimolybdenum *tetrakis*(μ -pivalate) **Mo₂** complexes.

MA-bridge-1				MA-bridge-2 <i>cis</i>			
Mo	-0.60881600	-0.02677100	-.09572100	Mo	-0.26237600	-0.81713900	-1.15894800
O	-1.70724000	-1.85179400	-1.06367500	O	-0.45164000	-2.91621900	-0.93955700
O	0.48755200	1.79531600	-1.22452900	O	-2.37261700	-0.60550000	-1.09141100
O	-2.42809700	1.06693600	-1.00886700	C	-2.93565200	-0.41579800	0.04384300
C	-1.94305700	-2.39954600	0.07046200	C	-4.45939800	-0.30408800	0.10407900
C	-2.73329800	-3.70942400	0.10802000	Mo	-0.12638600	-0.55755200	0.95110200
Mo	-0.44281100	-0.03013400	0.02336100	O	-2.23199100	-0.33730900	1.10913700
C	0.90119000	2.33656200	-0.14141700	O	-0.31538100	-2.65191600	1.26229900
C	-2.88511500	1.39281000	0.14351000	C	-0.43263300	-3.41345100	0.24199700
O	-1.52739900	-1.85906400	1.15292600	C	-0.53103000	-4.93034300	0.40792000
O	0.66141800	1.79034300	0.99257300	C	-4.91395500	0.80494000	-0.87252500
O	-2.25833000	1.06073700	1.20768000	H	-4.60390200	0.58181100	-1.89794600
C	1.68530000	3.65019800	-0.17657600	H	-6.00714200	0.88464200	-0.85157900
C	-4.18717700	2.19199800	0.22604400	H	-4.49737300	1.77896000	-0.58986800
C	0.88213300	4.71238500	0.61157400	C	-5.05373900	-1.66217400	-0.34356300
H	0.72975600	4.40357900	1.65050000	H	-4.73832800	-2.47361300	0.32307400
H	1.43115200	5.66147600	0.61056400	H	-6.14839400	-1.60761700	-0.31713100
H	-0.09944000	4.88828200	0.15533200	H	-4.74564500	-1.91284700	-1.36349600
C	1.89897900	4.12516600	-1.62363200	C	-1.79082800	-5.43044900	-0.33591100
H	2.45972500	5.06727400	-1.61793800	H	-2.70208400	-4.99035400	0.08650100
H	2.46846500	3.39359400	-2.20661500	H	-1.74881500	-5.18092900	-1.40040100
H	0.94618800	4.29856600	-2.13468500	H	-1.86429600	-6.51990900	-0.23860000
C	3.05226600	3.42284000	0.51005300	C	0.73138600	-5.56041800	-0.22973500
H	3.64125900	2.66334500	-0.01746800	H	1.64394900	-5.21567100	0.27099200
H	3.62393500	4.35845600	0.50631200	H	0.68371800	-6.65142700	-0.13315200
H	2.92563000	3.10051100	1.54817600	H	0.80483100	-5.31131600	-1.29307900
C	-3.97184900	3.54040300	-0.50196300	C	-0.61217800	-5.31544700	1.89480700
H	-4.89627800	4.12866600	-0.46367700	H	-0.68016700	-6.40589500	1.98433500
H	-3.17733400	4.12684700	-0.02516000	H	0.27316500	-4.98211500	2.44587600
H	-3.70467400	3.38603800	-1.55205400	H	-1.49471000	-4.87875200	2.37468000
C	-5.30138800	1.39119100	-0.48738300	C	-4.92963000	0.02631400	1.53059000
H	-5.46885100	0.42309100	-0.00029400	H	-4.52131800	0.98195000	1.87652900
H	-6.24006400	1.95641500	-0.44888000	H	-6.02342700	0.09788100	1.54475800
H	-5.05077000	1.21035100	-1.53720100	H	-4.62896600	-0.74892800	2.24284500
C	-4.58236200	2.44733100	1.69047300	C	5.34968200	0.30704300	1.36828000
H	-3.81413700	3.02029200	2.22014000	C	5.94738200	1.50023500	1.78876900
H	-5.51661100	3.02025700	1.72013900	C	5.95770000	2.61379400	0.94272700
H	-4.74036700	1.50941500	2.23343000	C	5.36991200	2.52747600	-0.32514900
C	-4.12823900	-3.44991200	-0.50916500	C	4.77083800	1.33564300	-0.74204200
H	-4.68427100	-2.70019800	0.06648100	C	4.75361800	0.21782300	0.10402100
H	-4.04560400	-3.09991900	-1.54286600	C	4.08088500	-1.07890500	-0.33523300
H	-4.70949200	-4.37957600	-0.50485200	C	2.55686100	-0.95377000	-0.23935600
C	-2.88742100	-4.21798100	1.55125800	O	1.88173300	-1.03506500	-1.32066300
H	-3.45581300	-5.15551600	1.54780200	O	2.01641800	-0.77159600	0.89410600
H	-1.91433800	-4.41122000	2.01512000	O	4.46041500	-1.45552100	-1.65274700
H	-3.42383100	-3.49655100	2.17646000	H	5.34997900	-0.55923700	2.02607000
C	-1.97945400	-4.75897400	-0.74198300	H	6.40937500	1.55615100	2.77102900
H	-0.98086400	-4.95739700	-0.33445700	H	6.42394700	3.54087100	1.26598700
H	-2.53897400	-5.70186400	-0.74086000	H	5.37876000	3.38757300	-0.98978000
H	-1.86896200	-4.42478900	-1.77819600	H	4.32366500	1.27213200	-1.73072700
C	4.92298700	-1.70221100	1.30688800	H	4.37742000	-1.87610700	0.35821600
C	6.04898600	-0.95723700	1.67504400	H	3.65139600	-1.44778400	-2.19825500
C	6.59038500	-0.02208100	0.78755900	C	-0.82653600	4.93264400	1.14638400
C	6.00047000	0.16480200	-0.46861100	C	-1.92390500	5.62863800	1.66490500
C	4.87423400	-0.57742900	-0.83303900	C	-3.10811900	5.71961100	0.92639400

C	4.32650600	-1.51567800	0.05375900	C	-3.18884300	5.11195900	-0.33230300
C	3.09537700	-2.32752700	-0.33840900	C	-2.09288000	4.41421300	-0.84735700
C	1.82062500	-1.48751600	-0.21148200	C	-0.90458700	4.31786400	-0.10966000
O	1.22036000	-1.15702900	-1.28920300	C	0.29033300	3.54442200	-0.66006000
O	1.40022500	-1.15434800	0.93963000	C	0.10775600	2.03889200	-0.44743400
O	3.20315200	-2.85239200	-1.65721000	O	-0.03190300	1.30366100	-1.48304400
H	4.51107700	-2.43615000	1.99591700	O	0.10326400	1.56857800	0.73174700
H	6.50595100	-1.11514500	2.64851000	O	0.51271100	3.82016000	-2.03779900
H	7.46839700	0.55347400	1.06891100	H	0.09534600	4.87176900	1.72030000
H	6.41874500	0.88704000	-1.16505200	H	-1.84960300	6.10519100	2.63895400
H	4.42672000	-0.43540100	-1.81322300	H	-3.95998100	6.26439400	1.32498600
H	2.99485500	-3.16653900	0.36022000	H	-4.10436700	5.18292600	-0.91404700
H	2.53357700	-2.39736100	-2.20193300	H	-2.15657800	3.95294300	-1.82910900
				H	1.18459600	3.83724000	-0.09595300
				H	0.36025700	2.98887900	-2.52535400
MA-bridge-2trans				MA-bridge-3			
Mo	-0.00374100	0.01725800	-1.30896000	Mo	0.09792700	-0.65187000	-1.32319800
O	1.06508100	1.85545000	-1.33906100	O	-0.87541700	-2.52861400	-1.21659700
O	-1.07482200	-1.81928200	-1.37231500	Mo	0.03534300	-0.43993400	.79675600
C	1.38521900	2.39428800	-0.22135900	C	-1.20140500	-2.98480000	-0.06573200
C	2.12365000	3.73388100	-0.22816500	O	-0.94633500	-2.30929100	0.99255100
Mo	0.00233500	-0.00720800	0.82035300	C	-1.88709900	-4.34420000	0.07037900
C	-1.38512100	-2.38504300	-0.26731800	C	-3.20768300	-4.15266900	0.85180100
O	1.07301300	1.82954000	0.88339400	H	-3.89274700	-3.48413500	0.31723600
O	-1.06505200	-1.84599100	0.85011700	H	-3.70460400	-5.12248800	0.97150300
C	-2.11740300	-3.72798500	-0.26058300	H	-3.02371000	-3.73420700	1.84598500
C	-5.18548400	1.74754000	1.76117800	C	-2.17795400	-4.95317800	-1.31162900
C	-6.21640600	1.03305100	2.38149600	H	-1.25820300	-5.10671400	-1.88547100
C	-6.88215900	0.01908700	1.68589400	H	-2.66722000	-5.92576100	-1.18382600
C	-6.51239900	-0.27638500	0.36797500	H	-2.84288600	-4.31238900	-1.90062900
C	-5.47994400	0.43529800	-0.24853400	C	-0.94399900	-5.27650600	0.86901900
C	-4.80746400	1.45104600	0.44591100	H	-0.73208700	-4.86941100	1.86270800
C	-3.67090600	2.22217400	-0.21628800	H	-1.41898300	-6.25685400	0.99206700
C	-2.37229900	1.40996100	-0.21337400	H	0.00743700	-5.42428400	0.34441300
O	-1.85376500	1.10633300	-1.34052300	C	1.36448900	5.01319100	1.07926100
O	-1.84274900	1.07910400	0.89258200	C	0.52439800	6.05397700	1.49137800
O	-4.00376400	2.60974100	-1.54379800	C	-0.52592600	6.47284700	0.66912500
H	-4.67627100	2.54156500	2.30272400	C	-0.73218700	5.84728900	-0.56689000
H	-6.50286900	1.27521000	3.40164200	C	0.10590400	4.80690900	-0.97542000
H	-7.68678200	-0.53368100	2.16377600	C	1.15917700	4.38108100	-0.15286600
H	-7.02916000	-1.06016200	-0.17998400	C	2.07031200	3.23891900	-0.59082900
H	-5.20286300	0.20959400	-1.27481200	C	1.35472800	1.89218400	-0.45958200
H	-3.47270000	3.12440800	0.37758000	O	1.10849000	1.24063200	-1.52996600
H	-3.33049000	2.22308600	-2.13457800	O	1.03025900	1.46468100	0.69177200
C	5.20137300	-1.85157200	1.70315000	O	2.53904300	3.41790400	-1.92266900
C	6.22744000	-1.16665300	2.36395400	H	2.18530600	4.69514900	1.71811800
C	6.86783900	-0.09272300	1.73834200	H	0.69669600	6.53990800	2.44819800
C	6.47801500	0.29261800	0.44957500	H	-1.17684400	7.28386100	0.98508300
C	5.45079400	-0.38984100	-0.20696200	H	-1.54434000	6.17103800	-1.21278000
C	4.80350800	-1.46588300	0.41741000	H	-0.05268900	4.33172300	-1.94010200
C	3.67344400	-2.20529400	-0.28894400	H	2.93534000	3.20500700	0.08307900
C	2.37303600	-1.39660700	-0.25908500	H	2.18294700	2.68238600	-2.45557200
O	1.84551400	-1.06953800	-1.37558700	C	-5.16284200	1.53280000	1.43777300
O	1.84983700	-1.09306700	0.85753600	C	-6.19252300	0.96369100	2.19560600
O	4.01997100	-2.52837500	-1.63059200	C	-6.84761300	-0.18293800	1.73630800
H	4.71128500	-2.69173600	2.19000600	C	-6.46877200	-0.75742900	0.51655800
H	6.52943500	-1.47783300	3.36061900	C	-5.43780100	-0.19030200	-0.23669700
H	7.66835300	0.43760200	2.24750700	C	-4.77595200	0.95796400	0.22135400
H	6.97492000	1.12384200	-0.04411500	C	-3.64541400	1.57400300	-0.59116600

H	5.15742300	-0.09309800	-1.21047000	C	-2.34502700	0.77567500	-0.45614500
H	3.47130100	-3.13463700	0.26069500	O	-1.78339500	0.36099300	-1.52607600
H	3.33231600	-2.14412900	-2.20627200	O	-1.84512600	0.58065100	0.69532300
C	-3.33609200	-3.63190800	0.68429100	O	-4.00795000	1.69594000	-1.96134100
H	-4.04655900	-2.87064600	0.34099300	H	-4.66115800	2.42962900	1.79416700
H	-3.85734200	-4.59612200	0.70764100	H	-6.48600800	1.42099800	3.13692500
H	-3.02939300	-3.38080200	1.70404900	H	-7.65109500	-0.62379600	2.32058500
C	-2.57919200	-4.10767300	-1.67789000	H	-6.97724200	-1.64631300	0.15200800
H	-1.73282300	-4.19773800	-2.36618800	H	-5.15241200	-0.63285700	-1.18730700
H	-3.09771300	-5.07300900	-1.64468100	H	-3.42955400	2.57177200	-0.18271700
H	-3.27165000	-3.36363300	-2.08670200	H	-3.27667300	1.32321600	-2.48843700
C	-1.13169600	-4.79691600	0.27313100	C	5.35571100	-1.57611500	1.87031300
H	-0.79526500	-4.55544000	1.28662200	C	6.31544800	-0.67351300	2.34191400
H	-1.63049500	-5.77295700	0.29917800	C	6.86289600	0.28068500	1.47872500
H	-0.25057600	-4.88399300	-0.37368100	C	6.44725300	0.32745400	0.14232200
C	3.36336000	3.61704100	-1.14346900	C	5.48671400	-0.57268600	-0.32624500
H	3.07840200	3.35330900	-2.16645500	C	4.93265500	-1.52942600	0.53635600
H	3.89129700	4.57756800	-1.16850500	C	3.86997700	-2.50317900	0.03475900
H	4.06071500	2.85661300	-0.77233400	C	2.50841200	-1.81082700	-0.05793200
C	2.55581400	4.12898500	1.19420800	O	1.99852400	-1.64502300	-1.21723500
H	3.07983100	5.09134300	1.16047400	O	1.93148700	-1.41945300	1.00397300
H	1.69458500	4.23212200	1.86205000	O	4.21844300	-3.07255800	-1.22112600
H	3.23472900	3.38679000	1.62794900	H	4.93783400	-2.32157200	2.54315900
C	1.15819600	4.80209400	-0.79833400	H	6.63891600	-0.72238600	3.37840900
H	1.66420800	5.77439100	-0.82524000	H	7.61168500	0.97981800	1.84176600
H	0.84331800	4.54979700	-1.81602400	H	6.87193700	1.06384700	-0.53511900
H	0.26301700	4.90345000	-0.17324800	H	5.17422800	-0.53797300	-1.36659200
				H	3.76554100	-3.31262300	0.76760500
				H	3.56381600	-2.76109200	-1.87367500
MA-bridge-4				MA-chel-1a			
Mo	0.08628200	-0.03724800	-1.45619500	Mo	1.43022000	-0.05135100	0.92936600
Mo	-0.0217220	-0.05694600	0.6740490	O	2.15612700	-1.98365000	0.46044000
C	-3.56247400	4.17085000	1.48699900	O	3.16561800	0.82150800	0.15494400
C	-4.80731400	4.08534900	2.12083500	C	3.19884500	1.17433500	-1.07719000
C	-5.88155200	3.46818800	1.47283900	C	4.46800100	1.81649100	-1.63378100
C	-5.70618600	2.93831100	0.18829700	Mo	0.45627600	0.09668700	-0.96593300
C	-4.46197400	3.02158700	-0.44164400	O	2.17276600	0.97888200	-1.81391600
C	-3.38057200	3.63629900	0.20607600	O	1.16614000	-1.82821000	-1.52309200
C	-2.01756000	3.71264700	-0.46967600	C	1.87660800	-2.48457600	-0.68649600
C	-1.29983300	2.36120400	-0.43000000	C	2.38834800	-3.88519600	-1.02619400
O	-0.94348900	1.83589600	-1.53906300	O	0.66031700	1.88120200	1.53295900
O	-1.05989800	1.81142700	0.69002500	O	-0.26855400	2.05832100	-0.47975000
O	-2.13200800	4.17165300	-1.81112000	C	-0.02162200	2.55609100	0.66148200
H	-2.73106400	4.65791000	1.99156400	C	-0.47263100	3.97590000	1.00670300
H	-4.93713400	4.50675600	3.11425200	O	-0.01091000	-0.99970200	2.34621400
H	-6.85025300	3.40418400	1.96152000	O	-0.66120200	0.71889700	3.63986300
H	-6.53868700	2.46135100	-0.32260100	C	-0.63430900	-0.56590300	3.32951900
H	-4.33205600	2.61763600	-1.44220900	C	-1.42462400	-1.46585600	4.27026100
H	-1.38644800	4.41014400	0.09872700	H	-0.16624300	1.25454400	2.96305400
H	-1.66101100	3.53364700	-2.37885700	C	4.79369400	3.07030700	-0.78817500
C	-4.37606200	-3.49870600	1.39067000	H	4.94330300	2.81144000	0.26458000
C	-4.35543000	-4.70001400	2.10850200	H	5.71305000	3.53477500	-1.16337700
C	-3.68342700	-5.81202600	1.59232300	H	3.98885400	3.81221900	-0.85086000
C	-3.03315000	-5.71827500	0.35538200	C	4.27959700	2.21202200	-3.10802500
C	-3.05213900	-4.51749500	-0.35827800	H	5.20299500	2.67008300	-3.48105600
C	-3.72215400	-3.39837400	0.15707100	H	4.05425100	1.34144000	-3.73264400
C	-3.73071800	-2.08317600	-0.60993900	H	3.46715600	2.93646400	-3.22853700
C	-2.37744900	-1.37283700	-0.51966000	C	5.62193300	0.79290000	-1.50489800
O	-1.78476300	-1.06552300	-1.60927400	H	5.41594000	-0.11415100	-2.08538800
O	-1.89483400	-1.08739900	0.62046000	H	6.54825000	1.23741900	-1.88724700

