Supporting Information

DFT investigations of 2D raft-type heterometallic clusters [MMoCp(or $C_5H_4NMe_2$)$(CO)_3]_n$ with triangular (n = 3) or square (n = 4) Cu, Ag, or Au cores.

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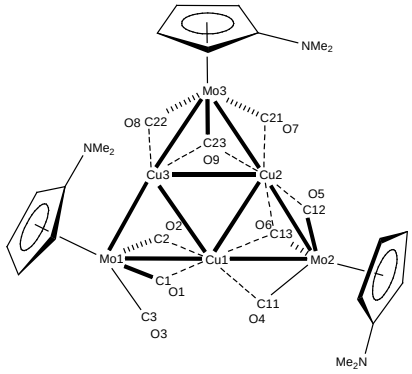
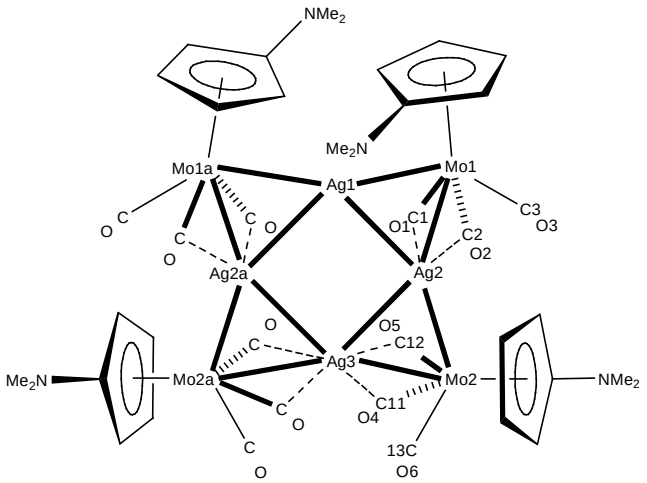


(E = −194049.4511517 eV) HOMO–LUMO gap (eV) = +2.30849 eV

Distances (Å)			**Angles**		
	Exp	**Calc**		**Exp**	**Calc**
Cu(1)–Cu(2)	2.6548(7)	2.642	Cu(1)–Cu(2)–Cu(3)	58.60(3)	57.965
Cu(2)–Cu(3)	2.6159(9)	2.580	Cu(1)–Cu(3)–Cu(2)	61.46(3)	62.256
Cu(1)–Cu(3)	2.5794(14)	2.531	Cu(2)–Cu(1)–Cu(3)	59.95(3)	59.779
Mo(1)–Cu(1)	2.6516(7)	2.683	Cu(1)–Mo(1)–Cu(3)	58.50(3)	56.480
Mo(1)–Cu(3)	2.6272(8)	2.665	Cu(1)–Mo(2)–Cu(2)	60.36(3)	59.346
Mo(2)–Cu(1)	2.6279(9)	2.668	Cu(2)–Mo(3)–Cu(3)	58.87(3)	57.458

Mo(2)–Cu(2)	2.6526(13)	2.669	Mo(1)–C(1)–O(1)	169.1(3)	165.164
Mo(3)–Cu(2)	2.6670(16)	2.678	Mo(1)–C(2)–O(2)	170.6(3)	169.729
Mo(3)–Cu(3)	2.6559(8)	2.689	Mo(1)–C(3)–O(3)	175.6(3)	175.775
Cu(1)–C(1)	2.331(4)	2.235	Mo(2)–C(11)–O(4)	168.6(3)	164.475
Cu(1)–C(2)	2.283(4)	2.384	Mo(2)–C(12)–O(5)	167.4(3)	165.331
Cu(1)–C(11)	2.259(4)	2.195	Mo(2)–C(13)–O(6)	166.9(3)	163.298
Cu(1)–C(13)	2.427(4)	2.358	Mo(3)–C(21)–O(7)	168.1(4)	164.304
Cu(2)–C(12)	2.314(4)	2.197	Mo(3)–C(22)–O(8)	168.7(4)	166.680
Cu(2)–C(13)	2.350(4)	2.283	Mo(3)–C(23)–O(9)	164.6(3)	161.590
Cu(2)–C(21)	2.187(5)	2.199			
Cu(2)–C(23)	2.311(4)	2.317			
Cu(3)–C(22)	2.190(5)	2.197			
Cu(3)–C(23)	2.227(4)	2.224			

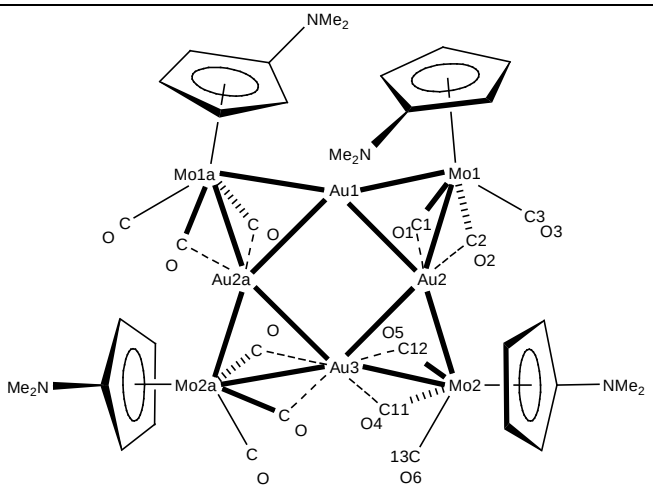
Table S2. Measured experimental and optimized geometric parameters of the complex $[Ag_4\{Mo(\eta^5\text{-}C_5H_4\text{-}NMe_2)(CO)_3\}_4]$ **A2** (distances in angstroms and angles in degrees).



(E = −96145.7651599 eV) HOMO–LUMO gap (eV) = +2.29816 eV

Distances (Å)			**Angles**		
	Exp	**Calc**		**Exp**	**Calc**
Ag(1)–Ag(2)	2.8287(7)	2.840	Ag(1)–Ag(2)–Ag(3)	86.80(2)	87.270
Ag(2)– Ag(3)	2.9088(7)	2.944	Ag(2)–Ag(3)–Ag(2a)	91.51(3)	90.567
Ag(1)–Ag(3)	3.943	3.992	Ag(2)–Ag(1)–Ag(2a)	94.89(3)	94.893
Ag(2)–Ag(2a)	4.167	4.184	Mo(1)–(1)–Mo(1a)	149.81(4)	150.092
Ag(1)–Mo(1)	2.8805(6)	2.911	Mo(1)–Ag(2)–Mo(2)	157.55(3)	159.096
Ag(2)–Mo(1)	2.8539(8)	2.913	Mo(1)–Ag(1)– Ag(2)	59.976(16)	60.857
Ag(2)–Mo(2)	2.7994(8)	2.834	Mo(1)–Ag(2)–Ag(1)	60.912(18)	60.769
Ag 3)–Mo(2)	2.8555(5)	2.890	Mo(2)–Ag(2)–Ag(3)	59.996(17)	59.980
Ag(1)–C(1)	2.850	2.674	Mo(2)–Ag(3)–Ag(2)	58.100(16)	58.109
Ag(1)–C(2)	3.300	3.400	Mo(1)–C(1)–O(1)	169.9(6)	167.728
Ag(2)–C(1)	2.529(7)	2.688	Mo(1)–C(2)–O(2)	168.5(6)	164.310
Ag(2)–C(2)	2.445(7)	2.389	Mo(1)–C(3)–O(3)	175.7(7)	177.018
Ag(2)–C(3)	3.313	3.330	Mo(2)–C(11)–O(4)	171.5(5)	167.010
Ag(2)–C(11)	2.842	2.977	Mo(2)–C(12)–O(5)	169.4(6)	167.762
Ag(2)–C(12)	2.735	2.755	Mo(2)–C(13)–O(6)	172.6(7)	174.056
Ag(3)–C(11)	2.587(6)	2.506			
Ag(3)–C(12)	2.575(7)	2.664			
Ag(3)–C(13)	2.947	3.06			

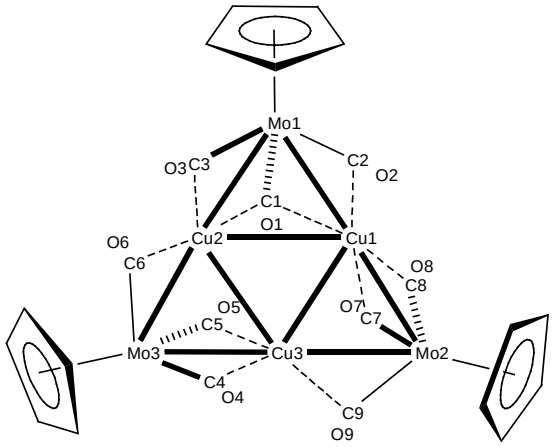
Table S3. Measured experimental and optimized geometric parameters of the complex $[Au_4\{Mo(\eta^5\text{-}C_5H_4\text{-}NMe_2)(CO)_3\}_4]$ **A3** (distances in angstroms and angles in degrees).



(E = −94927.5044792 eV) HOMO–LUMO gap (eV) = +2.01199 eV

Distances (Å)			**Angles**		
	Exp	**Calc**		**Exp**	**Calc**
Au(1)–Au(2)	2.7598(5)	2.883	Au(1)–Au(2)–Au(3)	87.874(18)	91.131
Au(2)–Au(3)	2.8248(5)	2.930	Au(2)–Au(3)–Au(2a)	90.74(2)	87.963
Au(1)–Au(3)	3.875	4.151	Au(2)–Au(1)–Au(2a)	93.51(2)	89.774
Au(2)–Au(2a)	4.021	4.070	Mo(1)–Au(1)–Mo(1a)	149.88(3)	154.525
Au(1)–Mo(1)	2.8437(7)	2.881	Mo(1)–Au(2)–Mo(2)	155.196(1)	156.896
Au(2)–Mo(1)	2.8140(8)	2.923	Mo(1)–Au(1)–Au(2)	60.267(17)	60.927
Au(2)–Mo(2)	2.7753(8)	2.837	Mo(1)–Au(2)–Au(1)	61.345(17)	59.506
Au(3)–Mo(2)	2.8114(7)	2.882	Mo(2)–Au(2)–Au(3)	60.262(18)	59.947
Au(1)–C(1)	2.868	2.616	Mo(2)–Au(3)–Au(2)	58.996(16)	58.418
Au(1)–C(2)	3.273	3.414	Mo(1)–C(1)–O(1)	171.2(6)	168.589
Au(2)–C(1)	2.564(6)	2.927	Mo(1)–C(2)–O(2)	167.4(6)	159.625
Au(2)–C(2)	2.413(6)	2.295	Mo(1)–C(3)–O(3)	176.3(6)	176.435
Au(2)–C(3)	3.285	3.294	Mo(2)–C(11)–O(4)	172.2(5)	163.800
Au(2)–C(11)	2.924	3.122	Mo(2)–C(12)–O(5)	169.6(6)	170.084
Au(2)–C(12)	2.808	2.816	Mo(2)–C(13)–O(6)	174.4(6)	174.002
Au(3)–C(11)	2.593(6)	2.412			
Au(3)–C(12)	2.566(7)	2.811			
Au(3)–C(13)	3.014	3.152			

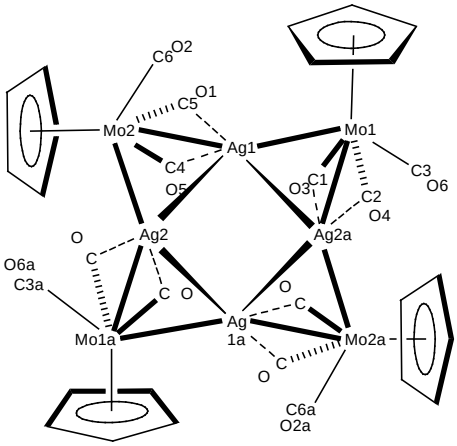
Table S4. Measured experimental and optimized geometric parameters of the complex $[Cu_3\{Mo(\eta^5\text{-}C5H_5)(CO)_3\}_3]$ **A4** (distances in angstroms and angles in degrees).



(E = −183108.9977034 eV) HOMO–LUMO gap (eV) = +2.25794 eV

Distances (Å)			**Angles**		
	Exp	**Calc**		**Exp**	**Calc**
Cu(1)–Cu(2)	2.6587(11)	2.614	Cu(1)–Cu(2)–Cu(3)	59.41(3)	59.943
Cu(2)–Cu(3)	2.6207(10)	2.599	Cu(1)–Cu(3)–Cu(2)	61.02(3)	60.317
Cu(1)–Cu(3)	2.6165(10)	2.604	Cu(2)–Cu(1)–Cu(3)	59.57(3)	59.740
Mo(1)–Cu(1)	2.6433(9)	2.646	Cu(1)–Mo(1)–Cu(2)	60.27(2)	58.739
Mo(1)–Cu(2)	2.6525(8)	2.683	Cu(1)–Mo(2)–Cu(3)	59.27(3)	58.537
Mo(2)–Cu(1)	2.6691(9)	2.684	Cu(2)–Mo(3)–Cu(3)	59.68(2)	58.419
Mo(2)–Cu(3)	2.6218(9)	2.642	Mo(1)–C(1)–O(1)	164.6(5)	163.559
Mo(3)–Cu(3)	2.6471(9)	2.682	Mo(1)–C(2)–O(2)	167.3(6)	164.672
Mo(3)–Cu(2)	2.6196(8)	2.643	Mo(1)–C(3)–O(3)	169.1(5)	165.239
Cu(1)–C(1)	2.382(7)	2.445	Mo(2)–C(7)–O(7)	168.0(6)	164.512
Cu(1)–C(2)	2.176(6)	2.180	Mo(2)–C(8)–O(8)	168.4(6)	165.00
Cu(1)–C(7)	2.284(6)	2.298	Mo(2)–C(9)–O(9)	166.4(7)	164.530
Cu(1)–C(8)	2.301(7)	2.220	Mo(3)–C(4)–O(4)	168.6(5)	164.647
Cu(2)–C(1)	2.261(6)	2.292	Mo(3)–C(5)–O(5)	167.7(5)	165.754
Cu(2)–C(3)	2.235(6)	2.202	Mo(3)–C(6)–O(6)	169.0(6)	164.136
Cu(2)–C(6)	2.203(7)	2.165			
Cu(3)–C(9)	2.141(7)	2.174			
Cu(3)–C(4)	2.266(6)	2.265			
Cu(3)–C(5)	2.304(7)	2.267			

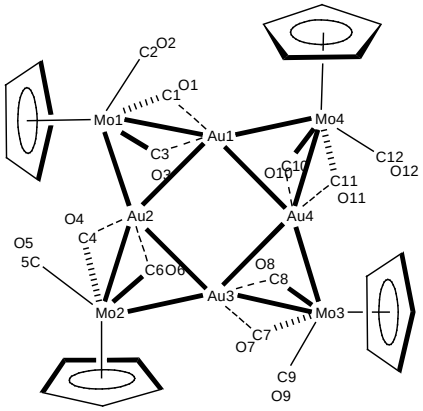
Table S5. Measured experimental and optimized geometric parameters of the complex $[Ag_4\{Mo(\eta^5\text{-}C_5H_5)(CO)_3\}_4]$ **A5** (distances in angstroms and angles in degrees).



(*E* = −81558.3428799 eV) HOMO–LUMO gap (eV) = +2.37743 eV

Distances (Å)			**Angles**		
	Exp	**Calc**		**Exp**	**Calc**
Ag(1)–Ag(2)	2.8408(9)	2.910	Ag(2)–Ag(1)–Ag(2a)	100.23(3)	88.760
Ag(2)–Ag(1a)	2.8999(9	2.889	Ag(1)–Ag(2)–Ag(1a)	75.92(3)	87.416
Ag(1)–Ag(1a)	3.531	4.001	Mo(1)–Ag(1)–Mo(2)	147.80(3)	152.452
Ag(2)–Ag(2a)	4.405	4.056	Mo(2)–Ag(2)–Mo(1)	163.56(3)	153.588
Ag(1)–Mo(1)	2.8115(9)	2.855	O(3)–C(1)–Mo(1)	167.0(7)	166.297
Ag(1)–Mo(2)	2.8868(9)	2.910	O(4)–C(2)–Mo(1)	169.1(7)	167.893
Ag(1)–C(4)	2.569(9)	2.627	O(6)–C(3)–Mo(1)	174.7(7)	175.804
Ag(1)–C(5)	2.584(8)	2.481	O(5)–C(4)–Mo2	168.8(7)	167.736
Ag(2)–C(1)	2.591(8)	2.471	O(1)–C(5)–Mo(2)	170.4(7)	166.348
Ag(2)–C(2)	2.596(9)	2.635	O(2)–C(6)–Mo(2)	177.4(7)	175.881
Ag(2)–Mo(2)	2.8216(10)	2.855			
Ag(2)–Mo(1)	2.8749(10)	2.908			

Table S6. Measured experimental and optimized geometric parameters of the complex $[Au_4\{Mo(\eta^5\text{-}C_5H_5)(CO)_3\}_4]$ **A6** (distances in angstroms and angles in degrees).



(E = −94927.5044792 eV) HOMO–LUMO gap (eV) = +2.01199 eV

Distances (Å)			**Angles**		
	Exp	**Calc**		**Exp**	**Calc**
Au(1)–Au(2)	2.7417(8)	2.897	Au(1)–Au(2)–Au(3)	90.53(2)	90.137
Au(2)–Au(3)	2.8030(9)	2.897	Au(3)–Au(4)–Au(1)	90.41(2)	90.047
Au(3)–Au(4)	2.7512(8)	2.899	Au(2)–Au(1)–Au(4)	89.58(2)	89.745
Au(1)–Au(4)	2.7995(8)	2.900	Au(4)–Au(3)–Au(2)	89.32(2)	89.789
Au(1)–Au(3)	3.939	4.102	Mo(1)–Au(1)–Mo(4)	154.29(3)	155.615
Au(2)–Au(4)	3.904	4.091	Mo(1)–Au(2)–Mo(2)	150.99(3)	155.143
Au(1)–Mo(1)	2.8527(12)	2.899	Mo(2)–Au(3)–Mo(3)	153.87(3)	155.654
Au(1)–Mo(4)	2.8243(12)	2.856	Mo(3)–Au(4)–Mo(4)	152.17(3)	155.489
Au(2)–Mo(1)	2.8054(12	2.857	Mo(1)–C(1)–O(1)	163.3(9)	165.024
Au(2)–Mo(2)	2.8114(11)	2.897	Mo(1)–C(2)–O(2)	175.9(11)	175.586
Au(3)–Mo(2)	2.7975(11)	2.859	Mo(1)–C(3)–O(3)	169.9(13)	168.889
Au(3)–Mo(3)	2.8259(12)	2.898	Mo(2)–C(4)–O(4)	169.3(10)	169.005
Au(1)–C(1)	2.336(11)	2.457	Mo(2)–C(5)–O(5)	175.4(11)	175.516
Au(2)–C(4)	2.511(13)	2.683	Mo(2)–C(6)–O(6)	172.5(11)	164.813
Au(2)–C(6)	2.584(12)	2.446	Mo(3)–C(7)–O(7)	163.3(10)	164.734
Au(3)–C(7)	2.329(11)	2.442	Mo(3)–C(8)–O(8)	168.8(12)	169.074
Au(4)–C(11)	2.513(15)	2.692	Mo(3)–C(9)–O(9)	173.6(13)	175.638

Au(4)–C(10)	2.524(12)	2.439	Mo(4)–C(10)–O(10)	170.4(10)	164.533
Au(4)–C(8)	2.672(14)	2.929	Mo(4)–C(11)–O(11)	169.8(13)	169.126
			Mo(4)–C(12)–O(12)	174.6(11)	175.649

Table S7. Energy decomposition in (kJ/mol) of BP86 functional obtained by interactions between the metal cores Cu_n and the metalloligand fragments $[MoC_5H_4NMe_2)(CO)_3]_n$ (n = 3 for **A1, A18, A21**, and n = 4 for **A7, A10, A13**)

Complex	ΔE_{Int}	ΔE_{Pauli}	ΔE_{ster}	ΔE_{elstat}	ΔE_{Orb}
A1	−4931.42	1954.20	−2502.96	−4457.16	−2428.42
A7	−7596.26	2273.48	−4110.52	−6384.00	−3485.75
A10	−7296.74	3010.49	−3936.70	−6947.19	−3360.06
A13	−7281.84	3005.73	−3938.55	−6944.28	−3343.26
A18	−4934.97	2006.97	−2519.74	−4526.72	−2415.25
A21	−4948.50	2040.77	−2519.4	−4560.27	−2428.9

Table S8. Energy decomposition in (kJ/mol) of BP86 functional obtained by interactions between the metal cores Ag_n and the metalloligand fragments $[MoC_5H_4NMe_2)(CO)_3]_n$ (n = 3 for **A14, A16, A19**, and n = 4 for **A2, A8, A11, A37**)

Complex	ΔE_{Int}	ΔE_{Pauli}	ΔE_{ster}	ΔE_{elstat}	ΔE_{Orb}
A14	−4467.87	1488.94	−2645.12	−4134.06	−1822.75
A16	−4447.01	1357.86	−2688.42	−4046.28	−1758.59
A19	−4471.83	1485.42	−2685.85	−4171.26	−1785.99
A2	−6967.21	1738.84	−4237.29	−5976.13	−2729.91
A8	−6968.46	1695.68	−4282.42	−5978.10	−2686.04
A11	−6944.37	1768.59	−4283.39	−6051.98	−2660.94
A37	−6662.59	2531.08	−4014.25	−6545.32	−2648.39

Table S9. Energy decomposition in (kJ/mol) of BP86 functional obtained by interactions between the metal cores Au_n and the metalloligand fragments $[MoC_5H_4NMe_2)(CO)_3]_n$ (n = 3 for **A14, A16, A19**, and n = 4 for **A2, A8, A11, A37**)

Complex	ΔE_{Int}	ΔE_{Pauli}	ΔE_{ster}	ΔE_{elstat}	ΔE_{Orb}
A15	−4987.91	2310.85	−2414.60	−4725.45	−2573.30
A17	−4963.35	2146.48	−2480.17	−4626.65	−2483.17
A20	−5005.04	2377.88	−2442.58	−4820.46	−2562.45
A3	−7679.67	3209.07	−3433.10	−6642.17	−4246.60
A9	−7586.28	2610.00	−3947.68	−6557.68	−3638.65
A12	−7606.89	2597.42	−3924.29	−6521.71	3682.54
A38	−7435.28	3717.70	−3716.81	−7434.50	−3718.41

Table S10. Energy decomposition in (kJ/mol) of BP86 functional obtained by interactions between the metal cores Cu_n and the metalloligand fragments $[MoCp)(CO)_3]_n$ (n = 3 for **A4, A34**, and n = 4 for **A24, A27, A29, A31, A41,A42**)

Complex	ΔE_{Int}	ΔE_{Pauli}	ΔE_{ster}	ΔE_{elstat}	ΔE_{Orb}
A4	−4879.49	2043.00	−2510.78	−4553.78	−2368.72

A34	−4862.47	1953.07	−2498.43	−4451.50	−2364.03
A24	−7508.49	2314.99	−4125.52	−6440.51	−3382.98
A27	−3308.37	1927.93	−4249.83	−6177.76	−3308.37
A29	−7466.56	2540.81	−4111.26	−6652.07	−3355.32
A31	−7490.22	2460.42	−4145.41	−6605.83	−3344.82
A40	−7344.99	3686.53	−3708.19	−7394.72	−3636.74
A41	−7257.68	3064.18	−3921.28	−6985.46	−3336.44

Table S11. Energy decomposition in (kJ/mol) of BP86 functional obtained by interactions between the metal cores Ag_n and the metalloligand fragments $[MoCp(CO)_3]_n$ (n = 3 for **A32, A35** and *n* = 4 for **A5, A22, A25, A28, A39**)

Complex	ΔE_{Int}	ΔE_{Pauli}	ΔE_{ster}	ΔE_{elstat}	ΔE_{Orb}
A32	−4398.84	1442.08	−2654.39	−4096.47	−1744.45
A35	−4393.05	1482.61	−2660.17	−4142.78	−1732.88
A5	−6894.09	1708.73	−4273.17	−5981.89	−2620.95
A22	−6879.73	1746.76	−4260.61	−6007.37	−2619.07
A25	−6917.62	1650.93	−4284.98	−5935.91	−2632.61
A28	−6869.50	1716.85	−4272.52	−5989.37	−2596.99
A39	−6599.34	2465.12	−4031.44	−6496.56	−2567.93

Table S12. Energy decomposition in (kJ/mol) of BP86 functional obtained by interactions between the metal cores Au_n and the metalloligand fragments $[MoCp(CO)_3]_n$ (*n* = 3 for **A33, A36** and *n* = 4 for **A6, A23, A26, A30, A40**)

Complex	ΔE_{Int}	ΔE_{Pauli}	ΔE_{ster}	ΔE_{elstat}	ΔE_{Orb}
A33	−4906.60	2297.54	−2401.26	−4698.80	−2505.30
A36	−2482.35	2342.24	−2424.86	−4767.10	−2482.35
A6	−7505.29	2553.78	−3932.93	−6486.71	−3572.38
A23	−7585.20	3125.25	−3473.32	−6598.57	−4111.87
A26	−7568.39	3087.75	−3472.69	−6560.44	−4095.66
A30	−7522.06	2632.34	−3901.59	−6533.94	−3620.48
A40	−7344.99	3686.53	−3708.19	−7394.72	−3636.74

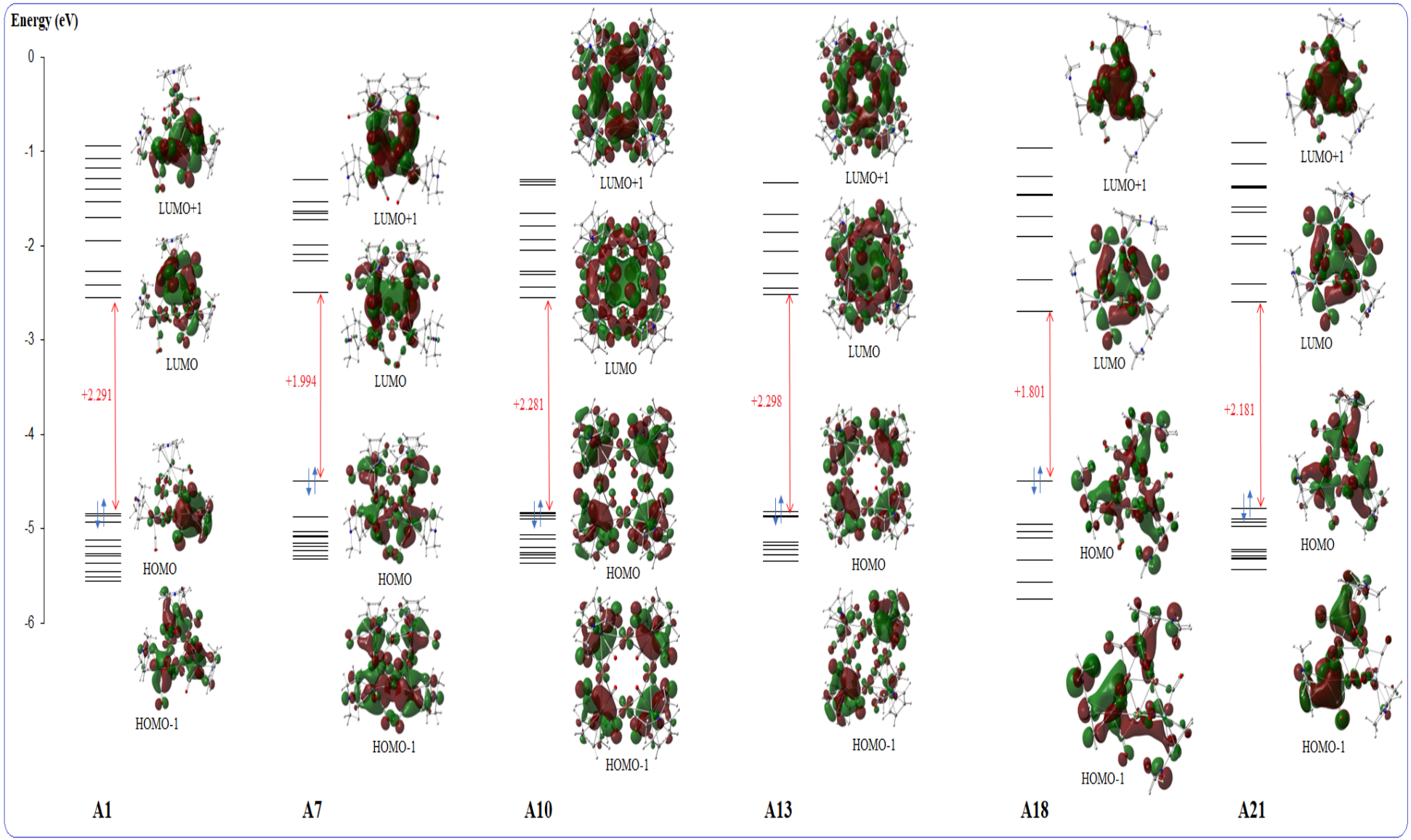


Figure S1. Molecular orbital energy (eV) of $[CuMoC_5H_4NMe_2(CO)_3]_n$ (n = 3 for **A1, A18, A21**, and n = 4 for **A7, A10, A13**)

