BONDING SITUATION IN HETEROMULTIMETALLIC CARBONYL COMPLEXES

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SUPPORTING INFORMATION

1 QTAIM Analysis

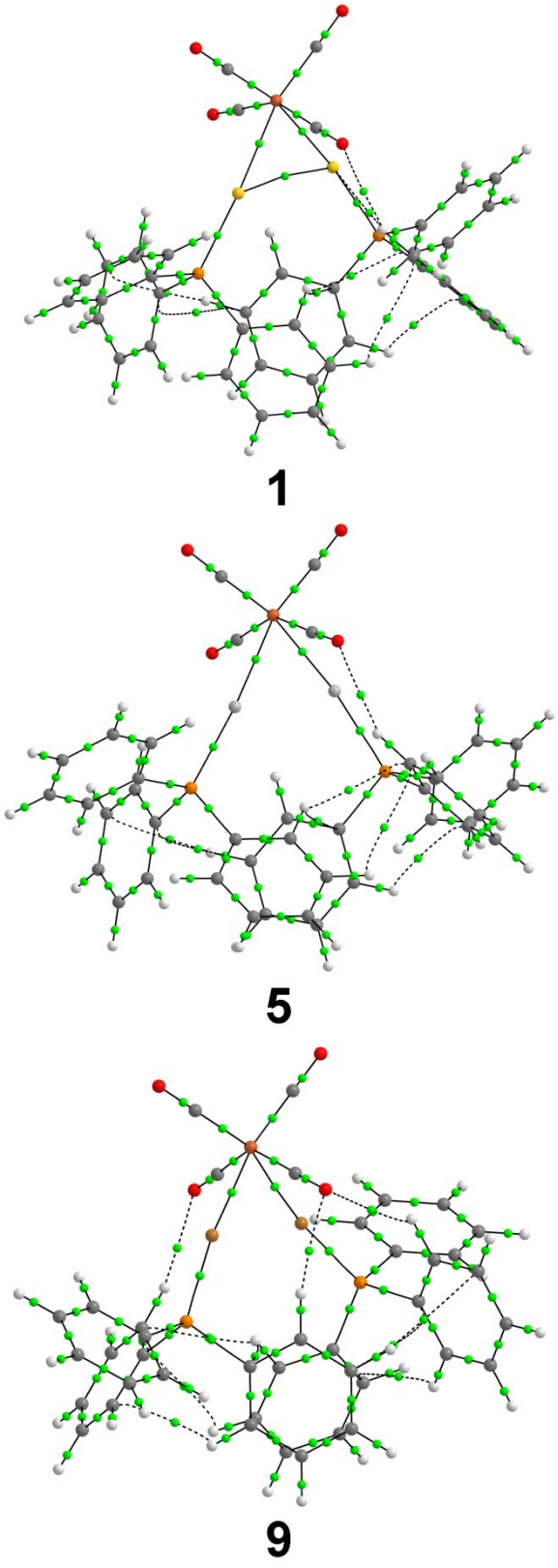

Fig. S1 Topological maps containing bond critical points (green dots) and bond paths (black lines) to selected complexes (**1**, **5** and **9**). Color code: H = white; C = gray; O = red; P = orange; Fe = brown; Cu = copper; Ag = silver; Au = yellow.

Table S1. Electron density, ρ_b, Laplacian of ρ_b, $\nabla^2\rho_b$, and $-G_b/V_b$, at M–M BCPs, and M–M fuzzy bond orders (FBOs) in the complexes **1**, **3**, **5**, **7**, **9** and **10**. The values of all the parameters are in a.u.

Complex	ρ_b	$\nabla^2\rho_b$	$-G_b/V_b$	FBO
1	0.039	0.082	0.828	0.592
3	0.040	0.080	0.820	0.618
5	–	–	–	0.489
7	–	–	–	0.522
9	–	–	–	0.446
10	–	–	–	0.471