O	-4.09206500	-2.28778700	-1.97064100	H	5.78299000	0.50625900	-0.46088500
H	-4.90521800	-2.63750300	1.79227300	C	3.91288400	-3.93340500	-0.77596600
H	-4.86917500	-4.76670000	3.06397000	H	4.44395200	-3.22376100	-1.42166800
H	-3.66929800	-6.74706200	2.14622400	H	4.15253700	-3.69748200	0.26525400
H	-2.51211900	-6.58041800	-0.05300700	H	4.28840400	-4.93922900	-0.99773100
H	-2.55350100	-4.45092100	-1.32169300	C	1.67741400	-4.88996100	-0.08672000
H	-4.45913000	-1.40957900	-0.13619500	H	2.03054800	-5.90509400	-0.30342900
H	-3.43407600	-1.82286800	-2.52022700	H	1.88956600	-4.66875000	0.96421600
C	3.89893400	3.83608200	1.59847700	H	0.59090800	-4.87050300	-0.23273000
C	3.67933200	5.14096200	2.05424700	C	2.08612600	-4.23839500	-2.49233000
C	3.09816100	6.08956900	1.20739900	H	1.01057700	-4.22686600	-2.69560500
C	2.73848600	5.72844300	-0.09705300	H	2.56915500	-3.53691700	-3.18124500
C	2.95584500	4.42467400	-0.54937100	H	2.46476700	-5.24412000	-2.70918600
C	3.53626300	3.46861500	0.29706200	C	-1.30703600	-2.93167300	3.82199500
C	3.76637300	2.03959600	-0.18866000	H	-1.70484000	-3.07680300	2.81263800
C	2.44022500	1.28116600	-0.24746700	H	-0.26678700	-3.27284500	3.83120300
O	1.96446600	0.99359100	-1.39762900	H	-1.88043800	-3.56335300	4.50903600
O	1.84451200	0.97324700	0.83226800	C	-2.90733000	-1.01774300	4.24289600
O	4.41475500	1.99609300	-1.45459600	H	-3.48515000	-1.66356600	4.91317000
H	4.35766800	3.10271500	2.25783100	H	-3.02086000	0.01709300	4.57898900
H	3.96886000	5.41532700	3.06528100	H	-3.33343400	-1.10695100	3.23722700
H	2.93019300	7.10455200	1.55789300	C	0.78948300	4.87593200	0.97439400
H	2.28987300	6.46225100	-0.76169700	H	1.25203800	4.87719700	-0.01928400
H	2.68136000	4.15373400	-1.56581300	H	0.50596700	5.90636200	1.21856400
H	4.40328200	1.52185100	0.53723600	H	1.53425300	4.54214500	1.70428900
H	3.75363700	1.71287700	-2.11302900	C	-1.49904600	4.48051300	-0.02276500
C	3.76839900	-4.03732500	1.58667300	H	-2.39760600	3.85374700	-0.03125400
C	5.03581500	-3.86125200	2.15331200	H	-1.79919000	5.50258600	0.23517000
C	6.05525800	-3.25448900	1.41332200	H	-1.08256800	4.49040200	-1.03445000
C	5.80234400	-2.82585300	0.10435400	C	-1.08894700	4.00841200	2.42194800
C	4.53569500	-3.00002500	-0.45891500	H	-1.96489000	3.35300900	2.49383300
C	3.50905900	-3.60532700	0.28033300	H	-0.36425700	3.71035500	3.18611200
C	2.11941700	-3.78470800	-0.32522400	H	-1.41497700	5.02944300	2.65038200
C	1.36589500	-2.45391000	-0.33632200	C	-0.85526100	-1.29822100	5.70091700
O	1.12467000	-1.91002800	-1.46696600	H	-0.94944100	-0.26675300	6.05286000
O	1.00922400	-1.92472000	0.76282800	H	-1.41432400	-1.94782700	6.38329300
O	2.17325700	-4.33042300	-1.63782600	H	0.20091000	-1.58793200	5.74632500
H	2.98024800	-4.51629500	2.16317900	C	-5.48387600	-0.87013100	-3.00951100
H	5.22620500	-4.20463900	3.16678500	C	-6.50852600	-0.02280400	-3.44570700
H	7.04145400	-3.12041700	1.84999100	C	-6.87723400	1.08452900	-2.67514000
H	6.59166000	-2.35725100	-0.47779300	C	-6.21669900	1.33676400	-1.46642700
H	4.34821000	-2.67330100	-1.47848100	C	-5.19130100	0.49033100	-1.03513100
H	1.54699600	-4.47031300	0.31083800	C	-4.81222300	-0.61856200	-1.80596000
H	1.87235100	-3.63823000	-2.25534600	C	-3.67376300	-1.52435600	-1.35889100
				C	-2.29591100	-0.90781200	-1.71287600
				O	-1.52674300	-0.72148400	-0.68528100
				O	-2.01163100	-0.65612500	-2.89065700
				O	-3.74966800	-1.81373500	0.03465600
				H	-5.20509100	-1.73333600	-3.60976800
				H	-7.02085300	-0.23231400	-4.38139800
				H	-7.67528300	1.74239000	-3.00966500
				H	-6.50067300	2.19287200	-0.85939700
				H	-4.68652600	0.68524200	-0.09281200
				H	-3.73795400	-2.46539100	-1.92216200
				H	-2.88544400	-1.53447100	0.39881300
MA-chel-1b				MA-chel-1c			
Mo	1.37095800	0.97618000	0.15687100	Mo	-0.98685300	0.18398400	-1.04737500
O	0.25730100	2.49132600	1.32052000	O	-0.25859100	-1.65852200	-1.80258200
O	2.34860300	-0.03986700	1.70318900	O	-2.95159700	-0.53849500	-1.08657100
C	1.95806800	-1.21450100	2.02971300	C	-3.43351600	-1.10947400	-0.04450600

C	2.56266300	-1.94593800	3.22515800	C	-4.87713900	-1.60797600	-0.05883000
Mo	0.08363500	-0.70425200	-.17606400	Mo	-0.73851100	-0.48764600	0.96719800
O	1.01642300	-1.76924100	1.35921000	O	-2.70196800	-1.23644600	0.99635700
O	0.48318700	2.77991900	-0.83654800	O	-0.02282900	-2.37633400	0.28835100
C	0.07313800	3.22936300	0.28802100	C	0.07729400	-2.57440700	-0.97060200
C	-0.60684600	4.58879700	0.42242200	C	0.59185500	-3.90905400	-1.51306100
O	2.73955600	0.24529300	-1.25794100	O	-1.65496600	2.13091600	-0.35888600
O	1.40851200	-1.48749000	-1.59086500	O	-1.45090400	1.38575900	1.72419000
C	2.47626500	-0.83985700	-1.88272200	C	-1.75685400	2.31776100	0.91666800
C	3.38114700	-1.34310700	-3.00450500	C	-2.22819600	3.66266300	1.47201200
C	-2.03190900	4.36002800	0.98041500	O	0.90467100	1.18064700	-1.73372500
H	-2.63489800	3.75188000	0.29575700	O	0.29671300	3.34452300	-1.82629200
H	-2.00170500	3.85902700	1.95295600	C	1.13224600	2.35150500	-2.08250600
H	-2.53337400	5.32695900	1.10514500	C	2.38544100	2.76172400	-2.84463000
C	-0.68171200	5.30036800	-0.93867600	H	-0.48612900	3.02287400	-1.30222500
H	-1.17791500	6.27017700	-0.81537000	C	-5.80580200	-0.37501000	-0.18201300
H	0.31593600	5.47859900	-1.35405700	H	-5.60281000	0.18461800	-1.10073300
H	-1.25277000	4.71511500	-1.66699500	H	-6.85067500	-0.70625600	-0.20391300
C	0.20967400	5.44070600	1.42283900	H	-5.68262500	0.30230300	0.67133100
H	1.23051500	5.61100600	1.06012700	C	-5.19951500	-2.37748900	1.23381900
H	-0.27226900	6.41741400	1.54791900	H	-6.23956100	-2.72220000	1.20059900
H	0.26722600	4.95634100	2.40247600	H	-4.55376800	-3.25462000	1.35017100
C	3.63502600	-2.85473700	-2.81447200	H	-5.07700200	-1.74596000	2.11961600
H	2.69804200	-3.41958700	-2.81713700	C	-5.07394500	-2.52894100	-1.28475800
H	4.26373800	-3.22480000	-3.63261500	H	-4.41905700	-3.40673500	-1.23109800
H	4.15523200	-3.05414200	-1.87007300	H	-6.11153000	-2.88149300	-1.31366100
C	2.63732900	-1.10544000	-4.34317900	H	-4.86385600	-1.99860500	-2.21857900
H	2.43320900	-0.03990100	-4.50132300	C	-0.53882000	-4.55655300	-2.34823800
H	3.26000100	-1.45863400	-5.17350600	H	-1.42294100	-4.75812400	-1.73160700
H	1.68699900	-1.64868700	-4.37089400	H	-0.83733800	-3.91055400	-3.17987700
C	4.71723000	-0.57990300	-3.00754700	H	-0.18879100	-5.51028400	-2.76056800
H	5.34915200	-0.95837400	-3.81926000	C	1.81176200	-3.63174700	-2.42212700
H	4.56780200	0.49318600	-3.16243500	H	2.18588200	-4.57790700	-2.83064800
H	5.25778600	-0.71570100	-2.06419300	H	1.54349700	-2.97756700	-3.25735700
C	3.00232500	-3.35815800	2.77594800	H	2.62616300	-3.15894300	-1.86058300
H	3.41711900	-3.90096500	3.63323300	C	0.99664300	-4.84920000	-0.36524000
H	2.15750600	-3.93088100	2.38146100	H	1.79924800	-4.41821800	0.24237400
H	3.77631000	-3.30557400	2.00107100	H	0.15034600	-5.06526200	0.29504900
C	1.46443600	-2.06596800	4.31090900	H	1.35575500	-5.79759500	-0.78195800
H	1.86945500	-2.59459100	5.18175900	C	3.27153200	1.53325600	-3.10584300
H	1.12265300	-1.07823200	4.64206700	H	3.59335300	1.06276200	-2.17162600
H	0.59965300	-2.62568800	3.94028700	H	2.74800100	0.78120400	-3.70505700
C	3.76870800	-1.17141300	3.78374000	H	4.16507000	1.84701800	-3.65658300
H	3.48209000	-0.17140400	4.12453700	C	3.15410000	3.80622000	-1.99802400
H	4.18583200	-1.71732900	4.63779900	H	4.05995800	4.10396100	-2.53751100
H	4.55767100	-1.06148500	3.03176300	H	2.55028600	4.70082400	-1.81921400
C	-5.47308000	-0.97484700	0.88928200	H	3.45654900	3.38992800	-1.03052100
C	-6.25986100	-2.08524500	1.21529300	C	-3.34884800	3.40113100	2.50473300
C	-6.36241000	-3.15701100	0.32308400	H	-2.99696700	2.76101200	3.31888800
C	-5.67598600	-3.11279600	-0.89670700	H	-3.67959300	4.35477700	2.93195200
C	-4.88849600	-2.00464800	-1.21955800	H	-4.21601400	2.92014700	2.03674800
C	-4.77996900	-0.92868600	-0.32655400	C	-1.02171000	4.33070400	2.17816500
C	-3.90924500	0.27531700	-0.66844600	H	-0.20094100	4.51994300	1.47637200
C	-2.42957200	-0.04830800	-0.45766000	H	-1.33479500	5.29289300	2.59987600
O	-1.64944300	-0.05575300	-1.46847900	H	-0.64382200	3.70415700	2.99235700
O	-1.96803000	-0.30719700	0.69594100	C	-2.75530300	4.57854300	0.35386700
O	-4.12019200	0.72341400	-2.00231400	H	-1.97566700	4.83178500	-0.37187800
H	-5.40251500	-0.13981400	1.58253400	H	-3.58769600	4.11527300	-0.18670200
H	-6.79673200	-2.10750700	2.16007800	H	-3.11558400	5.51481400	0.79525300
H	-6.97677700	-4.01822400	0.57235000	C	1.94835100	3.39769500	-4.18819900

H	-5.75497800	-3.94058100	-1.59675400	H	1.33768900	4.29152300	-4.03073500
H	-4.36550400	-1.96999500	-2.17164200	H	2.84245700	3.68557300	-4.75204800
H	-4.15350700	1.09171700	0.02314700	H	1.37727400	2.68804000	-4.79800800
H	-3.27275500	0.62236400	-2.47656200	C	4.83547900	0.63265300	1.12042500
				C	5.76578400	0.25575800	0.14439500
				C	6.08715700	-1.09301900	-0.03250700
				C	5.47383400	-2.06205100	0.77219100
				C	4.54521000	-1.68218600	1.74408800
				C	4.21408100	-0.33018500	1.92514200
				C	3.20812100	0.08431000	2.98861600
				C	1.77684100	-0.40874600	2.66150600
				O	1.23487900	-1.19734000	3.45998300
				O	1.26203900	0.06012400	1.58177600
				O	3.58027700	-0.40844600	4.27386100
				H	4.59411700	1.68436900	1.25850500
				H	6.24185900	1.01583600	-0.46991200
				H	6.81122300	-1.38853700	-0.78750700
				H	5.72021000	-3.11293500	0.64212900
				H	4.07922400	-2.43885300	2.37067100
				H	3.17062000	1.18089400	3.02530200
				H	2.82535800	-0.97047900	4.55141100
MA-chel-1d				MA-chel-2			
Mo	-1.19967900	0.54387000	-0.93374100	Mo	0.99998900	0.78798200	-0.32060000
O	-0.09842600	2.25076600	-1.04247400	O	0.51627700	2.28466100	-1.69698100
O	-2.22332800	1.41384900	0.70723500	C	-0.70354600	2.64861900	-1.83122100
C	-1.97552700	1.01704200	1.90115500	C	-1.11410700	3.66642500	-2.89161100
C	-2.67561000	1.69849800	3.07174100	Mo	-1.05067800	0.62329700	0.27341100
Mo	-0.18332800	-0.83985200	0.47384100	O	-1.59875500	2.12217700	-1.07968600
O	-1.15582500	0.05906000	2.10304100	O	1.34544900	2.23562200	1.13382500
O	2.04148100	1.88830500	-1.60395200	O	-0.76823400	2.06737900	1.76091300
C	1.13635400	2.64927500	-1.24292400	C	0.39182500	2.58520700	1.91846300
C	1.35215900	4.16108700	-1.03380700	C	0.66894500	3.58592900	3.03661700
O	-2.89211400	-0.73986200	-0.96721500	C	-2.03204700	2.94593900	-3.90974100
O	-1.85983900	-2.14196100	0.40963100	H	-2.92744200	2.54628800	-3.42322400
C	-2.88558000	-1.82237200	-0.27561600	H	-2.34746100	3.65676200	-4.68231000
C	-4.12100100	-2.71815700	-0.28914400	H	-1.50710800	2.11941600	-4.40319000
O	-0.74202700	-0.00007500	-2.78920900	C	-1.89734000	4.80932900	-2.20520200
O	0.80776400	-0.61843200	-4.26694100	H	-1.27309800	5.33385900	-1.47214000
C	-0.09716100	-0.92576400	-3.50066300	H	-2.21716700	5.53668300	-2.96037600
C	-0.60017900	-2.34187800	-3.33539900	H	-2.78707600	4.43023400	-1.69317800
H	-0.03724400	-3.01937200	-3.98011100	C	0.12238800	4.23303700	-3.61006400
H	-1.66411300	-2.39025000	-3.58986700	H	0.69033300	3.44541900	-4.11576300
H	-0.49571900	-2.65867900	-2.29229100	H	-0.19903200	4.96049000	-4.36428900
C	-2.20526500	1.10771000	4.41160000	H	0.79470200	4.74183800	-2.91093100
H	-1.12806200	1.24277400	4.55420100	C	-0.61832400	3.89957300	3.81798000
H	-2.72431200	1.61733400	5.23109400	H	-1.03695700	3.00010500	4.28113900
H	-2.42705200	0.03783500	4.48008300	H	-0.39260900	4.61961000	4.61292100
C	-2.35414500	3.21083900	3.01381700	H	-1.38512500	4.33698000	3.16979100
H	-2.69659000	3.65533000	2.07472300	C	1.23500300	4.88085500	2.40769500
H	-2.86201900	3.71692100	3.84240900	H	1.45957100	5.60319800	3.20102400
H	-1.27796300	3.39329300	3.11282300	H	2.15632000	4.68252900	1.85138200
C	-4.19995500	1.48422000	2.90218700	H	0.51043200	5.34078900	1.72532800
H	-4.45857500	0.41981800	2.93540300	C	1.72420400	2.96543700	3.98441800
H	-4.72524600	1.98590100	3.72262500	H	2.65554000	2.74655200	3.45273800
H	-4.55880800	1.90075700	1.95623800	H	1.94640700	3.67110700	4.79330000
C	-5.32370700	-1.88621000	0.21762900	H	1.35605200	2.03663400	4.43596900
H	-5.49771000	-1.01065000	-0.41493300	C	-4.51403600	-3.69813100	-0.83980600
H	-6.22406300	-2.51066100	0.20048900	C	-5.90948600	-3.69468200	-0.94485200
H	-5.16735000	-1.54633200	1.24776300	C	-6.69308300	-3.31107600	0.14788700
C	-4.37907600	-3.16567100	-1.74809000	C	-6.07529800	-2.93281200	1.34632800

H	-4.53364900	-2.30683200	-2.40811900	C	-4.68183900	-2.93403900	1.44882000
H	-3.54371200	-3.75971200	-2.13631400	C	-3.89142700	-3.31464700	0.35441200
H	-5.27913400	-3.79006000	-1.77711600	C	-2.36940500	-3.30157000	0.45765300
C	-3.91391800	-3.94894000	0.60979500	C	-1.84081200	-1.87021000	0.36485000
H	-4.81385700	-4.57336800	0.57820800	O	-1.30553200	-1.34159100	1.39471200
H	-3.06642300	-4.55484300	0.27303600	O	-1.93530800	-1.19971000	-0.71017300
H	-3.73505600	-3.66131500	1.65105000	O	-1.90779200	-3.90889100	1.65892300
C	1.00090100	4.51505400	0.42954300	H	-3.90856200	-4.00484200	-1.68964500
H	-0.04190500	4.27520800	0.65751100	H	-6.38125200	-3.99873300	-1.87561300
H	1.64257200	3.97342000	1.13529500	H	-7.77712100	-3.31193900	0.06968300
H	1.15124700	5.58897500	0.59372800	H	-6.67860000	-2.63782500	2.20104400
C	0.41279800	4.92960000	-1.99226300	H	-4.20766400	-2.64868500	2.38424100
H	0.55967800	6.00868300	-1.86280800	H	-1.95450900	-3.85142400	-0.39578100
H	0.62548200	4.68383200	-3.03999400	H	-1.49324500	-3.20668800	2.19572800
H	-0.63734900	4.69817800	-1.79040300	C	4.71340400	-3.34487100	0.79799500
C	2.81359000	4.53844800	-1.32533800	C	6.08173900	-3.27574700	1.08238600
H	3.09369500	4.29319400	-2.35530200	C	6.96945300	-2.76263200	0.13155300
H	2.94925200	5.61713000	-1.18194900	C	6.48278500	-2.32029800	-1.10471600
H	3.50519900	4.01842600	-0.65363400	C	5.11566700	-2.38694200	-1.38612200
C	5.24296200	-2.61077200	0.13165400	C	4.22123500	-2.89751500	-0.43430400
C	6.03132800	-3.39897200	0.97703100	C	2.72756000	-2.95692900	-0.73021600
C	6.29626100	-2.97573000	2.28330100	C	2.07766400	-1.58221400	-0.56357000
C	5.76908300	-1.76172900	2.74037300	O	1.51300600	-1.03930600	-1.57092100
C	4.97616900	-0.97797200	1.89804300	O	2.08054500	-0.98336500	0.55667900
C	4.70808300	-1.39856400	0.58662200	O	2.46756500	-3.45882300	-2.03554400
C	3.83920000	-0.55269000	-0.33118300	H	4.02739700	-3.75244100	1.53706600
C	2.36196900	-0.73494500	0.02838600	H	6.45221500	-3.62994900	2.04086100
O	1.78284200	0.03879400	0.86192400	H	8.03328900	-2.71282500	0.34847600
O	1.67202300	-1.65385800	-0.52609300	H	7.16805900	-1.92480100	-1.85005700
O	4.22284800	0.80836100	-0.23631000	H	4.74305800	-2.05247400	-2.35068100
H	5.04873400	-2.93781400	-0.88716600	H	2.25115700	-3.61482800	0.00901900
H	6.44365900	-4.33579100	0.61152700	H	1.95391200	-2.77621700	-2.50837400
H	6.91312400	-3.58397700	2.93967900				
H	5.97518500	-1.42539400	3.75330300				
H	4.57157000	-0.03444100	2.25208700				
H	3.94378400	-0.92501000	-1.35886900				
H	3.55742800	1.34072700	-0.72642300				

Table 3SI. The Cartesian Coordinates of *S*-1-amino-2-propanol (APol) substituted dimolybdenum *tetrakis*(μ -pivalate) Mo₂ complexes.