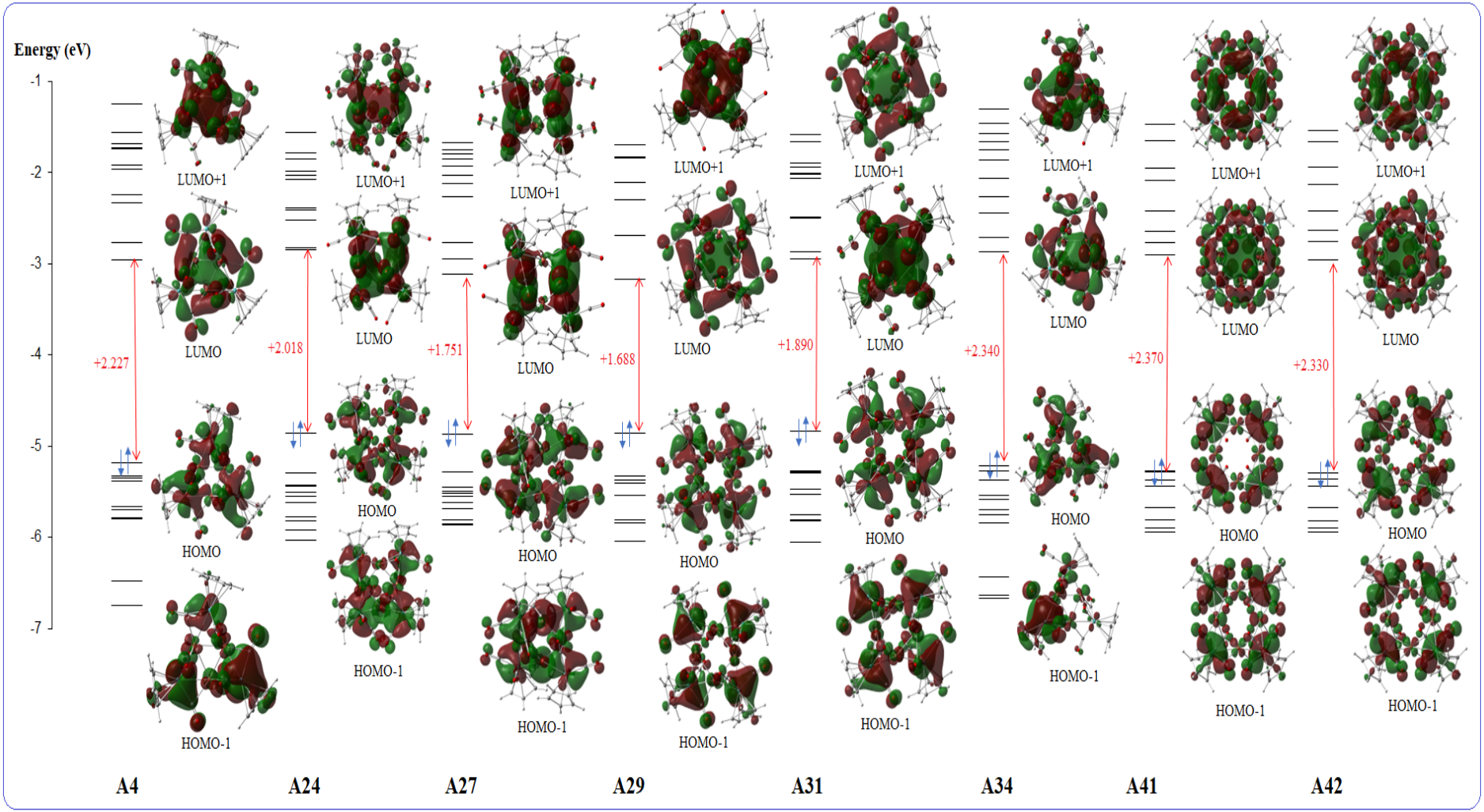


Figure S2. Molecular orbital energy (eV) of $[CuMoCp(CO)_3]_n$ (n = 3 for **A4, A34** and n = 4 for **A24, A27, A29, A31, A34, A41, A42**)

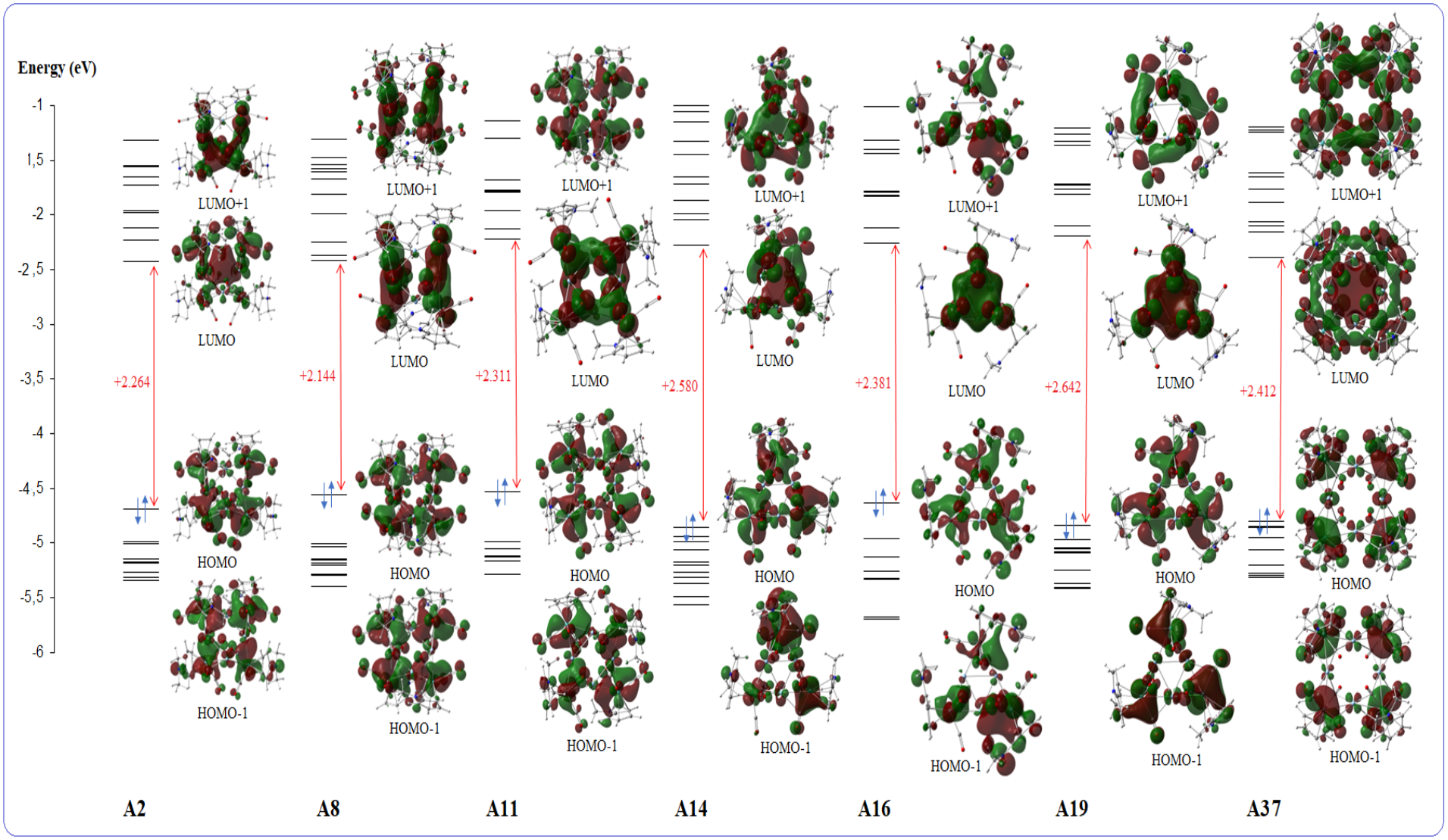


Figure S3. Molecular orbital energy (eV) of $[AgMoC_5H_4NMe_2(CO)_3]_n$ (n = 3 for **A14, A16, A19** and n = 4 for **A2, A8, A11, A37**)

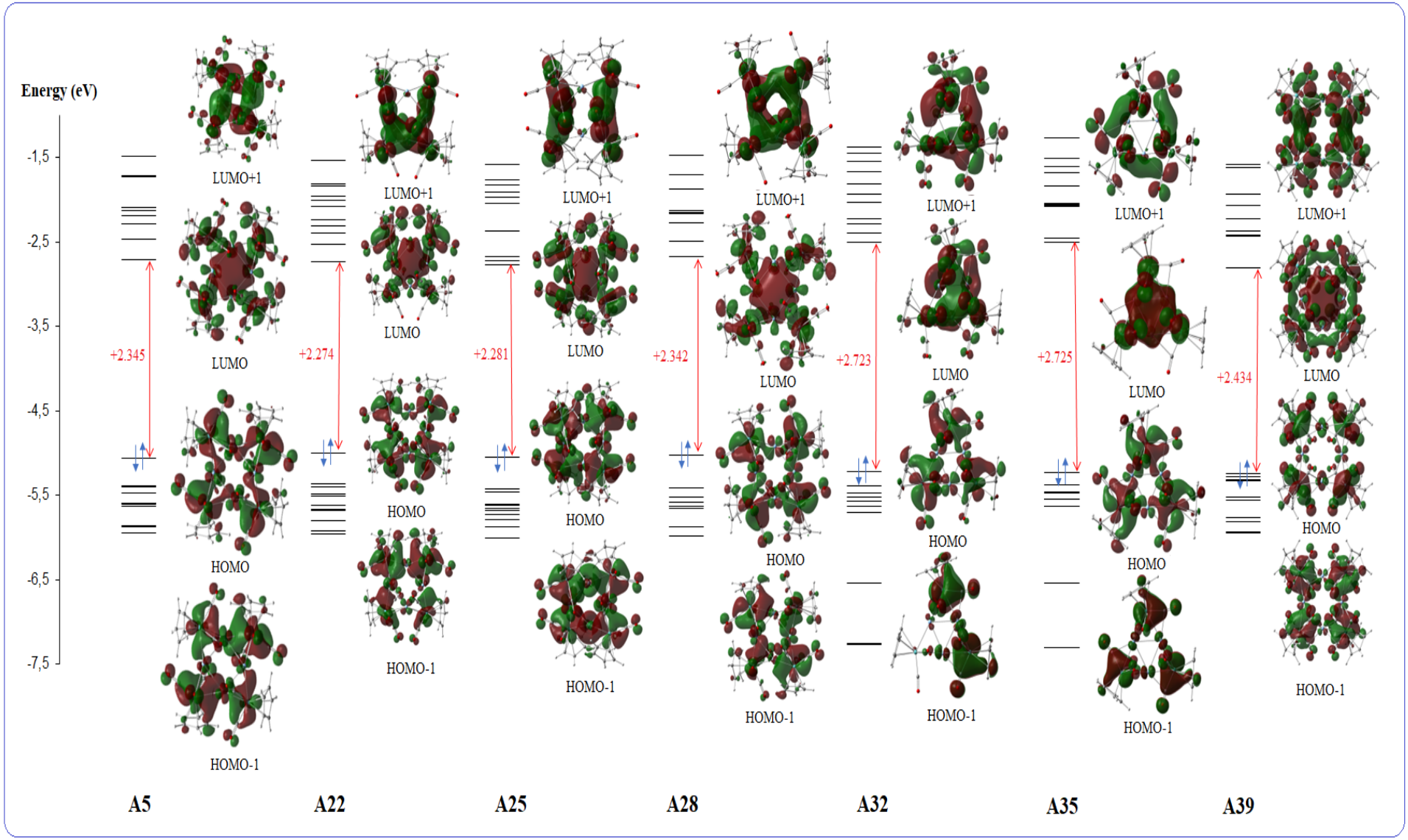


Figure S4. Molecular orbital energy (eV) of $[AgMoCp(CO)_3]_n$ (n = 3 for **A32, A35** and n = 4 for **A5, A22, A25, A28, A39**)

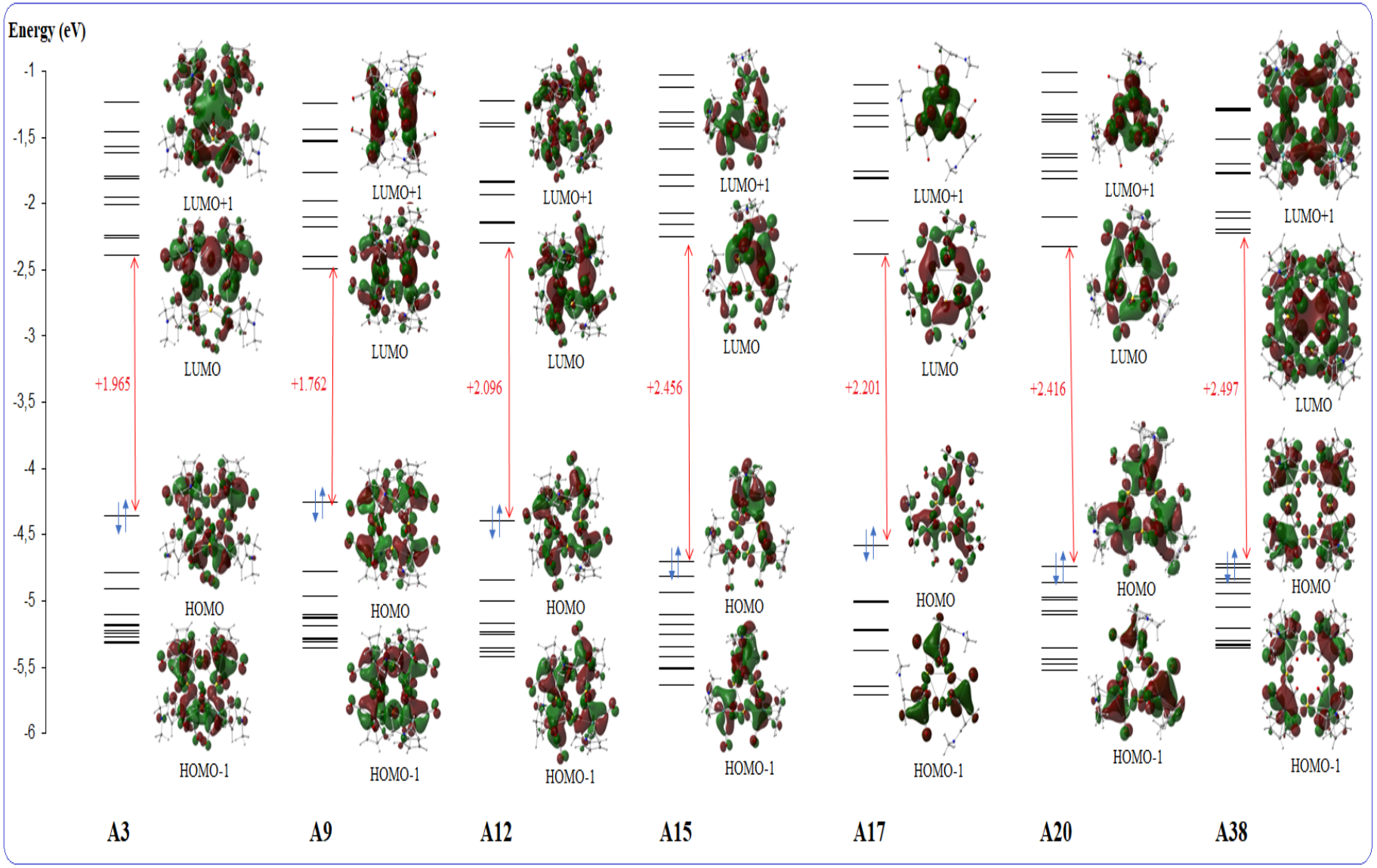


Figure S5. Molecular orbital energy (eV) of $[AuMoC_5H_4NMe_2(CO)_3]_n$ (n = 3 for **A15, A17, A20** and n = 4 for **A3, A9, A12, A38**)

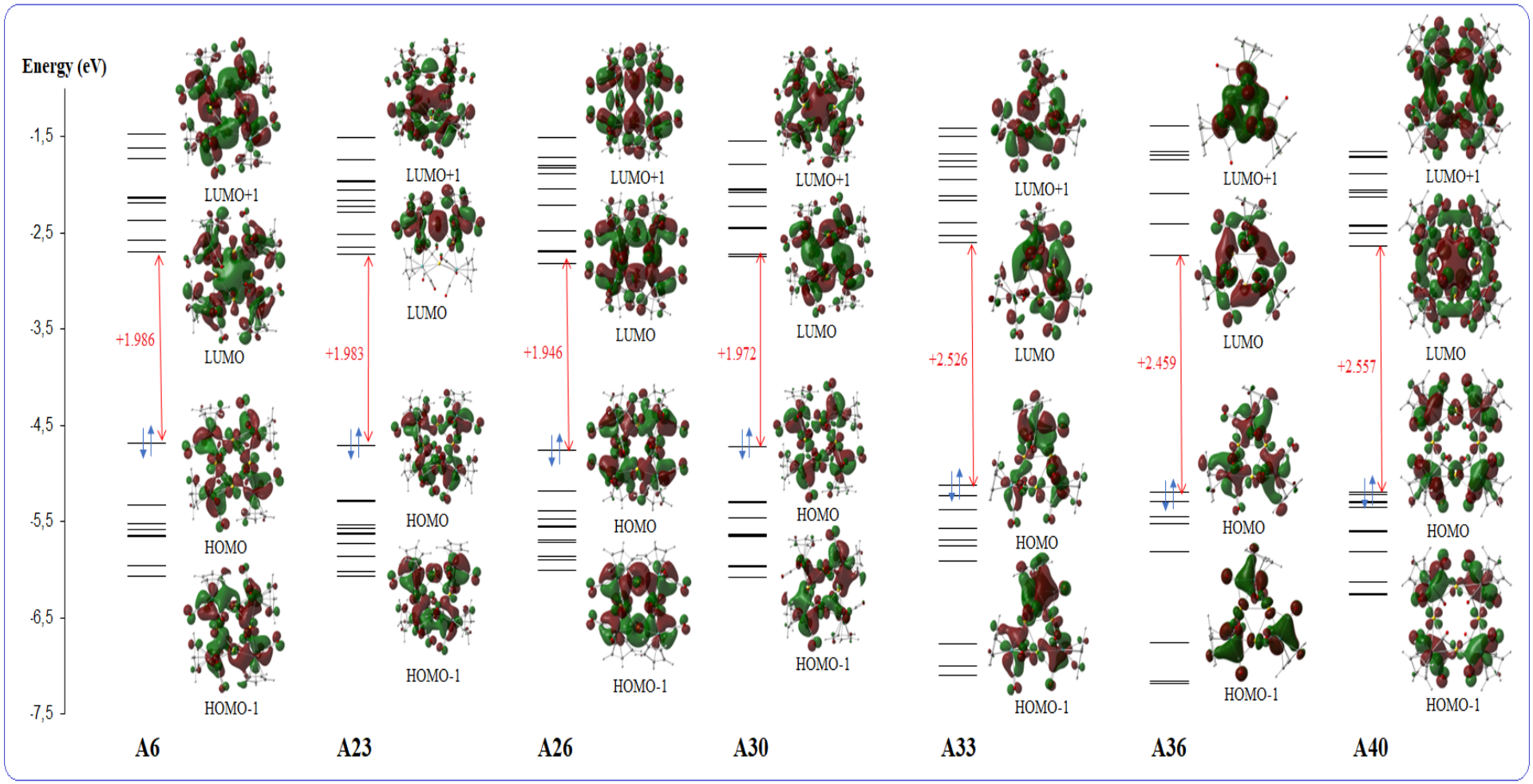


Figure S6. Molecular orbital energy (eV) of $[AuMoCp(CO)_3]_n$ (n = 3 for **A33, A36** and n = 4 for **A6, A23, A26, A30, A40**)

List of coordinates

$[CuMoC_5H_4NMe_2(CO)_3]_n$ (*n* = 3 for **A1, A18, A21**, and *n* = 4 for **A7, A10, A13**)

Complex A1			
H	5.1313065	-3.0897978	-2.8609307
H	4.8293295	-4.4680087	-1.7555488
C	4.4307390	-3.4894464	-2.0990732
H	3.4375785	-3.6622207	-2.5836791
H	5.1866596	-0.9848523	-2.1027822
N	4.3530801	-2.5541641	-0.9850795
H	4.1699049	3.5728391	-3.2155174
C	4.4345426	-1.1355804	-1.3005078
O	0.7681962	-2.0951198	-2.4618332
H	2.2574952	4.6758740	-3.5919210
H	3.3827131	-5.1733730	-0.1541839
H	3.4578736	-0.7110746	-1.6428954
H	4.7759677	-0.5635538	-0.4116006
O	-1.7842524	1.2865395	-2.9037464
C	3.8801277	3.1811415	-2.2180297
H	3.5839858	2.1099162	-2.3328406
C	0.8197062	-2.3927334	-1.3237994
C	3.2322052	-4.2796154	0.4623919
C	3.6627712	-2.9416021	0.1394232
C	1.7896929	4.4816723	-2.6047306
H	4.7749082	3.2408008	-1.5624078
H	0.9622560	3.7431694	-2.7418292
O	1.3578134	0.9365060	-2.0004274
O	-2.5629058	-3.2479169	-2.0133685
H	1.3560671	5.4389257	-2.2448088
O	-0.2968745	-5.7292002	-0.3651267
H	-5.3769488	-1.6610203	-2.5895928
N	2.8094611	4.0063708	-1.6786715
C	-2.1855886	0.6395985	-1.9979019
H	-4.9944144	1.0335049	-2.7794314
C	0.2092840	-4.7249445	-0.0495112
C	-2.6501226	-2.2072668	-1.4597065
Mo	1.1921061	-3.0934350	0.5140643
C	2.7084245	-4.2807670	1.8129623
C	3.2395769	-2.0871282	1.2390393
C	-5.3257067	-0.9492976	-1.7553193
C	1.0865637	1.2434856	-0.8810301
C	-5.1286892	0.4579397	-1.8539868
H	2.3926188	-5.1686536	2.3761103
H	3.4958950	-1.0275515	1.3671024
Cu	-1.0641835	-1.7410767	-0.0163365
C	2.4942564	3.9087212	-0.3459975
Mo	-3.2839672	-0.4582733	-0.7549313
C	2.7136661	-2.9355760	2.2837642
Cu	1.0206649	-0.4343933	0.5765569
H	4.1278701	2.5690379	0.5055092
Cu	-1.0748667	0.8991526	-0.1203512
C	-5.4796803	-1.2847593	-0.3573001
H	0.6138162	5.1679936	-0.1412164
C	3.2256839	3.1695391	0.6671365
C	-5.1537382	1.0110274	-0.5228128
H	-5.6850471	-2.2894724	0.0295828
C	1.3799074	4.5368680	0.3236969
H	2.3884544	-2.5836212	3.2714739
C	-0.3093172	-2.8138851	1.7927659
H	-5.0503427	2.0740931	-0.2772448
Mo	1.0289827	2.2397600	0.8546898
C	-5.4912905	-0.0526332	0.4030009
C	-2.5668626	-0.3147652	1.1087192
C	2.6669666	3.4934313	1.9541801
O	-1.0377451	-2.8437413	2.7194949
C	1.5315322	4.3292525	1.7473317
C	1.1740971	0.9010154	2.3138430
C	-0.8835883	2.6319754	1.2200617
H	3.0631722	3.1644667	2.9237356
O	-2.4764670	-0.1883149	2.2839465
N	-5.7726080	0.0888800	1.7357020
O	1.3431149	0.3189812	3.3319436
O	-1.8984778	3.1404122	1.5534648
H	0.8934082	4.7659023	2.5263043
H	-6.4704617	-1.8724264	2.1184686
H	-4.8037031	-1.5435145	2.7413705

Complex A18			
Cu	1.5108737	-0.0969200	-0.0354327
Cu	-0.6701591	1.3550999	-0.0392312
Mo	-3.0754263	0.2368209	-0.0217763
C	-4.9947521	-0.5688465	-1.1838126
C	-4.9745369	-1.4084513	-0.0040529
C	-5.0257369	-0.5096247	1.1311111
C	-5.2313767	0.8279648	0.6538889
C	-5.2113728	0.7930695	-0.7819097
H	-4.9429769	-0.9179892	-2.2219084
H	-4.9998067	-0.8031865	2.1871042
H	-5.3966962	1.7130522	1.2814922
H	-5.3634084	1.6448856	-1.4569309
C	-2.0791810	-0.3004992	-1.6659821
O	-1.7700946	-0.6022875	-2.7650721
C	-2.0849025	-0.3462058	1.6102976
O	-1.7717481	-0.6654977	2.7029857
C	-2.6641872	2.1685787	0.0293322
O	-2.7758615	3.3506195	0.0674675
N	-4.9638349	-2.7830804	0.0281268
C	-4.6621432	-3.4398864	1.2926852
H	-5.3361650	-3.0642831	2.0929909
H	-4.8383354	-4.5296596	1.1863331
H	-3.6029029	-3.2859553	1.6125769
C	-4.6501240	-3.4932626	-1.2038703
H	-4.7982246	-4.5805398	-1.0436709
H	-5.3358390	-3.1732061	-2.0184688
H	-3.5956949	-3.3288077	-1.5352135
Cu	-0.8404512	-1.2602107	-0.0372853
Mo	1.7443089	2.5457160	-0.0250646
Mo	1.3347741	-2.7823245	-0.0229268
C	1.9969264	4.6143605	-1.1834301
C	2.9998795	-4.0358867	-1.1807832
C	1.2650171	5.0121379	0.0007839
C	3.7105223	-3.5978346	0.0025290
C	2.0761046	4.6069136	1.1311865
C	2.9544319	-4.0957302	1.1340737
C	3.3352616	4.1183589	0.6464271
C	1.9019329	-4.9439483	0.6515146
C	3.2880108	4.1230701	-0.7896126
C	1.9286889	-4.9073022	-0.7847624
H	1.6639872	4.7459132	-2.2198869
H	3.2809949	-3.8130218	-2.2168786
H	1.8141376	4.7275776	2.1892435
H	3.1905904	-3.9249268	2.1912170
H	4.1885365	3.8190564	1.2686350
H	1.2161392	-5.5317442	1.2752616
H	4.0987174	3.8325934	-1.4699042
H	1.2706017	-5.4652104	-1.4630514
C	0.7791765	1.9529952	-1.6684773
C	1.3068358	-1.6487815	-1.6658534
O	0.3615564	1.8374305	-2.7668151
O	1.4184175	-1.2293274	-2.7640696
C	0.7432525	1.9752596	1.6057184
C	1.3332414	-1.6330659	1.6096958
O	0.3095028	1.8618253	2.6978687
O	1.4461933	-1.2028677	2.7034485
C	3.2136004	1.2254524	0.0181672
C	-0.5433375	-3.3945929	0.0176790
O	4.2928187	0.7304372	0.0480149
O	-1.5109868	-4.0829523	0.0488396
N	0.0658791	5.6838310	0.0410007
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H	5.3127731	-3.0875447	2.1066825
H	-1.5113924	6.4297894	1.2058761
H	6.3396211	-1.9231963	1.2089537
H	-1.0421803	4.7377596	1.6197820
H	4.6447333	-1.4718908	1.6319077
C	-0.7106200	5.7669401	-1.1879528
C	5.3573506	-2.2674003	-1.1861171