2 ETS–NOCV Density Flow Channels

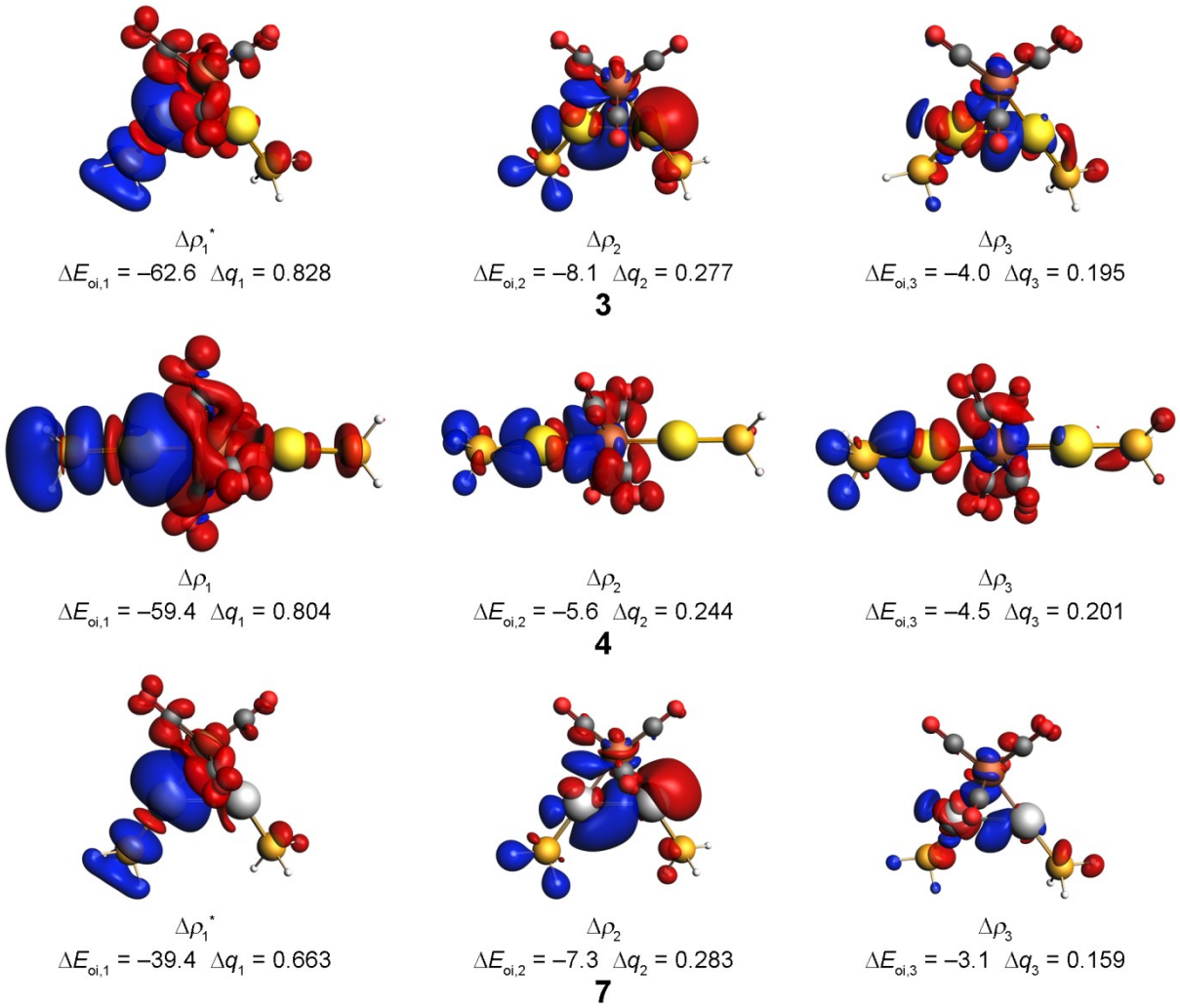

Fig. S2 Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions between the fragments $[M(PH_3)]^+$ and $[M(PH_3)Fe(CO)_4]^-$ (M = Au(I) and Ag(I)) in the complexes **3**, **4** and **7**). The values of the $\Delta E_{oi,i}$ (kcal mol^{-1}) energy and Δq_i charge transfer (a.u.) to each ($\Delta\rho_i$) channel are shown. Red and blue surfaces indicate the electron density outflow and inflow, respectively. The isovalue used to represent these surfaces is equal to 0.0003 (* 0.0008) a.u.