APol-bridge-1				APol-bridge-2cis-a			
Mo	-0.00572400	-0.39223700	-0.98156100	Mo	0.58217500	0.04335000	-0.91728600
O	-2.15389600	-0.30535700	-0.98567200	O	-1.04214000	-1.40451300	-1.13722600
O	2.14099400	-0.38058600	-1.03564600	O	-0.94834300	1.56412400	-1.08814400
O	0.02540000	1.74546600	-1.18033500	C	-1.61499800	-1.85064900	-0.08883700
C	-2.76701100	-0.22444800	0.13341500	C	-2.80729300	-2.81040700	-0.21053000
C	-4.29903200	-0.17659900	0.12744000	Mo	0.32267100	-0.00289800	1.20103900
Mo	0.02008300	-0.23582600	1.14034900	C	-1.52020700	1.98282800	-0.02447400
C	2.78014000	-0.33313300	0.06959200	O	-1.21542100	-1.51048100	1.07904500
C	0.03681500	2.45524700	-0.11449000	O	-1.18120900	1.53302100	1.12455700
O	-2.12288700	-0.20134600	1.23783300	C	-2.61656600	3.04811700	-0.14823900
O	2.15897200	-0.30466000	1.18924600	C	-1.96134900	4.35066200	-0.66722600
O	0.04986700	1.90003300	1.03573200	H	-2.72646400	5.12729200	-0.78970800
C	4.31123700	-0.26571400	0.07163500	H	-1.20974800	4.72583600	0.03837900
C	0.02925100	3.98140900	-0.24623700	H	-1.47411300	4.18900100	-1.63382200
C	4.71018000	1.18816400	0.42812600	C	-3.66784000	2.56170000	-1.17116600
H	4.32447000	1.47379100	1.41249900	H	-4.14798200	1.63435900	-0.83579200
H	5.80334400	1.27709900	0.44693600	H	-4.44846800	3.32302800	-1.29049000
H	4.32536800	1.89802700	-0.31355100	H	-3.21125400	2.37641100	-2.14781800
C	4.87810000	-0.63478600	-1.31018200	C	-3.29125000	3.30997100	1.20882900
H	5.97295500	-0.57387800	-1.28508600	H	-2.57300300	3.66889400	1.95339100
H	4.60020600	-1.65530500	-1.59655100	H	-4.07021000	4.07310900	1.09002200
H	4.51365200	0.04301500	-2.08791800	H	-3.76051800	2.40272300	1.60468700
C	4.86685900	-1.22780800	1.14323500	C	-4.04931000	-2.12271300	0.40306600
H	4.59377200	-2.26727200	0.92343200	H	-3.88336200	-1.87167500	1.45560200
H	5.96152100	-1.16457600	1.16437200	H	-4.29738000	-1.20040700	-0.13597400
H	4.48716800	-0.97642300	2.13798600	H	-4.91480000	-2.79398300	0.33945000
C	1.27332400	4.40703300	-1.06047600	C	-2.49094600	-4.09983800	0.58064700
H	1.27730700	5.49653400	-1.18750400	H	-3.34103300	-4.79050900	0.51978900
H	2.19994900	4.12268100	-0.54729600	H	-1.61229600	-4.61245100	0.16962400
H	1.27349700	3.94321700	-2.05169000	H	-2.29962500	-3.88035300	1.63573400
C	-1.25014600	4.39579800	-1.01062400	C	-3.08160700	-3.15900000	-1.68341000
H	-2.15324200	4.10105300	-0.46248900	H	-2.21483800	-3.63986900	-2.14896600
H	-1.27003400	5.48544900	-1.13487900	H	-3.93170700	-3.84971100	-1.74543600
H	-1.28464900	3.93381700	-2.00207800	H	-3.32222800	-2.26569000	-2.26864400
C	0.05288800	4.65437000	1.13618800	C	4.26480400	2.27606900	-1.15309500
H	0.94981500	4.37900800	1.70105000	C	3.17596100	1.50031100	-0.40335700
H	0.04694400	5.74427600	1.01334700	C	3.01641000	2.07763300	1.02499300
H	-0.82054500	4.37308600	1.73395600	O	1.97205800	1.52102200	-1.12771200
C	-4.75237500	1.00394800	-0.76161100	N	1.66401400	1.82257200	1.60917500
H	-4.39338500	1.96091600	-0.36398200	H	4.44791800	1.81661200	-2.13048100
H	-4.37809300	0.89545100	-1.78393300	H	3.95013900	3.31515000	-1.31378200
H	-5.84802400	1.04112500	-0.79507700	H	5.20993100	2.28351500	-0.59229300
C	-4.85225300	-0.00083000	1.55154400	H	3.51310300	0.45705700	-0.30500900
H	-5.94800100	0.03114500	1.51720000	H	3.76217900	1.62784900	1.69066500
H	-4.55581000	-0.82926100	2.20355800	H	3.19143400	3.16244000	1.01443000
H	-4.49777100	0.92958900	2.00791400	H	1.04094900	2.54205000	1.23873800
C	-4.81785900	-1.50328600	-0.47685500	H	1.71053100	2.01213000	2.61182900
H	-4.51183100	-2.36360700	0.13118700	C	3.98458300	-2.39211800	-0.52217400
H	-5.91399700	-1.48956600	-0.51339900	C	2.45435400	-2.51879400	-0.63867500
H	-4.43905100	-1.64882600	-1.49319100	C	1.79998100	-2.83576700	0.72010700
C	-0.18829800	-4.74798400	-1.37886000	O	1.91653200	-1.41372900	-1.31244800
C	-0.41376900	-3.44921900	-0.59310500	N	1.80317800	-1.68683800	1.67967400
C	0.37989400	-3.49273400	0.72497700	H	4.40962300	-2.18859100	-1.51027000
O	-0.07075600	-2.35665000	-1.40243300	H	4.28185200	-1.56639700	0.13665500
N	-0.04944900	-2.44575600	1.70269400	H	4.42885000	-3.31963500	-0.13751200

H	-0.72535400	-4.69572800	-2.33162300	H	2.25947400	-3.42111200	-1.24823800
H	0.87835600	-4.88507300	-1.59751400	H	0.75618700	-3.11926300	0.57602200
H	-0.54780700	-5.62435700	-0.82469700	H	2.32554800	-3.69334800	1.16242700
H	-1.48849000	-3.39008600	-0.32987100	H	2.75994800	-1.35073000	1.79552500
H	0.26477100	-4.48021700	1.19043800	H	1.53730600	-2.04644100	2.59837500
H	1.44111400	-3.33282500	0.51223800				
H	-1.00478200	-2.65279300	2.00163600				
H	0.52048800	-2.55232400	2.54453700				
APol-bridge-2cis-b							
Mo	-0.10249000	-0.44331300	-.05619600				
O	-1.66826600	1.00976300	-0.90219100				
O	1.32632200	1.15998300	-1.26581000				
C	-1.99622700	1.44991600	0.25280000				
C	-3.09650200	2.51259500	0.35451300				
Mo	0.14548000	-0.45636600	1.06143000				
C	1.85236500	1.63807700	-0.19995000				
O	-1.42773000	0.99901600	1.30586500				
O	1.56186900	1.15034500	0.94405900				
C	2.85371600	2.79238700	-0.32353900				
C	4.06672400	2.29354400	-1.14454800				
H	4.79683500	3.10419800	-1.25910700				
H	4.56858500	1.45685600	-0.64288300				
H	3.75940500	1.96463200	-2.14256100				
C	2.17349500	3.96056100	-1.07319400				
H	1.30670400	4.33698000	-0.51661000				
H	2.88356700	4.78803900	-1.19405200				
H	1.83328700	3.64826100	-2.06526700				
C	3.32420000	3.26501900	1.06226400				
H	3.82108300	2.46020100	1.61379000				
H	4.03599800	4.09158000	0.94580900				
H	2.48511200	3.61973000	1.67018800				
C	-2.71093900	3.71327600	-0.53918100				
H	-1.77535100	4.17479900	-0.20068700				
H	-2.58252000	3.40472700	-1.58106500				
H	-3.49894900	4.47536700	-0.49710600				
C	-3.27396700	2.98170100	1.80858100				
H	-4.06029600	3.74514600	1.85493400				
H	-3.56190400	2.15456200	2.46587500				
H	-2.35037500	3.41778600	2.20406100				
C	-4.41751000	1.89315600	-0.16070200				
H	-4.71799500	1.03296700	0.45035400				
H	-5.22119300	2.63831100	-0.11174000				
H	-4.31890800	1.55927200	-1.19849500				
C	3.48070600	-3.30024400	1.39083900				
C	2.61528500	-2.28026100	0.63679800				
C	2.10412900	-2.90681900	-0.67483000				
O	1.57475400	-1.84781600	1.46994600				
N	1.55544500	-1.90881900	-1.64140400				
H	3.81718400	-2.86623900	2.33852600				
H	2.90000400	-4.20372600	1.61876800				
H	4.36507000	-3.59201000	0.80987700				
H	3.26076400	-1.42132800	0.36392800				
H	2.91745900	-3.46209600	-1.16085900				
H	1.30079300	-3.61198200	-0.44113100				
H	-0.85179800	-2.61163300	2.37427600				
H	2.32949000	-1.36176100	-2.02233800				
C	-3.20883300	-3.52240100	-1.42368200				
C	-2.39436700	-2.47677200	-0.64912500				
C	-1.82712300	-3.10893400	0.63642400				
O	-1.39136800	-1.95832800	-1.48031500				

N	-1.33484100	-2.10659700	1.62865700				
H	-3.58182600	-3.08086600	-2.35409700				
H	-2.58053500	-4.38401700	-1.68499200				
H	-4.06734400	-3.88141100	-0.84154600				
H	-3.08330100	-1.66519600	-0.34192700				
H	-2.59478300	-3.73292600	1.11312400				
H	-0.98258400	-3.75210500	0.37125800				
H	1.16382400	-2.42242800	-2.43337300				
H	-2.14083500	-1.66177500	2.07123900				
APol-bridge-2trans-a				APol-bridge-2trans-b			
Mo	0.00957700	0.00741500	-0.94072700	Mo	0.01227300	-0.12904100	1.05164000
O	2.14695300	-0.22922200	-0.95604800	O	2.15795500	-0.40677300	1.05757800
O	-2.12848300	0.23987200	-0.98817200	O	-2.13190500	-0.21825000	1.05969500
C	2.76644600	-0.30505100	0.16105400	C	2.80172200	-0.20376400	-0.03928100
C	4.28471000	-0.51939100	0.14721800	C	4.32159100	-0.40998000	-0.03914000
Mo	-0.00655300	0.0113940	0.19173300	Mo	0.04443900	0.25470100	-0.05340600
C	-2.76623800	0.31312100	0.11655900	C	-2.75573400	0.09257700	-0.01653700
O	2.13687100	-0.19781100	1.27014800	O	2.20256200	0.18489700	-1.09161900
O	-2.15415800	0.21873600	1.23836900	O	-2.12437000	0.36352500	-1.09225500
C	-4.29042400	0.48459200	0.12016400	C	-4.28993600	0.12888300	-0.03132600
C	-4.64708000	1.74490100	0.94108600	C	-4.79489800	-0.93948600	-1.02940400
H	-4.21854400	2.64748800	0.48810200	H	-4.49567500	-1.94749500	-0.71754700
H	-5.73631300	1.86999600	0.97333300	H	-5.89058000	-0.91374900	-1.07803500
H	-4.27959800	1.66531400	1.96914000	H	-4.39939900	-0.75929700	-2.03387300
C	-4.83053900	0.62599500	-1.31289000	C	-4.86446100	-0.15252500	1.36732700
H	-4.60423900	-0.25928000	-1.91572000	H	-4.52735400	0.59168100	2.09691500
H	-5.91980500	0.75173200	-1.28299700	H	-5.96025200	-0.12008400	1.32725600
H	-4.39845700	1.49507800	-1.81981100	H	-4.56480000	-1.13995300	1.73313200
C	-4.91436200	-0.76019600	0.79470000	C	-4.74138900	1.52829700	-0.50925500
H	-4.55373200	-0.87623400	1.82181900	H	-4.35584000	1.74687600	-1.50995200
H	-6.00613800	-0.65852800	0.82101200	H	-5.83683000	1.57341500	-0.54376300
H	-4.67479400	-1.67488800	0.23892100	H	-4.39405200	2.31244000	0.17510600
C	4.57387500	-1.88048900	-0.52906200	C	4.95001700	0.67266400	0.87184600
H	4.16986100	-1.90984400	-1.54554500	H	4.56135000	0.60432400	1.89292200
H	5.65704000	-2.04605100	-0.58022700	H	6.03872800	0.54227000	0.90608500
H	4.13241800	-2.70829000	0.03974100	H	4.74248500	1.67988700	0.49066400
C	4.85705900	-0.51443600	1.57477300	C	4.89304300	-0.28625800	-1.46177700
H	5.94189900	-0.67098600	1.53525900	H	5.98019000	-0.42971300	-1.43474200
H	4.66882100	0.43919100	2.07974300	H	4.46628700	-1.04047700	-2.13209900
H	4.42034100	-1.31065500	2.18698000	H	4.68793000	0.69888900	-1.89245700
C	4.93542100	0.61250100	-0.68104300	C	4.64186400	-1.80885800	0.53358500
H	6.02142100	0.46401900	-0.72019500	H	5.72779800	-1.96157300	0.55399900
H	4.55014200	0.62472600	-1.70485900	H	4.26039800	-1.91665500	1.55357200
H	4.74560500	1.59452800	-0.23074100	H	4.20389700	-2.60148500	-0.08618300
C	1.47934300	4.03422400	-1.62549800	C	0.72378300	4.77095500	-0.42589800
C	1.14665400	2.82254300	-0.74744700	C	0.63661900	3.30461500	-0.01439500
C	0.67885600	3.30405600	0.64709400	C	-0.00959200	3.11099700	1.35720700
O	0.19441000	2.00479600	-1.38027900	O	-0.08438500	2.55699100	-1.04607100
N	-0.15850900	2.29663800	1.37068700	N	0.01487200	1.74259100	1.84531000
H	1.89935600	3.70137300	-2.58090800	H	1.13945400	4.85922300	-1.43484600
H	0.57160800	4.61527100	-1.83245200	H	-0.26506200	5.24801500	-0.41484900
H	2.21076900	4.69425700	-1.13885500	H	1.37229300	5.32324200	0.26358700
H	2.07686900	2.25012000	-0.60014800	H	1.62948600	2.84808600	-0.02268300
H	1.55271000	3.52473500	1.26992100	H	0.52696600	3.77710200	2.05351800
H	0.09581200	4.23006500	0.54792300	H	-1.04146000	3.51470900	1.29508500
H	-1.12028600	2.42187800	1.05144400	H	-1.01794400	2.83241800	-1.04563500
H	-0.17854600	2.55302900	2.35933100	H	-0.29216000	1.73079600	2.81966000
C	-1.45470700	-4.02387600	-1.63082800	C	-1.17408200	-4.37851700	0.66771200
C	-1.13785400	-2.80662000	-0.75453300	C	-0.17321900	-3.44802700	-0.00515500
C	-0.69575600	-3.27935200	0.65205600	C	-0.74096100	-2.75796600	-1.26380700

O	-0.17431600	-1.99303300	-1.37462700	O	0.26104700	-2.45918000	0.99775300
N	0.14079200	-2.27294700	1.37784800	N	0.06046400	-1.67856500	-1.80561900
H	-1.85588200	-3.69705100	-2.59639000	H	-0.71980000	-4.90517800	1.51396100
H	-0.54369300	-4.60698100	-1.81643000	H	-2.03554800	-3.80967000	1.03669500
H	-2.19584900	-4.68013800	-1.15384200	H	-1.53818000	-5.12503500	-0.04858700
H	-2.07122700	-2.23394700	-0.62772500	H	0.72745700	-4.00595000	-0.28921500
H	-1.58042500	-3.48545800	1.26436000	H	-0.89812900	-3.56803900	-2.00066000
H	-0.12009800	-4.21171200	0.57039300	H	-1.73659000	-2.36424600	-1.02322900
H	1.10388900	-2.40374500	1.06455200	H	1.23107600	-2.47868500	1.05016300
H	0.15346300	-2.52667700	2.36733600	H	0.97116600	-2.03331900	-2.10847700
APol-bridge-3				APol-bridge-4			
Mo	0.29300900	0.01613100	1.25714900	Mo	-0.00501200	-0.00261500	-0.85029900
O	-1.87931200	0.04088600	1.16642600	Mo	-0.00916600	0.00085100	1.31782800
C	-2.41688700	0.01363600	0.00382200	C	1.61906700	-4.07360300	-1.45010300
C	-3.95318000	0.01577400	-0.08534300	C	0.87585000	-3.01915300	-0.61285300
Mo	0.51981300	0.00289800	-0.88410500	C	1.53484700	-2.90545000	0.77361200
O	-1.71517600	-0.01237200	-1.05406700	O	0.84646700	-1.81402500	-1.29964900
C	-4.49595300	-1.20877400	0.68625600	N	0.68030900	-2.16535600	1.75178100
H	-4.18968000	-1.18121700	1.73701800	H	1.16658800	-4.12915900	-2.44595200
H	-5.59249600	-1.22035500	0.64667700	H	2.67297900	-3.79171000	-1.57438800
H	-4.13441700	-2.14618300	0.24537900	H	1.57421600	-5.07015300	-0.99008000
C	-4.42091200	-0.04580200	-1.54926200	H	-0.15941900	-3.39062700	-0.44796000
H	-5.51775900	-0.04006900	-1.58583300	H	1.74906400	-3.90851100	1.16889600
H	-4.05367900	0.81098100	-2.12342800	H	2.48124800	-2.36360400	0.67227300
H	-4.06626800	-0.95510700	-2.04580800	H	-0.14644400	-2.74308200	1.91947100
C	-4.48052300	1.31082000	0.57441600	C	-4.09262500	-1.58750600	-1.45364500
H	-5.57713100	1.32876900	0.53879700	C	-3.02808100	-0.86223900	-0.61346800
H	-4.16861700	1.37596300	1.62191700	C	-2.92079200	-1.53157300	0.76844000
H	-4.11308900	2.20095300	0.04894600	O	-1.82279900	-0.84340700	-1.30032100
C	0.17204400	4.32678700	-1.62658900	N	-2.17472800	-0.68958800	1.75235800
C	0.55047400	3.14552500	-0.72005700	H	-4.14473100	-1.12827500	-2.44651500
C	-0.28646600	3.19203600	0.56848300	H	-3.82383400	-2.64397400	-1.58475600
O	0.40628000	1.95270800	-1.42747300	H	-5.08781200	-1.53353500	-0.99161700
N	0.23966600	2.28294800	1.63082300	H	-3.38854100	0.17595400	-0.44117600
H	0.74996000	4.27231900	-2.55518100	H	-3.92564500	-1.74111300	1.16171700
H	-0.89297600	4.28408500	-1.88850900	H	-2.38609900	-2.48129400	0.66063000
H	0.37640300	5.29257800	-1.14572300	H	-2.74856500	0.13749700	1.93109100
H	1.61298600	3.27695800	-0.42300400	C	-1.53613600	4.09968800	-1.46365100
H	-0.30970500	4.22077400	0.95416700	C	-0.83859000	3.01979300	-0.61936900
H	-1.31100100	2.88167300	0.34556400	C	-1.51983100	2.92260500	0.75814400
H	-0.35908000	2.39644800	2.45176300	O	-0.84026700	1.81489000	-1.30673500
H	1.15089600	2.64305000	1.92282800	N	-0.69427800	2.16817700	1.75004400
C	4.89619300	-0.22842100	-1.02160800	H	-1.06753900	4.14509500	-2.45251900
C	3.55195200	-0.39649100	-0.29757200	H	-2.59651600	3.85171100	-1.60433300
C	3.56322100	0.40577000	1.01681500	H	-1.46695800	5.09277400	-0.99918700
O	2.51841000	-0.02394400	-1.15722000	H	0.20668300	3.35645200	-0.44166800
N	2.49223600	-0.02787000	1.96475000	H	-1.72153800	3.92978700	1.14953600
H	4.86767300	-0.77212800	-1.97156700	H	-2.47434300	2.39787800	0.64312800
H	5.08369900	0.83013900	-1.24348700	H	0.13569600	2.73529500	1.93678800
H	5.73207900	-0.61457500	-0.42353000	H	-1.20079000	2.16842900	2.63878700
H	3.44543300	-1.46732200	-0.02298200	C	4.09670000	1.54998200	-1.43536700
H	4.54078300	0.30128200	1.50711900	C	3.01254300	0.84946600	-0.59906700
H	3.40195200	1.46372500	0.78543000	C	2.90724000	1.52752700	0.77911800
H	2.72752700	-0.97200600	2.27776100	O	1.81058600	0.85211800	-1.29300700
H	2.57279100	0.54447000	2.80833100	N	2.15221100	0.69724300	1.76658500
C	-0.06056300	-4.31397500	-1.56119200	H	4.14737200	1.08442800	-2.42541500
C	-0.19939100	-3.04335600	-0.70852500	H	3.84927900	2.61071900	-1.57420700
C	0.42774200	-3.27634500	0.67714600	H	5.08738200	1.47979200	-0.96582700
O	0.37211000	-1.96447600	-1.38465800	H	3.35104100	-0.19524400	-0.42098800
N	0.03594300	-2.23051300	1.66823500	H	3.91174400	1.73288200	1.17543400