H	-6.0214576	2.1897361	1.7970450
C	-5.8155326	-1.1002554	2.5759681
H	-4.4415600	1.6159019	2.4629469
C	-5.5280808	1.3772453	2.3731753
H	-6.2475064	-0.8321214	3.5618569
H	-5.9724561	1.3654766	3.3891809

Complex A7

H	3.6843977	-5.5981399	-2.5084341
H	4.6004013	-4.3702112	-3.4392244
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H	1.4465398	-5.5671676	-2.3913670
H	4.1842227	-4.0614157	-1.7031497
H	-2.8177852	-4.0710479	3.8064612
N	2.5574530	-3.9320452	-3.1033341
C	1.3318049	-4.4707861	-2.5196702
H	-3.2828482	-3.9099181	1.1184947
H	1.0931482	-4.0121808	-1.5310241
C	-3.3425021	-3.2629240	3.2810137
H	4.7580942	-2.1311443	-3.7552871
H	0.4711065	-4.2954091	-3.1967100
C	-3.5922116	-3.1810209	1.8794978
O	2.9299918	-2.4270466	0.0426872
O	-0.0587705	-2.8185159	0.6136753
C	2.5520003	-2.6551094	-3.5987564
C	3.7107541	-1.8391677	-3.8947785
O	-1.5432489	-2.5341556	-2.1113332
C	-3.9389341	-2.0991063	3.9023080
O	-0.2586533	-1.7673963	4.9658095
C	-0.7900253	-2.1404105	1.2485796
H	-3.9457799	-1.8959552	4.9794942
C	2.6852134	-1.5543067	-0.7147450
C	-4.3452032	-1.9805177	1.6175588
H	6.3161396	-1.0836467	4.4534060
O	2.3884017	-1.7035190	2.9073326
C	-0.9021069	-1.5858614	4.0040950
H	6.6839662	-1.2208250	2.2487231
H	5.0101295	-1.1627040	1.5667473
H	-4.7423510	-1.6895819	0.6388664
C	-4.6564968	-1.3576490	2.8882080
Mo	-2.1730020	-1.4242927	2.4919453
C	1.3887147	-1.8556053	-3.9263144
H	4.5259267	-0.8966443	4.6202827
C	3.2673353	-0.6394391	-4.5733494
H	0.3459250	-2.1761168	-3.8260848
C	-1.7859028	-1.3730389	-2.0750123
C	5.8580165	-0.5431116	1.9486715
C	5.4799966	-0.3557609	4.4033402
H	3.9187795	0.1197961	-5.0250755
O	5.2986421	0.9022647	-1.6182219
Mo	2.5626780	-0.4438869	-2.3708993
C	4.2562571	0.4151473	-1.8565836
H	-1.1973103	-0.1092029	-5.0397165
C	2.1769097	-0.5699752	2.6633442
H	-5.6460516	-0.4023408	5.1983848
H	6.2285457	0.0937925	1.1185555
C	1.8427211	-0.6531501	-4.5852092
H	5.6460516	0.4023408	5.1983848
N	-5.4794691	-0.2780303	3.0921754
N	5.4794691	0.2780303	3.0921754
Cu	-1.8294774	-0.2631360	0.1253250
H	-6.2285457	-0.0937925	1.1185555
Cu	0.0000000	0.0000000	2.0276052
Cu	0.0000000	0.0000000	-1.6274272
C	-5.4799966	0.3557609	4.4033402
Cu	1.8294774	0.2631360	0.1253250
C	-1.8427211	0.6531501	-4.5852092
H	-3.9187795	-0.1197961	-5.0250755
O	-5.2986421	-0.9022647	-1.6182219
H	1.1973103	0.1092029	-5.0397165
C	-4.2562571	-0.4151473	-1.8565836
C	-5.8580165	0.5431116	1.9486715
H	-4.5259267	0.8966443	4.6202827
C	-2.1769097	0.5699752	2.6633442
C	-3.2673353	0.6394391	-4.5733494
Mo	-2.5626780	0.4438869	-2.3708993
H	-6.3161396	1.0836467	4.4534060
H	-6.6839662	1.2208250	2.2487231
C	4.6564968	1.3576490	2.8882080

H	-1.5826791	6.4308365	-1.0202176
H	6.3727614	-1.8540771	-1.0188912
H	-0.0973570	6.2097001	-2.0027689
H	5.4273737	-3.0188163	-2.0027381
H	-1.0893349	4.7704734	-1.5225351
H	4.6917558	-1.4345989	-1.5202182

Complex A10

H	3.8650156	1.7856431	-5.1580941
H	5.1717954	2.1712134	-3.9891506
C	4.0822981	1.9645143	-4.0860328
H	2.2041589	3.2051582	-5.4119845
H	3.8517594	1.0340491	-3.5154004
N	3.3041011	3.1086617	-3.6270575
C	2.0917708	3.4859846	-4.3447797
H	1.1791448	2.9916690	-3.9383995
H	5.3499201	2.4474547	-1.6546582
H	1.9457134	4.5870999	-4.2980603
O	1.1072706	0.9881635	-2.3564299
C	3.4926861	3.5583765	-2.3518512
C	4.5535412	3.1707275	-1.4458811
C	1.5542663	1.4618744	-1.3552442
C	2.6692530	4.5196414	-1.6406546
C	4.4897045	4.0305683	-0.2855105
H	1.7561743	4.9919488	-2.0207282
H	5.2210329	4.0499246	0.5331736
O	4.2883082	1.0306261	1.9763365
Mo	2.6245975	2.6553379	-0.1448736
C	3.5739157	1.5010648	1.1578076
C	3.3370920	4.8602347	-0.4107019
Cu	0.0000000	-2.2819683	0.0000000
Cu	0.0000000	2.2819683	0.0000000
Cu	2.4059330	0.0000000	0.0000000
H	3.0140935	5.6355882	0.2968485
C	1.4704219	3.2758903	1.3426061
O	0.9985796	3.8098984	2.2883748
H	-3.8650156	-1.7856431	-5.1580941
H	-5.1717954	-2.1712134	-3.9891506
C	-4.0822981	-1.9645143	-4.0860328
H	-2.2041589	-3.2051582	-5.4119845
H	-3.8517594	-1.0340491	-3.5154004
N	-3.3041011	-3.1086617	-3.6270575
C	-2.0917708	-3.4859846	-4.3447797
H	-1.1791448	-2.9916690	-3.9383995
H	-5.3499201	-2.4474547	-1.6546582
H	-1.9457134	-4.5870999	-4.2980603
O	-1.1072706	-0.9881635	-2.3564299
C	-3.4926861	-3.5583765	-2.3518512
C	-4.5535412	-3.1707275	-1.4458811
C	-1.5542663	-1.4618744	-1.3552442
C	-2.6692530	-4.5196414	-1.6406546
C	-4.4897045	-4.0305683	-0.2855105
H	-1.7561743	-4.9919488	-2.0207282
H	-5.2210329	-4.0499246	0.5331736
O	-4.2883082	-1.0306261	1.9763365
Mo	-2.6245975	-2.6553379	-0.1448736
C	-3.5739157	-1.5010648	1.1578076
C	-3.3370920	-4.8602347	-0.4107019
Cu	-2.4059330	0.0000000	0.0000000
H	-3.0140935	-5.6355882	0.2968485
C	-1.4704219	-3.2758903	1.3426061
O	-0.9985796	-3.8098984	2.2883748
H	3.8650156	-1.7856431	5.1580941
H	5.1717954	-2.1712134	3.9891506
C	4.0822981	-1.9645143	4.0860328
H	2.2041589	-3.2051582	5.4119845
H	3.8517594	-1.0340491	3.5154004
N	3.3041011	-3.1086617	3.6270575
C	2.0917708	-3.4859846	4.3447797
H	1.1791448	-2.9916690	3.9383995
H	5.3499201	-2.4474547	1.6546582
H	1.9457134	-4.5870999	4.2980603
O	1.1072706	-0.9881635	2.3564299
C	3.4926861	-3.5583765	2.3518512
C	4.5535412	-3.1707275	1.4458811
C	1.5542663	-1.4618744	1.3552442
C	2.6692530	-4.5196414	1.6406546
C	4.4897045	-4.0305683	0.2855105
H	1.7561743	-4.9919488	2.0207282

H	-0.3459250	2.1761168	-3.8260848
C	1.7859028	1.3730389	-2.0750123
C	-1.3887147	1.8556053	-3.9263144
H	-5.0101295	1.1627040	1.5667473
H	4.7423510	1.6895819	0.6388664
Mo	2.1730020	1.4242927	2.4919453
H	3.9457799	1.8959552	4.9794942
C	0.9021069	1.5858614	4.0040950
C	4.3452032	1.9805177	1.6175588
O	-2.3884017	1.7035190	2.9073326
C	3.9389341	2.0991063	3.9023080
O	0.2586533	1.7673963	4.9658095
C	-3.7107541	1.8391677	-3.8947785
C	-2.6852134	1.5543067	-0.7147450
C	0.7900253	2.1404105	1.2485796
O	1.5432489	2.5341556	-2.1113332
C	-2.5520003	2.6551094	-3.5987564
H	-4.7580942	2.1311443	-3.7552871
C	3.5922116	3.1810209	1.8794978
C	3.3425021	3.2629240	3.2810137
O	-2.9299918	2.4270466	0.0426872
O	0.0587705	2.8185159	0.6136753
H	-0.4711065	4.2954091	-3.1967100
H	-1.0931482	4.0121808	-1.5310241
H	3.2828482	3.9099181	1.1184947
N	-2.5574530	3.9320452	-3.1033341
H	2.8177852	4.0710479	3.8064612
C	-1.3318049	4.4707861	-2.5196702
H	-4.1842227	4.0614157	-1.7031497
H	-1.4465398	5.5671676	-2.3913670
C	-3.8195354	4.5073651	-2.6607915
H	-4.6004013	4.3702112	-3.4392244
H	-3.6843977	5.5981399	-2.5084341
H	5.2210329	-4.0499246	-0.5331736
O	4.2883082	-1.0306261	-1.9763365
Mo	2.6245975	-2.6553379	0.1448736
C	3.5739157	-1.5010648	-1.1578076
C	3.3370920	-4.8602347	0.4107019
H	3.0140935	-5.6355882	-0.2968485
C	1.4704219	-3.2758903	-1.3426061
O	0.9985796	-3.8098984	-2.2883748
H	-3.8650156	1.7856431	5.1580941
H	-5.1717954	2.1712134	3.9891506
C	-4.0822981	1.9645143	4.0860328
H	-2.2041589	3.2051582	5.4119845
H	-3.8517594	1.0340491	3.5154004
N	-3.3041011	3.1086617	3.6270575
C	-2.0917708	3.4859846	4.3447797
H	-1.1791448	2.9916690	3.9383995
H	-5.3499201	2.4474547	1.6546582
H	-1.9457134	4.5870999	4.2980603
O	-1.1072706	0.9881635	2.3564299
C	-3.4926861	3.5583765	2.3518512
C	-4.5535412	3.1707275	1.4458811
C	-1.5542663	1.4618744	1.3552442
C	-2.6692530	4.5196414	1.6406546
C	-4.4897045	4.0305683	0.2855105
H	-1.7561743	4.9919488	2.0207282
H	-5.2210329	4.0499246	-0.5331736
O	-4.2883082	1.0306261	-1.9763365
Mo	-2.6245975	2.6553379	0.1448736
C	-3.5739157	1.5010648	-1.1578076
C	-3.3370920	4.8602347	0.4107019
H	-3.0140935	5.6355882	-0.2968485
C	-1.4704219	3.2758903	-1.3426061
O	-0.9985796	3.8098984	-2.2883748

Complex A13

H	-1.1419150	-4.0155840	5.2460079
H	-0.9671742	-5.3469859	4.0569859
C	-1.1355580	-4.2524745	4.1626606
H	-2.9675453	-2.7842090	5.2924084
H	-0.2808557	-3.7180185	3.6850191
N	-2.4235276	-3.8818265	3.5882864
C	-3.1925087	-2.8082551	4.2067679
H	-2.9607229	-1.8080193	3.7717212
H	-1.0142029	-5.6672867	1.7572405
H	-4.2815562	-2.9982689	4.0889395
O	-0.8314587	-1.2487982	2.3424434
C	-2.6967379	-4.2359345	2.2978971
C	-1.9335191	-5.1448880	1.4679340
C	-1.1402765	-1.8216428	1.3413919
C	-3.8133992	-3.7759573	1.4926646
C	-2.6861608	-5.3873145	0.2581749
H	-4.5717392	-3.0460763	1.7975642
H	-2.4205122	-6.1113991	-0.5232967
O	0.0822505	-4.3214219	-1.9987847
Mo	-1.9566664	-3.1848493	0.1111090
C	-0.5677186	-3.7679119	-1.1777590
C	-3.8385183	-4.5491846	0.2766936
Cu	2.2968602	0.5550122	-0.0494460
Cu	-2.2968602	-0.5550122	-0.0494460
Cu	0.5550122	-2.2968602	0.0494460
H	-4.6208550	-4.5011939	-0.4923587
C	-2.8463873	-2.2390939	-1.3865564
O	-3.4705855	-1.9276359	-2.3433103
H	1.1419150	4.0155840	5.2460079
H	0.9671742	5.3469859	4.0569859
C	1.1355580	4.2524745	4.1626606
H	2.9675453	2.7842090	5.2924084
H	0.2808557	3.7180185	3.6850191
N	2.4235276	3.8818265	3.5882864
C	3.1925087	2.8082551	4.2067679
H	2.9607229	1.8080193	3.7717212
H	1.0142029	5.6672867	1.7572405
H	4.2815562	2.9982689	4.0889395
O	0.8314587	1.2487982	2.3424434
C	2.6967379	4.2359345	2.2978971
C	1.9335191	5.1448880	1.4679340
C	1.1402765	1.8216428	1.3413919
C	3.8133992	3.7759573	1.4926646
C	2.6861608	5.3873145	0.2581749

Complex A21

Cu	-0.0143516	-1.3959113	0.6791396
Cu	1.1419267	0.9131394	0.3565292
Mo	-0.1977435	3.0165273	-0.5103162
C	-1.1846564	4.5878157	-1.9279347
C	-2.0234375	4.5387200	-0.7576674
C	-1.2903812	5.1227001	0.3491667
C	0.0599478	5.3451623	-0.1180202
C	0.0957970	5.0783994	-1.5403433
H	-1.4927737	4.3003825	-2.9417838
H	0.8847607	5.7744996	0.4624388
H	0.9560406	5.2568259	-2.1977985
C	-0.6332280	1.6818155	-1.9250805
O	-0.8737512	1.1294871	-2.9406385
C	-0.6782286	2.3048032	1.2949277
O	-1.0366122	2.1988228	2.4181395
C	1.7716972	2.7810170	-0.5808576
O	2.9390070	2.9342947	-0.7234409
H	-3.0699329	4.2130534	-0.7441710
Cu	-1.4116786	0.6583704	-0.1186909
Mo	2.6125730	-1.2499020	0.9519819
Mo	-2.6756029	-1.5740593	0.4938157
C	4.8919771	-1.3761043	-0.1290569
C	-3.5450036	-3.7780107	-0.3697100
C	4.8468602	-0.3975399	0.9379252
C	-3.0505121	-3.8844463	0.9876378
C	4.5973983	-1.0926455	2.1768737
C	-3.8795573	-3.0620315	1.8332489
C	4.3670607	-2.4662875	1.8804721
C	-4.8044143	-2.3593569	1.0072354
C	4.4738213	-2.6373173	0.4472057
C	-4.5580273	-2.7445571	-0.3658855
H	4.5950224	-0.6324954	3.1741307
H	-3.8085841	-3.0067904	2.9278013
H	4.1644792	-3.2653885	2.6053221
H	-5.5898838	-1.6698654	1.3421766
H	4.3820616	-3.5944106	-0.0795361
H	-5.1357454	-2.4004214	-1.2314573
C	2.0133396	-0.7870964	-0.8938735
C	-1.4173883	-1.7401534	-1.0484263
O	1.9279291	-0.6390795	-2.0635412
O	-0.8935633	-2.0541974	-2.0630301
C	1.8525971	0.0219713	2.2880775
C	-1.6947470	-1.0782883	2.1568864
O	1.6378548	0.6854029	3.2402717

H	4.5717392	3.0460763	1.7975642
H	2.4205122	6.1113991	-0.5232967
O	-0.0822505	4.3214219	-1.9987847
Mo	1.9566664	3.1848493	0.1111090
C	0.5677186	3.7679119	-1.1777590
C	3.8385183	4.5491846	0.2766936
Cu	-0.5550122	2.2968602	0.0494460
H	4.6208550	4.5011939	-0.4923587
C	2.8463873	2.2390939	-1.3865564
O	3.4705855	1.9276359	-2.3433103
H	4.0155840	-1.1419150	-5.2460079
H	-4.0155840	1.1419150	-5.2460079
H	5.3469859	-0.9671742	-4.0569859
H	-5.3469859	0.9671742	-4.0569859
C	4.2524745	-1.1355580	-4.1626606
C	-4.2524745	1.1355580	-4.1626606
H	2.7842090	-2.9675453	-5.2924084
H	-2.7842090	2.9675453	-5.2924084
H	3.7180185	-0.2808557	-3.6850191
H	-3.7180185	0.2808557	-3.6850191
N	3.8818265	-2.4235276	-3.5882864
N	-3.8818265	2.4235276	-3.5882864
C	2.8082551	-3.1925087	-4.2067679
C	-2.8082551	3.1925087	-4.2067679
H	1.8080193	-2.9607229	-3.7717212
H	-1.8080193	2.9607229	-3.7717212
H	5.6672867	-1.0142029	-1.7572405
H	-5.6672867	1.0142029	-1.7572405
H	2.9982689	-4.2815562	-4.0889395
H	-2.9982689	4.2815562	-4.0889395
O	1.2487982	-0.8314587	-2.3424434
O	-1.2487982	0.8314587	-2.3424434
C	4.2359345	-2.6967379	-2.2978971
C	-4.2359345	2.6967379	-2.2978971
C	5.1448880	-1.9335191	-1.4679340
C	-5.1448880	1.9335191	-1.4679340
C	1.8216428	-1.1402765	-1.3413919
C	-1.8216428	1.1402765	-1.3413919
C	3.7759573	-3.8133992	-1.4926646
C	-3.7759573	3.8133992	-1.4926646
C	5.3873145	-2.6861608	-0.2581749
C	-5.3873145	2.6861608	-0.2581749
H	3.0460763	-4.5717392	-1.7975642
H	-3.0460763	4.5717392	-1.7975642
H	6.1113991	-2.4205122	0.5232967
H	-6.1113991	2.4205122	0.5232967
O	4.3214219	0.0822505	1.9987847
O	-4.3214219	-0.0822505	1.9987847
Mo	3.1848493	-1.9566664	-0.1111090
Mo	-3.1848493	1.9566664	-0.1111090
C	3.7679119	-0.5677186	1.1777590
C	-3.7679119	0.5677186	1.1777590
C	4.5491846	-3.8385183	-0.2766936
C	-4.5491846	3.8385183	-0.2766936
H	4.5011939	-4.6208550	0.4923587
H	-4.5011939	4.6208550	0.4923587
C	2.2390939	-2.8463873	1.3865564
C	-2.2390939	2.8463873	1.3865564
O	1.9276359	-3.4705855	2.3433103
O	-1.9276359	3.4705855	2.3433103
O	-1.3433624	-0.8938941	3.2669468
C	1.4680651	-2.8275174	1.3402042
C	-3.5176504	0.1923001	0.1469466
O	1.0723539	-3.9074799	1.6301749
O	-4.2836537	1.0810297	-0.0210336
H	5.0734500	0.6710070	0.8475072
H	-2.2624206	-4.5605542	1.3390286
N	-3.1233254	-4.5126545	-1.4449925
N	5.2666835	-1.1441254	-1.4263936
N	-1.7858956	5.4118566	1.5941506
C	-1.9200375	-5.3220007	-1.2988307
H	-1.0335324	-4.7112653	-1.0043135
H	-2.0691568	-6.1159466	-0.5325603
H	-1.6953459	-5.8175689	-2.2641128
C	-3.5781574	-4.1303718	-2.7753424
H	-3.1747412	-3.1398730	-3.0978951
H	-3.2511750	-4.8970845	-3.5067927
H	-4.6893763	-4.0873726	-2.8054405
C	5.0198490	-2.1674505	-2.4325786
H	5.6154659	-1.9352197	-3.3399004
H	5.3512276	-3.1595143	-2.0590841
H	3.9433173	-2.2340650	-2.7230280
C	5.4185743	0.2352032	-1.8740757
H	4.4475882	0.7833047	-1.9207406
H	6.0989293	0.7885085	-1.1916170
H	5.8769954	0.2372607	-2.8843246
C	-3.1089489	4.9227505	1.9617571
H	-3.8446788	5.1705856	1.1671506
H	-3.1293561	3.8199543	2.1355508
H	-3.4341153	5.4305855	2.8932284
C	-0.8483440	5.7196091	2.6659849
H	-1.4119307	6.0986403	3.5431351
H	-0.2555920	4.8271074	2.9841400
H	-0.1440499	6.5174010	2.3470072

$[CuMoCp(CO)_3]_n$ (n = 3 for **A4, A34** and n = 4 for **A24, A27, A29, A31, A34, A41, A42**)

Complex A4			
Mo	2.2500209	2.0901742	-0.0007083
Mo	-2.9304841	0.8966013	0.0054210
Mo	0.6936916	-2.9988833	-0.0085103
Cu	-0.3120224	1.4557254	0.1874408
Cu	1.4372691	-0.4646911	-0.1022521
Cu	-1.1035481	-1.0097942	-0.0875294
O	1.5427751	0.6134885	2.6883906
O	0.0308255	4.2083855	-0.6860031
O	2.1322642	0.5335268	-2.7324577
O	-0.2318376	-1.8525838	-2.7896053
O	-0.4567952	-1.8199798	2.6759988
O	3.7342502	-2.2157111	0.1524120

Complex A34			
O	-0.5328940	-2.0656475	-2.7119935
H	2.0980544	-5.3895295	-1.5259389
O	-1.9252904	1.3346669	-2.7910017
C	-0.1584444	-2.3538067	-1.6355444
C	2.3421030	-4.5944786	-0.8093197
C	2.7883518	-3.2756421	-1.1345630
O	1.2887468	0.5351158	-2.6635875
O	-3.7875803	-2.4676780	-0.6746121
O	-1.5164549	-5.3399986	-0.0817778
H	-6.0541422	-0.1104222	-0.9150736
C	-2.2142841	0.9992969	-1.6973254
H	-4.9860348	2.1780368	-1.9222461

O	-1.5905873	1.4223335	2.8032208
O	-1.2258098	1.0866212	-2.6370017
O	-3.7425019	-2.1110205	0.4265870
C	1.6443773	1.0577767	1.5988098
C	0.7147041	3.2853807	-0.4031483
C	2.0481427	0.9891855	-1.6482941
C	0.0841677	-2.0979069	-1.6800441
C	-0.0522425	-2.0916934	1.6040284
C	2.5566912	-2.3078892	0.0843837
C	-1.9147877	1.1739100	1.6972358
C	-1.6999081	0.9323791	-1.5680469
C	-3.2495908	-1.0489571	0.2566054
C	4.5210871	2.0094591	0.7048104
H	4.9651342	1.1000945	1.1310399
C	4.4981964	2.3644635	-0.6818132
H	4.9245213	1.7736234	-1.5037785
C	3.8371946	3.6333109	-0.8112052
H	3.6789593	4.1896086	-1.7443303
C	3.4570984	4.0657205	0.5092572
H	2.9491730	5.0072148	0.7576254
C	3.8763828	3.0670709	1.4397944
H	3.7386103	3.1002740	2.5290324
C	1.3053794	-5.0720770	-0.9652756
H	1.9952298	-5.1436509	-1.8161131
C	1.6675420	-5.1153884	0.4272614
H	2.6867101	-5.2103035	0.8252185
C	0.4705798	-5.0342535	1.2025221
H	0.4090029	-5.0472718	2.2990593
C	-0.6454097	-4.9384724	0.2975419
H	-1.7040112	-4.8728272	0.5815864
C	-0.1258590	-4.9645192	-1.0370951
H	-0.7228412	-4.9238119	-1.9583542
C	-4.3292991	2.6217626	0.8234536
H	-4.0886802	3.1668056	1.7463715
C	-5.1100874	1.4212932	0.7366860
H	-5.5843974	0.8932512	1.5741578
C	-5.1991582	1.0561464	-0.6550455
H	-5.7475845	0.1961814	-1.0620731
C	-4.4734923	2.0259082	-1.4119860
H	-4.3535106	2.0329594	-2.5038461
C	-3.9293641	2.9974110	-0.5001809
H	-3.3261704	3.8736384	-0.7712543

C	-0.7282028	-4.4806962	-0.0547558
C	-3.3611869	-1.3982757	-0.4109888
Mo	0.7081639	-3.1080627	-0.0034538
C	2.3107338	-4.7073771	0.6309958
C	3.0335257	-2.5615309	0.0930715
C	-5.5168475	0.6569052	-0.3419565
C	1.3629646	0.9927648	-1.5742323
C	-4.9574610	1.8607294	-0.8708658
H	2.0360552	-5.6035050	1.2029002
H	3.5106116	-1.5746833	0.1830251
Cu	-1.2382597	-1.2666160	0.0808660
C	3.5384446	2.9951249	-1.4743637
Mo	-3.1759039	0.5413791	-0.0111845
C	2.7382461	-3.4597434	1.1806442
Cu	1.1777735	-0.4938673	0.0880889
H	4.8867906	1.3713343	-0.6527834
Cu	-0.6201486	1.2868461	-0.2132918
C	-5.2721732	0.6344083	1.0782140
H	2.2641690	4.8565288	-1.3278596
C	4.2496840	2.2471667	-0.4737790
C	-4.3595881	2.5933782	0.2129814
H	-5.6011599	-0.1434453	1.7791866
C	2.8692064	4.0847481	-0.8340197
H	2.8327269	-3.2215140	2.2487569
C	-0.1688066	-2.4760591	1.6760676
H	-3.8593424	3.5681313	0.1395668
Mo	1.9187673	2.0841984	0.0066221
C	-4.5589673	1.8333336	1.4121935
C	-1.9185848	0.5522827	1.5418187
C	4.0140012	2.8810209	0.7922474
O	-0.5296713	-2.2893958	2.7805847
C	3.1635397	4.0107060	0.5767222
C	1.9178182	0.8882242	1.5980582
C	0.2904549	3.0977889	0.5320945
H	4.4264379	2.5622010	1.7591127
O	-1.4352368	0.6800306	2.6116034
O	2.1122981	0.3687223	2.6422189
O	-0.4482383	3.9479120	0.8944825
H	2.8167645	4.7153082	1.3443185
H	2.9328714	-2.8745846	-2.1472140
H	3.5224323	2.7705344	-2.5495494
H	-4.2268334	2.1277349	2.4168395