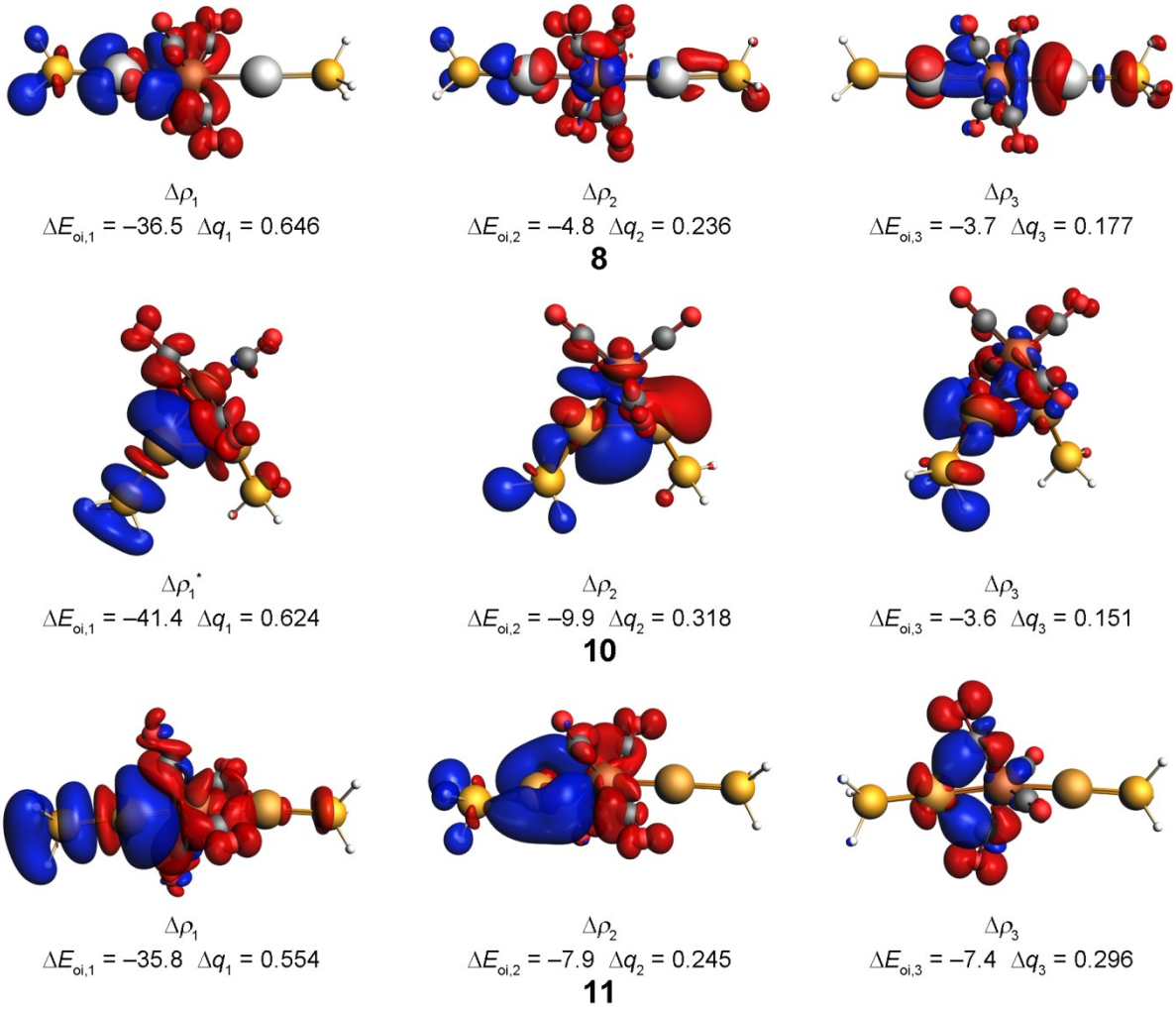

Fig. S3 Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions between the fragments $[M(PH_3)]^+$ and $[M(PH_3)Fe(CO)_4]^-$ (M = Ag(I) and Cu(I)) in the complexes **8**, **10** and **11**). The values of the $\Delta E_{oi,i}$ (kcal mol^{-1}) energy and Δq_i charge transfer (a.u.) to each ($\Delta\rho_i$) channel are shown. Red and blue surfaces indicate the electron density outflow and inflow, respectively. The isovalue used to represent these surfaces is equal to 0.0003 (* 0.0008) a.u.