H	-0.47893600	-4.13199700	-2.55679700	H	2.37929800	2.48008800	0.66296500
H	0.99685300	-4.58198200	-1.68312000	H	2.72458700	-0.12717900	1.96086000
H	-0.58826400	-5.16606600	-1.11264100	H	2.14068100	1.20672000	2.65395400
H	-1.28179900	-2.85893300	-0.55131000	H	-2.17071500	-1.18774600	2.64609200
H	0.12897100	-4.26272500	1.05846400	H	1.16944300	-2.16336100	2.65031600
H	1.51842200	-3.25825800	0.58119200				
H	-0.96761400	-2.32591100	1.84276400				
H	0.47763500	-2.46602400	2.55953000				
APol-chel-1				APol-chel-1b			
Mo	0.21919400	0.14173500	-0.84768900	Mo	-0.03996800	-0.91508500	0.57236800
O	-1.28449300	-1.16241700	-1.53311000	O	-1.81418500	-2.08559300	-0.08614900
O	-1.16172700	1.73286000	-0.85387100	O	1.61431400	-1.84011200	-0.36540500
C	-1.80149700	2.02541300	0.21540500	C	2.18199300	-1.26192700	-1.34697100
C	-2.69710000	3.26513300	0.23513000	C	3.29796700	-1.94383700	-2.13597900
Mo	-0.26390900	-0.30789100	1.19922400	Mo	0.15727100	0.78160900	-0.73175700
O	-1.65141800	1.30255300	1.26127900	O	1.78282600	-0.09237800	-1.71575200
O	-1.80177800	-1.62185200	0.57182800	O	-1.98612500	-0.75069000	1.63934800
C	-2.00360600	-1.79083700	-0.67839600	C	-2.51697700	-1.64048300	0.88841500
C	-3.08176100	-2.75252100	-1.17954000	C	-3.92187100	-2.18259300	1.14086600
O	2.18632800	-0.82061900	-1.38168400	O	1.32203000	-0.04516500	1.93265000
O	2.10693300	1.29334200	-0.80915300	O	1.47562600	1.72755400	0.61201400
C	2.78835200	0.29355200	-1.24971200	C	1.78085600	1.12201500	1.70721200
C	4.25420100	0.47414100	-1.64142600	C	2.64087700	1.84553500	2.74223400
C	-3.50000400	3.33821500	1.54521700	C	-4.75080900	-2.02361100	-0.15415900
H	-4.13631100	4.23122100	1.53406100	H	-4.86436100	-0.96711400	-0.42673900
H	-4.14514600	2.46163500	1.66961000	H	-4.28195700	-2.54818000	-0.99212200
H	-2.84206000	3.39877400	2.41813800	H	-5.75344300	-2.44019000	-0.00113300
C	-1.78566300	4.51055800	0.10792200	C	-4.59848200	-1.43193000	2.29976600
H	-1.20811800	4.48437600	-0.82165800	H	-5.60388000	-1.83893900	2.46100600
H	-2.40022400	5.41890700	0.10740900	H	-4.03310200	-1.53772300	3.23126200
H	-1.08459700	4.57798800	0.94878600	H	-4.69376400	-0.36235200	2.08407500
C	-3.66099500	3.20732800	-0.97120300	C	-3.78972900	-3.68561700	1.48780600
H	-4.31795200	2.33129300	-0.91203500	H	-3.19500600	-3.83316700	2.39730700
H	-4.29228700	4.10396900	-0.98143300	H	-4.78585200	-4.10896700	1.66329300
H	-3.11147200	3.16017900	-1.91613500	H	-3.31705900	-4.24040200	0.67129200
C	-4.04649200	-1.97400300	-2.10378100	C	4.52139200	-1.00018800	-2.18760000
H	-4.55203400	-1.16666900	-1.56014300	H	5.32131200	-1.46841800	-2.77342500
H	-3.51377900	-1.53513900	-2.95297400	H	4.26596600	-0.04383100	-2.65405300
H	-4.81491500	-2.65398600	-2.49098600	H	4.91087300	-0.79992200	-1.18224600
C	-2.38646800	-3.87524300	-1.98630500	C	3.68962100	-3.27794800	-1.47839300
H	-3.14024100	-4.57467600	-2.36777700	H	2.84326900	-3.97123400	-1.44141200
H	-1.83288000	-3.46593900	-2.83719000	H	4.49282100	-3.74758000	-2.05839400
H	-1.68608400	-4.43916400	-1.35895400	H	4.04981000	-3.12981900	-0.45462400
C	-3.86144300	-3.36053100	-0.00143600	C	2.77860400	-2.19650500	-3.57271300
H	-3.20253900	-3.92153100	0.66906100	H	1.90156800	-2.85463900	-3.56855900
H	-4.36335800	-2.58666800	0.58932400	H	2.50435400	-1.25831400	-4.06552300
H	-4.62584300	-4.04679500	-0.38538100	H	3.56319200	-2.68124900	-4.16586800
C	4.28176300	1.33130600	-2.93180600	C	3.91277800	2.38661600	2.05164100
H	3.82234800	2.31136700	-2.76688600	H	3.66135600	3.07010900	1.23513000
H	5.32095900	1.48563400	-3.24617500	H	4.52441500	2.92970100	2.78189000
H	3.75112600	0.83263000	-3.75157100	H	4.51973600	1.57006000	1.64237300
C	4.99636100	1.22111500	-0.51234300	C	3.02794700	0.89373600	3.88702800
H	6.03961200	1.38752900	-0.80602100	H	3.64636700	1.43195000	4.61507200
H	4.53606500	2.19259900	-0.30860500	H	2.14459400	0.50846600	4.40596400
H	4.99928000	0.63757500	0.41634100	H	3.60319300	0.03741600	3.51820500
C	4.91833800	-0.88806300	-1.90368300	C	1.81039600	3.02843900	3.29911500
H	4.89700200	-1.52254400	-1.01095900	H	2.40257000	3.57370800	4.04376600
H	4.41711800	-1.42956400	-2.71183100	H	1.53172400	3.72650700	2.50313000
H	5.96600100	-0.73521600	-2.18967600	H	0.89413900	2.67584500	3.78748700
C	2.71248900	-2.55579500	3.37665500	C	-3.29976900	4.32772800	-2.90721900

C	1.69207900	-1.45854600	3.07174100	C	-3.04073500	3.18355000	-1.93732300
C	2.36427900	-0.10251400	2.82489500	C	-1.99003200	2.18751700	-2.46242200
O	0.92991700	-1.78825900	1.93041200	O	-2.60791700	3.74604000	-0.69261200
N	1.31472100	0.85418800	2.35597500	N	-1.66192100	1.16156900	-1.47122700
H	2.19635000	-3.50762300	3.54215100	H	-4.04633600	5.01649100	-2.49708600
H	3.39943100	-2.68331100	2.53118600	H	-2.37793800	4.89138700	-3.09473200
H	3.29775300	-2.32069400	4.27537100	H	-3.67565700	3.94442700	-3.86314400
H	1.03068000	-1.35132600	3.95552800	H	-3.98049600	2.63007200	-1.76825600
H	2.87587200	0.28287500	3.71567800	H	-2.36780300	1.72982100	-3.39016500
H	3.09553800	-0.20602400	2.01811100	H	-1.07597800	2.74115400	-2.71701100
H	0.88095500	1.32053900	3.15455400	H	-2.24966800	3.00246200	-0.17180600
H	1.73165000	1.58991300	1.78518400	H	-2.46896600	0.56720500	-1.28259000
APol-chel-1sN				APol-chel-1sO			
Mo	-0.26261400	-0.26105400	-1.03679700	Mo	-0.08346800	-0.10000900	-1.07846500
O	-1.40737300	-2.06188600	-0.85037100	O	-0.76377700	-2.11563400	-1.15987700
O	-2.03583100	0.82136900	-1.43602500	O	-2.02359300	0.59059900	-1.53933800
C	-2.68581600	1.35374300	-0.47215500	C	-2.84742200	0.84279700	-0.59381800
C	-3.98565600	2.10394200	-0.78074500	C	-4.25290700	1.33793000	-0.94181300
Mo	-0.43900700	0.12343600	1.06275500	Mo	-0.50851100	0.00549700	1.01804400
O	-2.26893800	1.23579900	0.73054600	O	-2.49039900	0.67979000	0.62420500
O	-1.65490000	-1.60683500	1.31466400	O	-1.22238600	-1.99410400	1.01515000
C	-1.89202300	-2.34598500	0.29554600	C	-1.20547400	-2.64977400	-0.08540300
C	-2.76225400	-3.59894500	0.44289400	C	-1.72330200	-4.08992900	-0.13494000
O	0.92993400	1.55833900	-1.32516700	O	0.69142100	1.94149000	-1.07535000
O	0.58607600	2.04081300	0.82173600	O	0.07898800	2.09712000	1.05930700
C	1.03595600	2.36415400	-0.32174500	C	0.54858000	2.63237900	0.01008800
C	1.67366700	3.73855500	-0.54754800	C	0.91397600	4.11914000	-0.01049300
O	1.59146600	-1.50047800	-1.28021200	O	1.99448800	-0.88773200	-1.24689800
O	3.07499800	0.02369700	-2.01327900	O	3.20873400	0.97505300	-1.57796700
C	2.72017600	-1.21477600	-1.71157000	C	3.08440400	-0.33840400	-1.46644300
C	3.80994100	-2.25786100	-1.92916200	C	4.38305700	-1.11618300	-1.63860400
H	2.33741100	0.66379200	-1.80775300	H	2.33094800	1.42265500	-1.43234500
C	-4.46128500	2.89876700	0.44761500	C	-5.06935000	1.60376100	0.33434800
H	-5.39461900	3.42178500	0.20610300	H	-6.07030900	1.95791300	0.06013000
H	-4.64649400	2.24275700	1.30375800	H	-5.18092300	0.69585300	0.93621500
H	-3.72061500	3.64699800	0.75122100	H	-4.59666800	2.36705900	0.96142000
C	-3.75469000	3.06108000	-1.97015900	C	-4.12457400	2.64108300	-1.76488500
H	-3.42596500	2.51642500	-2.86021100	H	-3.55164500	2.47538200	-2.68252500
H	-4.68810700	3.58494300	-2.20940400	H	-5.12265900	3.00236800	-2.04062400
H	-2.99561200	3.81552000	-1.73073200	H	-3.62794600	3.42909500	-1.18615400
C	-5.05382500	1.05119300	-1.16717800	C	-4.95162500	0.25540000	-1.79803800
H	-5.23812200	0.35191900	-0.34296100	H	-5.05143800	-0.68570600	-1.24406000
H	-5.99978600	1.55417000	-1.40282500	H	-5.95767300	0.59515500	-2.07238900
H	-4.74184300	0.47562300	-2.04491400	H	-4.39178400	0.05573500	-2.71707900
C	0.70118500	4.56116400	-1.42972400	C	-0.17189500	4.84838400	-0.84160400
H	-0.26494800	4.70121400	-0.93103300	H	-1.16289300	4.73462800	-0.38694000
H	1.13061000	5.55208700	-1.62015700	H	0.05962600	5.91938000	-0.88518700
H	0.52608000	4.06989800	-2.39223300	H	-0.21400000	4.46293200	-1.86552900
C	1.90047500	4.46253300	0.79071200	C	0.94665200	4.68959700	1.41795700
H	2.58324900	3.90461300	1.44043600	H	1.70037300	4.18638100	2.03332100
H	2.34117400	5.44839200	0.60057200	H	1.19638500	5.75645700	1.37884600
H	0.96158700	4.60537000	1.33410700	H	-0.02149000	4.58208900	1.91619000
C	3.01882700	3.57127300	-1.28837200	C	2.29002800	4.31147300	-0.68423700
H	3.72455800	2.96609600	-0.70671100	H	3.08100800	3.78387400	-0.13796600
H	2.88401200	3.10318800	-2.26852500	H	2.28527900	3.95669700	-1.71961700
H	3.47303800	4.55659500	-1.44504300	H	2.54453200	5.37763400	-0.69442300
C	-3.94843600	-3.49487000	-0.54308300	C	-2.90846300	-4.14446500	-1.12779800
H	-4.57800200	-2.62616900	-0.31576200	H	-3.73483700	-3.50482900	-0.79496700
H	-3.59802300	-3.40353800	-1.57576400	H	-2.60282100	-3.81907600	-2.12704100
H	-4.57223300	-4.39384200	-0.46685900	H	-3.28375900	-5.17264500	-1.19768300

C	-1.89743600	-4.82960600	0.08128600	C	-0.58218700	-5.00160200	-0.64318200
H	-2.50052100	-5.74194100	0.16553100	H	-0.93699500	-6.03779200	-0.70042000
H	-1.51861900	-4.75868000	-0.94311100	H	-0.24491700	-4.69580600	-1.63829000
H	-1.04102000	-4.92564400	0.75956400	H	0.27901600	-4.97478400	0.03500400
C	-3.28965500	-3.73734800	1.88113800	C	-2.18612600	-4.55698100	1.25543300
H	-2.47076400	-3.82268800	2.60292300	H	-1.36619300	-4.53262800	1.98081600
H	-3.90210400	-2.87612200	2.16847600	H	-2.99565500	-3.92873700	1.64139800
H	-3.90961200	-4.63893700	1.95777700	H	-2.55446700	-5.58791700	1.18994300
C	4.27682900	-2.18795600	-3.40337400	C	4.95247700	-0.81215100	-3.04627000
H	4.68954600	-1.20514800	-3.64864500	H	5.16900200	0.25295000	-3.17098100
H	5.05619900	-2.94050900	-3.56714100	H	5.88449800	-1.37191300	-3.18318100
H	3.45167900	-2.40088800	-4.09306900	H	4.25480000	-1.12045300	-3.83390600
C	4.99403500	-1.91924100	-0.98913700	C	5.38321700	-0.64198300	-0.55559800
H	5.78327900	-2.66716700	-1.12462800	H	6.31741400	-1.20488700	-0.66204600
H	5.41245800	-0.93264600	-1.20929900	H	5.60917000	0.42363400	-0.65676300
H	4.68600800	-1.94005600	0.06279400	H	4.99136500	-0.82042800	0.45199300
C	3.26741800	-3.66077600	-1.61105300	C	4.11623200	-2.62268100	-1.48850600
H	2.93430700	-3.73739800	-0.57132500	H	3.70696400	-2.85986600	-0.50168800
H	2.42165700	-3.92077000	-2.25587100	H	3.40997900	-2.98346400	-2.24327000
H	4.06119300	-4.39852500	-1.77237800	H	5.05817800	-3.16877100	-1.61154200
C	2.85544900	0.14451700	5.28510200	C	2.01178100	-2.18105600	3.48975000
C	2.63243700	0.13762800	3.77839900	C	1.12487700	-0.93735600	3.35733500
C	1.45412300	-0.75944600	3.35092400	C	1.56460500	0.16841200	4.33933000
O	2.39906600	1.48854900	3.36043200	O	1.17154600	-0.45125000	2.02999600
N	1.20664400	-0.70684000	1.91726700	N	0.75055200	1.38925900	4.33783300
H	3.68686100	0.80766100	5.54955900	H	1.68156400	-2.95894700	2.79270600
H	1.95708100	0.49711400	5.80660400	H	3.05425200	-1.93155900	3.25420900
H	3.09416000	-0.86375600	5.64444600	H	1.97392400	-2.59042300	4.50807100
H	3.54301900	-0.23717500	3.27844500	H	0.08949500	-1.22703000	3.62540300
H	1.65617900	-1.78988300	3.69020600	H	1.57046000	-0.23611600	5.36051900
H	0.55608300	-0.41676000	3.88505300	H	2.59751000	0.45165200	4.09621600
H	1.98353600	1.45002000	2.47718600	H	0.70012700	1.76575000	3.39143400
H	1.92098200	-1.21546100	1.40026000	H	-0.20704500	1.17378300	4.61614300
APol-chel-2							
Mo	0.53276500	0.33089900	0.72212500				
O	-0.52996000	2.05932700	0.09893100				
C	-1.19581600	2.00045900	-0.99477000				
C	-1.91517400	3.25306800	-1.49983400				
Mo	-0.13887100	-0.76624500	-0.01009700				
O	-1.21784000	0.91825200	-1.67420800				
O	-1.19350200	-0.22603400	1.82780900				
O	-1.94262000	-1.35255700	0.06350700				
C	-2.07058500	-0.98788600	1.27873200				
C	-3.23516800	-1.49825000	2.13447000				
C	-2.85046800	3.77776500	-0.38698200				
H	-2.29044800	4.01097000	0.52379600				
H	-3.35427300	4.69078300	-0.72734600				
H	-3.62117100	3.03888400	-0.13624600				
C	-2.73190700	2.94138700	-2.76547200				
H	-3.23647900	3.85270000	-3.10879100				
H	-2.09243300	2.57717200	-3.57578000				
H	-3.49594300	2.18064000	-2.57175100				
C	-0.84237700	4.32250000	-1.81867600				
H	-0.15734700	3.97631000	-2.60184200				
H	-1.32894800	5.23905800	-2.17418700				
H	-0.25249200	4.56790300	-0.92975200				
C	-3.92491300	-0.29747500	2.81925200				
H	-4.74692700	-0.65370800	3.45235300				
H	-3.22134200	0.25874200	3.44591700				
H	-4.34382300	0.39391500	2.07801500				

C	-2.65386600	-2.44310600	3.21428100
H	-3.46369300	-2.82428500	3.84858600
H	-2.14788400	-3.30323300	2.75889500
H	-1.93451500	-1.91904100	3.85193600
C	-4.25407600	-2.26112500	1.27070900
H	-3.79886700	-3.13079300	0.78591100
H	-5.07947200	-2.61310500	1.90156700
H	-4.67326400	-1.62077600	0.48682800
C	5.49220700	1.65959500	2.66255900
C	4.53673400	1.28523300	1.52608700
C	3.36226700	0.42584100	2.03572200
O	4.09244200	2.45541500	0.82259700
N	2.46773900	-0.07321500	0.99956000
H	6.31557500	2.27271000	2.28107800
H	4.96938000	2.23379000	3.43968000
H	5.91681900	0.76435500	3.13314400
H	5.08321800	0.71374400	0.76537100
H	3.79398100	-0.40986700	2.61302200
H	2.77984100	1.02394000	2.75299600
H	3.51475500	2.97016800	1.41105900
H	2.97192200	-0.66544200	0.33992600
C	1.97321100	-4.55364300	-2.26198900
C	1.87756300	-3.11077800	-1.79257000
C	1.81838100	-2.05708900	-2.90410800
O	0.67572000	-2.92135300	-0.95794900
N	1.42077500	-0.76727600	-2.35082500
H	1.98689800	-5.24786500	-1.41447800
H	1.13401200	-4.81609000	-2.91992200
H	2.89832600	-4.69762200	-2.83189600
H	2.69964100	-2.87234100	-1.11056100
H	2.80056200	-2.00591100	-3.39509200
H	1.10218100	-2.41018400	-3.66927900
H	-0.01060700	-3.55774100	-1.22263200
H	2.12967700	-0.05319100	-2.47680800

Table 4SI. The Cartesian Coordinates of (1*S*,2*S*)-diaminocyclohexane (**11**, **DACH**) substituted dimolybdenum *tetrakis*(μ -pivalate) **Mo**₂ complexes.