Complex A24

H	-3.6022635	-3.2881331	4.1802184
H	1.3636649	-3.7414870	-2.9773274
H	-4.0922424	-3.2390873	1.5036606
C	-3.9513522	-2.4214232	3.6032450
H	4.0258107	-3.2765874	-3.3674808
C	-4.2162429	-2.3964720	2.1975655
O	2.1515831	-2.9853403	0.1041493
O	-0.7427305	-2.7282711	0.7477677
C	1.8018349	-2.8635524	-3.4707673
C	3.2021758	-2.6135529	-3.6636376
O	-1.8955361	-2.1984724	-2.0550013
C	-4.2575309	-1.1145965	4.1338579
O	-0.5858140	-1.6089612	5.0985455
C	-1.2762284	-1.9009367	1.3980948
H	-4.1874048	-0.8114287	5.1867620
C	2.1764687	-2.0593110	-0.6205970
C	-4.6930492	-1.0866994	1.8486850
O	1.9644826	-2.2163225	2.9839207
C	-1.1923532	-1.2937700	4.1487529
H	-5.0389469	-0.7638004	0.8584741
C	-4.7117479	-0.2989075	3.0468506
Mo	-2.4391689	-0.8845258	2.6662415
C	1.0668642	-1.7769091	-4.0438589
C	3.3313776	-1.3607052	-4.3649972
H	-0.0264260	-1.7042804	-4.0916747
C	-1.9663437	-1.0196386	-1.9841835
H	4.2721778	-0.8973087	-4.6912900
O	5.3088138	-0.1667546	-1.3081499
Mo	2.4096921	-0.9175377	-2.2415121
C	4.2035788	-0.4303287	-1.6019867
H	-1.7787729	-0.0853076	-5.1234916
C	2.0030126	-1.0604459	2.7734715
C	2.0171050	-0.8466852	-4.5935952
H	-5.0331813	0.7490134	3.1177129
H	5.0331813	-0.7490134	3.1177129

Complex A27

H	0.3104667	2.5653514	-3.9387106
H	2.9679673	3.0534507	-4.3524996
O	1.3761383	-0.4797770	-2.9237067
C	0.9676471	3.1715212	-3.3014908
C	2.3646561	3.4175937	-3.5103647
C	1.6618645	0.4268028	-2.2298094
C	0.5599102	3.8628221	-2.1132453
C	2.8271808	4.2665443	-2.4400103
H	-0.4668608	3.9153965	-1.7308389
H	3.8460924	4.6583709	-2.3202050
O	5.1977121	1.3039259	-1.7173584
Mo	2.1890514	2.2009212	-1.5087670
C	4.0706725	1.5900190	-1.6033231
C	1.7148453	4.5345590	-1.5816434
Cu	0.0000000	-1.4858748	0.0000000
Cu	0.0000000	1.4858748	0.0000000
Cu	2.0299351	0.0000000	0.0000000
H	1.7388352	5.1637410	-0.6817498
C	2.4440076	2.3079260	0.4632937
O	2.7090035	2.6429878	1.5628912
H	-0.3104667	-2.5653514	-3.9387106
H	-2.9679673	-3.0534507	-4.3524996
O	-1.3761383	0.4797770	-2.9237067
C	-0.9676471	-3.1715212	-3.3014908
C	-2.3646561	-3.4175937	-3.5103647
C	-1.6618645	-0.4268028	-2.2298094
C	-0.5599102	-3.8628221	-2.1132453
C	-2.8271808	-4.2665443	-2.4400103
H	0.4668608	-3.9153965	-1.7308389
H	-3.8460924	-4.6583709	-2.3202050
O	-5.1977121	-1.3039259	-1.7173584
Mo	-2.1890514	-2.2009212	-1.5087670
C	-4.0706725	-1.5900190	-1.6033231
C	-1.7148453	-4.5345590	-1.5816434
Cu	-2.0299351	0.0000000	0.0000000

Cu	-1.8722984	0.0929441	0.2612033
Cu	0.0000000	0.0000000	2.1727547
Cu	0.0000000	0.0000000	-1.4920110
Cu	1.8722984	-0.0929441	0.2612033
C	-2.0171050	0.8466852	-4.5935952
H	-4.2721778	0.8973087	-4.6912900
O	-5.3088138	0.1667546	-1.3081499
H	1.7787729	0.0853076	-5.1234916
C	-4.2035788	0.4303287	-1.6019867
C	-2.0030126	1.0604459	2.7734715
C	-3.3313776	1.3607052	-4.3649972
Mo	-2.4096921	0.9175377	-2.2415121
C	4.7117479	0.2989075	3.0468506
H	0.0264260	1.7042804	-4.0916747
C	1.9663437	1.0196386	-1.9841835
C	-1.0668642	1.7769091	-4.0438589
H	5.0389469	0.7638004	0.8584741
Mo	2.4391689	0.8845258	2.6662415
H	4.1874048	0.8114287	5.1867620
C	1.1923532	1.2937700	4.1487529
C	4.6930492	1.0866994	1.8486850
O	-1.9644826	2.2163225	2.9839207
C	4.2575309	1.1145965	4.1338579
O	0.5858140	1.6089612	5.0985455
C	-3.2021758	2.6135529	-3.6636376
C	-2.1764687	2.0593110	-0.6205970
C	1.2762284	1.9009367	1.3980948
O	1.8955361	2.1984724	-2.0550013
C	-1.8018349	2.8635524	-3.4707673
H	-4.0258107	3.2765874	-3.3674808
C	4.2162429	2.3964720	2.1975655
C	3.9513522	2.4214232	3.6032450
O	-2.1515831	2.9853403	0.1041493
O	0.7427305	2.7282711	0.7477677
H	4.0922424	3.2390873	1.5036606
H	-1.3636649	3.7414870	-2.9773274
H	3.6022635	3.2881331	4.1802184

H	-1.7388352	-5.1637410	-0.6817498
C	-2.4440076	-2.3079260	0.4632937
O	-2.7090035	-2.6429878	1.5628912
H	0.3104667	-2.5653514	3.9387106
H	2.9679673	-3.0534507	4.3524996
O	1.3761383	0.4797770	2.9237067
C	0.9676471	-3.1715212	3.3014908
C	2.3646561	-3.4175937	3.5103647
C	1.6618645	-0.4268028	2.2298094
C	0.5599102	-3.8628221	2.1132453
C	2.8271808	-4.2665443	2.4400103
H	-0.4668608	-3.9153965	1.7308389
H	3.8460924	-4.6583709	2.3202050
O	5.1977121	-1.3039259	1.7173584
Mo	2.1890514	-2.2009212	1.5087670
C	4.0706725	-1.5900190	1.6033231
C	1.7148453	-4.5345590	1.5816434
H	1.7388352	-5.1637410	0.6817498
C	2.4440076	-2.3079260	-0.4632937
O	2.7090035	-2.6429878	-1.5628912
H	-0.3104667	2.5653514	3.9387106
H	-2.9679673	3.0534507	4.3524996
O	-1.3761383	-0.4797770	2.9237067
C	-0.9676471	3.1715212	3.3014908
C	-2.3646561	3.4175937	3.5103647
C	-1.6618645	0.4268028	2.2298094
C	-0.5599102	3.8628221	2.1132453
C	-2.8271808	4.2665443	2.4400103
H	0.4668608	3.9153965	1.7308389
H	-3.8460924	4.6583709	2.3202050
O	-5.1977121	1.3039259	1.7173584
Mo	-2.1890514	2.2009212	1.5087670
C	-4.0706725	1.5900190	1.6033231
C	-1.7148453	4.5345590	1.5816434
H	-1.7388352	5.1637410	0.6817498
C	-2.4440076	2.3079260	-0.4632937
O	-2.7090035	2.6429878	-1.5628912

Complex A29

H	-2.1967109	-4.2342029	3.3636853
H	-0.9830541	-6.1251035	1.8344984
O	-0.8631382	-1.1658223	2.7767942
C	-2.4176187	-4.4508633	2.3098131
C	-1.7777197	-5.4421815	1.5049331
C	-0.9282410	-1.8315005	1.8047835
C	-3.4073975	-3.7897903	1.5006182
C	-2.3634965	-5.4016361	0.1921690
H	-4.0835143	-2.9898247	1.8264659
H	-2.1064857	-6.0565801	-0.6507432
O	1.5066832	-4.7468704	0.3707902
Mo	-1.2818718	-3.3335054	0.5346913
C	0.5522624	-4.0502261	0.3889211
C	-3.3740629	-4.3778631	0.1960487
Cu	1.7794381	0.7704778	-0.0733531
Cu	-1.7794381	-0.7704778	-0.0733531
Cu	0.7704778	-1.7794381	0.0733531
H	-4.0218224	-4.0988559	-0.6450620
C	-1.3886336	-2.6885511	-1.3504085
O	-1.5649011	-2.5510251	-2.5055078
H	2.1967109	4.2342029	3.3636853
H	0.9830541	6.1251035	1.8344984
O	0.8631382	1.1658223	2.7767942
C	2.4176187	4.4508633	2.3098131
C	1.7777197	5.4421815	1.5049331
C	0.9282410	1.8315005	1.8047835
C	3.4073975	3.7897903	1.5006182
C	2.3634965	5.4016361	0.1921690
H	4.0835143	2.9898247	1.8264659
H	2.1064857	6.0565801	-0.6507432
O	-1.5066832	4.7468704	0.3707902
Mo	1.2818718	3.3335054	0.5346913
C	-0.5522624	4.0502261	0.3889211
C	3.3740629	4.3778631	0.1960487
Cu	-0.7704778	1.7794381	0.0733531
H	4.0218224	4.0988559	-0.6450620
C	1.3886336	2.6885511	-1.3504085
O	1.5649011	2.5510251	-2.5055078
H	4.2342029	-2.1967109	-3.3636853
H	-4.2342029	2.1967109	-3.3636853

Complex A31

H	6.0778600	1.0349353	-1.9923584
H	-6.0778600	-1.0349353	-1.9923584
H	4.7802887	-0.9430562	-3.3298638
H	-4.7802887	0.9430562	-3.3298638
C	5.7088337	0.0967934	-1.5559227
C	-5.7088337	-0.0967934	-1.5559227
C	5.0291424	-0.9444153	-2.2598907
C	-5.0291424	0.9444153	-2.2598907
O	-1.4646844	0.3034696	-2.9869895
O	1.4646844	-0.3034696	-2.9869895
C	5.8408768	-0.3030344	-0.1803521
C	-5.8408768	0.3030344	-0.1803521
H	-6.3413000	-0.2666596	0.6134048
H	6.3413000	0.2666596	0.6134048
C	2.0792545	-0.2244029	-1.9865404
C	-2.0792545	0.2244029	-1.9865404
C	-4.7389440	2.0005595	-1.3267339
C	4.7389440	-2.0005595	-1.3267339
O	0.4789644	2.7658434	-2.4071044
O	-0.4789644	-2.7658434	-2.4071044
H	4.2445019	-2.9523333	-1.5571043
H	-4.2445019	2.9523333	-1.5571043
C	-5.2388535	1.6021254	-0.0460395
C	5.2388535	-1.6021254	-0.0460395
Mo	3.5374827	-0.0621004	-0.6267578
Mo	-3.5374827	0.0621004	-0.6267578
O	-3.8084337	-3.0515157	-0.8182413
O	3.8084337	3.0515157	-0.8182413
C	3.5488061	1.9082043	-0.6896412
C	-3.5488061	-1.9082043	-0.6896412
C	-0.2647161	-2.8575712	-1.2513270
C	0.2647161	2.8575712	-1.2513270
H	-5.1769016	2.1987774	0.8730216
H	5.1769016	-2.1987774	0.8730216
Cu	-1.2577768	1.4127113	-0.2499063
Cu	1.2577768	-1.4127113	-0.2499063
H	2.1942152	5.1576432	-0.8756628
H	-2.1942152	-5.1576432	-0.8756628
Cu	1.4310549	1.2406793	0.2552494
Cu	-1.4310549	-1.2406793	0.2552494

H	6.1251035	-0.9830541	-1.8344984
H	-6.1251035	0.9830541	-1.8344984
O	1.1658223	-0.8631382	-2.7767942
O	-1.1658223	0.8631382	-2.7767942
C	4.4508633	-2.4176187	-2.3098131
C	-4.4508633	2.4176187	-2.3098131
C	5.4421815	-1.7777197	-1.5049331
C	-5.4421815	1.7777197	-1.5049331
C	1.8315005	-0.9282410	-1.8047835
C	-1.8315005	0.9282410	-1.8047835
C	3.7897903	-3.4073975	-1.5006182
C	-3.7897903	3.4073975	-1.5006182
C	5.4016361	-2.3634965	-0.1921690
C	-5.4016361	2.3634965	-0.1921690
H	2.9898247	-4.0835143	-1.8264659
H	-2.9898247	4.0835143	-1.8264659
H	6.0565801	-2.1064857	0.6507432
H	-6.0565801	2.1064857	0.6507432
O	4.7468704	1.5066832	-0.3707902
O	-4.7468704	-1.5066832	-0.3707902
Mo	3.3335054	-1.2818718	-0.5346913
Mo	-3.3335054	1.2818718	-0.5346913
C	4.0502261	0.5522624	-0.3889211
C	-4.0502261	-0.5522624	-0.3889211
C	4.3778631	-3.3740629	-0.1960487
C	-4.3778631	3.3740629	-0.1960487
H	4.0988559	-4.0218224	0.6450620
H	-4.0988559	4.0218224	0.6450620
C	2.6885511	-1.3886336	1.3504085
C	-2.6885511	1.3886336	1.3504085
O	2.5510251	-1.5649011	2.5055078
O	-2.5510251	1.5649011	2.5055078

C	-2.8855991	0.2582717	1.2526496
C	2.8855991	-0.2582717	1.2526496
O	-3.0496048	3.7930613	0.8106794
O	3.0496048	-3.7930613	0.8106794
C	1.9074515	-3.5268875	0.6842960
C	-1.9074515	3.5268875	0.6842960
C	1.5989493	5.2172091	0.0444325
C	-1.5989493	-5.2172091	0.0444325
Mo	0.0636368	3.5123698	0.6261649
Mo	-0.0636368	-3.5123698	0.6261649
H	-0.2725558	6.3171684	-0.6100287
H	0.2725558	-6.3171684	-0.6100287
H	2.9540896	4.2234538	1.5513408
H	-2.9540896	-4.2234538	1.5513408
C	0.2993122	5.8167557	0.1821230
C	-0.2993122	-5.8167557	0.1821230
O	2.7965429	-0.4712818	2.4090731
O	-2.7965429	0.4712818	2.4090731
C	2.0008357	4.7164203	1.3238619
C	-2.0008357	-4.7164203	1.3238619
C	0.2255309	2.0571964	1.9886958
C	-0.2255309	-2.0571964	1.9886958
O	-0.3045461	-1.4463600	2.9912911
O	0.3045461	1.4463600	2.9912911
C	-0.0975956	5.6821531	1.5584284
C	0.0975956	-5.6821531	1.5584284
C	0.9461879	5.0036289	2.2595554
C	-0.9461879	-5.0036289	2.2595554
H	-1.0356148	6.0489322	1.9970022
H	1.0356148	-6.0489322	1.9970022
H	-0.9473305	-4.7533780	3.3291948
H	0.9473305	4.7533780	3.3291948

Complex A41

H	4.2900938	2.4038409	-2.6799417
H	5.7097492	2.5649430	-0.3659966
O	1.1104770	1.1121225	-2.3752626
C	4.1189221	3.1212797	-1.8659150
C	4.8593633	3.2010391	-0.6462694
C	1.5428529	1.5435635	-1.3521341
C	3.1102210	4.1493467	-1.8436285
C	4.3085160	4.2726550	0.1405172
H	2.3779119	4.3514205	-2.6369477
H	4.6703625	4.6056051	1.1222354
O	3.9888678	0.9054084	2.1842871
Mo	2.6349323	2.6342518	-0.0655162
C	3.3739676	1.4136979	1.3143789
C	3.2314523	4.8608020	-0.6098435
Cu	0.0000000	-2.2859484	0.0000000
Cu	0.0000000	2.2859484	0.0000000
Cu	2.2792415	0.0000000	0.0000000
H	2.6182387	5.7163637	-0.2958833
C	1.4146964	3.3763697	1.3130983
O	0.9077807	3.9940864	2.1822036
H	-4.2900938	-2.4038409	-2.6799417
H	-5.7097492	-2.5649430	-0.3659966
O	-1.1104770	-1.1121225	-2.3752626
C	-4.1189221	-3.1212797	-1.8659150
C	-4.8593633	-3.2010391	-0.6462694
C	-1.5428529	-1.5435635	-1.3521341
C	-3.1102210	-4.1493467	-1.8436285
C	-4.3085160	-4.2726550	0.1405172
H	-2.3779119	-4.3514205	-2.6369477
H	-4.6703625	-4.6056051	1.1222354
O	-3.9888678	-0.9054084	2.1842871
Mo	-2.6349323	-2.6342518	-0.0655162
C	-3.3739676	-1.4136979	1.3143789
C	-3.2314523	-4.8608020	-0.6098435
Cu	-2.2792415	0.0000000	0.0000000
H	-2.6182387	-5.7163637	-0.2958833
C	-1.4146964	-3.3763697	1.3130983
O	-0.9077807	-3.9940864	2.1822036
H	4.2900938	-2.4038409	2.6799417
H	5.7097492	-2.5649430	0.3659966
O	1.1104770	-1.1121225	2.3752626
C	4.1189221	-3.1212797	1.8659150
C	4.8593633	-3.2010391	0.6462694
C	1.5428529	-1.5435635	1.3521341
C	3.1102210	-4.1493467	1.8436285

Complex A42

H	-1.6611954	-4.3657553	2.9921459
H	-1.0875998	-6.0676461	0.9480879
O	-0.8290405	-1.2685528	2.3845177
C	-2.2629015	-4.5117638	2.0848686
C	-1.9556147	-5.3975086	1.0065215
C	-1.1194990	-1.8300733	1.3744648
C	-3.5004305	-3.8420609	1.7790248
C	-3.0006113	-5.2746290	0.0217894
H	-4.0043987	-3.0956757	2.4075422
H	-3.0719810	-5.8389787	-0.9173712
O	0.1870298	-4.3234732	-1.9292887
Mo	-1.9020609	-3.1989029	0.1306339
C	-0.4844426	-3.7611620	-1.1365853
C	-3.9545838	-4.3190298	0.5088903
Cu	2.1994666	0.5648496	-0.0458902
Cu	-2.1994666	-0.5648496	-0.0458902
Cu	0.5648496	-2.1994666	0.0458902
H	-4.8769146	-4.0113768	-0.0017936
C	-2.8020317	-2.2504962	-1.3640467
O	-3.4522378	-1.9371527	-2.2977990
H	1.6611954	4.3657553	2.9921459
H	1.0875998	6.0676461	0.9480879
O	0.8290405	1.2685528	2.3845177
C	2.2629015	4.5117638	2.0848686
C	1.9556147	5.3975086	1.0065215
C	1.1194990	1.8300733	1.3744648
C	3.5004305	3.8420609	1.7790248
C	3.0006113	5.2746290	0.0217894
H	4.0043987	3.0956757	2.4075422
H	3.0719810	5.8389787	-0.9173712
O	-0.1870298	4.3234732	-1.9292887
Mo	1.9020609	3.1989029	0.1306339
C	0.4844426	3.7611620	-1.1365853
C	3.9545838	4.3190298	0.5088903
Cu	-0.5648496	2.1994666	0.0458902
H	4.8769146	4.0113768	-0.0017936
C	2.8020317	2.2504962	-1.3640467
O	3.4522378	1.9371527	-2.2977990
H	4.3657553	-1.6611954	-2.9921459
H	-4.3657553	1.6611954	-2.9921459
H	6.0676461	-1.0875998	-0.9480879
H	-6.0676461	1.0875998	-0.9480879
O	1.2685528	-0.8290405	-2.3845177
O	-1.2685528	0.8290405	-2.3845177
C	4.5117638	-2.2629015	-2.0848686

C	4.3085160	-4.2726550	-0.1405172	C	-4.5117638	2.2629015	-2.0848686
H	2.3779119	-4.3514205	2.6369477	C	5.3975086	-1.9556147	-1.0065215
H	4.6703625	-4.6056051	-1.1222354	C	-5.3975086	1.9556147	-1.0065215
O	3.9888678	-0.9054084	-2.1842871	C	1.8300733	-1.1194990	-1.3744648
Mo	2.6349323	-2.6342518	0.0655162	C	-1.8300733	1.1194990	-1.3744648
C	3.3739676	-1.4136979	-1.3143789	C	3.8420609	-3.5004305	-1.7790248
C	3.2314523	-4.8608020	0.6098435	C	-3.8420609	3.5004305	-1.7790248
H	2.6182387	-5.7163637	0.2958833	C	5.2746290	-3.0006113	-0.0217894
C	1.4146964	-3.3763697	-1.3130983	C	-5.2746290	3.0006113	-0.0217894
O	0.9077807	-3.9940864	-2.1822036	H	3.0956757	-4.0043987	-2.4075422
H	-4.2900938	2.4038409	2.6799417	H	-3.0956757	4.0043987	-2.4075422
H	-5.7097492	2.5649430	0.3659966	H	5.8389787	-3.0719810	0.9173712
O	-1.1104770	1.1121225	2.3752626	H	-5.8389787	3.0719810	0.9173712
C	-4.1189221	3.1212797	1.8659150	O	4.3234732	0.1870298	1.9292887
C	-4.8593633	3.2010391	0.6462694	O	-4.3234732	-0.1870298	1.9292887
C	-1.5428529	1.5435635	1.3521341	Mo	3.1989029	-1.9020609	-0.1306339
C	-3.1102210	4.1493467	1.8436285	Mo	-3.1989029	1.9020609	-0.1306339
C	-4.3085160	4.2726550	-0.1405172	C	3.7611620	-0.4844426	1.1365853
H	-2.3779119	4.3514205	2.6369477	C	-3.7611620	0.4844426	1.1365853
H	-4.6703625	4.6056051	-1.1222354	C	4.3190298	-3.9545838	-0.5088903
O	-3.9888678	0.9054084	-2.1842871	C	-4.3190298	3.9545838	-0.5088903
Mo	-2.6349323	2.6342518	0.0655162	H	4.0113768	-4.8769146	0.0017936
C	-3.3739676	1.4136979	-1.3143789	H	-4.0113768	4.8769146	0.0017936
C	-3.2314523	4.8608020	0.6098435	C	2.2504962	-2.8020317	1.3640467
H	-2.6182387	5.7163637	0.2958833	C	-2.2504962	2.8020317	1.3640467
C	-1.4146964	3.3763697	-1.3130983	O	1.9371527	-3.4522378	2.2977990
O	-0.9077807	3.9940864	-2.1822036	O	-1.9371527	3.4522378	2.2977990

$[AgMoC_5H_4NMe_2(CO)_3]_n$ (n = 3 for **A14, A16, A19** and n = 4 for **A2, A8, A11, A37**)

Complex A2				**Complex A8**			
H	2.8346395	-5.9964403	-2.5366018	H	1.4349214	2.6446519	-6.4406534
H	3.9283592	-4.9893416	-3.5394521	H	2.8300389	3.5383747	-5.7530828
C	3.1728176	-4.9566242	-2.7251579	C	2.0175332	2.8186438	-5.5128702
H	0.6234831	-5.5521710	-2.4281997	H	-0.6182347	2.9695865	-5.5837271
H	3.6604382	-4.5716058	-1.7967189	H	2.4803938	1.8505076	-5.2008502
H	-3.4392457	-4.1205064	3.8138726	N	1.1337324	3.3698381	-4.4957098
N	2.0266805	-4.1540268	-3.1303493	C	-0.2688303	2.9680980	-4.5295232
C	0.7490253	-4.4505729	-2.4893151	H	-0.4400462	1.9542057	-4.0964470
H	-3.6281549	-3.8096701	1.1045629	H	3.9176317	3.7741032	-3.7510857
H	0.6788030	-4.0239623	-1.4599273	H	-0.8931075	3.6907535	-3.9675473
C	-3.8277661	-3.2425460	3.2820562	O	1.5708757	0.1431887	-3.0822601
H	4.5111994	-2.8190791	-3.8627728	C	1.6852437	3.8255793	-3.3290507
H	-0.0924476	-4.0465889	-3.0865725	C	3.0970348	3.9997054	-3.0603250
C	-3.9350344	-3.0820435	1.8678937	C	1.8952495	0.9334506	-2.2695419
O	2.8453188	-2.6858851	-0.0373262	C	0.9804144	4.2470771	-2.1329545
O	-0.2900364	-3.0982061	0.9911047	C	3.2436108	4.6928819	-1.7986906
C	2.2487905	-2.9084757	-3.6541531	H	-0.1076082	4.2635113	-2.0019343
C	3.5361683	-2.3347006	-3.9918377	H	4.1845052	5.0738158	-1.3815290
O	-2.2019093	-2.4177338	-2.4069189	O	5.4855011	1.5758733	-1.2917939
C	-4.3747685	-2.0538242	3.8997529	Mo	2.5004824	2.5694686	-1.2807254
O	-0.7475917	-2.1223880	5.2884404	C	4.3566837	1.8825019	-1.2454730
C	-1.0076924	-2.3744032	1.5811603	C	1.9404557	4.8336465	-1.2312431
H	-4.4677149	-1.8936444	4.9801733	Ag	0.0000000	-1.8726438	0.0000000
C	2.7245205	-1.8128079	-0.8211908	Ag	0.0000000	1.8726438	0.0000000
C	-4.5577264	-1.8108615	1.5941287	Ag	2.2313830	0.0000000	0.0000000
H	6.6156562	-1.2277391	4.3968790	H	1.6977395	5.3350672	-0.2850007
O	2.5068505	-1.5912643	3.3719086	C	2.5311584	2.5603279	0.7191066
C	-1.3118929	-1.8527010	4.2991929	O	2.6912300	2.7852020	1.8662481
H	6.7474644	-1.5004236	2.1624373	H	-1.4349214	-2.6446519	-6.4406534
H	4.9903238	-1.4672697	1.7351583	H	-2.8300389	-3.5383747	-5.7530828
H	-4.8580066	-1.4612125	0.6000176	C	-2.0175332	-2.8186438	-5.5128702
C	-4.9329555	-1.2127023	2.8610463	H	0.6182347	-2.9695865	-5.5837271
Mo	-2.4255075	-1.5049492	2.6974484	H	-2.4803938	-1.8505076	-5.2008502
C	1.2503758	-1.9145202	-3.9974927	N	-1.1337324	-3.3698381	-4.4957098
H	4.8618210	-0.9546431	4.7366658	C	0.2688303	-2.9680980	-4.5295232
C	3.3159934	-1.0907766	-4.6969485	H	0.4400462	-1.9542057	-4.0964470
H	0.1653714	-2.0420695	-3.9074411	H	-3.9176317	-3.7741032	-3.7510857
C	-2.2970164	-1.2430379	-2.3155947	H	0.8931075	-3.6907535	-3.9675473
C	5.8898082	-0.8343034	1.9317894	O	-1.5708757	-0.1431887	-3.0822601
C	5.8059254	-0.4686602	4.3888187	C	-1.6852437	-3.8255793	-3.3290507
H	4.0896853	-0.4840042	-5.1847924	C	-3.0970348	-3.9997054	-3.0603250
O	5.6608688	0.1544777	-1.7905385	C	-1.8952495	-0.9334506	-2.2695419
Mo	2.7222017	-0.7055268	-2.4952741	C	-0.9804144	-4.2470771	-2.1329545
C	4.5499461	-0.1515387	-2.0212188	C	-3.2436108	-4.6928819	-1.7986906
H	-1.4100639	-0.0189011	-5.1622268	H	0.1076082	-4.2635113	-2.0019343
C	2.3268689	-0.4724284	3.0510689	H	-4.1845052	-5.0738158	-1.3815290