3. KS–MO Diagrams

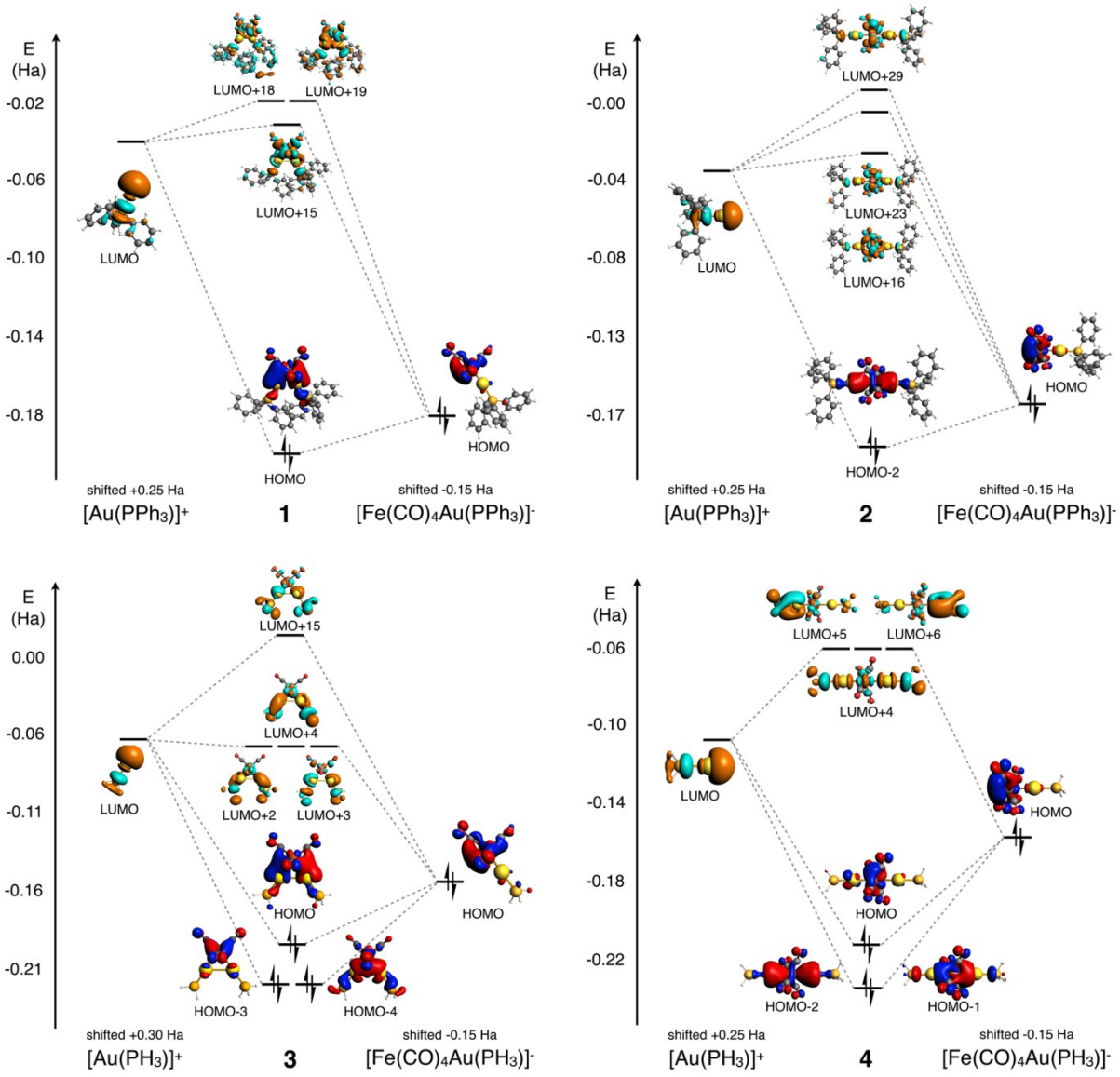

Fig. S4 Schematic orbital–interaction diagram for complexes **1**, **2**, **3** and **4**, based on quantitative Kohn–Sham MO analyses. MOs shown in blue/red indicates double occupied whereas in cyan/orange empty virtual orbitals.