DACH-bridge-1				DACH-bridge-2-trans			
Mo	-0.06476600	-0.11096400	-1.02981000	Mo	-0.07091700	0.05196600	1.06056600
O	-1.22388300	-1.92396800	-1.04761000	O	0.12724700	-2.09973600	1.09086700
O	0.86414400	1.83405600	-1.08368700	O	-0.13568800	2.20020400	1.13529500
O	-1.95870100	0.94810900	-1.14266100	C	0.18294900	-2.71522200	-0.02935400
C	-1.55372100	-2.44607100	0.07430300	C	0.27799500	-4.24702400	-0.01906400
C	-2.40353600	-3.72307700	0.06175000	Mo	0.03681400	0.08256000	-0.06119300
Mo	-0.11738000	-0.05520000	1.09799700	C	-0.17502900	2.84004600	0.02809200
C	1.14782400	2.40562500	0.02406400	O	0.15180400	-2.07684900	-1.13477400
C	-2.52179400	1.28404100	-0.04200100	O	-0.16027800	2.22264900	-1.09306900
O	-1.18906000	-1.92412900	1.18067100	C	-0.21682000	4.37376600	0.02032400
O	0.91659500	1.83361700	1.14326800	C	1.09181900	4.88748300	-0.62705700
O	-1.98676700	1.00369600	1.08145500	H	1.20111600	4.50958000	-1.64864200
C	1.76700400	3.80969400	0.02862800	H	1.08460400	5.98402900	-0.66274500
C	-3.85447600	2.04138400	-0.09886400	H	1.96961600	4.57464700	-0.04836600
C	0.74663000	4.78298000	0.66554100	C	-0.34121200	4.93128400	1.44829300
H	0.49648000	4.47965400	1.68726100	H	-0.36726300	6.02741800	1.41377300
H	1.16962400	5.79474300	0.69853900	H	-1.25809600	4.58332800	1.93636500
H	-0.18045500	4.82298000	0.08125400	H	0.50617600	4.62914600	2.07235400
C	2.10157600	4.26927800	-1.40057600	C	-1.42270800	4.83646600	-0.82830300
H	2.54531300	5.27207200	-1.36915900	H	-2.36858900	4.48450000	-0.39840600
H	2.81775400	3.59353500	-1.88049200	H	-1.45467500	5.93248700	-0.86178000
H	1.20636300	4.31016600	-2.02913600	H	-1.35100800	4.46193400	-1.85400500
C	3.05329900	3.78384000	0.88450400	C	1.53009700	-4.65805600	0.78929000
H	3.79717300	3.09688000	0.46233200	H	2.44595800	-4.27035600	0.32622900
H	3.49885300	4.78575100	0.91439300	H	1.47700900	-4.28366800	1.81640600
H	2.83937000	3.47046000	1.91093900	H	1.60751900	-5.75178100	0.82431600
C	-3.61990000	3.37888200	-0.83972300	C	0.37675500	-4.80526500	-1.44860000
H	-4.56351400	3.93388900	-0.91176300	H	0.44401200	-5.89964900	-1.41177600
H	-2.89816800	4.00724900	-0.30377300	H	-0.50175500	-4.53760400	-2.04518800
H	-3.24075100	3.20818100	-1.85212900	H	1.26255200	-4.42468200	-1.96802200
C	-4.87209200	1.18865200	-0.89059500	C	-0.98562400	-4.80703500	0.67541100
H	-5.05921700	0.22996600	-0.39169000	H	-1.89440300	-4.53642100	0.12367400
H	-5.82698600	1.72373100	-0.96449200	H	-0.93192800	-5.90195400	0.72011900
H	-4.51090600	0.98269200	-1.90275400	H	-1.07783800	-4.42154700	1.69544600
C	-4.39364000	2.31778400	1.31456000	C	-3.21549400	-0.55829000	0.67388000
H	-3.69414000	2.92477200	1.89876400	C	-4.52984300	-0.45805600	1.48461100
H	-5.34416200	2.86119400	1.24551800	C	-5.79312200	-0.88506300	0.72725900
H	-4.57141500	1.38746300	1.86457700	C	-5.93891800	-0.07970500	-0.56870700
C	-3.72376300	-3.42258500	-0.68527900	C	-4.68264400	-0.24277100	-1.43210100
H	-4.29982200	-2.64219000	-0.17354800	C	-3.38214800	0.15179900	-0.70152700
H	-3.53073100	-3.08971900	-1.70961500	N	-2.10824100	-0.06889400	1.48424400
H	-4.34147200	-4.32825900	-0.72462700	N	-2.21969100	-0.12953400	-1.60516300
C	-2.71116600	-4.19690200	1.49207700	H	-3.03340100	-1.62464900	0.45557000
H	-3.31670500	-5.11072500	1.45343300	H	-4.40338900	-1.04886900	2.40007000
H	-1.79369100	-4.41924300	2.04748400	H	-4.65019200	0.58986400	1.80577000
H	-3.26923000	-3.44073700	2.05418300	H	-6.67626900	-0.75176200	1.36646500
C	-1.62332800	-4.82185000	-0.69703100	H	-5.73941800	-1.95741700	0.48515100
H	-0.67850500	-5.05856600	-0.19221400	H	-6.82326800	-0.40133100	-1.13430500
H	-2.22213100	-5.73999600	-0.73967800	H	-6.08828300	0.98330400	-0.32628200
H	-1.39630200	-4.50873800	-1.72067900	H	-4.77097200	0.34504500	-2.35715700
C	2.79382100	-1.65916100	-0.73154100	H	-4.60291400	-1.29777400	-1.74043700
C	4.09497400	-1.52076300	-1.55747800	H	-3.37573500	1.23449300	-0.52037100
C	5.32638300	-2.11519800	-0.86153200	H	-2.41517600	0.78828700	1.95163100
C	5.51921400	-1.48434300	0.52330200	H	-2.29409200	-1.10282900	-1.91221600
C	4.24097300	-1.62142100	1.36209200	H	-2.35481200	0.41927600	-2.45758500

C	3.00358300	-1.03032800	0.66006000	C	3.21184500	-0.21559500	-0.68896700
N	1.66780000	-1.08627200	-1.45458700	C	4.51892400	-0.01361600	-1.49343300
N	1.79196500	-1.20775700	1.52643500	C	5.80219500	-0.41093900	-0.75337600
H	2.63592000	-2.74573100	-0.56182800	C	5.91149400	0.34690100	0.57448100
H	3.93770500	-2.00465400	-2.53127600	C	4.66445100	0.09303400	1.42937800
H	4.25985800	-0.45241800	-1.75987200	C	3.34584800	0.45136000	0.71237400
H	6.21898400	-1.96089100	-1.48154900	N	2.07774800	0.24879500	-1.47604200
H	5.20211100	-3.20313400	-0.75336900	N	2.19982400	0.09315200	1.61139200
H	6.36116500	-1.95046100	1.05083900	H	3.08399700	-1.29765300	-0.51652700
H	5.76880100	-0.41919900	0.40851900	H	4.42086200	-0.56893600	-2.43408300
H	4.37121400	-1.12794800	2.33556600	H	4.58576000	1.05184000	-1.76902900
H	4.05548400	-2.68662300	1.57027200	H	6.67800400	-0.21106300	-1.38537400
H	3.13529200	0.05072400	0.53584400	H	5.79866300	-1.49371300	-0.55507900
H	1.74900500	-1.32810900	-2.44398200	H	6.80959600	0.04304400	1.12822300
H	1.55713800	-2.20315600	1.55648900	H	6.01260300	1.42443400	0.37520700
H	2.06067100	-0.97231900	2.48556800	H	4.72594300	0.64949700	2.37581400
				H	4.63452800	-0.97536400	1.69794900
				H	3.29238900	1.53823800	0.56541600
				H	2.29670100	1.18881900	-1.81692300
				H	2.34955700	-0.86628400	1.93413700
				H	2.28163400	0.66421500	2.45555100
DACH-bridge-2-cis-a				DACH-bridge-2-cis-b			
Mo	-0.19286200	-0.19362200	-0.05344500	Mo	-0.11957600	-0.03591100	-1.04003900
O	-1.88399200	-1.51610500	-0.99688600	O	-1.05746200	2.00761600	-1.10406700
O	-1.60186000	1.46507000	-1.18563100	O	1.71961600	1.23174400	-1.10920400
C	-2.37591500	-1.86411600	0.13568100	C	-1.33900800	2.56074700	0.00858000
C	-3.60460600	-2.78593500	0.13803000	C	-2.00507000	3.94839700	-0.01050100
Mo	-0.15807700	-0.06851200	1.07858900	Mo	-0.07927600	0.06976300	1.10298900
C	-2.00413700	1.98794400	-0.08272000	C	2.27813100	1.53607300	-0.00353200
O	-1.86943600	-1.45370200	1.22900000	O	-1.10216900	1.98887600	1.12560100
O	-1.55288300	1.58314900	1.03539700	O	1.82455200	1.12123600	1.11462700
C	-3.03174200	3.12671700	-0.14038400	C	3.53380000	2.42511900	-0.04036500
C	-2.40659700	4.30812600	-0.91884500	C	4.60550800	1.72684200	-0.90837900
H	-3.12669900	5.13310800	-0.98758800	H	5.50603000	2.35156700	-0.96586700
H	-1.50964600	4.68587100	-0.41233800	H	4.89355800	0.75843400	-0.48053000
H	-2.12952000	4.00828200	-1.93477900	H	4.23713600	1.55458400	-1.92424500
C	-4.28622200	2.62588200	-0.89183500	C	3.15563600	3.77702700	-0.68764800
H	-4.75451100	1.78623100	-0.36406500	H	2.39985100	4.30330300	-0.09193300
H	-5.02486600	3.43408500	-0.96478400	H	4.04219500	4.42058800	-0.75400300
H	-4.03393600	2.29438100	-1.90383400	H	2.75532900	3.63235000	-1.69581600
C	-3.42222400	3.58799900	1.27398700	C	4.08997300	2.66706400	1.37290600
H	-2.55360600	3.95645300	1.82965300	H	4.37140800	1.72692500	1.85981900
H	-4.15718600	4.39997500	1.20704000	H	4.98359300	3.30147400	1.31440500
H	-3.86650300	2.77103100	1.85246400	H	3.35604200	3.16889300	2.01230000
C	-4.77673400	-2.03216500	-0.53380100	C	-1.15091600	4.90088900	-0.87547900
H	-5.03204100	-1.12182900	0.02198800	H	-0.14825000	5.03005400	-0.45030100
H	-4.52634700	-1.74752300	-1.56061200	H	-1.04083500	4.51462900	-1.89300800
H	-5.66641200	-2.67403700	-0.55926800	H	-1.62717100	5.88828400	-0.92605700
C	-3.99683100	-3.17688500	1.57287300	C	-2.14425700	4.52199500	1.40969700
H	-4.87875900	-3.82919500	1.54895800	H	-2.62247200	5.50876400	1.36451100
H	-3.18773600	-3.71712700	2.07687100	H	-2.75631300	3.87480800	2.04667500
H	-4.23780600	-2.29602900	2.17659400	H	-1.16743600	4.63840800	1.89180500
C	-3.27851800	-4.05701600	-0.67858300	C	-3.40580100	3.79792000	-0.64980600
H	-2.44794000	-4.61532500	-0.22869700	H	-4.04202900	3.12673600	-0.05922400
H	-4.15362500	-4.71848900	-0.70538600	H	-3.90203700	4.77556800	-0.69956300
H	-3.00299200	-3.80538900	-1.70723400	H	-3.33261900	3.39515800	-1.66507400
C	1.95630800	-2.63970100	-0.74952800	C	-3.13315900	-1.26488900	-0.68750900
C	3.20487300	-3.05257600	-1.56660400	C	-3.89213100	-2.34170000	-1.50030500
C	4.09534400	-4.08336400	-0.86153400	C	-5.14370000	-2.88032900	-0.79537200
C	4.52906900	-3.56137900	0.51364700	C	-4.78214500	-3.43668100	0.58749100

C	3.30354400	-3.16843700	1.34933400	C	-4.04606000	-2.37606600	1.41707700
C	2.39522500	-2.14234300	0.64304900	C	-2.79407400	-1.82046000	0.70988500
N	1.16883000	-1.66382500	-1.48992900	N	-1.96371900	-0.80996800	-1.42233100
N	1.21638900	-1.82981700	1.51581400	N	-2.15089900	-0.77263600	1.56479200
H	1.36744800	-3.56593800	-0.57469000	H	-3.84770600	-0.42931500	-0.51992700
H	2.86562300	-3.44177400	-2.53666500	H	-4.16057000	-1.91025600	-2.47460000
H	3.78824500	-2.14460400	-1.77998500	H	-3.19589100	-3.16852500	-1.70435000
H	4.97235500	-4.30993200	-1.48195300	H	-5.61741000	-3.65667800	-1.41039200
H	3.54487900	-5.02792200	-0.73701700	H	-5.88315100	-2.07332300	-0.68223500
H	5.11865900	-4.31555800	1.05056400	H	-5.68085400	-3.76988900	1.12243600
H	5.18111400	-2.68474500	0.38329200	H	-4.13892300	-4.32141800	0.46862900
H	3.62093800	-2.75778100	2.31837000	H	-3.75184900	-2.79234500	2.39132500
H	2.71195300	-4.07077900	1.56938600	H	-4.73151000	-1.54034400	1.62722800
H	2.93685300	-1.19773900	0.51435100	H	-2.05518000	-2.62260100	0.58800500
H	1.09692600	-1.98045800	-2.45945700	H	-2.20821200	-0.73206800	-2.41153900
H	0.62697000	-2.66385500	1.57297900	H	-2.76722100	0.04520800	1.57876100
H	1.56503500	-1.69384000	2.46862200	H	-2.15481200	-1.11584200	2.52886100
C	1.87140900	2.36459000	0.77867500	C	1.72611200	-2.71242100	-0.69014100
C	2.94664400	3.14263800	1.57492600	C	2.93481700	-3.22597200	-1.51011000
C	3.53417400	4.35891800	0.84825100	C	3.73076200	-4.33622200	-0.81261300
C	4.11513200	3.94496300	-0.50878400	C	4.20639700	-3.86620900	0.56760800
C	3.04221200	3.24518100	-1.35169900	C	3.01846800	-3.37377000	1.40485600
C	2.40921800	2.02930300	-0.64370500	C	2.20537900	-2.26631700	0.70547900
N	1.43302100	1.20026200	1.53484900	N	1.02906200	-1.66937300	-1.42350200
N	1.34110400	1.46070400	-1.53152900	N	1.05141100	-1.86257400	1.57318200
H	1.00117600	3.02846200	0.64514400	H	1.05885400	-3.58769200	-0.51992100
H	2.50528600	3.43687000	2.53522000	H	2.56460500	-3.57713300	-2.48340600
H	3.76597200	2.44344900	1.81192000	H	3.59376100	-2.36980900	-1.71585700
H	4.30579100	4.83277800	1.47004300	H	4.58594200	-4.63351400	-1.43373400
H	2.74907400	5.11448100	0.69241800	H	3.09994800	-5.23058500	-0.69635500
H	4.50491300	4.81622100	-1.05147200	H	4.72709400	-4.67374000	1.09854500
H	4.96575700	3.26446100	-0.35180700	H	4.93245800	-3.04889600	0.44511600
H	3.45846600	2.92762600	-2.31870900	H	3.36850200	-3.00054300	2.37797600
H	2.24468700	3.97071900	-1.57933300	H	2.34946000	-4.22318400	1.61572600
H	3.16298300	1.23866300	-0.53214500	H	2.82463000	-1.37057000	0.58882300
H	2.27089900	0.72012500	1.87701800	H	0.96667200	-1.94920600	-2.40407000
H	0.73226500	2.23150400	-1.81867700	H	0.42125100	-2.66458800	1.64453700
H	1.79750600	1.14610400	-2.39047700	H	1.41666800	-1.73560700	2.52106500
DACH-bridge-3				DACH-bridge-4			
Mo	0.00454600	-0.29793100	-1.03347000	Mo	0.00014500	-0.00019300	-1.02281700
O	-0.94025700	-2.25101100	-0.97364000	Mo	0.00011000	-0.00021700	1.11524500
C	-1.23208200	-2.77372500	0.15902100	C	2.27056200	-2.28466000	-0.94300800
C	-1.89576300	-4.16128900	0.16444100	C	3.38142200	-2.95805300	-1.78945700
Mo	0.00051900	-0.19493500	1.10021400	C	4.13331300	-4.10205900	-1.09747500
O	-0.97339900	-2.17752300	1.25507300	C	4.73880400	-3.62014800	0.22557200
C	-3.16192300	-4.11571500	-0.72014700	C	3.64083300	-3.04044600	1.12459700
H	-3.89330400	-3.39764400	-0.32870000	C	2.83689400	-1.90240000	0.45839300
H	-2.91444500	-3.82522900	-1.74565200	N	1.67717600	-1.17676100	-1.67856800
H	-3.63860000	-5.10401900	-0.74397200	N	1.75886800	-1.46663700	1.40297400
C	-2.27706400	-4.58669900	1.59245600	H	1.48694400	-3.04407900	-0.76139300
H	-2.74834600	-5.57752400	1.56987400	H	2.92330000	-3.30085000	-2.72596800
H	-1.39818300	-4.64098700	2.24347600	H	4.10886300	-2.17832500	-2.07033100
H	-2.98468200	-3.88292000	2.04444100	H	4.91615700	-4.49567600	-1.76052200
C	-0.89588600	-5.18147300	-0.43013000	H	3.44309300	-4.93638700	-0.89771500
H	0.01618000	-5.24248700	0.17676500	H	5.25327800	-4.43978400	0.74492900
H	-1.35020600	-6.18028200	-0.45718100	H	5.49791000	-2.84954300	0.02207800
H	-0.61011000	-4.90428000	-1.44985600	H	4.06891600	-2.67715600	2.07057200
C	3.04013100	-1.56620400	-0.80794500	H	2.94183100	-3.84996800	1.39131900
C	4.32588000	-1.32586700	-1.63748000	H	3.49031900	-1.03080900	0.31649000
C	5.60592500	-1.82477700	-0.95390500	H	2.45977100	-0.60682200	-2.01947600

C	5.75576500	-1.18777200	0.43349900	H	1.23335300	-2.29516700	1.69214500
C	4.49597400	-1.42887500	1.27673800	H	2.22037000	-1.12552100	2.24945100
C	3.20931300	-0.93329100	0.58726300	C	-2.27018300	2.28444300	-0.94314000
N	1.86625100	-1.08224200	-1.51682700	C	-3.38105100	2.95779300	-1.78961300
N	2.02226500	-1.20691600	1.45915600	C	-4.13294600	4.10183600	-1.09769900
H	2.97479800	-2.66409000	-0.63910300	C	-4.73841700	3.61999500	0.22538300
H	4.20014100	-1.81416000	-2.61398000	C	-3.64041600	3.04039500	1.12443500
H	4.40657200	-0.24657500	-1.83565100	C	-2.83646300	1.90230200	0.45832200
H	6.48088400	-1.59807500	-1.57762600	N	-1.67680600	1.17649500	-1.67865900
H	5.56875900	-2.91973000	-0.85022800	N	-1.75836100	1.46668000	1.40287800
H	6.63545500	-1.58754700	0.95454200	H	-1.48656000	3.04388000	-0.76158400
H	5.91977100	-0.10534400	0.32246500	H	-2.92293500	3.30054000	-2.72614600
H	4.59389600	-0.93361500	2.25348400	H	-4.10849700	2.17805200	-2.07044000
H	4.39591200	-2.50667700	1.47966000	H	-4.91580500	4.49539000	-1.76076500
H	3.25501000	0.15603000	0.46845400	H	-3.44274400	4.93619200	-0.89799500
H	1.91171900	-1.42562100	-2.47870900	H	-5.25291500	4.43965000	0.74468700
H	1.86260300	-2.21691900	1.47566600	H	-5.49750000	2.84935100	0.02194700
H	2.28479200	-0.96891800	2.41948500	H	-4.06847800	2.67717900	2.07044900
C	-2.82132200	1.37921500	-0.84154600	H	-2.94142800	3.84995500	1.39107800
C	-4.09214000	1.56571100	-1.70222300	H	-3.48987400	1.03068500	0.31654200
C	-5.22899100	2.33130500	-1.01441500	H	-2.45941400	0.60660300	-2.01963600
C	-5.60756000	1.65450800	0.30829100	H	-1.23265200	2.29519000	1.69172800
C	-4.37358800	1.53155800	1.21033000	H	-2.21978700	1.12596100	2.24956200
C	-3.20214900	0.78237500	0.54176400	C	1.89976100	2.70602400	0.90937900
N	-1.82226100	0.62215300	-1.58316700	C	3.08652500	3.25691800	1.73711500
N	-2.02705300	0.78761800	1.46675500	C	3.84455100	4.40635400	1.06077300
H	-2.42054700	2.39051700	-0.62358200	C	4.34201800	3.97430800	-0.32418300
H	-3.79896100	2.06371600	-2.63576600	C	3.17558800	3.45188400	-1.17304300
H	-4.45983600	0.56556100	-1.98404100	C	2.39785500	2.30418600	-0.49577600
H	-6.09946200	2.38902900	-1.68175600	N	1.24368200	1.61705200	1.61593600
H	-4.91524800	3.36755900	-0.81641200	N	1.27383300	1.86660200	-1.37504900
H	-6.39432600	2.21890500	0.82599400	H	1.20314200	3.56167400	0.74591500
H	-6.01855900	0.65441500	0.10362000	H	2.70279200	3.57864400	2.71601400
H	-4.63436500	1.02877000	2.15294900	H	3.77895800	2.42364100	1.93123900
H	-4.03166700	2.54333100	1.48176100	H	4.68572400	4.72601900	1.69048600
H	-3.47181400	-0.27023400	0.39008400	H	3.18189000	5.27862800	0.95441800
H	-2.28815700	0.09525000	-2.32336000	H	4.83636700	4.80800500	-0.84001000
H	-1.79064800	1.75753500	1.69177900	H	5.09692300	3.18181300	-0.20980400
H	-2.34181600	0.39036300	2.35564100	H	3.54113300	3.10824400	-2.15130200
C	0.78053900	2.90249600	0.83475700	H	2.47720600	4.27963600	-1.37387100
C	1.36968400	4.08700600	1.64062100	H	3.05423100	1.43223800	-0.38359200
C	1.40017100	5.42859400	0.89702400	H	1.24901200	1.83289200	2.61498700
C	2.16268900	5.29195500	-0.42590200	H	0.61340400	2.63928200	-1.48420000
C	1.53905800	4.18319800	-1.28172000	H	1.65713100	1.72661000	-2.31335900
C	1.46811200	2.82014000	-0.56033600	C	-1.90032400	-2.70600200	0.90945600
N	0.85769100	1.67255100	1.61273800	C	-3.08762700	-3.25587400	1.73710600
N	0.79739500	1.83298900	-1.45926400	C	-3.84624800	-4.40499900	1.06089100
H	-0.28460500	3.12498000	0.64201000	C	-4.34308600	-3.97303200	-0.32431700
H	0.80161700	4.17165100	2.57571500	C	-3.17614200	-3.45151300	-1.17303300
H	2.39986100	3.81965300	1.92919600	C	-2.39795700	-2.30407700	-0.49582900
H	1.85891300	6.20069900	1.52989700	N	-1.24344700	-1.61742300	1.61591800
H	0.37192100	5.76328700	0.68994300	N	-1.27360000	-1.86705800	-1.37492700
H	2.15897400	6.23963600	-0.98073700	H	-1.20434600	-3.56220900	0.74625100
H	3.21664600	5.05215700	-0.21800000	H	-2.70431000	-3.57760900	2.71616400
H	2.09261800	4.06578100	-2.22475000	H	-3.77953900	-2.42208000	1.93086900
H	0.51541800	4.48349400	-1.55795200	H	-4.68779400	-4.72393800	1.69047300
H	2.48792800	2.44516600	-0.39594700	H	-3.18412500	-5.27773400	0.95496100
H	1.82694400	1.59495200	1.93946200	H	-4.83780200	-4.80657600	-0.84004000
H	-0.08562100	2.22419900	-1.79877700	H	-5.09754800	-3.18005300	-0.21035700
H	1.38402300	1.71756200	-2.28780300	H	-3.54128000	-3.10789800	-2.15145400