H	-6.0828993	-0.3274671	5.1118990
H	6.1369091	-0.2775280	1.0048046
C	1.9130368	-0.8345364	-4.6890104
H	6.0828993	0.3274671	5.1118990
N	-5.6902521	-0.0848319	3.0462701
N	5.6902521	0.0848319	3.0462701
Ag	-2.0760308	-0.2592028	0.1765284
H	-6.1369091	0.2775280	1.0048046
Ag	0.0000000	0.0000000	2.2480815
Ag	0.0000000	0.0000000	-1.7441755
C	-5.8059254	0.4686602	4.3888187
Ag	2.0760308	0.2592028	0.1765284
C	-1.9130368	0.8345364	-4.6890104
H	-4.0896853	0.4840042	-5.1847924
O	-5.6608688	-0.1544777	-1.7905385
H	1.4100639	0.0189011	-5.1622268
C	-4.5499461	0.1515387	-2.0212188
C	-5.8898082	0.8343034	1.9317894
H	-4.8618210	0.9546431	4.7366658
C	-2.3268689	0.4724284	3.0510689
C	-3.3159934	1.0907766	-4.6969485
Mo	-2.7222017	0.7055268	-2.4952741
H	-6.6156562	1.2277391	4.3968790
H	-6.7474644	1.5004236	2.1624373
C	4.9329555	1.2127023	2.8610463
H	-0.1653714	2.0420695	-3.9074411
C	2.2970164	1.2430379	-2.3155947
C	-1.2503758	1.9145202	-3.9974927
H	-4.9903238	1.4672697	1.7351583
H	4.8580066	1.4612125	0.6000176
Mo	2.4255075	1.5049492	2.6974484
H	4.4677149	1.8936444	4.9801733
C	1.3118929	1.8527010	4.2991929
C	4.5577264	1.8108615	1.5941287
O	-2.5068505	1.5912643	3.3719086
C	4.3747685	2.0538242	3.8997529
O	0.7475917	2.1223880	5.2884404
C	-3.5361683	2.3347006	-3.9918377
C	-2.7245205	1.8128079	-0.8211908
C	1.0076924	2.3744032	1.5811603
O	2.2019093	2.4177338	-2.4069189
C	-2.2487905	2.9084757	-3.6541531
H	-4.5111994	2.8190791	-3.8627728
C	3.9350344	3.0820435	1.8678937
C	3.8277661	3.2425460	3.2820562
O	-2.8453188	2.6858851	-0.0373262
O	0.2900364	3.0982061	0.9911047
H	0.0924476	4.0465889	-3.0865725
H	-0.6788030	4.0239623	-1.4599273
H	3.6281549	3.8096701	1.1045629
N	-2.0266805	4.1540268	-3.1303493
H	3.4392457	4.1205064	3.8138726
C	-0.7490253	4.4505729	-2.4893151
H	-3.6604382	4.5716058	-1.7967189
H	-0.6234831	5.5521710	-2.4281997
C	-3.1728176	4.9566242	-2.7251579
H	-3.9283592	4.9893416	-3.5394521
H	-2.8346395	5.9964403	-2.5366018

O	-5.4855011	-1.5758733	-1.2917939
Mo	-2.5004824	-2.5694686	-1.2807254
C	-4.3566837	-1.8825019	-1.2454730
C	-1.9404557	-4.8336465	-1.2312431
Ag	-2.2313830	0.0000000	0.0000000
H	-1.6977395	-5.3350672	-0.2850007
C	-2.5311584	-2.5603279	0.7191066
O	-2.6912300	-2.7852020	1.8662481
H	1.4349214	-2.6446519	6.4406534
H	2.8300389	-3.5383747	5.7530828
C	2.0175332	-2.8186438	5.5128702
H	-0.6182347	-2.9695865	5.5837271
H	2.4803938	-1.8505076	5.2008502
N	1.1337324	-3.3698381	4.4957098
C	-0.2688303	-2.9680980	4.5295232
H	-0.4400462	-1.9542057	4.0964470
H	3.9176317	-3.7741032	3.7510857
H	-0.8931075	-3.6907535	3.9675473
O	1.5708757	-0.1431887	3.0822601
C	1.6852437	-3.8255793	3.3290507
C	3.0970348	-3.9997054	3.0603250
C	1.8952495	-0.9334506	2.2695419
C	0.9804144	-4.2470771	2.1329545
C	3.2436108	-4.6928819	1.7986906
H	-0.1076082	-4.2635113	2.0019343
H	4.1845052	-5.0738158	1.3815290
O	5.4855011	-1.5758733	1.2917939
Mo	2.5004824	-2.5694686	1.2807254
C	4.3566837	-1.8825019	1.2454730
C	1.9404557	-4.8336465	1.2312431
H	1.6977395	-5.3350672	0.2850007
C	2.5311584	-2.5603279	-0.7191066
O	2.6912300	-2.7852020	-1.8662481
H	-1.4349214	2.6446519	6.4406534
H	-2.8300389	3.5383747	5.7530828
C	-2.0175332	2.8186438	5.5128702
H	0.6182347	2.9695865	5.5837271
H	-2.4803938	1.8505076	5.2008502
N	-1.1337324	3.3698381	4.4957098
C	0.2688303	2.9680980	4.5295232
H	0.4400462	1.9542057	4.0964470
H	-3.9176317	3.7741032	3.7510857
H	0.8931075	3.6907535	3.9675473
O	-1.5708757	0.1431887	3.0822601
C	-1.6852437	3.8255793	3.3290507
C	-3.0970348	3.9997054	3.0603250
C	-1.8952495	0.9334506	2.2695419
C	-0.9804144	4.2470771	2.1329545
C	-3.2436108	4.6928819	1.7986906
H	0.1076082	4.2635113	2.0019343
H	-4.1845052	5.0738158	1.3815290
O	-5.4855011	1.5758733	1.2917939
Mo	-2.5004824	2.5694686	1.2807254
C	-4.3566837	1.8825019	1.2454730
C	-1.9404557	4.8336465	1.2312431
H	-1.6977395	5.3350672	0.2850007
C	-2.5311584	2.5603279	-0.7191066
O	-2.6912300	2.7852020	-1.8662481

Complex A11

H	-2.7366871	-3.7336362	5.8037148
H	-2.2516610	-5.1882973	4.8751678
C	-2.2964151	-4.0785180	4.8454843
H	-4.0868614	-2.1858237	4.9375744
H	-1.2539684	-3.6821690	4.7735591
N	-3.1431952	-3.6354867	3.7470774
C	-3.8068522	-2.3431645	3.8753892
H	-3.1664279	-1.4901617	3.5467765
H	-1.4936249	-5.8774336	2.8632064
H	-4.7408360	-2.3301155	3.2753459
O	-0.2313118	-1.6749900	3.0661540
C	-2.9358199	-4.1577367	2.4981778
C	-2.0953176	-5.2878157	2.1618478
C	-0.4928533	-2.3009884	2.1045874
C	-3.5327638	-3.6997273	1.2586198
C	-2.3250124	-5.6303289	0.7744974
H	-4.2433125	-2.8740766	1.1418658
H	-1.9266892	-6.5138956	0.2593719
O	1.4851852	-5.3211070	0.7770733

Complex A37

H	3.9243854	1.9185847	-5.3522256
H	5.2524263	2.2789494	-4.1989513
C	4.1579440	2.0956203	-4.2833964
H	2.2869643	3.3724614	-5.5869542
H	3.9120953	1.1709961	-3.7085179
N	3.4092537	3.2560321	-3.8169968
C	2.1961154	3.6586984	-4.5192311
H	1.2778707	3.1842196	-4.1005890
H	5.4898029	2.5794755	-1.8894293
H	2.0770057	4.7630671	-4.4744712
O	1.2935239	1.1709960	-2.5346306
C	3.6307551	3.7105394	-2.5490377
C	4.7074958	3.3134804	-1.6662639
C	1.7373780	1.6422080	-1.5349517
C	2.8343818	4.6855667	-1.8246118
C	4.6816884	4.1807606	-0.5104450
H	1.9222154	5.1732496	-2.1875527
H	5.4366699	4.2004414	0.2864836
O	4.5912676	1.3505939	1.8317230

Mo	-1.1684761	-3.6344240	0.7584361
C	0.5420973	-4.6177140	0.7502193
C	-3.2020992	-4.6459451	0.2248607
Ag	1.8481897	0.9846145	-0.0737394
Ag	-1.8481897	-0.9846145	-0.0737394
Ag	0.9846145	-1.8481897	0.0737394
H	-3.5932334	-4.6181537	-0.8007575
C	-0.9407873	-3.2317830	-1.1905461
O	-0.8889866	-3.2364969	-2.3686750
H	2.7366871	3.7336362	5.8037148
H	2.2516610	5.1882973	4.8751678
C	2.2964151	4.0785180	4.8454843
H	4.0868614	2.1858237	4.9375744
H	1.2539684	3.6821690	4.7735591
N	3.1431952	3.6354867	3.7470774
C	3.8068522	2.3431645	3.8753892
H	3.1664279	1.4901617	3.5467765
H	1.4936249	5.8774336	2.8632064
H	4.7408360	2.3301155	3.2753459
O	0.2313118	1.6749900	3.0661540
C	2.9358199	4.1577367	2.4981778
C	2.0953176	5.2878157	2.1618478
C	0.4928533	2.3009884	2.1045874
C	3.5327638	3.6997273	1.2586198
C	2.3250124	5.6303289	0.7744974
H	4.2433125	2.8740766	1.1418658
H	1.9266892	6.5138956	0.2593719
O	-1.4851852	5.3211070	0.7770733
Mo	1.1684761	3.6344240	0.7584361
C	-0.5420973	4.6177140	0.7502193
C	3.2020992	4.6459451	0.2248607
Ag	-0.9846145	1.8481897	0.0737394
H	3.5932334	4.6181537	-0.8007575
C	0.9407873	3.2317830	-1.1905461
O	0.8889866	3.2364969	-2.3686750
H	3.7336362	-2.7366871	-5.8037148
H	-3.7336362	2.7366871	-5.8037148
H	5.1882973	-2.2516610	-4.8751678
H	-5.1882973	2.2516610	-4.8751678
C	4.0785180	-2.2964151	-4.8454843
C	-4.0785180	2.2964151	-4.8454843
H	2.1858237	-4.0868614	-4.9375744
H	-2.1858237	4.0868614	-4.9375744
H	3.6821690	-1.2539684	-4.7735591
H	-3.6821690	1.2539684	-4.7735591
N	3.6354867	-3.1431952	-3.7470774
N	-3.6354867	3.1431952	-3.7470774
C	2.3431645	-3.8068522	-3.8753892
C	-2.3431645	3.8068522	-3.8753892
H	1.4901617	-3.1664279	-3.5467765
H	-1.4901617	3.1664279	-3.5467765
H	5.8774336	-1.4936249	-2.8632064
H	-5.8774336	1.4936249	-2.8632064
H	2.3301155	-4.7408360	-3.2753459
H	-2.3301155	4.7408360	-3.2753459
O	1.6749900	-0.2313118	-3.0661540
O	-1.6749900	0.2313118	-3.0661540
C	4.1577367	-2.9358199	-2.4981778
C	-4.1577367	2.9358199	-2.4981778
C	5.2878157	-2.0953176	-2.1618478
C	-5.2878157	2.0953176	-2.1618478
C	2.3009884	-0.4928533	-2.1045874
C	-2.3009884	0.4928533	-2.1045874
C	3.6997273	-3.5327638	-1.2586198
C	-3.6997273	3.5327638	-1.2586198
C	5.6303289	-2.3250124	-0.7744974
C	-5.6303289	2.3250124	-0.7744974
H	2.8740766	-4.2433125	-1.1418658
H	-2.8740766	4.2433125	-1.1418658
H	6.5138956	-1.9266892	-0.2593719
H	-6.5138956	1.9266892	-0.2593719
O	5.3211070	1.4851852	-0.7770733
O	-5.3211070	-1.4851852	-0.7770733
Mo	3.6344240	-1.1684761	-0.7584361
Mo	-3.6344240	1.1684761	-0.7584361
C	4.6177140	0.5420973	-0.7502193
C	-4.6177140	-0.5420973	-0.7502193
C	4.6459451	-3.2020992	-0.2248607

Mo	2.8105612	2.8345208	-0.3029843
C	3.8346514	1.7593582	1.0213302
C	3.5347989	5.0233985	-0.6123332
Ag	0.0000000	-2.3721375	0.0000000
Ag	0.0000000	2.3721375	0.0000000
Ag	2.4921319	0.0000000	0.0000000
H	3.2408022	5.8099708	0.0951492
C	1.7433864	3.5345871	1.2234795
O	1.3393864	4.1195538	2.1676906
H	-3.9243854	-1.9185847	-5.3522256
H	-5.2524263	-2.2789494	-4.1989513
C	-4.1579440	-2.0956203	-4.2833964
H	-2.2869643	-3.3724614	-5.5869542
H	-3.9120953	-1.1709961	-3.7085179
N	-3.4092537	-3.2560321	-3.8169968
C	-2.1961154	-3.6586984	-4.5192311
H	-1.2778707	-3.1842196	-4.1005890
H	-5.4898029	-2.5794755	-1.8894293
H	-2.0770057	-4.7630671	-4.4744712
O	-1.2935239	-1.1709960	-2.5346306
C	-3.6307551	-3.7105394	-2.5490377
C	-4.7074958	-3.3134804	-1.6662639
C	-1.7373780	-1.6422080	-1.5349517
C	-2.8343818	-4.6855667	-1.8246118
C	-4.6816884	-4.1807606	-0.5104450
H	-1.9222154	-5.1732496	-2.1875527
H	-5.4366699	-4.2004414	0.2864836
O	-4.5912676	-1.3505939	1.8317230
Mo	-2.8105612	-2.8345208	-0.3029843
C	-3.8346514	-1.7593582	1.0213302
C	-3.5347989	-5.0233985	-0.6123332
Ag	-2.4921319	0.0000000	0.0000000
H	-3.2408022	-5.8099708	0.0951492
C	-1.7433864	-3.5345871	1.2234795
O	-1.3393864	-4.1195538	2.1676906
H	3.9243854	-1.9185847	5.3522256
H	5.2524263	-2.2789494	4.1989513
C	4.1579440	-2.0956203	4.2833964
H	2.2869643	-3.3724614	5.5869542
H	3.9120953	-1.1709961	3.7085179
N	3.4092537	-3.2560321	3.8169968
C	2.1961154	-3.6586984	4.5192311
H	1.2778707	-3.1842196	4.1005890
H	5.4898029	-2.5794755	1.8894293
H	2.0770057	-4.7630671	4.4744712
O	1.2935239	-1.1709960	2.5346306
C	3.6307551	-3.7105394	2.5490377
C	4.7074958	-3.3134804	1.6662639
C	1.7373780	-1.6422080	1.5349517
C	2.8343818	-4.6855667	1.8246118
C	4.6816884	-4.1807606	0.5104450
H	1.9222154	-5.1732496	2.1875527
H	5.4366699	-4.2004414	-0.2864836
O	4.5912676	-1.3505939	-1.8317230
Mo	2.8105612	-2.8345208	0.3029843
C	3.8346514	-1.7593582	-1.0213302
C	3.5347989	-5.0233985	0.6123332
H	3.2408022	-5.8099708	-0.0951492
C	1.7433864	-3.5345871	-1.2234795
O	1.3393864	-4.1195538	-2.1676906
H	-3.9243854	1.9185847	5.3522256
H	-5.2524263	2.2789494	4.1989513
C	-4.1579440	2.0956203	4.2833964
H	-2.2869643	3.3724614	5.5869542
H	-3.9120953	1.1709961	3.7085179
N	-3.4092537	3.2560321	3.8169968
C	-2.1961154	3.6586984	4.5192311
H	-1.2778707	3.1842196	4.1005890
H	-5.4898029	2.5794755	1.8894293
H	-2.0770057	4.7630671	4.4744712
O	-1.2935239	1.1709960	2.5346306
C	-3.6307551	3.7105394	2.5490377
C	-4.7074958	3.3134804	1.6662639
C	-1.7373780	1.6422080	1.5349517
C	-2.8343818	4.6855667	1.8246118
C	-4.6816884	4.1807606	0.5104450
H	-1.9222154	5.1732496	2.1875527
H	-5.4366699	4.2004414	-0.2864836

C	-4.6459451	3.2020992	-0.2248607
H	4.6181537	-3.5932334	0.8007575
H	-4.6181537	3.5932334	0.8007575
C	3.2317830	-0.9407873	1.1905461
C	-3.2317830	0.9407873	1.1905461
O	3.2364969	-0.8889866	2.3686750
O	-3.2364969	0.8889866	2.3686750

Complex A14

H	5.4240582	-2.3828708	-2.9386023
H	5.2640221	-3.9395204	-2.0671535
C	4.7789247	-2.9550153	-2.2407491
H	3.7892295	-3.1264709	-2.7293068
H	5.1938025	-0.4248113	-1.9306894
N	4.6642628	-2.2225823	-0.9859637
H	4.0837203	3.8335273	-3.2217131
C	4.6477272	-0.7697173	-1.0294288
O	1.1071188	-2.5001449	-2.4431912
H	2.1896016	4.9455969	-3.6299462
H	3.9540888	-5.0253954	-0.5376332
H	3.6061706	-0.3557848	-1.0627161
H	5.1592880	-0.3456005	-0.1374815
O	-1.7621132	-0.2681578	-3.1062166
C	3.7753081	3.4251682	-2.2365011
H	3.5060707	2.3494200	-2.3720117
C	1.1758695	-2.7232456	-1.2883880
C	3.7731932	-4.2515094	0.2170291
C	4.0800183	-2.8447765	0.0892394
C	1.6899551	4.7320662	-2.6622646
H	4.6510229	3.4943848	-1.5562384
H	0.8599487	4.0071178	-2.8439652
O	1.1752467	1.2463384	-2.1203069
O	-3.2903222	-4.1516429	-0.8735420
H	1.2551073	5.6842697	-2.2903892
O	0.2365885	-6.0449260	-0.0219445
H	-5.6703296	-2.2859015	-2.3211141
N	2.6738182	4.2229977	-1.7168727
C	-2.2760491	-0.5239256	-2.0781794
H	-4.9340701	0.2633736	-2.9687115
C	0.7059815	-4.9941368	0.1874378
C	-3.2033447	-2.9845840	-0.7314049
Mo	1.6450565	-3.2956320	0.5767356
C	3.3470468	-4.4999534	1.5771508
C	3.6798407	-2.2090065	1.3316528
C	-5.5576685	-1.4430323	-1.6269182
C	0.9308105	1.5048826	-0.9897669
C	-5.1781373	-0.1089612	-1.9648587
H	3.1464470	-5.4868349	2.0145983
H	3.8525401	-1.1623289	1.6092166
Ag	-0.9733136	-2.2071703	-0.0100855
C	2.3262346	4.1107774	-0.3952752
Mo	-3.5283037	-1.0279931	-0.5988258
C	3.2838568	-3.2462200	2.2527946
Ag	1.2489216	-0.4587567	0.6093073
H	3.9596193	2.7906505	0.4893783
Ag	-1.3496853	0.7610721	-0.0902536
C	-5.8178199	-1.4828219	-0.2037819
H	0.4207463	5.3398109	-0.2283357
C	3.0464074	3.3786897	0.6313641
C	-5.2010048	0.6876800	-0.7651061
H	-6.1706285	-2.3609039	0.3493721
C	1.1843896	4.7162835	0.2509259
H	3.0045310	-3.0858432	3.3029236
C	0.2775635	-2.9876016	2.0065378
H	-4.9859747	1.7608791	-0.7138610
Mo	0.8510222	2.4259292	0.7950658
C	-5.7155362	-0.1337227	0.3126668
C	-2.9125190	-0.7298995	1.2904111
C	2.4586565	3.6945189	1.9064112
O	-0.3567711	-2.9577267	2.9969109
C	1.3135029	4.5144808	1.6780788
C	0.9447262	1.1911251	2.3614075
C	-1.0654308	2.8220743	1.1343763
H	2.8460696	3.3740900	2.8827149
O	-2.8203285	-0.5571711	2.4528400
N	-6.0440771	0.2892613	1.5717961
O	1.0410905	0.7163497	3.4378357
O	-2.0903653	3.3244085	1.4458325
H	0.6587944	4.9482312	2.4458789

O	-4.5912676	1.3505939	-1.8317230
Mo	-2.8105612	2.8345208	0.3029843
C	-3.8346514	1.7593582	-1.0213302
C	-3.5347989	5.0233985	0.6123332
H	-3.2408022	5.8099708	-0.0951492
C	-1.7433864	3.5345871	-1.2234795
O	-1.3393864	4.1195538	-2.1676906

Complex A16

Ag	-0.6721118	-1.6084094	0.0000000
Ag	1.7173351	0.2191841	0.0000000
Mo	1.2812770	3.0865932	0.0000000
C	0.7222576	5.0856063	-1.1586381
C	-0.1451476	5.1488143	0.0000000
C	0.7222576	5.0856063	1.1586381
C	2.0884954	5.1467514	0.7185934
C	2.0884954	5.1467514	-0.7185934
H	0.3984726	5.0863507	-2.2060807
H	0.3984726	5.0863507	2.2060807
H	2.9695153	5.2184615	1.3695782
H	2.9695153	5.2184615	-1.3695782
C	0.7943637	2.1705486	-1.7171376
O	0.5904072	1.8812016	-2.8391698
C	0.7943637	2.1705486	1.7171376
O	0.5904072	1.8812016	2.8391698
C	3.1459955	2.4537050	0.0000000
O	4.3174892	2.3119015	0.0000000
N	-1.5131158	5.2821521	0.0000000
C	-2.2133123	4.9991586	1.2444490
H	-1.8207580	5.6397093	2.0634096
H	-3.2915182	5.2197070	1.1188929
H	-2.1057069	3.9252565	1.5468961
C	-2.2133123	4.9991586	-1.2444490
H	-3.2915182	5.2197070	-1.1188929
H	-1.8207580	5.6397093	-2.0634096
H	-2.1057069	3.9252565	-1.5468961
Ag	-1.0563616	1.3752986	0.0000000
Mo	2.0377998	-2.6563453	0.0000000
Mo	-3.3232229	-0.4364003	0.0000000
C	4.0510123	-3.1641755	-1.1586285
C	-4.7783114	-1.9175365	-1.1591959
C	4.5387970	-2.4436069	0.0000000
C	-4.4005727	-2.7010941	0.0000000
C	4.0510123	-3.1641755	1.1586285
C	-4.7783114	-1.9175365	1.1591959
C	3.4247772	-4.3802195	0.7184694
C	-5.5129146	-0.7642714	0.7186066
C	3.4247772	-4.3802195	-0.7184694
C	-5.5129146	-0.7642714	-0.7186066
H	4.2178926	-2.8859558	-2.2059139
H	-4.6172781	-2.1976680	-2.2070805
H	4.2178926	-2.8859558	2.2059139
H	-4.6172781	-2.1976680	2.2070805
H	3.0471414	-5.1789026	1.3699648
H	-6.0118051	-0.0343818	1.3690162
H	3.0471414	-5.1789026	-1.3699648
H	-6.0118051	-0.0343818	-1.3690162
C	1.4878141	-1.7782935	-1.7184909
C	-2.2842784	-0.3955977	-1.7160117
O	1.3414475	-1.4559972	-2.8402761
O	-1.9280656	-0.4234442	-2.8368327
C	1.4878141	-1.7782935	1.7184909
C	-2.2842784	-0.3955977	1.7160117
O	1.3414475	-1.4559972	2.8402761
O	-1.9280656	-0.4234442	2.8368327
C	0.5624811	-3.9617429	0.0000000
C	-3.7112901	1.4944101	0.0000000
O	-0.1436078	-4.9067833	0.0000000
O	-4.1728874	2.5801557	0.0000000
N	5.3394784	-1.3262350	0.0000000
N	-3.8362711	-3.9551648	0.0000000
C	5.4521282	-0.5801596	1.2444732
C	-3.2372730	-4.4176483	1.2435062
H	5.8088159	-1.2427202	2.0619870
H	-3.9850657	-4.3922147	2.0650411
H	6.1868735	0.2388167	1.1159729
H	-2.8937293	-5.4631302	1.1197576
H	4.4734083	-0.1286346	1.5515198
H	-2.3578387	-3.7888334	1.5407334

H	-7.1137254	-1.4168965	2.2272249
H	-5.4383148	-1.2892497	2.8996030
H	-6.0041092	2.3827889	1.2520646
C	-6.3406601	-0.7068632	2.5932511
H	-4.5485211	1.7431097	2.1071764
C	-5.6531012	1.6302730	1.9908438
H	-6.7496811	-0.1973305	3.4894222
H	-6.1361119	1.8610124	2.9622176

Complex A19

Ag	-0.1736091	-1.6253791	0.7263002
Ag	1.5420731	0.7888136	0.3242886
Mo	0.2789831	3.2606480	-0.4028286
C	-0.7121354	4.7642292	-1.8836171
C	-1.5811450	4.7447188	-0.7352985
C	-0.8830755	5.3736913	0.3693694
C	0.4771565	5.5980193	-0.0711998
C	0.5542173	5.2879228	-1.4831973
H	-0.9957615	4.4479352	-2.8962053
H	1.2799543	6.0582439	0.5159282
H	1.4222631	5.4676859	-2.1302038
C	0.0360221	1.9269086	-1.8785913
O	-0.0675486	1.3633221	-2.9066566
C	-0.1230227	2.6581729	1.4690589
O	-0.3849486	2.5872736	2.6161892
C	2.2545486	3.0980749	-0.3331100
O	3.4257453	3.2509574	-0.3538018
H	-2.6275533	4.4193465	-0.7405538
Ag	-1.4151615	0.9737154	-0.0093738
Mo	2.6890491	-1.7703602	0.9403447
Mo	-3.0253067	-1.3483302	0.4894686
C	4.9505185	-1.8964831	-0.1794730
C	-4.0620125	-3.4874613	-0.3615533
C	4.9233989	-0.8883955	0.8611162
C	-3.4532830	-3.6677828	0.9413287
C	4.6923905	-1.5490055	2.1202947
C	-4.1561176	-2.8356280	1.8837276
C	4.4636097	-2.9345991	1.8688642
C	-5.1190657	-2.0598973	1.1706490
C	4.5507832	-3.1442693	0.4392527
C	-5.0158580	-2.4071664	-0.2311274
H	4.7130008	-1.0589763	3.1026402
H	-3.9871670	-2.8270943	2.9686916
H	4.2881906	-3.7142613	2.6208045
H	-5.8406530	-1.3551332	1.6034266
H	4.4593446	-4.1159789	-0.0601911
H	-5.6538447	-2.0071242	-1.0277776
C	2.0532847	-1.4140033	-0.9273375
C	-1.9132674	-1.5122915	-1.1722927
O	1.9112226	-1.3465570	-2.0958390
O	-1.4791276	-1.7699291	-2.2377498
C	1.9062340	-0.6680929	2.4209965
C	-2.1000465	-0.7702370	2.1705738
O	1.6513208	-0.1316228	3.4361599
O	-1.7991643	-0.5062277	3.2769814
C	1.5673995	-3.3733144	1.2683797
C	-3.8416332	0.4151486	0.0894566
O	1.1165326	-4.4411071	1.4927646
O	-4.5537655	1.3322888	-0.1290528
H	5.1599863	0.1751202	0.7425219
H	-2.6807758	-4.4014144	1.1999801
N	-3.7882259	-4.2086644	-1.4932025
N	5.3019142	-1.7024490	-1.4900704
N	-1.4104911	5.6998659	1.5904640
C	-2.6113268	-5.0678399	-1.5067585
H	-1.6573872	-4.4888165	-1.4530079
H	-2.6392546	-5.7773509	-0.6515415
H	-2.6091527	-5.6643394	-2.4414545
C	-4.3497909	-3.7633096	-2.7618580
H	-3.9036740	-2.8028058	-3.1172770
H	-4.1670477	-4.5402655	-3.5313875
H	-5.4494867	-3.6293643	-2.6684909
C	5.0817588	-2.7784867	-2.4470904
H	5.6276910	-2.5459255	-3.3849131
H	5.4863889	-3.7328678	-2.0486439
H	4.0016033	-2.9214972	-2.6934859
C	5.3869329	-0.3385062	-1.9973417
H	4.3875718	0.1570786	-2.0636078
H	6.0386216	0.2786076	-1.3429660
C	5.4521282	-0.5801596	-1.2444732
C	-3.2372730	-4.4176483	-1.2435062
H	6.1868735	0.2388167	-1.1159729
H	-2.8937293	-5.4631302	-1.1197576
H	5.8088159	-1.2427202	-2.0619870
H	-3.9850657	-4.3922147	-2.0650411
H	4.4734083	-0.1286346	-1.5515198
H	-2.3578387	-3.7888334	-1.5407334

H	5.8422441	-0.3563687	-3.0082326
C	-2.7223325	5.1839523	1.9598712
H	-3.4529839	5.3681709	1.1436194
H	-2.7087210	4.0895262	2.1826354
H	-3.0822574	5.7224270	2.8606324
C	-0.5072322	6.1197475	2.6536598
H	-1.1047629	6.4949448	3.5095279
H	0.1454729	5.2884788	3.0146496
H	0.1417480	6.9519439	2.3037438

$[AgMoCp(CO)_3]_n$ (n = 3 for **A32, A35** and n = 4 for **A5, A22, A25, A28, A39**)

Complex A5			
H	0.7481440	-5.8742199	-3.0800020
H	-0.7481440	5.8742199	-3.0800020
H	-1.1532413	-4.0207670	-3.6812961
H	1.1532413	4.0207670	-3.6812961
C	-0.0387914	-5.5137856	-2.4041065
C	0.0387914	5.5137856	-2.4041065
C	-1.0433124	-4.5457799	-2.7226971
C	1.0433124	4.5457799	-2.7226971
O	-0.9064136	1.3226481	-2.9779723
O	0.9064136	-1.3226481	-2.9779723
C	-0.2684443	-5.9639604	-1.0538143
C	0.2684443	5.9639604	-1.0538143
H	-0.3083003	6.7314244	-0.5211880
H	0.3083003	-6.7314244	-0.5211880
C	0.6986016	-2.0931266	-2.1181506
C	-0.6986016	2.0931266	-2.1181506
C	1.9060038	4.3959595	-1.5824699
C	-1.9060038	-4.3959595	-1.5824699
O	3.6384773	0.5291492	-2.1792304
O	-3.6384773	-0.5291492	-2.1792304
H	-2.8201491	-3.7899988	-1.5369074
H	2.8201491	3.7899988	-1.5369074
C	1.4170007	5.2661928	-0.5509191
C	-1.4170007	-5.2661928	-0.5509191
Mo	0.3209789	-3.6956917	-0.9674926
Mo	-0.3209789	3.6956917	-0.9674926
O	-3.3939198	4.3535103	-1.0734988
O	3.3939198	-4.3535103	-1.0734988
C	2.2597592	-4.0615045	-1.0121220
C	-2.2597592	4.0615045	-1.0121220
C	-3.4947566	-0.4912248	-1.0111440
C	3.4947566	0.4912248	-1.0111440
H	1.8709969	5.3934129	0.4409687
H	-1.8709969	-5.3934129	0.4409687
Ag	1.3635772	1.5013626	-0.2613555
Ag	-1.3635772	-1.5013626	-0.2613555
H	5.2937165	-1.9737675	-0.4223331
H	-5.2937165	1.9737675	-0.4223331
Ag	1.4934049	-1.3358867	0.2682703
Ag	-1.4934049	1.3358867	0.2682703
C	-0.4832988	3.4750058	1.0168656
C	0.4832988	-3.4750058	1.0168656
O	4.4004341	3.3799844	1.0928022
O	-4.4004341	-3.3799844	1.0928022
C	-4.0969431	-2.2492210	1.0262157
C	4.0969431	2.2492210	1.0262157
C	5.2189373	-1.4804093	0.5557739
C	-5.2189373	1.4804093	0.5557739
Mo	3.7147099	0.3140724	0.9718251
Mo	-3.7147099	-0.3140724	0.9718251
H	6.7290258	0.2010354	0.4056166
H	-6.7290258	-0.2010354	0.4056166
H	3.7439760	-2.8022145	1.6505228
H	-3.7439760	2.8022145	1.6505228
C	5.9690176	-0.3348543	0.9891552
C	-5.9690176	0.3348543	0.9891552
O	0.5155204	-3.6179630	2.1852231
O	-0.5155204	3.6179630	2.1852231
C	4.3799957	-1.9075424	1.6389729
C	-4.3799957	1.9075424	1.6389729
C	2.1185381	0.6960805	2.1308368
C	-2.1185381	-0.6960805	2.1308368
O	-1.3500390	-0.9034769	2.9926487

Complex A22			
H	-4.0971032	-3.2444977	4.3774203
H	-4.2984971	-3.3227167	1.6633967
C	-4.3366686	-2.3960571	3.7225474
H	3.9712111	-3.4887031	-3.6104276
C	-4.4509883	-2.4374223	2.2958325
O	2.0077106	-3.0909723	-0.0851649
O	-0.9145135	-3.0157494	1.2060880
C	1.8070459	-2.8372252	-3.7043143
C	3.2263869	-2.7286445	-3.8803571
O	-2.5315084	-2.1364992	-2.1905645
C	-4.6341713	-1.0512060	4.1508131
O	-1.0383082	-1.7274879	5.4743817
C	-1.4569780	-2.1488897	1.7839413
H	-4.6633853	-0.6933875	5.1881093
C	2.1857850	-2.1823076	-0.8075836
C	-4.8302843	-1.1312851	1.8310381
O	2.1784885	-2.1059661	3.3468171
C	-1.5724015	-1.4183411	4.4812880
H	-5.0707200	-0.8523439	0.7972942
C	-4.9316518	-0.2775575	2.9796692
Mo	-2.6651224	-0.9830411	2.8872439
C	1.1937580	-1.6551881	-4.2346826
C	3.4952633	-1.4636999	-4.5180984
H	0.1141576	-1.4708981	-4.3080923
C	-2.4788737	-0.9610824	-2.1316552
H	4.4825191	-1.0897691	-4.8202015
O	5.5620353	-0.7753125	-1.3276992
Mo	2.6161657	-1.0242758	-2.3866256
C	4.4451789	-0.8538218	-1.6767128
H	-2.1091349	-0.1721647	-5.2149762
C	2.2031554	-0.9576968	3.0997718
C	2.2429306	-0.8036720	-4.7282543
H	-5.2139942	0.7837401	2.9636462
H	5.2139942	-0.7837401	2.9636462
Ag	-2.0916057	0.0271711	0.2936737
Ag	0.0000000	0.0000000	2.3775865
Ag	0.0000000	0.0000000	-1.6901305
Ag	2.0916057	-0.0271711	0.2936737
C	-2.2429306	0.8036720	-4.7282543
H	-4.4825191	1.0897691	-4.8202015
O	-5.5620353	0.7753125	-1.3276992
H	2.1091349	0.1721647	-5.2149762
C	-4.4451789	0.8538218	-1.6767128
C	-2.2031554	0.9576968	3.0997718
C	-3.4952633	1.4636999	-4.5180984
Mo	-2.6161657	1.0242758	-2.3866256
C	4.9316518	0.2775575	2.9796692
H	-0.1141576	1.4708981	-4.3080923
C	2.4788737	0.9610824	-2.1316552
C	-1.1937580	1.6551881	-4.2346826
H	5.0707200	0.8523439	0.7972942
Mo	2.6651224	0.9830411	2.8872439
H	4.6633853	0.6933875	5.1881093
C	1.5724015	1.4183411	4.4812880
C	4.8302843	1.1312851	1.8310381
O	-2.1784885	2.1059661	3.3468171
C	4.6341713	1.0512060	4.1508131
O	1.0383082	1.7274879	5.4743817
C	-3.2263869	2.7286445	-3.8803571
C	-2.1857850	2.1823076	-0.8075836
C	1.4569780	2.1488897	1.7839413
O	2.5315084	2.1364992	-2.1905645
C	-1.8070459	2.8372252	-3.7043143

O	1.3500390	0.9034769	2.9926487
C	5.5814927	-0.0464917	2.3469656
C	-5.5814927	0.0464917	2.3469656
C	4.6009974	-1.0109432	2.7409158
C	-4.6009974	1.0109432	2.7409158
H	5.9901726	0.7532326	2.9792449
H	-5.9901726	-0.7532326	2.9792449
H	-4.1144651	1.0720272	3.7238759
H	4.1144651	-1.0720272	3.7238759

Complex A25

H	0.3681727	2.6240232	-4.0475585
H	2.9885672	3.2213925	-4.5319250
O	1.5312486	-0.3748510	-3.0346377
C	1.0158940	3.2563473	-3.4257875
C	2.3948760	3.5609402	-3.6728475
C	1.8296428	0.5505315	-2.3721987
C	0.6063460	3.9406003	-2.2330599
C	2.8497353	4.4329500	-2.6177633
H	-0.4171472	3.9758896	-1.8374339
H	3.8513642	4.8749230	-2.5307755
O	5.3511239	1.5384906	-2.0731368
Mo	2.3409330	2.3501980	-1.6676964
C	4.2260622	1.7945725	-1.8868759
C	1.7489722	4.6560157	-1.7303878
Ag	0.0000000	-1.7913219	0.0000000
Ag	0.0000000	1.7913219	0.0000000
Ag	2.2206851	0.0000000	0.0000000
H	1.7681406	5.2924741	-0.8355702
C	2.7499237	2.5128136	0.2876488
O	3.0700266	2.8483347	1.3698081
H	-0.3681727	-2.6240232	-4.0475585
H	-2.9885672	-3.2213925	-4.5319250
O	-1.5312486	0.3748510	-3.0346377
C	-1.0158940	-3.2563473	-3.4257875
C	-2.3948760	-3.5609402	-3.6728475
C	-1.8296428	-0.5505315	-2.3721987
C	-0.6063460	-3.9406003	-2.2330599
C	-2.8497353	-4.4329500	-2.6177633
H	0.4171472	-3.9758896	-1.8374339
H	-3.8513642	-4.8749230	-2.5307755
O	-5.3511239	-1.5384906	-2.0731368
Mo	-2.3409330	-2.3501980	-1.6676964
C	-4.2260622	-1.7945725	-1.8868759
C	-1.7489722	-4.6560157	-1.7303878
Ag	-2.2206851	0.0000000	0.0000000
H	-1.7681406	-5.2924741	-0.8355702
C	-2.7499237	-2.5128136	0.2876488
O	-3.0700266	-2.8483347	1.3698081
H	0.3681727	-2.6240232	4.0475585
H	2.9885672	-3.2213925	4.5319250
O	1.5312486	0.3748510	3.0346377
C	1.0158940	-3.2563473	3.4257875
C	2.3948760	-3.5609402	3.6728475
C	1.8296428	-0.5505315	2.3721987
C	0.6063460	-3.9406003	2.2330599
C	2.8497353	-4.4329500	2.6177633
H	-0.4171472	-3.9758896	1.8374339
H	3.8513642	-4.8749230	2.5307755
O	5.3511239	-1.5384906	2.0731368
Mo	2.3409330	-2.3501980	1.6676964
C	4.2260622	-1.7945725	1.8868759
C	1.7489722	-4.6560157	1.7303878
H	1.7681406	-5.2924741	0.8355702
C	2.7499237	-2.5128136	-0.2876488
O	3.0700266	-2.8483347	-1.3698081
H	-0.3681727	2.6240232	4.0475585
H	-2.9885672	3.2213925	4.5319250
O	-1.5312486	-0.3748510	3.0346377
C	-1.0158940	3.2563473	3.4257875
C	-2.3948760	3.5609402	3.6728475
C	-1.8296428	0.5505315	2.3721987
C	-0.6063460	3.9406003	2.2330599
C	-2.8497353	4.4329500	2.6177633
H	0.4171472	3.9758896	1.8374339
H	-3.8513642	4.8749230	2.5307755
O	-5.3511239	1.5384906	2.0731368
Mo	-2.3409330	2.3501980	1.6676964
C	-4.2260622	1.7945725	1.8868759

H	-3.9712111	3.4887031	-3.6104276
C	4.4509883	2.4374223	2.2958325
C	4.3366686	2.3960571	3.7225474
O	-2.0077106	3.0909723	-0.0851649
O	0.9145135	3.0157494	1.2060880
H	4.2984971	3.3227167	1.6633967
H	-1.2741241	3.6898864	-3.2612902
H	4.0971032	3.2444977	4.3774203
H	1.2741241	-3.6898864	-3.2612902

Complex A28

H	-3.0220050	-3.2728666	3.2310600
H	-1.6254376	-5.6109415	3.1208474
O	-0.0311224	-1.6480820	3.0701153
C	-2.8961890	-3.9091066	2.3443608
C	-2.1542595	-5.1339817	2.2852091
C	-0.3402031	-2.2849713	2.1342732
C	-3.4763841	-3.6667970	1.0540588
C	-2.2654387	-5.6513018	0.9431652
H	-4.1655417	-2.8546216	0.7912179
H	-1.8375294	-6.5944001	0.5778393
O	1.5586361	-5.3309749	1.1523490
Mo	-1.0699836	-3.6380299	0.8436218
C	0.6151258	-4.6452167	1.0209132
C	-3.0742515	-4.7404679	0.1888397
Ag	1.8038992	1.0127202	-0.0232649
Ag	-1.8038992	-1.0127202	-0.0232649
Ag	1.0127202	-1.8038992	0.0232649
H	-3.3647439	-4.8528280	-0.8646686
C	-0.6590717	-3.3807950	-1.1037027
O	-0.5423207	-3.4538433	-2.2719235
H	3.0220050	3.2728666	3.2310600
H	1.6254376	5.6109415	3.1208474
O	0.0311224	1.6480820	3.0701153
C	2.8961890	3.9091066	2.3443608
C	2.1542595	5.1339817	2.2852091
C	0.3402031	2.2849713	2.1342732
C	3.4763841	3.6667970	1.0540588
C	2.2654387	5.6513018	0.9431652
H	4.1655417	2.8546216	0.7912179
H	1.8375294	6.5944001	0.5778393
O	-1.5586361	5.3309749	1.1523490
Mo	1.0699836	3.6380299	0.8436218
C	-0.6151258	4.6452167	1.0209132
C	3.0742515	4.7404679	0.1888397
Ag	-1.0127202	1.8038992	0.0232649
H	3.3647439	4.8528280	-0.8646686
C	0.6590717	3.3807950	-1.1037027
O	0.5423207	3.4538433	-2.2719235
H	3.2728666	-3.0220050	-3.2310600
H	-3.2728666	3.0220050	-3.2310600
H	5.6109415	-1.6254376	-3.1208474
H	-5.6109415	1.6254376	-3.1208474
O	1.6480820	-0.0311224	-3.0701153
O	-1.6480820	0.0311224	-3.0701153
C	3.9091066	-2.8961890	-2.3443608
C	-3.9091066	2.8961890	-2.3443608
C	5.1339817	-2.1542595	-2.2852091
C	-5.1339817	2.1542595	-2.2852091
C	2.2849713	-0.3402031	-2.1342732
C	-2.2849713	0.3402031	-2.1342732
C	3.6667970	-3.4763841	-1.0540588
C	-3.6667970	3.4763841	-1.0540588
C	5.6513018	-2.2654387	-0.9431652
C	-5.6513018	2.2654387	-0.9431652
H	2.8546216	-4.1655417	-0.7912179
H	-2.8546216	4.1655417	-0.7912179
H	6.5944001	-1.8375294	-0.5778393
H	-6.5944001	1.8375294	-0.5778393
O	5.3309749	1.5586361	-1.1523490
O	-5.3309749	-1.5586361	-1.1523490
Mo	3.6380299	-1.0699836	-0.8436218
Mo	-3.6380299	1.0699836	-0.8436218
C	4.6452167	0.6151258	-1.0209132
C	-4.6452167	-0.6151258	-1.0209132
C	4.7404679	-3.0742515	-0.1888397
C	-4.7404679	3.0742515	-0.1888397
H	4.8528280	-3.3647439	0.8646686
H	-4.8528280	3.3647439	0.8646686

C	-1.7489722	4.6560157	1.7303878
H	-1.7681406	5.2924741	0.8355702
C	-2.7499237	2.5128136	-0.2876488
O	-3.0700266	2.8483347	-1.3698081

Complex A39

H	3.8780789	2.7961285	-3.3045947
H	5.7412882	2.8874457	-1.3275530
O	1.2409719	1.1500937	-2.5698952
C	3.8574183	3.4591958	-2.4290422
C	4.8339925	3.5032724	-1.3880931
C	1.7001111	1.6265476	-1.5846726
C	2.8440794	4.4427681	-2.1393119
C	4.4297603	4.5136999	-0.4437986
H	1.9607405	4.6596700	-2.7546405
H	4.9783994	4.8100132	0.4601585
O	4.6981400	1.3437340	1.6370884
Mo	2.8015104	2.8268498	-0.3872817
C	3.8871144	1.7424806	0.8800536
C	3.2031639	5.0938840	-0.9171708
Ag	0.0000000	-2.3432716	0.0000000
Ag	0.0000000	2.3432716	0.0000000
Ag	2.4458275	0.0000000	0.0000000
H	2.6468647	5.9086590	-0.4342514
C	1.7793152	3.5014827	1.1834232
O	1.3973751	4.0904310	2.1310017
H	-3.8780789	-2.7961285	-3.3045947
H	-5.7412882	-2.8874457	-1.3275530
O	-1.2409719	-1.1500937	-2.5698952
C	-3.8574183	-3.4591958	-2.4290422
C	-4.8339925	-3.5032724	-1.3880931
C	-1.7001111	-1.6265476	-1.5846726
C	-2.8440794	-4.4427681	-2.1393119
C	-4.4297603	-4.5136999	-0.4437986
H	-1.9607405	-4.6596700	-2.7546405
H	-4.9783994	-4.8100132	0.4601585
O	-4.6981400	-1.3437340	1.6370884
Mo	-2.8015104	-2.8268498	-0.3872817
C	-3.8871144	-1.7424806	0.8800536
C	-3.2031639	-5.0938840	-0.9171708
Ag	-2.4458275	0.0000000	0.0000000
H	-2.6468647	-5.9086590	-0.4342514
C	-1.7793152	-3.5014827	1.1834232
O	-1.3973751	-4.0904310	2.1310017
H	3.8780789	-2.7961285	3.3045947
H	5.7412882	-2.8874457	1.3275530
O	1.2409719	-1.1500937	2.5698952
C	3.8574183	-3.4591958	2.4290422
C	4.8339925	-3.5032724	1.3880931
C	1.7001111	-1.6265476	1.5846726
C	2.8440794	-4.4427681	2.1393119
C	4.4297603	-4.5136999	0.4437986
H	1.9607405	-4.6596700	2.7546405
H	4.9783994	-4.8100132	-0.4601585
O	4.6981400	-1.3437340	-1.6370884
Mo	2.8015104	-2.8268498	0.3872817
C	3.8871144	-1.7424806	-0.8800536
C	3.2031639	-5.0938840	0.9171708
H	2.6468647	-5.9086590	0.4342514
C	1.7793152	-3.5014827	-1.1834232
O	1.3973751	-4.0904310	-2.1310017
H	-3.8780789	2.7961285	3.3045947
H	-5.7412882	2.8874457	1.3275530
O	-1.2409719	1.1500937	2.5698952
C	-3.8574183	3.4591958	2.4290422
C	-4.8339925	3.5032724	1.3880931
C	-1.7001111	1.6265476	1.5846726
C	-2.8440794	4.4427681	2.1393119
C	-4.4297603	4.5136999	0.4437986
H	-1.9607405	4.6596700	2.7546405
H	-4.9783994	4.8100132	-0.4601585
O	-4.6981400	1.3437340	-1.6370884
Mo	-2.8015104	2.8268498	0.3872817
C	-3.8871144	1.7424806	-0.8800536
C	-3.2031639	5.0938840	0.9171708
H	-2.6468647	5.9086590	0.4342514
C	-1.7793152	3.5014827	-1.1834232
O	-1.3973751	4.0904310	-2.1310017

C	3.3807950	-0.6590717	1.1037027
C	-3.3807950	0.6590717	1.1037027
O	3.4538433	-0.5423207	2.2719235
O	-3.4538433	0.5423207	2.2719235

Complex A32

O	0.4959700	-2.3297980	-2.8307192
H	3.5919546	-4.9535713	-1.3999887
O	-2.2001804	-0.0479554	-2.8592084
C	0.8335888	-2.4711024	-1.7144461
C	3.6646705	-4.0869953	-0.7299722
C	3.8360034	-2.7230147	-1.1298456
O	1.0292794	1.3609110	-2.7988726
O	-3.5034900	-3.6211408	0.0037770
O	0.1600081	-5.6521155	-0.0309619
H	-6.0411053	-1.5327286	-1.3020522
C	-2.5025524	-0.2051406	-1.7339939
H	-5.2007317	0.9175024	-2.1451783
C	0.6983903	-4.6152514	-0.0199734
C	-3.3241034	-2.4584077	0.0025245
Mo	1.7580776	-2.9412812	0.0009593
C	3.6494723	-4.1256890	0.7125408
C	3.9397246	-1.9111352	0.0533972
C	-5.7067094	-0.7073112	-0.6599008
C	1.0160464	1.7492807	-1.6874887
C	-5.2722827	0.5843601	-1.1007112
H	3.5622291	-5.0269504	1.3334748
H	4.1856207	-0.8413636	0.0849237
Ag	-0.9013725	-1.7735136	-0.0217978
C	2.7048898	4.1598753	-1.3241947
Mo	-3.4627126	-0.4756376	0.0047705
C	3.8116128	-2.7858215	1.1887796
Ag	1.4393022	-0.0923405	0.0166243
H	4.3087454	2.7028070	-0.6657568
Ag	-1.1752847	1.2393203	-0.0890571
C	-5.6702151	-0.7149727	0.7828035
H	1.1195936	5.7318957	-0.9940671
C	3.5255812	3.4243033	-0.3992820
C	-4.9697297	1.3816032	0.0548969
H	-5.9727988	-1.5454903	1.4342961
C	1.8491702	5.0251925	-0.5763273
H	3.8537342	-2.4790885	2.2425685
C	0.8072090	-2.4920886	1.7076381
H	-4.6384659	2.4279887	0.0536650
Mo	1.2494552	2.8133751	-0.0006848
C	-5.2142338	0.5716056	1.2155188
C	-2.4023475	-0.1743080	1.6797903
C	3.1679768	3.8407131	0.9251463
O	0.4520948	-2.3593182	2.8191133
C	2.1333474	4.8299627	0.8239025
C	1.2402781	1.7427096	1.6909319
C	-0.5814986	3.5479006	0.2289027
H	3.6236095	3.4804878	1.8573152
O	-2.0310170	0.0166158	2.7784122
O	1.3541786	1.3565040	2.7967563
O	-1.5145885	4.2548013	0.3885776
H	1.6667153	5.3690558	1.6589002
H	3.9037559	-2.3608229	-2.1647548
H	2.7428446	4.0803319	-2.4194438
H	-5.0897106	0.8952517	2.2577724

Complex A35			
Ag	1.6401389	0.5267433	0.0000000
Ag	-0.3741357	-1.6573261	0.0000000
Ag	-1.2742370	1.1687907	0.0000000
Mo	2.4520133	-2.2342565	0.0000000
Mo	-3.1779618	-0.9958429	0.0000000
Mo	0.7129602	3.2462992	0.0000000
C	4.4075191	-3.5785818	0.0000000
C	3.6454249	-3.9247060	-1.1622117
C	2.3954224	-4.4871569	-0.7159509
C	2.3954224	-4.4871569	0.7159509
C	3.6454249	-3.9247060	1.1622117
H	5.4128759	-3.1361223	0.0000000
H	3.9666913	-3.8023003	-2.2049872
H	1.5952860	-4.8745302	-1.3609460
H	1.5952860	-4.8745302	1.3609460
H	3.9666913	-3.8023003	2.2049872
C	-5.3158065	-2.0223421	0.0000000
C	-5.2368098	-1.1885628	-1.1618513
C	-5.1036801	0.1757309	-0.7157890
C	-5.1036801	0.1757309	0.7157890
C	-5.2368098	-1.1885628	1.1618513
H	-5.4324362	-3.1145844	0.0000000
H	-5.2865977	-1.5281100	-2.2047157
H	-5.0392248	1.0625731	-1.3604087
H	-5.0392248	1.0625731	1.3604087
H	-5.2865977	-1.5281100	2.2047157
C	2.9246994	4.1571059	0.0000000
C	2.2341323	4.6498878	1.1584423
C	1.1249852	5.4450273	0.7217208
C	1.1249852	5.4450273	-0.7217208
C	2.2341323	4.6498878	-1.1584423
H	3.8315862	3.5384220	0.0000000
H	2.5202754	4.4595956	2.2017990
H	0.4238702	5.9885740	1.3689305
H	0.4238702	5.9885740	-1.3689305
H	2.5202754	4.4595956	-2.2017990
C	1.5288188	-1.7456796	1.7112958
O	1.1615958	-1.6504656	2.8235959
C	1.5288188	-1.7456796	-1.7112958
O	1.1615958	-1.6504656	-2.8235959
C	3.7540797	-0.7328029	0.0000000
O	4.7142270	-0.0469270	0.0000000
C	-2.5187800	-2.8712845	0.0000000
O	-2.3976333	-4.0446776	0.0000000
C	-2.2953271	-0.4421724	-1.7123360
O	-2.0335094	-0.1748444	-2.8265071
C	-2.2953271	-0.4421724	1.7123360
O	-2.0335094	-0.1748444	2.8265071
C	-1.2258010	3.6691153	0.0000000
O	-2.2958112	4.1641875	0.0000000
C	0.7040110	2.1939624	-1.7080812
O	0.7758869	1.8252193	-2.8218613
C	0.7040110	2.1939624	1.7080812
O	0.7758869	1.8252193	2.8218613

$[AuMoC_5H_4NMe_2(CO)_3]_n$ (n = 3 for **A15, A17, A20** and n = 4 for **A3, A9, A12, A38**)

Complex A3			
H	3.1578271	5.9972280	2.3029784
H	3.8575308	4.5044543	1.5686925
C	3.4512082	4.9471680	2.5095627
H	4.2569077	4.9667938	3.2750767
H	0.9460134	5.6673861	2.2907169
H	-3.4819907	4.2485429	-3.4431155
N	2.2915865	4.2267888	3.0172833
C	0.9844536	4.5721630	2.4671289
H	0.1791724	4.3150514	3.1851050
H	-3.7778847	3.6366506	-0.7946707
C	-3.8427430	3.2983512	-3.0285540
H	4.7324991	2.7652549	3.6621366
C	-4.0083111	2.9810362	-1.6447793
H	0.7732026	4.0464058	1.5051813
O	2.8961450	2.6171668	0.0864587
O	-0.2790991	3.2158590	-0.8155995

Complex A9			
H	1.5097039	2.4127543	-6.4551960
H	2.9424329	3.2423525	-5.7676787
C	2.0848092	2.5793168	-5.5210546
H	-0.5305382	2.7659221	-5.6129240
H	2.4826073	1.5962291	-5.1707965
N	1.2176722	3.2146148	-4.5390719
C	-0.2013331	2.8714117	-4.5579844
H	-0.4234284	1.9223386	-4.0155609
H	4.0099564	3.5569597	-3.7755209
H	-0.8015138	3.6816699	-4.0966969
O	1.5862877	0.1349865	-3.0495903
C	1.7738127	3.7201174	-3.3971131
C	3.1886608	3.8545575	-3.1132555
C	1.9129530	0.9000615	-2.2132067
C	1.0688364	4.2422740	-2.2438365
C	3.3420454	4.6202846	-1.8951265