				H	-2.47818000	-4.27970400	-1.37350100
				H	-3.05400400	-1.43186700	-0.38386300
				H	-1.24850200	-1.83342200	2.61493600
				H	-0.61320000	-2.63984500	-1.48346900
				H	-1.65649900	-1.72742400	-2.31344700
DACH-chel-1a				DACH-chel-1b			
Mo	-0.37778500	0.16707600	1.08040500	Mo	-0.41024100	-0.47935400	1.02790400
O	-0.94046700	-1.86821200	1.54067300	O	1.33231300	0.05806400	2.32042200
O	-2.49537700	0.50148900	0.80288700	O	-1.99305100	0.79498100	1.62577700
C	-3.03247200	0.38956700	-0.35271100	C	-2.39195000	1.70332100	0.82373700
C	-4.53675200	0.66250500	-0.48067700	C	-3.53068500	2.64765700	1.21383800
Mo	-0.21417000	-0.25269700	-1.08999900	Mo	-0.21966800	0.56566500	-0.83671800
O	-2.35885300	0.05962800	-1.38037100	O	-1.82214000	1.85147500	-0.31649800
O	-1.17717100	-2.22911400	-0.64506100	O	1.36603900	-1.82414500	1.19915800
C	-1.32134900	-2.59813400	0.56613700	C	1.92224300	-1.04245700	2.04756300
C	-1.92701800	-3.97349800	0.87886200	C	3.21672000	-1.43263100	2.76144400
O	-0.14689000	2.26674000	0.91617600	O	-1.85212100	-1.79241500	0.18875200
O	-0.67665200	2.06081100	-1.23816800	O	-1.62169800	-0.79049600	-1.77836900
C	-0.43444000	2.77773300	-0.23227500	C	-2.13811200	-1.71312500	-1.05309400
C	-0.42369100	4.30890700	-0.34788700	C	-3.07774400	-2.73541900	-1.70012500
O	1.41070300	-0.03536400	2.12873000	C	4.11804200	-0.19037100	2.91197600
O	3.09625300	0.86532600	0.93887100	H	4.40162200	0.21601800	1.93345700
C	2.62672000	0.42598900	1.99670800	H	3.61426500	0.60008000	3.47546500
C	3.46681800	0.36932200	3.29653000	H	5.03721900	-0.46512100	3.44330600
C	-5.00011600	0.52132900	-1.94031600	C	3.95630300	-2.53759000	1.98656300
H	-4.81948600	-0.48850300	-2.32304200	H	4.86704800	-2.81875000	2.52882500
H	-6.07627300	0.72340900	-2.00200300	H	3.33586200	-3.43128200	1.86951900
H	-4.48108600	1.22798600	-2.59616500	H	4.25029000	-2.19727200	0.98710400
C	-5.28953600	-0.35232200	0.41084100	C	2.81761100	-1.95584400	4.16464200
H	-4.98092900	-0.26725300	1.45723800	H	2.16683900	-2.83516300	4.09147100
H	-6.36804000	-0.16313300	0.35115700	H	3.71922200	-2.24606600	4.71751300
H	-5.10992300	-1.38216900	0.07910600	H	2.29542800	-1.18431500	4.74040400
C	-4.81419900	2.09760400	0.02341400	C	-4.62545700	2.58300700	0.12498000
H	-4.28044300	2.84085600	-0.58057900	H	-5.43736900	3.27618900	0.37655300
H	-5.88749100	2.31007800	-0.05067600	H	-4.22561600	2.85990300	-0.85538000
H	-4.50852100	2.21740200	1.06706300	H	-5.05154500	1.57516900	0.05058100
C	-1.20569600	4.92137100	0.83324600	C	-4.12370300	2.25629000	2.57827900
H	-0.77052600	4.62735900	1.79262400	H	-3.37111000	2.30720100	3.37188700
H	-1.18267800	6.01570500	0.76209700	H	-4.93831600	2.94470200	2.83380200
H	-2.25573600	4.60459600	0.82206000	H	-4.52875100	1.23865900	2.56312000
C	1.05626800	4.75972000	-0.28109100	C	-2.95822800	4.08401100	1.28377100
H	1.52074900	4.45783200	0.66309900	H	-2.17157700	4.16027400	2.04390700
H	1.63911100	4.32941400	-1.10386500	H	-2.53565100	4.38781300	0.32084700
H	1.11015600	5.85249300	-0.36095300	H	-3.75686100	4.78739300	1.54985100
C	-1.04386600	4.76110200	-1.68083500	C	-4.23051900	-1.97610400	-2.39572400
H	-1.01296300	5.85560700	-1.74684100	H	-3.84845300	-1.28190300	-3.15044800
H	-0.50011800	4.34832000	-2.53585700	H	-4.90075100	-2.69086600	-2.88877400
H	-2.09004000	4.44503100	-1.76336600	H	-4.82118400	-1.40348500	-1.67050200
C	-3.02669400	-3.80706600	1.95049900	C	-3.64901700	-3.70206800	-0.64889500
H	-2.62519600	-3.36266300	2.86563400	H	-4.32226900	-4.41715900	-1.13716700
H	-3.84167700	-3.16947600	1.58865800	H	-2.85525200	-4.26637600	-0.14843300
H	-3.44935400	-4.78843000	2.19655600	H	-4.21787600	-3.16782400	0.11961600
C	-0.79084200	-4.86216800	1.44235900	C	-2.27209000	-3.52896400	-2.75629800
H	-1.19159600	-5.85113700	1.69451800	H	-2.92554800	-4.25996100	-3.24788500
H	0.00987100	-5.00355400	0.70590500	H	-1.86281800	-2.86349700	-3.52313800
H	-0.35732400	-4.42472400	2.34719700	H	-1.44208300	-4.07641600	-2.29296600
C	-2.51744000	-4.62014200	-0.38548000	C	2.36581600	1.73938400	-1.66481000
H	-1.75524000	-4.76778700	-1.15711900	C	3.61974400	2.60387600	-1.46734200
H	-2.94036600	-5.59922000	-0.13062600	C	4.65586300	2.35839100	-2.57940400
H	-3.31617200	-4.00564400	-0.81485700	C	5.02025700	0.86921400	-2.70822000

C	2.32049100	-0.23282500	-2.58972400	C	3.77021400	-0.00817900	-2.90505100
C	3.62865900	0.41894800	-3.05634400	C	2.75902800	0.25165900	-1.78354100
C	4.43137600	-0.55789700	-3.93773600	N	1.34770200	1.88877500	-0.62456200
C	4.67788400	-1.90752100	-3.23872300	N	1.48319800	-0.52008900	-1.91820000
C	3.36633700	-2.55595700	-2.75218200	H	1.91329900	2.02795700	-2.63015700
C	2.60153600	-1.56238700	-1.87355400	H	3.33036500	3.66155500	-1.43380900
N	1.50990200	0.57688500	-1.68703800	H	4.06472400	2.36477100	-0.48840600
N	1.26889900	-2.02134700	-1.39814200	H	5.56037200	2.94949500	-2.38611000
H	1.72050100	-0.46049400	-3.48780100	H	4.24869200	2.71489200	-3.53741000
H	3.40770100	1.34308000	-3.60423600	H	5.71460700	0.71863500	-3.54450700
H	4.22119800	0.70137400	-2.17396600	H	5.54887500	0.54422800	-1.79973100
H	5.39052400	-0.10417100	-4.21791300	H	4.04628400	-1.07111700	-2.93542500
H	3.88247900	-0.73202400	-4.87537100	H	3.30471600	0.22964000	-3.87455800
H	5.20012600	-2.59398000	-3.91696200	H	3.19199400	-0.05218300	-0.82213100
H	5.34205000	-1.75335200	-2.37574900	H	1.78813700	2.01088800	0.28753900
H	3.57679100	-3.48250800	-2.20140000	H	1.22731700	-0.60077400	-2.90552000
H	2.74565200	-2.82968000	-3.61952600	H	1.60497400	-1.47586200	-1.58246600
H	3.18583200	-1.33612000	-0.97397300				
H	2.08652900	0.98042400	-0.94283700				
H	0.81702000	-2.61757900	-2.09572600				
H	1.34867800	-2.59283900	-0.55835900				
C	2.77405800	1.23749900	4.37130800				
H	1.76736500	0.86835000	4.59034200				
H	3.35863700	1.21885900	5.30008400				
H	2.69302700	2.28207000	4.04568900				
C	3.53686100	-1.09505200	3.78449000				
H	4.01828900	-1.73970200	3.03778900				
H	4.12766100	-1.15366800	4.70765500				
H	2.53789300	-1.49259500	3.98768300				
C	4.88751300	0.89881900	3.04275500				
H	5.40533900	0.30567000	2.28131800				
H	4.87142800	1.93859500	2.69952700				
H	5.47229700	0.85206600	3.97034100				
DACH-chel-1s				DACH-chel-2			
Mo	0.55290000	0.22633000	1.13304800	Mo	-0.39464500	-0.49921600	0.94686600
O	-0.99284600	1.39468100	1.61428200	O	-1.88864800	0.86522900	1.71630600
O	1.48037100	1.89802800	0.28019700	C	-2.32712700	1.77752300	0.93282700
C	1.48865300	2.05892000	-1.00031000	C	-3.35599600	2.78149900	1.46738100
C	2.10975700	3.34219700	-1.55142000	Mo	-0.39464600	0.49920700	-0.94686800
Mo	0.12408700	-0.65748800	-0.89465400	O	-1.90305900	1.86506400	-0.26942200
O	1.00689700	1.18367200	-1.77311700	O	-1.90305200	-1.86507900	0.26941700
O	-1.70798300	2.67587100	-0.08546700	O	-1.88864200	-0.86524400	-1.71631100
C	-1.89065200	2.17323000	1.01706900	C	-2.32706800	-1.77758100	-0.93285300
C	-3.15071200	2.42613400	1.86855200	C	-3.35603900	-2.78147500	-1.46736800
O	2.54126100	-0.55961900	0.98504600	C	-4.58122900	1.99984900	1.99427500
O	2.14283900	-1.41433800	-1.03457800	H	-4.29285800	1.29887400	2.78368800
C	2.91623300	-1.23480300	-0.03628700	H	-5.32011700	2.69943400	2.40437600
C	4.32420900	-1.82992600	-0.03190100	H	-5.06378300	1.43122900	1.19002700
O	0.21863600	-1.12978100	2.58085300	C	-3.79655500	3.75943000	0.36498500
O	-1.27448800	-2.79037100	2.28118000	H	-4.53567600	4.46133800	0.77063200
C	-0.41398600	-2.22455200	2.95669300	H	-2.95047200	4.33848700	-0.01977500
C	-0.00403600	-2.71864500	4.32830900	H	-4.25332500	3.23206000	-0.47921500
H	-0.53702600	-3.63723700	4.58004400	C	-2.70736100	3.56619500	2.63227800
H	-0.22189700	-1.94873300	5.07707100	H	-1.82835000	4.12739100	2.29178900
H	1.07673100	-2.89627100	4.35175000	H	-3.42769300	4.28435400	3.04325000
C	2.02773700	3.37106100	-3.08681400	H	-2.39559900	2.89244600	3.43678000
H	0.98995100	3.33539000	-3.43341300	C	-3.79678200	-3.75925100	-0.36490800
H	2.48095400	4.29840100	-3.45643100	H	-4.53596700	-4.46110400	-0.77053300
H	2.56234400	2.52684700	-3.53467700	H	-2.95079300	-4.33837700	0.01995200
C	1.34067800	4.54577700	-0.95633400	H	-4.25353500	-3.23174900	0.47921800

H	1.41300600	4.56137200	0.13515000	C	-2.70744400	-3.56635500	-2.63216100
H	1.77020500	5.47577800	-1.34722400	H	-3.42784200	-4.28447100	-3.04309300
H	0.28043400	4.51274300	-1.22839100	H	-2.39557100	-2.89272000	-3.43671400
C	3.58822400	3.39595100	-1.09835700	H	-1.82851300	-4.12762000	-2.29158000
H	4.16026500	2.55147900	-1.50102000	C	-4.58114500	-1.99971500	-1.99439500
H	4.04682800	4.32040400	-1.46841500	H	-4.29263900	-1.29883300	-2.78384200
H	3.67073400	3.38166000	-0.00746400	H	-5.32009500	-2.69923800	-2.40449000
C	5.33458800	-0.66389800	0.09123400	H	-5.06367900	-1.43097600	-1.19021900
H	5.16777700	-0.08785300	1.00620600	C	2.10087800	1.77861400	-1.92136300
H	6.35253800	-1.06969400	0.11695300	C	3.33047800	2.70355700	-1.88339000
H	5.26411500	0.01658300	-0.76546500	C	4.26304100	2.43891000	-3.07976200
C	4.44903900	-2.75625200	1.20156800	C	4.68025600	0.95953300	-3.15942900
H	4.28054800	-2.20451400	2.13106900	C	3.46283100	0.01554200	-3.14665200
H	3.73055400	-3.58305700	1.15323800	C	2.56342700	0.31513300	-1.94320000
H	5.45705100	-3.18572700	1.23046400	N	1.17617900	1.93117700	-0.79124200
C	4.58993100	-2.62572800	-1.32028300	N	1.36842600	-0.58129300	-1.84236000
H	5.60592400	-3.03607400	-1.28871800	H	1.59462000	1.96935000	-2.89190700
H	3.88842500	-3.45918200	-1.42999400	H	3.00204900	3.75231500	-1.87921100
H	4.50442000	-1.99244400	-2.20917400	H	3.87013200	2.53636600	-0.93879700
C	-2.72900300	3.17201300	3.15631300	H	5.15509000	3.07577100	-3.01400600
H	-2.02966400	2.57574800	3.75029200	H	3.74699300	2.71966700	-4.01018400
H	-2.25211800	4.13150600	2.92145400	H	5.28082200	0.78134300	-4.06085800
H	-3.61525000	3.37744700	3.76938700	H	5.32572000	0.71987000	-2.30114800
C	-3.79413400	1.07191800	2.24182000	H	3.79281900	-1.03193900	-3.11864800
H	-4.69432400	1.24552100	2.84417000	H	2.88468500	0.14534900	-4.07475400
H	-4.09221200	0.51253900	1.34653100	H	3.14181400	0.14780500	-1.02625200
H	-3.10720900	0.44829300	2.82159700	H	0.85757900	2.90181500	-0.74532700
C	-4.15335400	3.28097200	1.07646400	H	1.17909600	-1.03940800	-2.73457700
H	-4.46446700	2.77986200	0.15339100	H	1.53801100	-1.31679700	-1.12391900
H	-5.04710400	3.46027300	1.68651600	C	2.10088000	-1.77862400	1.92135700
H	-3.72402700	4.25000900	0.80194200	C	3.33048000	-2.70356700	1.88338200
C	-2.15239900	-2.25403000	-1.58028500	C	4.26304600	-2.43892000	3.07975200
C	-3.27609900	-3.25179100	-1.29835500	C	4.68026100	-0.95954200	3.15941900
C	-4.26685400	-3.24261700	-2.48128500	C	3.46283500	-0.01555200	3.14664400
C	-4.78195200	-1.82769100	-2.81075100	C	2.56342900	-0.31514300	1.94319300
C	-3.63465100	-0.81961800	-3.03392100	N	1.17618000	-1.93118700	0.79123800
C	-2.69736500	-0.82752600	-1.82062300	N	1.36842800	0.58128300	1.84235500
N	-1.13871700	-2.08320900	-0.52970800	H	1.59462300	-1.96935900	2.89190200
N	-1.49925900	0.01336800	-1.90877500	H	3.00205200	-3.75232500	1.87920400
H	-1.63498800	-2.55748800	-2.50368400	H	3.87013300	-2.53637600	0.93878800
H	-2.86699700	-4.25909300	-1.14923400	H	5.15509500	-3.07578000	3.01399500
H	-3.79417400	-2.97165000	-0.36991200	H	3.74700000	-2.71967700	4.01017600
H	-5.11236800	-3.90654700	-2.26110100	H	5.28082700	-0.78135200	4.06084700
H	-3.76545900	-3.65923600	-3.36750900	H	5.32572300	-0.71987900	2.30113700
H	-5.42387600	-1.86554700	-3.70014400	H	3.79282300	1.03192900	3.11864000
H	-5.41495800	-1.47299500	-1.98384200	H	2.88469000	-0.14536000	4.07474700
H	-4.03905000	0.18856400	-3.19573300	H	3.14181500	-0.14781500	1.02624400
H	-3.06162500	-1.08560800	-3.93403800	H	0.85757600	-2.90182400	0.74532600
H	-3.29638400	-0.55054200	-0.93224900	H	1.17910000	1.03939900	2.73457200
H	-1.42905700	-2.36586200	0.41470100	H	1.53801300	1.31678700	1.12391400
H	-1.70681300	1.01074200	-1.94101500				

Table 5SI. The Cartesian Coordinates of 3-phenyl-propane-1,2-diamine (**13**, **PhPDA**) substituted dimolybdenum *tetrakis*(μ -pivalate) **Mo2** complexes.