C	2.4710831	3.0059361	3.6065061
C	3.7393270	2.3613957	3.8914443
O	-2.0477007	2.4081718	2.8426505
C	-4.2930746	2.1562960	-3.7942279
C	-0.9959338	2.5100895	-1.4164087
O	-0.7404619	2.5193909	-5.0884864
H	-4.3254246	2.1070641	-4.8885994
C	2.7303762	1.7251495	0.8452710
H	6.3037198	1.1899274	-4.7277128
C	-4.5805433	1.6647556	-1.5400305
O	2.3897065	1.4075324	-3.6068862
C	-1.2850658	2.1355709	-4.1283212
H	6.4773257	1.7219317	-2.5752079
H	4.8079400	1.5059722	-1.9118477
H	-4.8973486	1.1912401	-0.6043930
C	-4.8567958	1.1839720	-2.8779850
Mo	-2.3753546	1.5915249	-2.5621276
C	1.4374517	2.1128467	4.0848790
C	-2.1858100	1.2547666	2.6527696
H	0.3579950	2.2905782	4.0265993
C	3.4873730	1.1889448	4.7008278
C	5.7500447	0.9764396	-2.1923968
C	5.5716490	0.3644535	-4.6119572
H	4.5800149	0.7185909	-4.9842504
H	4.2509200	0.5654543	5.1836621
O	5.5790716	-0.3755884	1.8184474
H	-1.5440023	-0.2493706	5.3574037
Mo	2.7251883	0.6873289	2.5881429
C	4.4940328	-0.0008316	2.0707661
C	2.1900427	0.3397051	-3.1513732
H	-5.9116952	0.4797572	-5.2499743
H	6.1823566	0.5222467	-1.2762243
H	5.9116952	-0.4797572	-5.2499743
C	2.0713224	1.0357229	4.8017356
N	-5.5344150	0.0435304	-3.2135567
N	5.5344150	-0.0435304	-3.2135567
H	-6.1823566	-0.5222467	-1.2762243
Au	-2.0197685	0.2464623	-0.0899605
Au	0.0000000	0.0000000	-2.1983833
C	-5.5716490	-0.3644535	-4.6119572
Au	0.0000000	0.0000000	1.9528243
C	-2.0713224	-1.0357229	4.8017356
H	-4.2509200	-0.5654543	5.1836621
Au	2.0197685	-0.2464623	-0.0899605
H	-4.5800149	-0.7185909	-4.9842504
O	-5.5790716	0.3755884	1.8184474
H	1.5440023	0.2493706	5.3574037
C	-4.4940328	0.0008316	2.0707661
C	-5.7500447	-0.9764396	-2.1923968
C	-2.1900427	-0.3397051	-3.1513732
C	-3.4873730	-1.1889448	4.7008278
Mo	-2.7251883	-0.6873289	2.5881429
C	4.8567958	-1.1839720	-2.8779850
H	-6.4773257	-1.7219317	-2.5752079
H	-6.3037198	-1.1899274	-4.7277128
H	-0.3579950	-2.2905782	4.0265993
C	-1.4374517	-2.1128467	4.0848790
H	-4.8079400	-1.5059722	-1.9118477
H	4.8973486	-1.1912401	-0.6043930
C	2.1858100	-1.2547666	2.6527696
Mo	2.3753546	-1.5915249	-2.5621276
H	4.3254246	-2.1070641	-4.8885994
C	4.5805433	-1.6647556	-1.5400305
C	1.2850658	-2.1355709	-4.1283212
O	-2.3897065	-1.4075324	-3.6068862
C	4.2930746	-2.1562960	-3.7942279
O	0.7404619	-2.5193909	-5.0884864
C	-3.7393270	-2.3613957	3.8914443
C	-2.7303762	-1.7251495	0.8452710
C	0.9959338	-2.5100895	-1.4164087
C	-2.4710831	-3.0059361	3.6065061
O	2.0477007	-2.4081718	2.8426505
H	-4.7324991	-2.7652549	3.6621366
C	4.0083111	-2.9810362	-1.6447793
C	3.8427430	-3.2983512	-3.0285540
H	-0.7732026	-4.0464058	1.5051813
O	-2.8961450	-2.6171668	0.0864587
O	0.2790991	-3.2158590	-0.8155995
H	-0.0187370	4.2914276	-2.1245775
H	4.2893891	4.9953832	-1.4874947
O	5.5060091	1.5686413	-1.1861386
Mo	2.5219387	2.5698157	-1.2555781
C	4.3771747	1.8730011	-1.1659728
C	2.0350123	4.8427848	-1.3605015
Au	0.0000000	-2.0337114	0.0000000
Au	0.0000000	2.0337114	0.0000000
Au	2.1417144	0.0000000	0.0000000
H	1.7959087	5.4066009	-0.4493545
C	2.5454696	2.7021449	0.7533882
O	2.6936265	2.9614956	1.8892364
H	-1.5097039	-2.4127543	-6.4551960
H	-2.9424329	-3.2423525	-5.7676787
C	-2.0848092	-2.5793168	-5.5210546
H	0.5305382	-2.7659221	-5.6129240
H	-2.4826073	-1.5962291	-5.1707965
N	-1.2176722	-3.2146148	-4.5390719
C	0.2013331	-2.8714117	-4.5579844
H	0.4234284	-1.9223386	-4.0155609
H	-4.0099564	-3.5569597	-3.7755209
H	0.8015138	-3.6816699	-4.0966969
O	-1.5862877	-0.1349865	-3.0495903
C	-1.7738127	-3.7201174	-3.3971131
C	-3.1886608	-3.8545575	-3.1132555
C	-1.9129530	-0.9000615	-2.2132067
C	-1.0688364	-4.2422740	-2.2438365
C	-3.3420454	-4.6202846	-1.8951265
H	0.0187370	-4.2914276	-2.1245775
H	-4.2893891	-4.9953832	-1.4874947
O	-5.5060091	-1.5686413	-1.1861386
Mo	-2.5219387	-2.5698157	-1.2555781
C	-4.3771747	-1.8730011	-1.1659728
C	-2.0350123	-4.8427848	-1.3605015
Au	-2.1417144	0.0000000	0.0000000
H	-1.7959087	-5.4066009	-0.4493545
C	-2.5454696	-2.7021449	0.7533882
O	-2.6936265	-2.9614956	1.8892364
H	1.5097039	-2.4127543	6.4551960
H	2.9424329	-3.2423525	5.7676787
C	2.0848092	-2.5793168	5.5210546
H	-0.5305382	-2.7659221	5.6129240
H	2.4826073	-1.5962291	5.1707965
N	1.2176722	-3.2146148	4.5390719
C	-0.2013331	-2.8714117	4.5579844
H	-0.4234284	-1.9223386	4.0155609
H	4.0099564	-3.5569597	3.7755209
H	-0.8015138	-3.6816699	4.0966969
O	1.5862877	-0.1349865	3.0495903
C	1.7738127	-3.7201174	3.3971131
C	3.1886608	-3.8545575	3.1132555
C	1.9129530	-0.9000615	2.2132067
C	1.0688364	-4.2422740	2.2438365
C	3.3420454	-4.6202846	1.8951265
H	-0.0187370	-4.2914276	2.1245775
H	4.2893891	-4.9953832	1.4874947
O	5.5060091	-1.5686413	1.1861386
Mo	2.5219387	-2.5698157	1.2555781
C	4.3771747	-1.8730011	1.1659728
C	2.0350123	-4.8427848	1.3605015
H	1.7959087	-5.4066009	0.4493545
C	2.5454696	-2.7021449	-0.7533882
O	2.6936265	-2.9614956	-1.8892364
H	-1.5097039	2.4127543	6.4551960
H	-2.9424329	3.2423525	5.7676787
C	-2.0848092	2.5793168	5.5210546
H	0.5305382	2.7659221	5.6129240
H	-2.4826073	1.5962291	5.1707965
N	-1.2176722	3.2146148	4.5390719
C	0.2013331	2.8714117	4.5579844
H	0.4234284	1.9223386	4.0155609
H	-4.0099564	3.5569597	3.7755209
H	0.8015138	3.6816699	4.0966969
O	-1.5862877	0.1349865	3.0495903
C	-1.7738127	3.7201174	3.3971131
C	-3.1886608	3.8545575	3.1132555
C	-1.9129530	0.9000615	2.2132067
C	-1.0688364	4.2422740	2.2438365

H	3.7778847	-3.6366506	-0.7946707
H	-0.1791724	-4.3150514	3.1851050
N	-2.2915865	-4.2267888	3.0172833
C	-0.9844536	-4.5721630	2.4671289
H	3.4819907	-4.2485429	-3.4431155
H	-4.2569077	-4.9667938	3.2750767
H	-0.9460134	-5.6673861	2.2907169
C	-3.4512082	-4.9471680	2.5095627
H	-3.8575308	-4.5044543	1.5686925
H	-3.1578271	-5.9972280	2.3029784

Complex A12

H	-1.5981365	-2.7414999	6.3944675
H	-1.5640892	-4.3634293	5.6300583
C	-1.4004103	-3.2801371	5.4445986
H	-2.8517487	-1.0871179	5.5271033
H	-0.3299193	-3.1218297	5.1659243
N	-2.3203800	-2.7949108	4.4253320
C	-2.6853508	-1.3822055	4.4695632
H	-1.9005664	-0.7223302	4.0305767
H	-1.2243467	-5.3765628	3.6368713
H	-3.6301170	-1.2061780	3.9175298
O	0.6234385	-1.5156772	3.1362478
C	-2.4249369	-3.4854303	3.2489456
C	-1.8395198	-4.7776265	2.9548500
C	0.1689279	-2.1496390	2.2512820
C	-3.1481335	-3.0798594	2.0598322
C	-2.3534967	-5.2379299	1.6832176
H	-3.7263786	-2.1575891	1.9409730
H	-2.1941071	-6.2337429	1.2499883
O	1.5283241	-5.4772088	1.3298985
Mo	-0.9223885	-3.5030188	1.2053445
C	0.6531458	-4.7020714	1.2536170
C	-3.1489704	-4.1844227	1.1344864
Au	1.7298996	1.0937052	-0.1062037
Au	-1.7298996	-1.0937052	-0.1062037
Au	1.0937052	-1.7298996	0.1062037
H	-3.7005931	-4.2075166	0.1856212
C	-0.7752897	-3.6456521	-0.7936975
O	-0.7286825	-3.9270514	-1.9327403
H	1.5981365	2.7414999	6.3944675
H	1.5640892	4.3634293	5.6300583
C	1.4004103	3.2801371	5.4445986
H	2.8517487	1.0871179	5.5271033
H	0.3299193	3.1218297	5.1659243
N	2.3203800	2.7949108	4.4253320
C	2.6853508	1.3822055	4.4695632
H	1.9005664	0.7223302	4.0305767
H	1.2243467	5.3765628	3.6368713
H	3.6301170	1.2061780	3.9175298
O	-0.6234385	1.5156772	3.1362478
C	2.4249369	3.4854303	3.2489456
C	1.8395198	4.7776265	2.9548500
C	-0.1689279	2.1496390	2.2512820
C	3.1481335	3.0798594	2.0598322
C	2.3534967	5.2379299	1.6832176
H	3.7263786	2.1575891	1.9409730
H	2.1941071	6.2337429	1.2499883
O	-1.5283241	5.4772088	1.3298985
Mo	0.9223885	3.5030188	1.2053445
C	-0.6531458	4.7020714	1.2536170
C	3.1489704	4.1844227	1.1344864
Au	-1.0937052	1.7298996	0.1062037
H	3.7005931	4.2075166	0.1856212
C	0.7752897	3.6456521	-0.7936975
O	0.7286825	3.9270514	-1.9327403
H	2.7414999	-1.5981365	-6.3944675
H	-2.7414999	1.5981365	-6.3944675
H	4.3634293	-1.5640892	-5.6300583
H	-4.3634293	1.5640892	-5.6300583
C	3.2801371	-1.4004103	-5.4445986
C	-3.2801371	1.4004103	-5.4445986
H	1.0871179	-2.8517487	-5.5271033
H	-1.0871179	2.8517487	-5.5271033
H	3.1218297	-0.3299193	-5.1659243
H	-3.1218297	0.3299193	-5.1659243
N	2.7949108	-2.3203800	-4.4253320
N	-2.7949108	2.3203800	-4.4253320
C	1.3822055	-2.6853508	-4.4695632

C	-3.3420454	4.6202846	1.8951265
H	0.0187370	4.2914276	2.1245775
H	-4.2893891	4.9953832	1.4874947
O	-5.5060091	1.5686413	1.1861386
Mo	-2.5219387	2.5698157	1.2555781
C	-4.3771747	1.8730011	1.1659728
C	-2.0350123	4.8427848	1.3605015
H	-1.7959087	5.4066009	0.4493545
C	-2.5454696	2.7021449	-0.7533882
O	-2.6936265	2.9614956	-1.8892364

Complex A38

H	4.1440812	1.8012245	-5.2288064
H	5.4206574	2.2533018	-4.0498354
C	4.3360032	2.0300145	-4.1615991
H	2.4909166	3.2007566	-5.5897138
H	4.1009117	1.1220125	-3.5567673
N	3.5333074	3.1815914	-3.7679162
C	2.3519826	3.5427559	-4.5440574
H	1.4169624	3.0867718	-4.1433870
H	5.5576707	2.6579441	-1.7287819
H	2.2291924	4.6481835	-4.5627585
O	1.2962084	1.1595865	-2.5304160
C	3.6801247	3.6789418	-2.5059246
C	4.7297183	3.3566553	-1.5630796
C	1.7365174	1.6101634	-1.5228502
C	2.8077734	4.6366609	-1.8468886
C	4.6070538	4.2541406	-0.4348747
H	1.8875676	5.0642663	-2.2614530
H	5.3173900	4.3300085	0.3987706
O	4.6707606	1.3733028	1.8088318
Mo	2.8066830	2.8216735	-0.2807785
C	3.8828698	1.7566327	1.0172393
C	3.4299412	5.0410084	-0.6156877
Au	0.0000000	-2.5018185	0.0000000
Au	0.0000000	2.5018185	0.0000000
Au	2.5445398	0.0000000	0.0000000
H	3.0651047	5.8303094	0.0549659
C	1.7755284	3.4731898	1.2984629
O	1.4274501	4.0260743	2.2830714
H	-4.1440812	-1.8012245	-5.2288064
H	-5.4206574	-2.2533018	-4.0498354
C	-4.3360032	-2.0300145	-4.1615991
H	-2.4909166	-3.2007566	-5.5897138
H	-4.1009117	-1.1220125	-3.5567673
N	-3.5333074	-3.1815914	-3.7679162
C	-2.3519826	-3.5427559	-4.5440574
H	-1.4169624	-3.0867718	-4.1433870
H	-5.5576707	-2.6579441	-1.7287819
H	-2.2291924	-4.6481835	-4.5627585
O	-1.2962084	-1.1595865	-2.5304160
C	-3.6801247	-3.6789418	-2.5059246
C	-4.7297183	-3.3566553	-1.5630796
C	-1.7365174	-1.6101634	-1.5228502
C	-2.8077734	-4.6366609	-1.8468886
C	-4.6070538	-4.2541406	-0.4348747
H	-1.8875676	-5.0642663	-2.2614530
H	-5.3173900	-4.3300085	0.3987706
O	-4.6707606	-1.3733028	1.8088318
Mo	-2.8066830	-2.8216735	-0.2807785
C	-3.8828698	-1.7566327	1.0172393
C	-3.4299412	-5.0410084	-0.6156877
Au	-2.5445398	0.0000000	0.0000000
H	-3.0651047	-5.8303094	0.0549659
C	-1.7755284	-3.4731898	1.2984629
O	-1.4274501	-4.0260743	2.2830714
H	4.1440812	-1.8012245	5.2288064
H	5.4206574	-2.2533018	4.0498354
C	4.3360032	-2.0300145	4.1615991
H	2.4909166	-3.2007566	5.5897138
H	4.1009117	-1.1220125	3.5567673
N	3.5333074	-3.1815914	3.7679162
C	2.3519826	-3.5427559	4.5440574
H	1.4169624	-3.0867718	4.1433870
H	5.5576707	-2.6579441	1.7287819
H	2.2291924	-4.6481835	4.5627585
O	1.2962084	-1.1595865	2.5304160
C	3.6801247	-3.6789418	2.5059246
C	4.7297183	-3.3566553	1.5630796

C	-1.3822055	2.6853508	-4.4695632
H	0.7223302	-1.9005664	-4.0305767
H	-0.7223302	1.9005664	-4.0305767
H	5.3765628	-1.2243467	-3.6368713
H	-5.3765628	1.2243467	-3.6368713
H	1.2061780	-3.6301170	-3.9175298
H	-1.2061780	3.6301170	-3.9175298
O	1.5156772	0.6234385	-3.1362478
O	-1.5156772	-0.6234385	-3.1362478
C	3.4854303	-2.4249369	-3.2489456
C	-3.4854303	2.4249369	-3.2489456
C	4.7776265	-1.8395198	-2.9548500
C	-4.7776265	1.8395198	-2.9548500
C	2.1496390	0.1689279	-2.2512820
C	-2.1496390	-0.1689279	-2.2512820
C	3.0798594	-3.1481335	-2.0598322
C	-3.0798594	3.1481335	-2.0598322
C	5.2379299	-2.3534967	-1.6832176
C	-5.2379299	2.3534967	-1.6832176
H	2.1575891	-3.7263786	-1.9409730
H	-2.1575891	3.7263786	-1.9409730
H	6.2337429	-2.1941071	-1.2499883
H	-6.2337429	2.1941071	-1.2499883
O	5.4772088	1.5283241	-1.3298985
O	-5.4772088	-1.5283241	-1.3298985
Mo	3.5030188	-0.9223885	-1.2053445
Mo	-3.5030188	0.9223885	-1.2053445
C	4.7020714	0.6531458	-1.2536170
C	-4.7020714	-0.6531458	-1.2536170
C	4.1844227	-3.1489704	-1.1344864
C	-4.1844227	3.1489704	-1.1344864
H	4.2075166	-3.7005931	-0.1856212
H	-4.2075166	3.7005931	-0.1856212
C	3.6456521	-0.7752897	0.7936975
C	-3.6456521	0.7752897	0.7936975
O	3.9270514	-0.7286825	1.9327403
O	-3.9270514	0.7286825	1.9327403

C	1.7365174	-1.6101634	1.5228502
C	2.8077734	-4.6366609	1.8468886
C	4.6070538	-4.2541406	0.4348747
H	1.8875676	-5.0642663	2.2614530
H	5.3173900	-4.3300085	-0.3987706
O	4.6707606	-1.3733028	-1.8088318
Mo	2.8066830	-2.8216735	0.2807785
C	3.8828698	-1.7566327	-1.0172393
C	3.4299412	-5.0410084	0.6156877
H	3.0651047	-5.8303094	-0.0549659
C	1.7755284	-3.4731898	-1.2984629
O	1.4274501	-4.0260743	-2.2830714
H	-4.1440812	1.8012245	5.2288064
H	-5.4206574	2.2533018	4.0498354
C	-4.3360032	2.0300145	4.1615991
H	-2.4909166	3.2007566	5.5897138
H	-4.1009117	1.1220125	3.5567673
N	-3.5333074	3.1815914	3.7679162
C	-2.3519826	3.5427559	4.5440574
H	-1.4169624	3.0867718	4.1433870
H	-5.5576707	2.6579441	1.7287819
H	-2.2291924	4.6481835	4.5627585
O	-1.2962084	1.1595865	2.5304160
C	-3.6801247	3.6789418	2.5059246
C	-4.7297183	3.3566553	1.5630796
C	-1.7365174	1.6101634	1.5228502
C	-2.8077734	4.6366609	1.8468886
C	-4.6070538	4.2541406	0.4348747
H	-1.8875676	5.0642663	2.2614530
H	-5.3173900	4.3300085	-0.3987706
O	-4.6707606	1.3733028	-1.8088318
Mo	-2.8066830	2.8216735	0.2807785
C	-3.8828698	1.7566327	-1.0172393
C	-3.4299412	5.0410084	0.6156877
H	-3.0651047	5.8303094	-0.0549659
C	-1.7755284	3.4731898	-1.2984629
O	-1.4274501	4.0260743	-2.2830714

Complex A15

H	5.4625001	-2.5869206	-2.9703123
H	5.1037064	-4.1382796	-2.1504535
C	4.7370497	-3.1015947	-2.3066881
H	3.7499019	-3.1468532	-2.8279810
H	5.3744097	-0.6273567	-1.9195820
N	4.6681940	-2.3947197	-1.0346009
H	3.9375679	4.0836906	-3.3773209
C	4.7573010	-0.9411887	-1.0531437
O	1.1374124	-2.3152316	-2.5344558
H	2.0058055	5.1857276	-3.5781013
H	3.6987072	-5.1315693	-0.6781327
H	3.7519501	-0.4538451	-1.1255102
H	5.2542119	-0.5707084	-0.1301547
O	-1.9206499	0.2833737	-3.1108392
C	3.7040979	3.6117893	-2.3997335
H	3.4272055	2.5451135	-2.5817722
C	1.1776285	-2.5846190	-1.3937006
C	3.5858590	-4.3700545	0.1022527
C	4.0217372	-2.9923286	0.0184566
C	1.5864459	4.9212540	-2.5857473
H	4.6287005	3.6436330	-1.7842971
H	0.7445853	4.2011677	-2.7333661
O	1.2560560	1.2537992	-2.1555399
O	-3.2752434	-3.8143204	-1.2683020
H	1.1788381	5.8506604	-2.1336593
O	0.0419015	-5.9087848	-0.2724275
H	-5.5273059	-1.8595975	-2.5037026
N	2.6451862	4.3714903	-1.7503020
C	-2.3448458	-0.0486343	-2.0640017
H	-5.0034898	0.8192127	-2.6822550
C	0.5430772	-4.8875648	-0.0084875
C	-3.1077912	-2.6903272	-0.9414743
Mo	1.5550832	-3.2487688	0.4767531
C	3.1280114	-4.6203029	1.4520241
C	3.6743430	-2.3644101	1.2791742
C	-5.4782206	-1.1459345	-1.6717347
C	1.0247505	1.5379583	-1.0332525
C	-5.2104162	0.2549934	-1.7637207
H	2.8395949	-5.5975924	1.8599688
H	3.9050062	-1.3352573	1.5751613

Complex A17

Au	1.7597159	-0.5069040	0.0000000
Au	-0.4412537	1.7756952	0.0000000
Mo	-3.1874790	0.8662758	0.0000000
C	-5.1437869	0.1799549	-1.1580728
C	-5.1571129	-0.6912132	0.0000000
C	-5.1437869	0.1799549	1.1580728
C	-5.2874889	1.5407188	0.7180997
C	-5.2874889	1.5407188	-0.7180997
H	-5.1293933	-0.1426412	-2.2057830
H	-5.1293933	-0.1426412	2.2057830
H	-5.4157195	2.4147933	1.3687467
H	-5.4157195	2.4147933	-1.3687467
C	-2.2758303	0.4328134	-1.7461514
O	-1.9898664	0.2382534	-2.8667092
C	-2.2758303	0.4328134	1.7461514
O	-1.9898664	0.2382534	2.8667092
C	-2.7092448	2.7907718	0.0000000
O	-2.7391747	3.9722475	0.0000000
N	-5.1975673	-2.0635474	0.0000000
C	-4.8785949	-2.7521221	1.2435101
H	-5.5303433	-2.3895541	2.0662009
H	-5.0579345	-3.8379398	1.1152161
H	-3.8085747	-2.6028175	1.5357506
C	-4.8785949	-2.7521221	-1.2435101
H	-5.0579345	-3.8379398	-1.1152161
H	-5.5303433	-2.3895541	-2.0662009
H	-3.8085747	-2.6028175	-1.5357506
Au	-1.3165189	-1.2740312	0.0000000
Mo	2.3470224	2.3249999	0.0000000
Mo	0.8438830	-3.1965283	0.0000000
C	2.7236934	4.3612122	-1.1581265
C	2.4241551	-4.5370265	-1.1580679
C	1.9744490	4.8056578	0.0000000
C	3.1826464	-4.1077236	0.0000000
C	2.7236934	4.3612122	1.1581265
C	2.4241551	-4.5370265	1.1580679
C	3.9764936	3.8089776	0.7183947
C	1.3217547	-5.3485536	0.7185162
C	3.9764936	3.8089776	-0.7183947
C	1.3217547	-5.3485536	-0.7185162

Au	-1.0351268	-2.1117874	-0.0669960	H	2.4340136	4.5049073	-2.2062002
C	2.4015702	4.1819684	-0.4141065	H	2.6924852	-4.3574722	-2.2062130
Mo	-3.4933555	-0.7557697	-0.5706377	H	2.4340136	4.5049073	2.2062002
C	3.1738473	-3.3833511	2.1639834	H	2.6924852	-4.3574722	2.2062130
Au	1.2718853	-0.4123763	0.6607736	H	4.7971408	3.4812552	1.3685261
H	4.0506158	2.7524018	0.2350368	H	0.6316866	-5.9013028	1.3688984
Au	-1.3658148	1.0510424	-0.1073979	H	4.7971408	3.4812552	-1.3685261
C	-5.7290968	-1.4592759	-0.2803298	H	0.6316866	-5.9013028	-1.3688984
H	0.5512123	5.4372126	-0.0082633	C	1.5182566	1.7483773	-1.7472858
C	3.1798579	3.3629473	0.4998351	C	0.7608347	-2.1910389	-1.7476742
C	-5.2895010	0.8173782	-0.4421373	O	1.2042504	1.5929333	-2.8662488
H	-6.0049481	-2.4482985	0.1026791	O	0.7843172	-1.8424261	-2.8671248
C	1.3336596	4.7650045	0.3624751	C	1.5182566	1.7483773	1.7472858
H	2.9014133	-3.2270613	3.2162954	C	0.7608347	-2.1910389	1.7476742
C	0.2016283	-2.9789168	1.9448279	O	1.2042504	1.5929333	2.8662488
H	-5.1396089	1.8746470	-0.1957254	O	0.7843172	-1.8424261	2.8671248
Mo	0.9838532	2.4569970	0.7706080	C	3.7772942	0.9524057	0.0000000
C	-5.7350988	-0.2210547	0.4684643	C	-1.0592081	-3.7542437	0.0000000
C	-2.8746022	-0.5569769	1.3450627	O	4.8156137	0.3889522	0.0000000
C	2.7085512	3.6003517	1.8369624	O	-2.0675430	-4.3706503	0.0000000
O	-0.4105387	-2.9828683	2.9463417	N	0.8036379	5.5222388	0.0000000
C	1.5707344	4.4600060	1.7578766	N	4.3850161	-3.4483346	0.0000000
C	1.0488684	1.2266573	2.3540866	C	0.0489801	5.5879474	1.2447082
C	-0.9104047	2.9556341	1.1654192	C	4.8207114	-2.8293015	1.2441584
H	3.1621933	3.2046151	2.7551344	H	0.6904456	5.9739293	2.0653519
O	-2.7637947	-0.4349445	2.5074905	H	4.8319797	-3.5775407	2.0651542
N	-6.0884021	-0.0610993	1.7794389	H	-0.8040169	6.2837030	1.1178024
O	1.1382059	0.8182709	3.4591201	H	5.8510557	-2.4402590	1.1185671
O	-1.8538915	3.5638859	1.5442276	H	-0.3528475	4.5855274	1.5400703
H	0.9874780	4.8495963	2.6022054	H	4.1550544	-1.9783421	1.5397752
H	-6.9792631	-1.9500118	2.1351971	C	0.0489801	5.5879474	-1.2447082
H	-5.2931243	-1.7937543	2.7672336	C	4.8207114	-2.8293015	-1.2441584
H	-6.2429529	2.0501891	1.8124342	H	-0.8040169	6.2837030	-1.1178024
C	-6.2551732	-1.2494011	2.6057016	H	5.8510557	-2.4402590	-1.1185671
H	-4.7578988	1.4080300	2.6192230	H	0.6904456	5.9739293	-2.0653519
C	-5.8421944	1.2194925	2.4320667	H	4.8319797	-3.5775407	-2.0651542
H	-6.6627940	-0.9523556	3.5928882	H	-0.3528475	4.5855274	-1.5400703
H	-6.3768524	1.2358765	3.4034659	H	4.1550544	-1.9783421	-1.5397752