PhPDA-bridge-1				PhPDA-bridge-2-cis-a			
C	4.91383400	-1.00104100	0.21825000	C	-3.30295800	-3.89761700	-0.02559800
C	4.95628000	-1.53397000	1.51622300	C	-2.73969500	-4.91695700	-0.81040100
C	5.82494800	-1.01248200	2.48234500	C	-3.41055600	-5.42004300	-1.93137500
C	6.66999100	0.05445100	2.16406100	C	-4.66310200	-4.91135400	-2.28788200
C	6.64187600	0.59330400	0.87211400	C	-5.23995400	-3.89826000	-1.51234500
C	5.77302900	0.06859000	-0.08794600	C	-4.56546400	-3.40016900	-0.39426300
C	3.96330000	-1.54706000	-0.82601600	C	-2.57363200	-3.33226300	1.17368000
C	2.70072200	-0.66203700	-1.04899900	C	-1.87228600	-1.96798500	0.89346200
C	1.89355200	-1.26866400	-2.20429700	C	-1.25358900	-1.46998500	2.20830100
N	1.91282000	-0.52392900	0.15982600	N	-0.88684400	-2.06538200	-0.16092500
N	0.80136900	-0.37372400	-2.69089200	N	-0.88588000	-0.02404100	2.17027100
H	4.30696700	-2.36880500	1.77082300	H	-1.76861500	-5.32347000	-0.53674800
H	5.84144600	-1.44264100	3.48081700	H	-2.95524100	-6.21172300	-2.52167700
H	7.34733300	0.45950100	2.91159200	H	-5.18837100	-5.30405000	-3.15488500
H	7.29968800	1.41911800	0.61185500	H	-6.21802200	-3.50165100	-1.77460200
H	5.76414200	0.49058200	-1.09126200	H	-5.02698300	-2.61898300	0.20715900
H	4.49582300	-1.63759200	-1.78242500	H	-3.28985300	-3.19363200	1.99530100
H	3.63259400	-2.55262200	-0.53706200	H	-1.81259300	-4.04524900	1.51511000
H	3.07048200	0.32486100	-1.39934000	H	-2.68842200	-1.25052600	0.64135800
H	2.57472700	-1.48552400	-3.03726200	H	-1.96612700	-1.63227200	3.02838200
H	1.43067100	-2.20641200	-1.88329800	H	-0.34407700	-2.03867900	2.42296300
H	2.53180800	-0.37763000	0.95863500	H	-1.27652900	-2.60416900	-0.93621100
H	0.41803200	-0.78504100	-3.54471300	H	-0.58675300	0.24717100	3.10944600
H	1.21091600	0.51567700	-2.98416600	H	-1.72393000	0.52918600	1.98120000
Mo	-0.97426400	0.06146600	-1.32572900	Mo	0.70846000	0.75597500	0.73135300
O	-1.51236200	-2.02602800	-1.26906300	O	2.17974800	-0.32815100	1.89894200
O	-0.52514500	2.16718600	-1.47840900	O	2.32807100	1.72785100	-0.30724000
O	-2.86095100	0.54800100	-0.42709000	C	2.61978400	-1.42887500	1.41311200
C	-1.26268000	-2.66886800	-0.19266200	C	3.71810300	-2.18613500	2.17140500
C	-1.73886700	-4.12291200	-0.07712300	Mo	0.65371300	-0.77722400	-0.75030700
Mo	-0.03135600	-0.06157400	0.58170100	C	2.76106700	1.23195200	-1.40128700
C	0.01845600	2.72956800	-0.46966000	O	2.15898000	-1.88705700	0.31608900
C	-2.93210900	0.63393000	0.84576200	O	2.23919100	0.17165900	-1.89199600
O	-0.63292900	-2.12099400	0.77546500	C	3.91064700	1.94335400	-2.12810200
O	0.36282900	2.05446400	0.56220200	C	3.42184600	3.34926800	-2.55048100
O	-1.90311200	0.42942700	1.57644900	H	4.23341900	3.89222100	-3.05123400
C	0.27417800	4.24195600	-0.46849100	H	2.57900900	3.28258600	-3.24963500
C	-4.27835200	0.99942400	1.48513200	H	3.09970400	3.93124000	-1.68130400
C	-0.48796200	4.86291900	0.72548100	C	5.10075900	2.08780000	-1.15260600
H	-0.15995000	4.42583700	1.67356700	H	5.46955300	1.10659000	-0.82982100
H	-0.30496800	5.94397900	0.75966300	H	5.92652500	2.61366300	-1.64813800
H	-1.56918700	4.70579700	0.63019900	H	4.81390100	2.65462600	-0.26163000
C	-0.20369900	4.88418200	-1.78157100	C	4.35135800	1.15278000	-3.37161600
H	-0.01247400	5.96390700	-1.75279100	H	3.53105000	1.04151600	-4.08857300
H	0.32278100	4.46804600	-2.64728800	H	5.17287900	1.68104900	-3.87149900
H	-1.27689100	4.73091700	-1.93582600	H	4.70201200	0.14977900	-3.10555600
C	1.79143300	4.48112400	-0.28923000	C	4.96648700	-1.27732900	2.25996700
H	2.36222900	4.05060300	-1.12133500	H	5.35199500	-1.03641500	1.26186300
H	1.99660700	5.55839400	-0.26113500	H	4.73548300	-0.33831200	2.77279100
H	2.15389300	4.03497100	0.64182800	H	5.76218800	-1.78951300	2.81555200
C	-4.66444500	2.42355700	1.02019600	C	4.08093600	-3.49675600	1.45287600
H	-5.63185900	2.70598600	1.45384400	H	4.86791200	-4.01761000	2.01263300
H	-3.92064300	3.16141800	1.34451900	H	3.21602900	-4.16430700	1.37617000
H	-4.74696100	2.47472800	-0.07016400	H	4.44946500	-3.30892100	0.43893400
C	-5.34716400	-0.00652300	1.00085600	C	3.20971600	-2.49662000	3.59794200

O	1.50069600	1.49618600	-1.06961300	H	-1.23811500	-5.64951500	0.03620400
C	3.40924900	3.00286500	-0.86746200	H	-1.81289300	-4.18941700	0.87279900
C	3.36670900	4.18226000	0.13129500	C	-5.48160000	-0.45941800	-0.51833700
H	4.03198000	4.98556300	-0.20982900	C	-5.97867300	0.10077500	0.66943800
H	2.35376000	4.59616900	0.21238600	C	-6.79811800	-0.63901300	1.52986700
H	3.69114200	3.86662600	1.12805400	C	-7.13705900	-1.95860500	1.21578900
C	4.84871900	2.44462300	-0.93880400	C	-6.65174900	-2.53016200	0.03349900
H	4.91243000	1.60376000	-1.64005100	C	-5.83492300	-1.78584500	-0.82200900
H	5.53603900	3.22643100	-1.28651300	C	-4.58234800	0.32981000	-1.44459300
H	5.18762800	2.09746600	0.04237500	C	-3.06765100	-0.01725000	-1.30342100
C	2.97391000	3.49040200	-2.25962200	C	-2.29578000	0.79926500	-2.34800100
H	1.95749500	3.89779900	-2.24222300	N	-2.57720200	0.22455700	0.03735200
H	3.65439400	4.27996200	-2.60321300	N	-0.91196600	0.29027000	-2.57477800
H	2.99492500	2.67750700	-2.99285000	H	-5.72346700	1.12807900	0.91911700
C	5.03430700	-2.08318600	-1.30008400	H	-7.17322100	-0.18201100	2.44262800
H	5.07327100	-1.07548100	-1.73113900	H	-7.77639100	-2.53414700	1.88054900
H	5.30114700	-2.01106100	-0.24112000	H	-6.91395000	-3.55359600	-0.22439500
H	5.78915400	-2.69715100	-1.80782000	H	-5.46940600	-2.23791200	-1.74231800
C	3.29708800	-2.80555000	-2.97784100	H	-4.88733600	0.14190200	-2.48361100
H	4.04606900	-3.42539700	-3.48705200	H	-4.70544500	1.40342600	-1.25302900
H	2.31203400	-3.25535700	-3.13908500	H	-2.96754700	-1.08540800	-1.60045700
H	3.29372900	-1.81694800	-3.44884500	H	-2.84426600	0.78400800	-3.29941700
C	3.62606200	-4.12830100	-0.85837600	H	-2.21479800	1.83728200	-2.01217700
H	2.64220700	-4.60205500	-0.96418400	H	-3.18137100	-0.27739500	0.69186200
H	4.36229600	-4.76401900	-1.36651500	H	-0.50110500	0.82404100	-3.34306000
H	3.87868900	-4.09347800	0.20635500	H	-0.96620900	-0.67208500	-2.91283700
C	-3.25800400	3.55743700	0.27539000	C	5.48096400	-0.27957200	0.53597800
C	-4.10671800	2.92686900	-0.64837600	C	5.99084400	0.30065200	-0.63657500
C	-4.54684100	3.59452500	-1.79726100	C	6.82349300	-0.42345800	-1.49797000
C	-4.14466100	4.91073000	-2.04187900	C	7.16348600	-1.74642100	-1.19983600
C	-3.30123300	5.55373800	-1.12789400	C	6.66640200	-2.33743600	-0.03206300
C	-2.86518900	4.88219600	0.01723300	C	5.83623200	-1.60910900	0.82408500
C	-2.76609400	2.83348400	1.51035300	C	4.56382900	0.48783800	1.46333700
C	-1.30306300	2.30489600	1.39641700	C	3.05568100	0.13018700	1.29104600
C	-0.93208900	1.66999600	2.74266700	C	2.25747500	0.87797900	2.36801100
N	-1.14229500	1.38679200	0.28915700	N	2.57354000	0.43817600	-0.04021900
N	0.51958400	1.34715800	2.86089600	N	0.89436600	0.30871600	2.57651900
H	-4.42914000	1.90461200	-0.46317700	H	5.73567900	1.33101300	-0.87371400
H	-5.20467600	3.08564200	-2.49773900	H	7.20790300	0.04838300	-2.39921200
H	-4.48694100	5.43248500	-2.93202600	H	7.81274300	-2.30971400	-1.86546000
H	-2.98654200	6.57934700	-1.30559500	H	6.92965100	-3.36355800	0.21390500
H	-2.21438800	5.39381400	0.72404100	H	5.46129300	-2.07607400	1.73310300
H	-2.82194200	3.51467900	2.37052100	H	4.85523700	0.28107900	2.50252200
H	-3.42279100	1.98015000	1.72283300	H	4.68140900	1.56597500	1.29489500
H	-0.65716300	3.20163800	1.27717200	H	2.96724700	-0.95352800	1.52992800
H	-1.21488900	2.36144100	3.54806800	H	2.80664400	0.84797300	3.31869700
H	-1.49164500	0.73821000	2.87317200	H	2.13739100	1.92362700	2.07100100
H	-1.64394000	1.74548500	-0.52471100	H	3.21373200	0.01277200	-0.71490500
H	0.70378400	1.09916900	3.83518400	H	0.45114000	0.82245600	3.34045400
H	1.05475800	2.20452300	2.70174300	H	0.98782400	-0.65071900	2.91425500
PhPDA-bridge-2-trans-b				PhPDA-bridge-3a			
Mo	0.00546300	0.01339400	0.01366300	Mo	-0.59842400	0.33062800	-0.08738400
O	0.51322900	2.14631200	0.01137300	O	-1.92457800	0.60686400	1.61805400
O	-0.50783700	-2.12375400	0.01104100	C	-1.75709500	-0.10470600	2.66731500
C	0.63093700	2.74692000	-1.10876500	C	-2.70798300	0.10970200	3.85547300
C	0.97782900	4.24492400	-1.09470900	Mo	0.44068100	-1.21227400	0.95827900
Mo	-0.00177300	0.01360600	-1.12753400	O	-0.82749700	-0.97811300	2.73075200
C	-0.63775700	-2.72123300	-1.10653600	C	-2.61910800	1.58719800	4.30211300
O	0.45922700	2.14057800	-2.21944200	H	-1.60614700	1.83872200	4.64021200
O	-0.46918400	-2.11602800	-2.22021400	H	-2.88206500	2.26200400	3.48192400

C	-0.99945500	-4.21635900	-1.13708500	H	-3.30858900	1.76868000	5.13658600
C	-2.29780200	-4.39497900	-1.95662700	C	-2.34015500	-0.80872700	5.03310600
H	-2.17361500	-4.02330800	-2.97876300	H	-3.03090600	-0.63363600	5.86762800
H	-2.56627900	-5.45782400	-2.00579500	H	-2.40482400	-1.86578200	4.75341700
H	-3.13507900	-3.85828400	-1.49313600	H	-1.32151200	-0.61832300	5.38833100
C	-1.20588300	-4.76487700	0.28489600	C	-4.15095000	-0.19623100	3.39073000
H	-1.46082500	-5.83110100	0.23504900	H	-4.24992300	-1.23961800	3.06596400
H	-0.30082900	-4.65631700	0.89127300	H	-4.85374300	-0.03228900	4.21767600
H	-2.01780000	-4.24234700	0.80165600	H	-4.44125400	0.44955800	2.55635600
C	0.15163500	-4.98325500	-1.82836300	C	-4.81384600	-1.43026600	-2.33315200
H	1.09072400	-4.87332600	-1.27210600	C	-4.82250800	-0.43354600	-3.32200400
H	-0.08780300	-6.05308400	-1.87632300	C	-5.90366100	0.44604100	-3.45304300
H	0.31150400	-4.61986100	-2.84868700	C	-7.00162200	0.34239000	-2.59392000
C	-0.15711000	4.99957900	-0.36354800	C	-7.00956400	-0.64887600	-1.60524700
H	-1.11350100	4.88246300	-0.88816700	C	-5.92740300	-1.52385400	-1.48006400
H	-0.28051600	4.62952400	0.65881500	C	-3.64035200	-2.37172800	-2.17130300
H	0.07472200	6.07128600	-0.32008000	C	-2.67934000	-1.98559700	-1.00551000
C	1.12794600	4.79564000	-2.52275300	C	-1.60587900	-3.07606700	-0.89937100
H	1.37390600	5.86419500	-2.48192600	N	-2.08912000	-0.67499400	-1.18661600
H	1.92753600	4.28317200	-3.06891000	N	-0.82639900	-3.02032300	0.36874800
H	0.20290100	4.68018300	-3.09752700	H	-3.97458600	-0.34912800	-3.99830000
C	2.30114900	4.43832600	-0.31975200	H	-5.88785900	1.20878200	-4.22807700
H	3.13051200	3.91777600	-0.81487100	H	-7.84400400	1.02207600	-2.69525300
H	2.55364900	5.50514100	-0.27168700	H	-7.86050600	-0.74260400	-0.93460300
H	2.21909900	4.05429500	0.70144900	H	-5.94649500	-2.29424300	-0.71134700
C	4.58897900	-1.06191900	1.93449700	H	-4.02055900	-3.38654400	-1.98867600
C	3.97929300	-1.53643000	3.10690900	H	-3.05772900	-2.40139700	-3.10153900
C	4.33969300	-1.03372200	4.36266100	H	-3.28636800	-2.04222800	-0.07482600
C	5.32185500	-0.04451100	4.46791800	H	-2.07982900	-4.06386500	-0.98568600
C	5.94201500	0.43528600	3.30805400	H	-0.89214800	-2.96594600	-1.72081400
C	5.57789900	-0.07034400	2.05734300	H	-2.82720000	-0.01817300	-1.44815900
C	4.18626100	-1.58268800	0.57185300	H	-0.11966100	-3.75782900	0.32083700
C	3.21184700	-0.63771300	-0.19702600	H	-1.44388400	-3.26757600	1.14400800
C	3.00242800	-1.21907700	-1.60001900	C	1.94938500	4.72844400	0.07116700
N	1.96300700	-0.44120000	0.50705300	C	0.80830900	5.51228500	-0.16400400
N	2.22440200	-0.31243900	-2.49377000	C	0.72470400	6.35008500	-1.28258500
H	3.21767100	-2.30962600	3.03476500	C	1.78703500	6.42043700	-2.18852200
H	3.85378500	-1.41742400	5.25660600	C	2.93402100	5.64894600	-1.96460500
H	5.60538100	0.34573700	5.44216800	C	3.01138900	4.81439300	-0.84641700
H	6.71158800	1.20041500	3.37845400	C	2.03603500	3.80227800	1.26514600
H	6.07043700	0.30587100	1.16247200	C	1.79265500	2.30386200	0.91420100
H	5.08932400	-1.72419600	-0.03799900	C	1.98916600	1.47604300	2.19347800
H	3.70143700	-2.56146400	0.67697000	N	0.49363200	2.07606100	0.32471800
H	3.75753000	0.32227400	-0.32871500	N	2.11219300	0.01452600	1.92634000
H	3.98496900	-1.41805800	-2.04940700	H	-0.02069500	5.46914600	0.53910100
H	2.45384800	-2.16337400	-1.53534700	H	-0.16889800	6.94888900	-1.44200900
H	2.15641500	-0.26863800	1.49464800	H	1.72652900	7.07341000	-3.05558600
H	2.30820700	-0.66911400	-3.44799400	H	3.77006800	5.70246900	-2.65805700
H	2.68133700	0.60262200	-2.51108700	H	3.91067900	4.22475600	-0.67764500
C	-4.58274200	1.01335800	1.96182600	H	3.03161700	3.89633700	1.72016600
C	-3.97830100	1.49128100	3.13559000	H	1.29917100	4.10353500	2.02080300
C	-4.32399800	0.97232900	4.38886600	H	2.62162100	2.01128100	0.22557000
C	-5.28601100	-0.03685900	4.49032600	H	2.89281200	1.82201400	2.71511500
C	-5.90112000	-0.52005200	3.32917800	H	1.12958200	1.62031400	2.85497700
C	-5.55177400	0.00188000	2.08095000	H	0.23830700	2.86640700	-0.26782200
C	-4.19501500	1.55152200	0.60154400	H	2.31537400	-0.44409400	2.81689900
C	-3.20724200	0.62998000	-0.17829800	H	2.93994600	-0.14672600	1.34848600
C	-3.01293600	1.22579800	-1.57756800	C	4.77016500	-2.44270500	-1.42721700
N	-1.95262100	0.45203500	0.52009600	C	4.92065700	-3.72531100	-0.87561100
N	-2.23021600	0.33630500	-2.48429400	C	6.02223500	-4.04266500	-0.07198800

H	-3.23241400	2.27995300	3.06651700	C	6.99895400	-3.07848900	0.19513700
H	-3.84230200	1.35888400	5.28386300	C	6.86614000	-1.79632900	-0.35168000
H	-5.55797800	-0.43993400	5.46264700	C	5.76446600	-1.48623200	-1.15380800
H	-6.65531500	-1.30060100	3.39671000	C	3.57192700	-2.08155600	-2.27713200
H	-6.04036600	-0.37723300	1.18513300	C	2.49044600	-1.25770000	-1.51254200
H	-5.10293600	1.68220300	-0.00346600	C	1.39709800	-0.85213400	-2.51337600
H	-3.72604800	2.53727500	0.71217000	N	1.93380400	-1.98502400	-0.38771700
H	-3.73591000	-0.33882500	-0.31555200	N	0.57753900	0.30515600	-2.05873700
H	-4.00020500	1.41756500	-2.01970900	H	4.16867600	-4.48348000	-1.08279300
H	-2.47485700	2.17578700	-1.50696000	H	6.11800700	-5.04425900	0.34078900
H	-2.13891200	0.27308500	1.50790900	H	7.85792400	-3.32397600	0.81465100
H	-2.31832700	0.70518200	-3.43345500	H	7.62458100	-1.04092400	-0.15931600
H	-2.68086000	-0.58156900	-2.51286000	H	5.67607300	-0.48936500	-1.58214300
				H	3.91294000	-1.49488700	-3.14174500
				H	3.09982700	-2.99452200	-2.66292200
				H	2.99451300	-0.30816700	-1.20773100
				H	1.85532400	-0.60276900	-3.48082600
				H	0.71835100	-1.69651400	-2.66488100
				H	2.71874700	-2.35411200	0.15744700
				H	-0.15070600	0.46467700	-2.75721400
				H	1.15774000	1.14493700	-2.04277900
PhPDA-bridge-3b				PhPDA- bridge-4			
C	3.23179100	-3.25175700	2.14186400	Mo	-0.00005600	1.06292400	-0.00009100
C	2.89312500	-2.71694300	3.39530000	Mo	0.00001800	-1.06302600	-0.00006400
C	3.86165700	-2.12405000	4.21369100	C	-3.98437200	2.93753800	-2.57390200
C	5.19295100	-2.05639700	3.79199600	C	-3.41467700	4.19264800	-2.84279500
C	5.54703500	-2.58848300	2.54634600	C	-3.99167400	5.36965000	-2.35130200
C	4.57539800	-3.17943700	1.73416500	C	-5.15583600	5.31262400	-1.57908100
C	2.18694200	-3.87213200	1.24023700	C	-5.73891800	4.06920300	-1.30613900
C	1.69434100	-2.92103800	0.10471600	C	-5.15808900	2.89796100	-1.80018900
C	0.74390800	-3.71445200	-0.79992200	C	-3.35394300	1.65865800	-3.07928200
N	1.08151900	-1.71981500	0.61928600	C	-2.52601500	0.90054400	-1.99651900
N	0.47610100	-3.02924200	-2.09932500	C	-2.03258100	-0.41992700	-2.60638600
H	1.86046300	-2.76734000	3.73263200	N	-1.42078000	1.68593700	-1.48874000
H	3.57441600	-1.71714500	5.18042100	N	-1.61362700	-1.42243700	-1.58795500
H	5.94750000	-1.59884000	4.42710000	H	-2.51229800	4.24697000	-3.44772300
H	6.58045500	-2.54667700	2.20987300	H	-3.53300000	6.32982600	-2.57588800
H	4.86269200	-3.59469300	0.76978000	H	-5.60874300	6.22548300	-1.20030500
H	2.60666800	-4.77808200	0.78040500	H	-6.64964000	4.01295700	-0.71431000
H	1.31565000	-4.17523400	1.83477900	H	-5.62448300	1.93718200	-1.58957100
H	2.59618300	-2.69389800	-0.51254300	H	-4.14637200	0.99092200	-3.44545100
H	1.17969800	-4.70404600	-0.99853400	H	-2.69163900	1.88039400	-3.92633200
H	-0.21762300	-3.85138100	-0.29886400	H	-3.25419700	0.61950000	-1.19747400
H	1.68931700	-1.32578200	1.33897900	H	-2.82271900	-0.85654100	-3.23381800
H	-0.06974300	-3.67461800	-2.67451400	H	-1.16451300	-0.21701100	-3.24097200
H	1.36884900	-2.93438800	-2.58943700	H	-1.76669200	2.62397600	-1.27225000
Mo	-0.76556300	-1.09598900	-.06399300	H	-1.22867500	-2.22557400	-2.09007800
O	-2.40264700	-2.21416100	-1.12388900	H	-2.44116200	-1.76182900	-1.09515600
C	-2.59534900	-2.03519800	0.13410400	C	3.98411600	2.93783300	2.57394900
C	-3.77662100	-2.79273900	0.78088500	C	3.41439300	4.19293600	2.84281200
Mo	-0.03357500	-0.18774600	-.24311700	C	3.99141000	5.36994500	2.35136000
O	-1.85818800	-1.29096500	0.83495600	C	5.15562000	5.31293300	1.57921200
C	-5.07418200	-2.46104000	0.01131900	C	5.73873000	4.06951900	1.30630000
H	-5.29855600	-1.38776800	0.05935600	C	5.15788200	2.89827000	1.80031000
H	-4.99315700	-2.74794100	-1.04195000	C	3.35367100	1.65894300	3.07928800
H	-5.92265700	-3.00068800	0.45193000	C	2.52595600	0.90075400	1.99642600
C	-3.93965600	-2.39910000	2.25857300	C	2.03259600	-0.41977000	2.60622600
H	-4.78233200	-2.94853800	2.69850200	N	1.42070000	1.68602000	1.48851400
H	-3.03861700	-2.63140100	2.83511700	N	1.61377100	-1.42227200	1.58776300
H	-4.13493100	-1.32681600	2.36691300	H	2.51197400	4.24724800	3.44768100