Complex A20

Au	-0.0514127	-1.6633603	0.8135463
Au	1.5267752	0.9859113	0.3093055
Mo	-0.0384663	3.2762203	-0.3908009
C	-1.1515369	4.8138074	-1.7312228
C	-1.8489216	4.8390868	-0.4736317
C	-0.9780885	5.4420168	0.5176270
C	0.3178004	5.5946269	-0.1070586
C	0.1837098	5.2765676	-1.5144856
H	-1.5889264	4.5083816	-2.6903591
H	1.2147816	6.0157454	0.3618152
H	0.9602797	5.4112611	-2.2782839
C	-0.4115777	2.0132890	-1.9138554
O	-0.5583222	1.5301966	-2.9772674
C	-0.3662558	2.6609855	1.5061173
O	-0.6006295	2.5513038	2.6516732
C	1.9520049	3.1398156	-0.5231338
O	3.0859299	3.4229839	-0.7114318
H	-2.8962683	4.5495118	-0.3284061
Au	-1.5894211	0.9179747	-0.0823825
Mo	2.8054393	-1.4853972	0.8764662
Mo	-2.8801225	-1.5548555	0.5708628
C	4.9957280	-1.8453578	-0.3360658
C	-3.9931182	-3.6267333	-0.3508823
C	5.0440171	-0.6939013	0.5437981
C	-3.2763917	-3.8960402	0.8805368
C	4.8697625	-1.1541734	1.8955584
C	-3.8928160	-3.1382848	1.9364606
C	4.5936643	-2.5561085	1.8644776
C	-4.9076626	-2.3108627	1.3623493
C	4.5942092	-2.9728416	0.4780085
C	-4.9220986	-2.5555410	-0.0649752
H	4.9571247	-0.5284837	2.7934738
H	-3.6337173	-3.2116886	3.0012940
H	4.4477979	-3.2141563	2.7303879
H	-5.5883184	-1.6397387	1.9011099
H	4.4514354	-4.0026344	0.1306926
H	-5.6222920	-2.0985837	-0.7736126
C	2.1432684	-1.1725247	-1.0033601
C	-1.7972752	-1.7139461	-1.1253708

O	1.9795335	-1.1119679	-2.1654667
O	-1.3611329	-1.9766397	-2.1851577
C	2.1325708	-0.3270844	2.3807640
C	-1.9573946	-1.0040393	2.2736184
O	1.9433396	0.2243339	3.4004770
O	-1.6750959	-0.7506152	3.3858976
C	1.7398544	-3.1155919	1.3295980
C	-3.8064704	0.1899658	0.2596110
O	1.4510080	-4.2219182	1.6332776
O	-4.6547807	1.0053410	0.1346674
H	5.2744507	0.3374296	0.2537687
H	-2.4701512	-4.6261806	1.0175630
N	-3.8215650	-4.2650542	-1.5489077
N	5.2831146	-1.8641794	-1.6742553
N	-1.3189243	5.7984450	1.7936210
C	-2.6989261	-5.1819969	-1.7040662
H	-1.7118049	-4.6600069	-1.6983288
H	-2.7044131	-5.9369736	-0.8879134
H	-2.8062021	-5.7235583	-2.6658408
C	-4.4347409	-3.6897994	-2.7393390
H	-3.9886900	-2.7030277	-3.0141796
H	-4.2996551	-4.3862785	-3.5911366
H	-5.5271011	-3.5512990	-2.5848424
C	4.9541665	-3.0537863	-2.4478446
H	5.4296655	-2.9782438	-3.4470454
H	5.3575042	-3.9611280	-1.9492345
H	3.8537144	-3.1836355	-2.5884733
C	5.4487908	-0.6020558	-2.3845571
H	4.4840964	-0.0588709	-2.5300482
H	6.1466961	0.0613185	-1.8314401
H	5.8926199	-0.8043686	-3.3814921
C	-2.6107464	5.3823908	2.3270132
H	-3.4224503	5.6517838	1.6178812
H	-2.6611902	4.2850112	2.5259324
H	-2.7998351	5.9219986	3.2778590
C	-0.2570074	6.1595743	2.7237958
H	-0.7095529	6.5326652	3.6646046
H	0.4086731	5.2967661	2.9693343
H	0.3679434	6.9768035	2.3013107

$[AuMoCp(CO)_3]_n$ (n = 3 for **A33, A36** and n = 4 for **A6, A23, A26, A30, A40**)

Complex A33			
O	2.2847386	-0.4144337	-2.8478917
H	5.8696841	1.3186934	-1.5288292
O	-1.2294707	-2.0453572	-2.8479328
C	2.5568064	-0.1635137	-1.7376397
C	5.1535798	1.7479535	-0.8157650
C	3.9709986	2.4860440	-1.1522568
O	-0.9053581	1.3679236	-2.7914668
O	1.9637271	-4.4955027	-0.3178294
O	5.2281953	-2.0282644	-0.0361410
H	-0.7905130	-5.9909592	-1.4311017
C	-1.0848758	-2.3213935	-1.7152482
H	-3.0046114	-4.4749102	-1.9105182
C	4.4807591	-1.1336507	-0.0260900
C	1.0069191	-3.8174752	-0.1745023
Mo	3.3508697	0.5038282	-0.0072835
C	5.2511685	1.7072132	0.6231892
C	3.3443602	2.9189566	0.0657222
C	-1.4011194	-5.4810396	-0.6739998
C	-1.2463447	1.5443575	-1.6810791
C	-2.5702973	-4.6891040	-0.9246725
H	6.0604003	1.2410967	1.2005999
H	2.4665429	3.5724996	0.1469769
Au	1.3114055	-1.5362333	0.0377230
C	-3.0421040	3.8748221	-1.4731179
Mo	-0.9221870	-3.3016702	0.0390993
C	4.1310080	2.4214453	1.1600157
Au	0.6196926	1.3249103	0.0648291
H	-1.0798180	4.9602691	-1.1442342
Au	-1.7717128	-0.6009564	-0.1077611
C	-1.1958290	-5.5244648	0.7546338
H	-5.0013770	2.9654486	-0.8228612
C	-1.9946632	4.5201187	-0.7258380
C	-3.0915157	-4.2419256	0.3338878

Complex A36			
Au	1.1714933	-1.3846455	0.0000000
Au	0.6139887	1.7097027	0.0000000
Mo	-2.1404151	2.4963694	0.0000000
C	-4.0975492	3.1577737	-1.1578999
C	-4.5281230	2.4278160	0.0000000
C	-4.0975492	3.1577737	1.1578999
C	-3.4048318	4.3343003	0.7217192
C	-3.4048318	4.3343003	-0.7217192
H	-4.2824347	2.8683156	-2.2013876
H	-4.2824347	2.8683156	2.2013876
H	-2.9828005	5.1144697	1.3685069
H	-2.9828005	5.1144697	-1.3685069
C	-1.7255767	1.5559324	-1.7353359
O	-1.6484659	1.2034763	-2.8506845
C	-1.7255767	1.5559324	1.7353359
O	-1.6484659	1.2034763	2.8506845
C	-0.5811327	3.7482648	0.0000000
O	0.0659186	4.7365851	0.0000000
H	-5.0926841	1.4863279	0.0000000
Au	-1.7848137	-0.3214744	0.0000000
Mo	3.2315113	0.6061680	0.0000000
Mo	-1.0915380	-3.1012163	0.0000000
C	4.7870905	1.9660894	-1.1579449
C	-0.6865283	-5.1271075	-1.1578420
C	4.3726689	2.7055407	0.0000000
C	0.1609593	-5.1351554	0.0000000
C	4.7870905	1.9660894	1.1579449
C	-0.6865283	-5.1271075	1.1578420
C	5.4562909	0.7757840	0.7218198
C	-2.0520867	-5.1146555	0.7218039
C	5.4562909	0.7757840	-0.7218198
C	-2.0520867	-5.1146555	-0.7218039
H	4.6296829	2.2715233	-2.2013999

H	-0.4029866	-6.0747503	1.2780938
C	-4.0595075	3.4642281	-0.5597297
H	3.9188243	2.5833749	2.2259634
C	2.6182088	-0.1579579	1.7532251
H	-3.9826709	-3.6185531	0.4831276
Mo	-2.1080083	2.2577559	0.0060439
C	-2.2401430	-4.7625429	1.3674371
C	-0.8383262	-2.2158506	1.7404232
C	-2.3733648	4.5090561	0.6552216
O	2.3865988	-0.4006891	2.8751291
C	-3.6470510	3.8551230	0.7662205
C	-0.9694822	2.1338284	1.6577691
C	-3.3912287	0.8637524	0.6472934
H	-1.8000530	4.9407989	1.4859027
O	-0.8804378	-1.7972528	2.8332299
O	-0.5398683	2.2882624	2.7447695
O	-4.3711455	0.3796749	1.1015551
H	-4.2212664	3.7040616	1.6898434
H	-2.3784994	-4.6053699	2.4457006
H	-3.0561291	3.7282941	-2.5619142
H	3.6174784	2.7100296	-2.1679217

Complex A6

H	-3.1477942	-3.1622655	3.1583789
H	-1.7542177	-5.5072742	3.2033759
O	0.0312727	-1.6021891	3.1421478
C	-2.9683202	-3.8250345	2.3009424
C	-2.2258390	-5.0518323	2.3226279
C	-0.3056283	-2.2508200	2.2302959
C	-3.4714345	-3.6242515	0.9716606
C	-2.2512268	-5.6042589	0.9903291
H	-4.1380296	-2.8183986	0.6420529
H	-1.8039114	-6.5565094	0.6755597
O	1.5256090	-5.3210016	1.5190484
Mo	-1.0421939	-3.6055100	0.9269124
C	0.6030249	-4.6380903	1.2844961
C	-3.0129265	-4.7153753	0.1624299
Au	1.7968647	0.9924255	0.0680685
Au	-1.7968647	-0.9924255	0.0680685
Au	0.9924255	-1.7968647	-0.0680685
H	-3.2332517	-4.8551944	-0.9046495
C	-0.4562056	-3.5315097	-1.0047254
O	-0.3006011	-3.7397276	-2.1514062
H	3.1477942	3.1622655	3.1583789
H	1.7542177	5.5072742	3.2033759
O	-0.0312727	1.6021891	3.1421478
C	2.9683202	3.8250345	2.3009424
C	2.2258390	5.0518323	2.3226279
C	0.3056283	2.2508200	2.2302959
C	3.4714345	3.6242515	0.9716606
C	2.2512268	5.6042589	0.9903291
H	4.1380296	2.8183986	0.6420529
H	1.8039114	6.5565094	0.6755597
O	-1.5256090	5.3210016	1.5190484
Mo	1.0421939	3.6055100	0.9269124
C	-0.6030249	4.6380903	1.2844961
C	3.0129265	4.7153753	0.1624299
Au	-0.9924255	1.7968647	-0.0680685
H	3.2332517	4.8551944	-0.9046495
C	0.4562056	3.5315097	-1.0047254
O	0.3006011	3.7397276	-2.1514062
H	3.1622655	-3.1477942	-3.1583789
H	-3.1622655	3.1477942	-3.1583789
H	5.5072742	-1.7542177	-3.2033759
H	-5.5072742	1.7542177	-3.2033759
O	1.6021891	0.0312727	-3.1421478
O	-1.6021891	-0.0312727	-3.1421478
C	3.8250345	-2.9683202	-2.3009424
C	-3.8250345	2.9683202	-2.3009424
C	5.0518323	-2.2258390	-2.3226279
C	-5.0518323	2.2258390	-2.3226279
C	2.2508200	-0.3056283	-2.2302959
C	-2.2508200	0.3056283	-2.2302959
C	3.6242515	-3.4714345	-0.9716606
C	-3.6242515	3.4714345	-0.9716606
C	5.6042589	-2.2512268	-0.9903291
C	-5.6042589	2.2512268	-0.9903291
H	2.8183986	-4.1380296	-0.6420529
H	-2.8183986	4.1380296	-0.6420529

H	-0.3432640	-5.1419370	-2.2010577
H	4.6296829	2.2715233	2.2013999
H	-0.3432640	-5.1419370	2.2010577
H	5.9181604	0.0185601	1.3684521
H	-2.9387680	-5.1388403	1.3686650
H	5.9181604	0.0185601	-1.3684521
H	-2.9387680	-5.1388403	-1.3686650
C	2.2084848	0.7203937	-1.7345628
C	-0.4851148	-2.2711391	-1.7355497
O	1.8636003	0.8312460	-2.8494487
O	-0.2186822	-2.0277474	-2.8509455
C	2.2084848	0.7203937	1.7345628
C	-0.4851148	-2.2711391	1.7355497
O	1.8636003	0.8312460	2.8494487
O	-0.2186822	-2.0277474	2.8509455
C	3.5315974	-1.3709316	0.0000000
C	-2.9548449	-2.3758111	0.0000000
O	4.0635255	-2.4257838	0.0000000
O	-4.1341615	-2.3086484	0.0000000
H	3.8431138	3.6672740	0.0000000
H	1.2585223	-5.1532575	0.0000000

Complex A23

H	-4.2344722	3.3973791	-3.9856377
H	1.3663583	3.7814340	3.1043100
H	-4.4479354	3.0312776	-1.2937346
C	-4.4112871	2.4410737	-3.4756117
H	4.0491349	3.4833344	3.4911122
C	-4.5342632	2.2488259	-2.0598750
O	2.1335368	3.0963375	0.0528887
O	-0.9061997	3.1317357	-1.2038034
C	1.8565679	2.9325804	3.5996584
C	3.2697603	2.7697933	3.7903533
O	-2.5408642	2.1572972	2.3082791
C	-4.6107429	1.1613741	-4.1107496
C	-1.4583213	2.2765457	-1.7767514
O	-1.1879814	2.1172950	-5.4347959
H	-4.6132364	0.9677211	-5.1913480
C	2.2581146	2.1547693	0.7466212
C	-4.8306345	0.8662008	-1.8123325
O	2.0347241	1.9227543	-3.7607424
C	-1.6636951	1.6963367	-4.4557927
H	-5.0572101	0.4155895	-0.8379043
C	-4.8606994	0.1960187	-3.0785135
Mo	-2.6469038	1.0505963	-2.8585951
C	1.1889006	1.8115598	4.1896676
C	-2.4833561	0.9886263	2.2272736
H	0.1028802	1.6705321	4.2503546
C	3.4784635	1.5284659	4.4938803
H	4.4454873	1.1277628	4.8249466
O	5.5734540	0.6952856	1.4049721
H	-2.0107426	0.0085434	5.2549622
Mo	2.6080507	1.0200714	2.3837046
C	4.4498255	0.7999686	1.7253488
C	2.0629481	0.8225436	-3.3514572
C	2.1945959	0.9372255	4.7269305
H	-5.0648135	-0.8724166	-3.2315924
H	5.0648135	0.8724166	-3.2315924
Au	-2.0605606	-0.0767313	-0.3250629
Au	0.0000000	0.0000000	-2.3948235
Au	0.0000000	0.0000000	1.7328967
C	-2.1945959	-0.9372255	4.7269305
H	-4.4454873	-1.1277628	4.8249466
Au	2.0605606	0.0767313	-0.3250629
O	-5.5734540	-0.6952856	1.4049721
H	2.0107426	-0.0085434	5.2549622
C	-4.4498255	-0.7999686	1.7253488
C	-2.0629481	-0.8225436	-3.3514572
C	-3.4784635	-1.5284659	4.4938803
Mo	-2.6080507	-1.0200714	2.3837046
C	4.8606994	-0.1960187	-3.0785135
H	-0.1028802	-1.6705321	4.2503546
C	-1.1889006	-1.8115598	4.1896676
H	5.0572101	-0.4155895	-0.8379043
C	2.4833561	-0.9886263	2.2272736
Mo	2.6469038	-1.0505963	-2.8585951
H	4.6132364	-0.9677211	-5.1913480
C	4.8306345	-0.8662008	-1.8123325
C	1.6636951	-1.6963367	-4.4557927

H	6.5565094	-1.8039114	-0.6755597
H	-6.5565094	1.8039114	-0.6755597
O	5.3210016	1.5256090	-1.5190484
O	-5.3210016	-1.5256090	-1.5190484
Mo	3.6055100	-1.0421939	-0.9269124
Mo	-3.6055100	1.0421939	-0.9269124
C	4.6380903	0.6030249	-1.2844961
C	-4.6380903	-0.6030249	-1.2844961
C	4.7153753	-3.0129265	-0.1624299
C	-4.7153753	3.0129265	-0.1624299
H	4.8551944	-3.2332517	0.9046495
H	-4.8551944	3.2332517	0.9046495
C	3.5315097	-0.4562056	1.0047254
C	-3.5315097	0.4562056	1.0047254
O	3.7397276	-0.3006011	2.1514062
O	-3.7397276	0.3006011	2.1514062

Complex A26

H	0.6616225	2.7123827	-4.1173282
H	3.3333251	3.2139390	-4.3515275
O	1.5471720	-0.2341157	-3.0421217
C	1.2653472	3.3337595	-3.4423714
C	2.6726630	3.5864988	-3.5575014
C	1.8531507	0.6338405	-2.3110497
C	0.7664010	4.0528002	-2.3081206
C	3.0537886	4.4602016	-2.4746823
H	-0.2854468	4.1116901	-2.0015107
H	4.0560059	4.8717565	-2.2961050
O	5.3974807	1.5146139	-1.8231008
Mo	2.3966627	2.4192044	-1.5530822
C	4.2733232	1.7987231	-1.6834497
C	1.8780735	4.7324340	-1.7013453
Au	0.0000000	-1.9741487	0.0000000
Au	0.0000000	1.9741487	0.0000000
Au	2.1201361	0.0000000	0.0000000
H	1.8285308	5.3768298	-0.8135821
C	2.7430334	2.6226147	0.4241126
O	3.0338729	2.9430469	1.5130120
H	-0.6616225	-2.7123827	-4.1173282
H	-3.3333251	-3.2139390	-4.3515275
O	-1.5471720	0.2341157	-3.0421217
C	-1.2653472	-3.3337595	-3.4423714
C	-2.6726630	-3.5864988	-3.5575014
C	-1.8531507	-0.6338405	-2.3110497
C	-0.7664010	-4.0528002	-2.3081206
C	-3.0537886	-4.4602016	-2.4746823
H	0.2854468	-4.1116901	-2.0015107
H	-4.0560059	-4.8717565	-2.2961050
O	-5.3974807	-1.5146139	-1.8231008
Mo	-2.3966627	-2.4192044	-1.5530822
C	-4.2733232	-1.7987231	-1.6834497
C	-1.8780735	-4.7324340	-1.7013453
Au	-2.1201361	0.0000000	0.0000000
H	-1.8285308	-5.3768298	-0.8135821
C	-2.7430334	-2.6226147	0.4241126
O	-3.0338729	-2.9430469	1.5130120
H	0.6616225	-2.7123827	4.1173282
H	3.3333251	-3.2139390	4.3515275
O	1.5471720	0.2341157	3.0421217
C	1.2653472	-3.3337595	3.4423714
C	2.6726630	-3.5864988	3.5575014
C	1.8531507	-0.6338405	2.3110497
C	0.7664010	-4.0528002	2.3081206
C	3.0537886	-4.4602016	2.4746823
H	-0.2854468	-4.1116901	2.0015107
H	4.0560059	-4.8717565	2.2961050
O	5.3974807	-1.5146139	1.8231008
Mo	2.3966627	-2.4192044	1.5530822
C	4.2733232	-1.7987231	1.6834497
C	1.8780735	-4.7324340	1.7013453
H	1.8285308	-5.3768298	0.8135821
C	2.7430334	-2.6226147	-0.4241126
O	3.0338729	-2.9430469	-1.5130120
H	-0.6616225	2.7123827	4.1173282
H	-3.3333251	3.2139390	4.3515275
O	-1.5471720	-0.2341157	3.0421217
C	-1.2653472	3.3337595	3.4423714
C	-2.6726630	3.5864988	3.5575014
C	-1.8531507	0.6338405	2.3110497

O	-2.0347241	-1.9227543	-3.7607424
C	4.6107429	-1.1613741	-4.1107496
O	1.1879814	-2.1172950	-5.4347959
C	-3.2697603	-2.7697933	3.7903533
C	-2.2581146	-2.1547693	0.7466212
C	1.4583213	-2.2765457	-1.7767514
C	-1.8565679	-2.9325804	3.5996584
O	2.5408642	-2.1572972	2.3082791
H	-4.0491349	-3.4833344	3.4911122
C	4.5342632	-2.2488259	-2.0598750
C	4.4112871	-2.4410737	-3.4756117
O	-2.1335368	-3.0963375	0.0528887
O	0.9061997	-3.1317357	-1.2038034
H	4.4479354	-3.0312776	-1.2937346
H	-1.3663583	-3.7814340	3.1043100
H	4.2344722	-3.3973791	-3.9856377

Complex A30

H	5.9542457	0.9724465	-2.9530052
H	-5.9542457	-0.9724465	-2.9530052
H	4.3490388	-1.1769228	-3.4289998
H	-4.3490388	1.1769228	-3.4289998
C	5.6266106	0.2335436	-2.2097193
C	-5.6266106	-0.2335436	-2.2097193
C	4.7915455	-0.9016968	-2.4616440
C	-4.7915455	0.9016968	-2.4616440
O	-1.4132585	-0.8647242	-3.1404828
O	1.4132585	0.8647242	-3.1404828
C	5.9946916	0.2100701	-0.8158346
C	-5.9946916	-0.2100701	-0.8158346
H	-6.6569983	-0.9241562	-0.3091333
H	6.6569983	0.9241562	-0.3091333
C	2.1561673	0.7466192	-2.2473620
C	-2.1561673	-0.7466192	-2.2473620
C	-4.6557883	1.6443197	-1.2401267
C	4.6557883	-1.6443197	-1.2401267
O	-1.1651694	3.6015189	-2.1630077
O	1.1651694	-3.6015189	-2.1630077
H	4.1380283	-2.6034295	-1.1206494
H	-4.1380283	2.6034295	-1.1206494
C	-5.3854329	0.9477425	-0.2222917
C	5.3854329	-0.9477425	-0.2222917
Mo	3.6906464	0.5608739	-0.9442788
Mo	-3.6906464	-0.5608739	-0.9442788
O	-4.1815396	-3.6366760	-1.3754852
O	4.1815396	3.6366760	-1.3754852
C	3.9477244	2.5023340	-1.1985758
C	-3.9477244	-2.5023340	-1.1985758
C	0.9984146	-3.3968906	-1.0142587
C	-0.9984146	3.3968906	-1.0142587
H	-5.4845331	1.2679864	0.8235409
H	5.4845331	-1.2679864	0.8235409
Au	-1.5885679	1.2362714	-0.2779955
Au	1.5885679	-1.2362714	-0.2779955
H	1.1121764	5.5901646	-0.8496193
H	-1.1121764	-5.5901646	-0.8496193
Au	1.2473523	1.5924361	0.2491435
Au	-1.2473523	-1.5924361	0.2491435
C	-3.4029432	-0.9717687	1.0157623
C	3.4029432	0.9717687	1.0157623
O	-3.6427620	4.1056859	1.4330098
O	3.6427620	-4.1056859	1.4330098
C	2.5080526	-3.8944098	1.2323990
C	-2.5080526	3.8944098	1.2323990
C	0.8563426	5.4378259	0.2077529
C	-0.8563426	-5.4378259	0.2077529
Mo	-0.5669690	3.6718509	0.9434846
Mo	0.5669690	-3.6718509	0.9434846
H	-1.0389548	6.6505197	0.4498580
H	1.0389548	-6.6505197	0.4498580
H	2.5926641	4.2030798	0.9558666
H	-2.5926641	-4.2030798	0.9558666
C	-0.2811879	5.9881398	0.8887143
C	0.2811879	-5.9881398	0.8887143
O	3.5894629	1.1246588	2.1687967
O	-3.5894629	-1.1246588	2.1687967
C	1.6289455	4.6874109	1.1522915
C	-1.6289455	-4.6874109	1.1522915
C	-0.7170469	2.1256428	2.2358718

C	-0.7664010	4.0528002	2.3081206	C	0.7170469	-2.1256428	2.2358718
C	-3.0537886	4.4602016	2.4746823	O	0.8185412	-1.3746194	3.1239620
H	0.2854468	4.1116901	2.0015107	O	-0.8185412	1.3746194	3.1239620
H	-4.0560059	4.8717565	2.2961050	C	-0.2181410	5.5628479	2.2652785
O	-5.3974807	1.5146139	1.8231008	C	0.2181410	-5.5628479	2.2652785
Mo	-2.3966627	2.4192044	1.5530822	C	0.9520026	4.7502562	2.4174937
C	-4.2733232	1.7987231	1.6834497	C	-0.9520026	-4.7502562	2.4174937
C	-1.8780735	4.7324340	1.7013453	H	-0.9219432	5.8398549	3.0613918
H	-1.8285308	5.3768298	0.8135821	H	0.9219432	-5.8398549	3.0613918
C	-2.7430334	2.6226147	-0.4241126	H	-1.2926646	-4.2758761	3.3478519
O	-3.0338729	2.9430469	-1.5130120	H	1.2926646	4.2758761	3.3478519
Complex A40							
H	3.8778190	2.7248287	-3.2649774				
H	5.7398768	2.8032049	-1.2842482				
O	1.2284349	1.1415168	-2.5389315				
C	3.8725739	3.4027292	-2.4005801				
C	4.8459359	3.4368963	-1.3556694				
C	1.6788173	1.6039025	-1.5452159				
C	2.8800029	4.4099290	-2.1260972				
C	4.4577627	4.4667293	-0.4249656				
H	1.9991024	4.6328163	-2.7428926				
H	5.0060037	4.7594845	0.4805174				
O	4.6644301	1.4122147	1.7585456				
Mo	2.8009311	2.8173575	-0.3531086				
C	3.8661915	1.7660978	0.9667755				
C	3.2466619	5.0685710	-0.9105952				
Au	0.0000000	-2.4631644	0.0000000				
Au	0.0000000	2.4631644	0.0000000				
Au	2.5456467	0.0000000	0.0000000				
H	2.7041647	5.8988116	-0.4386614				
C	1.7904607	3.5376436	1.2114002				
O	1.4460985	4.1523632	2.1565374				
H	-3.8778190	-2.7248287	-3.2649774				
H	-5.7398768	-2.8032049	-1.2842482				
O	-1.2284349	-1.1415168	-2.5389315				
C	-3.8725739	-3.4027292	-2.4005801				
C	-4.8459359	-3.4368963	-1.3556694				
C	-1.6788173	-1.6039025	-1.5452159				
C	-2.8800029	-4.4099290	-2.1260972				
C	-4.4577627	-4.4667293	-0.4249656				
H	-1.9991024	-4.6328163	-2.7428926				
H	-5.0060037	-4.7594845	0.4805174				
O	-4.6644301	-1.4122147	1.7585456				
Mo	-2.8009311	-2.8173575	-0.3531086				
C	-3.8661915	-1.7660978	0.9667755				
C	-3.2466619	-5.0685710	-0.9105952				
Au	-2.5456467	0.0000000	0.0000000				
H	-2.7041647	-5.8988116	-0.4386614				
C	-1.7904607	-3.5376436	1.2114002				
O	-1.4460985	-4.1523632	2.1565374				
H	3.8778190	-2.7248287	3.2649774				
H	5.7398768	-2.8032049	1.2842482				
O	1.2284349	-1.1415168	2.5389315				
C	3.8725739	-3.4027292	2.4005801				
C	4.8459359	-3.4368963	1.3556694				
C	1.6788173	-1.6039025	1.5452159				
C	2.8800029	-4.4099290	2.1260972				
C	4.4577627	-4.4667293	0.4249656				
H	1.9991024	-4.6328163	2.7428926				
H	5.0060037	-4.7594845	-0.4805174				
O	4.6644301	-1.4122147	-1.7585456				
Mo	2.8009311	-2.8173575	0.3531086				
C	3.8661915	-1.7660978	-0.9667755				
C	3.2466619	-5.0685710	0.9105952				
H	2.7041647	-5.8988116	0.4386614				
C	1.7904607	-3.5376436	-1.2114002				
O	1.4460985	-4.1523632	-2.1565374				
H	-3.8778190	2.7248287	3.2649774				
H	-5.7398768	2.8032049	1.2842482				
O	-1.2284349	1.1415168	2.5389315				
C	-3.8725739	3.4027292	2.4005801				
C	-4.8459359	3.4368963	1.3556694				
C	-1.6788173	1.6039025	1.5452159				
C	-2.8800029	4.4099290	2.1260972				
C	-4.4577627	4.4667293	0.4249656				
H	-1.9991024	4.6328163	2.7428926				
H	-5.0060037	4.7594845	-0.4805174				
O	-4.6644301	1.4122147	-1.7585456				

Mo	-2.8009311	2.8173575	0.3531086
C	-3.8661915	1.7660978	-0.9667755
C	-3.2466619	5.0685710	0.9105952
H	-2.7041647	5.8988116	0.4386614
C	-1.7904607	3.5376436	-1.2114002
O	-1.4460985	4.1523632	-2.1565374