C	-3.49666400	-4.30977600	0.67875900	H	3.53271300	6.33011600	2.57592200
H	-2.57692000	-4.57911100	1.21277200	H	5.60854100	6.22579800	1.20046500
H	-4.32335600	-4.87643300	1.12685400	H	6.64948900	4.01328200	0.71452600
H	-3.39164000	-4.62220300	-0.36551200	H	5.62430000	1.93749700	1.58971800
C	3.60326000	3.12733800	-1.24147500	H	4.14607600	0.99126000	3.44560800
C	4.15443000	3.00320000	0.04390200	H	2.69122800	1.88068300	3.92622800
C	4.26188800	4.11028700	0.89371500	H	3.25426800	0.61978800	1.19746500
C	3.82004600	5.36701100	0.46975400	H	2.82274100	-0.85633000	3.23369000
C	3.27249900	5.50742500	-0.81109700	H	1.16448800	-0.21692500	3.24078300
C	3.16777500	4.39844500	-1.65473800	H	1.76654100	2.62407900	1.27200500
C	3.46463100	1.93047100	-2.15758200	H	1.22893700	-2.22549100	2.08984300
C	2.02446700	1.33349500	-2.20624100	H	2.44132500	-1.76151200	1.09489500
C	2.01932200	0.19645100	-3.23677700	C	3.98437700	-2.93759900	-2.57385100
N	1.57730000	0.89242800	-0.90637300	C	3.41487100	-4.19279200	-2.84275800
N	0.64388900	-0.20175700	-3.65728300	C	3.99200600	-5.36970700	-2.35121900
H	4.50421700	2.02990300	0.38075800	C	5.15611600	-5.31250800	-1.57893300
H	4.69187100	3.98892500	1.88510300	C	5.73901000	-4.06900300	-1.30597500
H	3.90434700	6.22891200	1.12698900	C	5.15804600	-2.89784900	-1.80007400
H	2.93031900	6.48130000	-1.15347900	C	3.35381100	-1.65881100	-3.07930400
H	2.74454400	4.51982800	-2.65025500	C	2.52588200	-0.90068900	-1.99656000
H	3.75196000	2.22610500	-3.17613600	C	2.03228800	0.41970200	-2.60647900
H	4.15377900	1.13832900	-1.83749700	N	1.42072300	-1.68615900	-1.48868900
H	1.37040900	2.13671500	-2.61846700	N	1.61349400	1.42232000	-1.58808900
H	2.59039600	0.50910600	-4.12239100	H	2.51252900	-4.24724900	-3.44772900
H	2.50419100	-0.68367200	-2.80230700	H	3.53347700	-6.32995000	-2.57581700
H	1.83521200	1.59358900	-0.21070200	H	5.60912900	-6.22529900	-1.20011700
H	0.74090700	-0.88707300	-4.41056300	H	6.64969100	-4.01262200	-0.71409500
H	0.21352300	0.60971500	-4.10537700	H	5.62429800	-1.93700300	-1.58944600
C	-3.18128200	3.46499800	1.33258100	H	4.14616500	-0.99104300	-3.44558100
C	-2.17818100	4.07632000	2.10178800	H	2.69148300	-1.88067900	-3.92629900
C	-2.32974800	4.24692300	3.48287900	H	3.25406800	-0.61954400	-1.19755900
C	-3.49360300	3.80883300	4.12149400	H	2.82228900	0.85626400	-3.23412300
C	-4.50436100	3.20093000	3.36730300	H	1.16410100	0.21667700	-3.24086500
C	-4.34706900	3.03350600	1.98900700	H	1.76673200	-2.62414900	-1.27213700
C	-3.01520100	3.25700000	-0.15690000	H	1.22837500	2.22537100	-2.09022700
C	-2.58149200	1.81023800	-0.54844600	H	2.44110300	1.76181000	-1.09548800
C	-2.55424300	1.72695000	-2.08035200	C	-3.98415000	-2.93765900	2.57400800
N	-1.30611100	1.44588900	0.02403800	C	-3.41457300	-4.19281300	2.84294200
N	-2.48345100	0.32550200	-2.58330200	C	-3.99169600	-5.36977900	2.35150900
H	-1.27086900	4.42357200	1.61253800	C	-5.15586400	-5.31267100	1.57930600
H	-1.53853900	4.72303600	4.05725900	C	-5.73882900	-4.06920400	1.30632200
H	-3.61459900	3.94156400	5.19372300	C	-5.15787600	-2.89799900	1.80031300
H	-5.41586400	2.85983300	3.85264900	C	-3.35360500	-1.65882000	3.07935400
H	-5.14093800	2.56320400	1.41155300	C	-2.52578700	-0.90070200	1.99652100
H	-3.96778600	3.48279200	-0.65626100	C	-2.03219800	0.41972900	2.60637200
H	-2.26433500	3.95674900	-0.54673600	N	-1.42065600	-1.68614100	1.48857600
H	-3.40051700	1.13858000	-0.20618400	N	-1.61355000	1.42235200	1.58794500
H	-3.45498300	2.20942000	-2.48633500	H	-2.51218200	-4.24719900	3.44784600
H	-1.67377100	2.26050300	-2.45217900	H	-3.53311100	-6.32999100	2.57612500
H	-1.28107900	1.75079500	0.99868400	H	-5.60887000	-6.22550100	1.20057700
H	-2.59540000	0.35869900	-3.59879200	H	-6.64955400	-4.01289200	0.71450300
H	-3.31050800	-0.17419400	-2.24393100	H	-5.62418100	-1.93718300	1.58966300
				H	-4.14596400	-0.99107300	3.44566100
				H	-2.69120500	-1.88062000	3.92631200
				H	-3.25405200	-0.61959200	1.19757300
				H	-2.82217100	0.85624300	3.23408800
				H	-1.16394800	0.21676200	3.24068900
				H	-1.76665200	-2.62413700	1.27203000
				H	-1.22834200	2.22539700	2.09001600
				H	-2.44121700	1.76184100	1.09544300

PhPDA-chel-1				PhPDA-chel-1s			
Mo	1.06063400	0.07183300	0.68368800	Mo	1.18512300	0.74673200	0.70412500
O	2.85365200	-0.92890900	0.16022400	O	-0.34765300	2.00708600	1.72475300
O	0.57533000	-1.53947800	1.97490900	O	1.47740700	-0.92268100	1.97349900
C	-0.11952300	-2.51911500	1.53464100	C	1.05694800	-2.06610300	1.59644500
C	-0.48078900	-3.66197600	2.48533200	C	1.23030000	-3.29957900	2.48428100
Mo	0.03410300	-0.90221500	-0.93611000	Mo	0.17446800	-0.48059800	-0.74287300
O	-0.51360000	-2.52739100	0.31839400	O	0.44919900	-2.18828500	0.47266600
O	1.80600500	-1.90471400	-1.52894500	O	0.87695500	2.89026200	0.13690400
C	2.87209000	-1.71663200	-0.84501500	C	-0.00536400	3.03978000	1.05464400
C	4.15678200	-2.44134400	-1.25009700	C	-0.57352800	4.42325200	1.37262600
O	-0.19183700	1.30038300	1.85911600	O	3.06174300	0.31522400	-0.18747400
O	-2.27805000	1.69795100	1.11878600	O	2.04736700	-0.90560700	-1.73823500
C	-1.36072000	1.83647100	1.95535300	C	3.11627400	-0.39373500	-1.24689800
C	-1.57507800	2.70644300	3.21876000	C	4.44907500	-0.61045500	-1.96944200
O	1.97986200	1.87409800	0.08833200	C	-1.89089100	4.30083300	2.15865300
O	2.38606800	2.08972600	-2.11461900	H	-2.65673300	3.77653600	1.57545700
C	2.54549100	2.43969300	-0.92698400	H	-1.74936400	3.75489500	3.09605300
C	3.45652900	3.64084600	-0.57389100	H	-2.27132200	5.30183400	2.39526000
C	-1.27325700	-4.75655300	1.75092200	C	-0.80352300	5.20764200	0.06505400
H	-0.69567800	-5.18509400	0.92492600	H	-1.17797700	6.21140300	0.29908000
H	-1.51686300	-5.56344900	2.45238200	H	0.12308100	5.30908900	-0.50736500
H	-2.21083600	-4.36720200	1.34045900	H	-1.54712800	4.71191800	-0.57099500
C	0.82713600	-4.25372000	3.06008400	C	0.48490800	5.15593800	2.23637100
H	1.40628300	-3.49205400	3.59095700	H	1.43274700	5.26044200	1.69742000
H	0.58803400	-5.06024400	3.76361000	H	0.12072500	6.15915900	2.48874500
H	1.45593700	-4.67314900	2.26541800	H	0.67469600	4.61837100	3.17271300
C	-1.33336900	-3.07918100	3.63779500	C	1.91802500	-4.41387800	1.66330800
H	-2.26650900	-2.64357900	3.26072000	H	2.02696900	-5.31330100	2.28150900
H	-1.59328900	-3.87772600	4.34321200	H	1.33108900	-4.67268300	0.77683900
H	-0.78620200	-2.30242400	4.18068100	H	2.91814800	-4.10537800	1.33542400
C	-1.31823400	1.83947200	4.47143400	C	2.07540100	-2.96537400	3.72518000
H	-0.29859900	1.44289600	4.47649700	H	1.60700700	-2.18289500	4.33080500
H	-1.46084000	2.44195300	5.37768500	H	2.18295000	-3.86241500	4.34696200
H	-2.01485900	0.99287100	4.51803500	H	3.07725600	-2.62091600	3.44659500
C	-0.56564400	3.87607700	3.18671400	C	-0.17755700	-3.77383100	2.91996100
H	0.46469900	3.50839800	3.17014400	H	-0.69416800	-3.00067200	3.50114000
H	-0.71816300	4.50797800	2.30281100	H	-0.79684400	-4.02196600	2.05229600
H	-0.69545100	4.50538500	4.07652600	H	-0.08713600	-4.66787400	3.54905500
C	-3.00793700	3.26226400	3.26036300	C	4.67121500	-2.12814100	-2.15896500
H	-3.13989300	3.87961000	4.15816500	H	3.85493400	-2.57925000	-2.73123300
H	-3.22290200	3.88215500	2.38355700	H	5.61034800	-2.30041400	-2.69882500
H	-3.74910900	2.45615800	3.28830500	H	4.73737100	-2.64232400	-1.19256100
C	5.31606300	-2.06525000	-0.31193000	C	5.61401300	-0.00786100	-1.16588400
H	5.52228300	-0.99041000	-0.34054500	H	6.55584300	-0.17921400	-1.70121700
H	5.09767800	-2.33841900	0.72569900	H	5.49060000	1.07095400	-1.02654600
H	6.22365400	-2.59681200	-0.62227200	H	5.69647700	-0.46734800	-0.17504400
C	4.50427900	-2.04125400	-2.70328900	C	4.35962300	0.07439200	-3.35456000
H	5.41874500	-2.55840800	-3.01792100	H	5.29919100	-0.07176900	-3.90123000
H	3.69922300	-2.31473700	-3.39260700	H	3.54534000	-0.34790700	-3.95235900
H	4.67820000	-0.96206900	-2.78711900	H	4.19270500	1.15385100	-3.25366800
C	3.89762600	-3.96487500	-1.18129100	C	-4.92590800	-0.51067700	-0.98171800
H	3.07763600	-4.25746700	-1.84459800	C	-5.25052300	-0.67659500	0.37273100
H	4.80076800	-4.50614900	-1.48798200	C	-6.06492900	-1.73305700	0.79475500
H	3.64520900	-4.27889600	-0.16128100	C	-6.57213600	-2.64472400	-0.13622200
C	-4.88499600	0.61029600	-2.05767200	C	-6.26095900	-2.48851200	-1.49167400
C	-5.42170600	0.53823800	-0.76231600	C	-5.44776200	-1.43007200	-1.90662700
C	-6.56813400	-0.22119000	-0.50282800	C	-4.03266400	0.61989700	-1.44727900
C	-7.19710700	-0.92113000	-1.53711300	C	-2.56376600	0.20641900	-1.69148400
C	-6.67340600	-0.85475300	-2.83328800	C	-1.79020200	1.33459100	-2.40231000

C	-5.52810100	-0.09490200	-3.08849400	N	-1.83983600	-0.16417500	-0.47677700
C	-3.62892700	1.41131000	-2.33587700	N	-0.35806100	0.91977400	-2.48726400
C	-2.34114400	0.55804900	-2.34389500	H	-4.86372100	0.02801900	1.10568500
C	-1.10720100	1.39094800	-2.70014100	H	-6.30208800	-1.84235400	1.85026300
N	-2.07267400	-0.10751900	-1.03675800	H	-7.20654400	-3.46533500	0.18920300
N	0.10452300	0.53364000	-2.66863600	H	-6.65516800	-3.18711700	-2.22589900
H	-4.93920900	1.08341500	0.04594900	H	-5.21793100	-1.31335200	-2.96439500
H	-6.97024800	-0.26147800	0.50648600	H	-4.43421600	1.03526800	-2.38190100
H	-8.09001400	-1.50803400	-1.33756400	H	-4.04438000	1.43458100	-0.70969200
H	-7.15986000	-1.38857700	-3.64601500	H	-2.57316700	-0.66096500	-2.37279200
H	-5.13436000	-0.04109100	-4.10199100	H	-2.19014000	1.56021700	-3.40007800
H	-3.71357500	1.90154000	-3.31434500	H	-1.83261700	2.24497800	-1.79581200
H	-3.51684800	2.20409800	-1.58630800	H	-2.17124900	0.37515500	0.32228100
H	-2.45005700	-0.24000100	-3.09051400	H	0.25203000	1.73576400	-2.52263000
H	-1.23439800	1.86434500	-3.68099000	H	-0.19171700	0.40730400	-3.35542200
H	-0.96750000	2.18351400	-1.95770200				
H	-2.17052200	0.57422100	-0.25832000				
H	0.96063500	1.11041200	-2.56718600				
H	0.19010300	0.01531100	-3.54512200				
C	4.13022900	4.20326900	-1.83622500				
H	3.39007800	4.55048800	-2.56480600				
H	4.77103900	5.05252600	-1.56672600				
H	4.75281700	3.44783400	-2.32786900				
C	4.53611600	3.17446900	0.42774100				
H	5.18918200	4.01632300	0.69101800				
H	4.08371500	2.78749700	1.34550800				
H	5.16356100	2.38442700	-0.00367400				
C	2.58508900	4.73654700	0.08157500				
H	3.20934700	5.59847600	0.34997700				
H	1.80569000	5.08796400	-0.60652700				
H	2.09891300	4.36512700	0.98863500				
H	-2.77189400	-0.83265500	-0.86963000				
PhPDA-chel-2							
Mo	-0.71756100	0.48401700	0.80211000				
O	0.42229200	1.97278600	1.87755900				
C	1.49684600	2.41143900	1.33945900				
C	2.38540400	3.40025600	2.10393100				
Mo	0.70586200	0.48752900	-0.79775500				
O	1.87234000	1.98857200	0.19208800				
O	-1.87602700	2.00080900	-0.17590600				
O	-0.42722300	1.98729100	-1.86295600				
C	-1.49856100	2.42997100	-1.31880700				
C	-2.34007100	3.46509700	-2.07503600				
C	3.09647700	4.34731000	1.11755800				
H	3.74344500	5.03916200	1.67082400				
H	3.71272300	3.79154400	0.40509200				
H	2.37290300	4.94250600	0.54778000				
C	1.54607500	4.21784700	3.10340600				
H	1.04695900	3.57142400	3.83126900				
H	2.19582400	4.91436100	3.64742900				
H	0.77555800	4.80402100	2.58895000				
C	3.44256000	2.56802800	2.87328700				
H	2.96670800	1.88331200	3.58524600				
H	4.05993600	1.97915300	2.18560200				
H	4.10372500	3.23801500	3.43698900				
C	-1.43582400	4.65819100	-2.45879100				
H	-0.59338200	4.33345400	-3.07706400				
H	-2.01681400	5.39756000	-3.02384400				
H	-1.03463900	5.15384100	-1.56641900				
C	-3.51410700	3.95705900	-1.21169600				

H	-4.09857200	4.69590100	-1.77381900
H	-4.18003500	3.13427400	-0.93211000
H	-3.16167700	4.43142000	-0.28935300
C	-2.88233200	2.79625400	-3.36105200
H	-3.48081700	3.51775300	-3.93096200
H	-2.06429600	2.44757200	-3.99983800
H	-3.52439300	1.93947100	-3.12231800
C	4.48964400	-2.96615400	-0.79810900
C	4.97264200	-2.87445900	0.51689600
C	6.31041000	-2.55360100	0.77484600
C	7.19305100	-2.31818400	-0.28354500
C	6.72703700	-2.40917000	-1.60040700
C	5.39037500	-2.73101800	-1.85138300
C	3.03769200	-3.28601600	-1.08195800
C	2.18225000	-2.03841700	-1.42431300
C	0.76686200	-2.46662300	-1.83274000
N	2.04186800	-1.09490400	-0.31216500
N	-0.13454500	-1.27764800	-1.91561600
H	4.29452600	-3.06114900	1.34670300
H	6.66173400	-2.49075000	1.80208400
H	8.23325700	-2.07164100	-0.08617300
H	7.40582800	-2.23445000	-2.43183800
H	5.04060300	-2.80594300	-2.87942600
H	2.98086300	-3.98930200	-1.92544200
H	2.58816700	-3.78133000	-0.21150800
H	2.65397800	-1.56556700	-2.30967400
H	0.77563600	-3.00850100	-2.78523100
H	0.36068200	-3.14006700	-1.06989300
H	2.96740000	-0.79797800	0.00219300
H	-1.00472800	-1.44863400	-1.36540600
H	-0.39904700	-1.08394700	-2.88041000
C	-4.51768100	-2.95225200	0.77731800
C	-5.00146200	-2.84490500	-0.53621200
C	-6.33808400	-2.51576300	-0.78959500
C	-7.21881000	-2.28774600	0.27201000
C	-6.75203300	-2.39441900	1.58742100
C	-5.41650100	-2.72437300	1.83381300
C	-3.06674500	-3.28064100	1.05645900
C	-2.20576100	-2.03963600	1.40890900
C	-0.79220000	-2.47761000	1.81341300
N	-2.06173400	-1.08731800	0.30475000
N	0.11506000	-1.29373900	1.90551900
H	-4.32481500	-3.02584300	-1.36848600
H	-6.69003300	-2.44066300	-1.81579600
H	-8.25814100	-2.03476900	0.07819600
H	-7.42935500	-2.22550700	2.42124800
H	-5.06611000	-2.81131100	2.86070000
H	-3.01184000	-3.99171000	1.89352800
H	-2.62021300	-3.76989100	0.18105000
H	-2.67520100	-1.57217400	2.29833200
H	-0.80339900	-3.02690000	2.76162500
H	-0.38943100	-3.14709100	1.04525800
H	-2.98617400	-0.78348600	-0.00634000
H	0.98369500	-1.46416800	1.35254500
H	0.38177700	-1.11011000	2.87164000