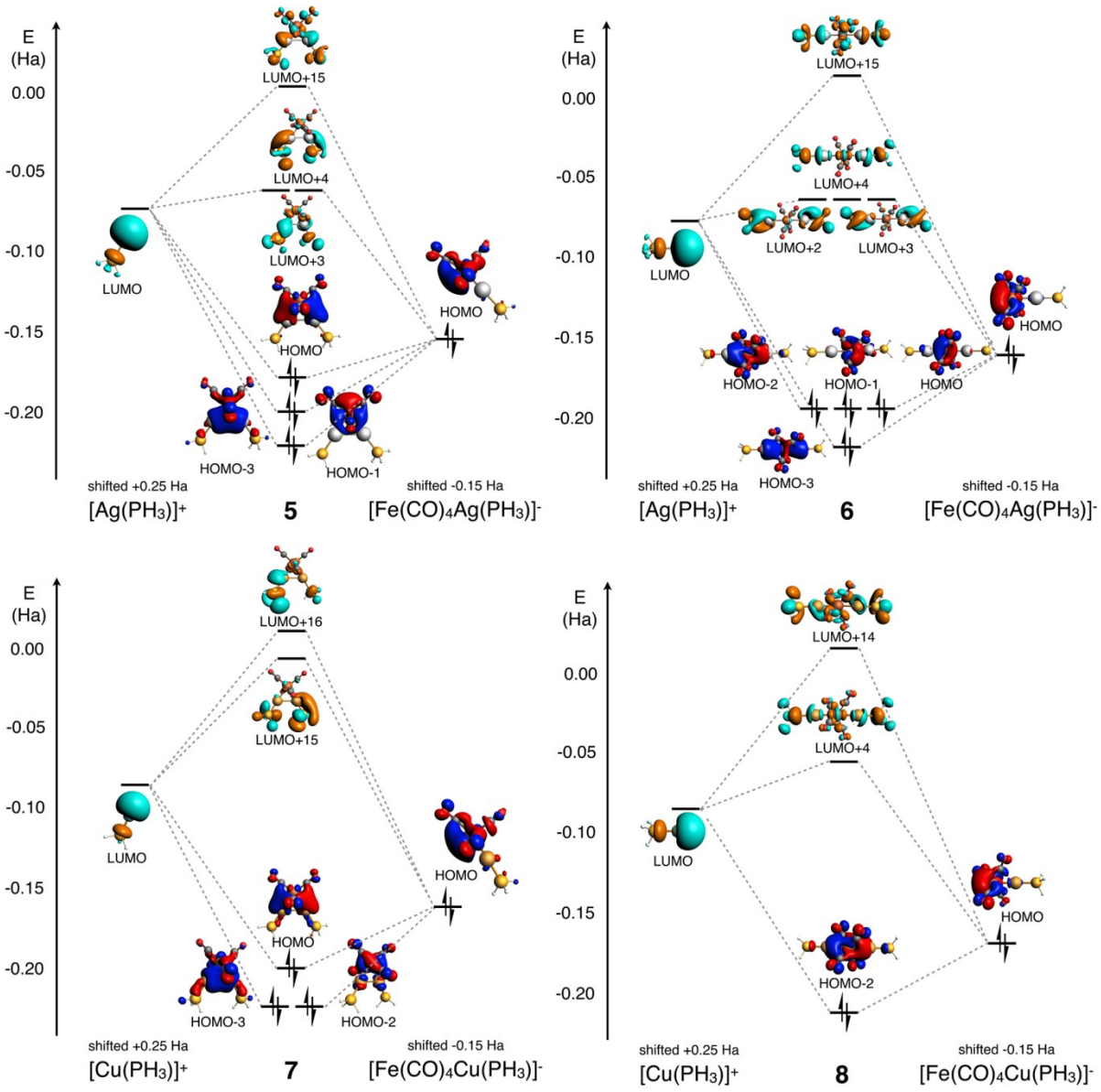

Fig. S5 Schematic orbital–interaction diagram for complexes **5**, **6**, **7** and **8**, based on quantitative Kohn–Sham MO analyses. MOs shown in blue/red indicates double occupied whereas in cyan/orange empty virtual orbitals.

4. XYZ Cartesian Coordinates

Complex		**1**	
Atom	X	Y	Z
Au	12.876316	–3.577879	5.215368
Au	15.307734	–2.833860	6.658846
Fe	13.603400	–1.182571	5.699914
P	12.525727	–5.803452	4.818543
P	16.857438	–4.196523	7.636461
C	12.178487	–0.489329	4.902153
O	11.251457	–0.019506	4.382338
C	14.476653	0.268610	6.226753
O	15.037933	1.227820	6.566285
C	14.592492	–1.595288	4.270451
O	15.235178	–1.826573	3.321990
C	12.887370	–1.659994	7.266659
O	12.409205	–1.930396	8.298241
C	18.436575	–3.369177	8.022017
C	18.990146	–2.548512	7.026897
C	20.211487	–1.915784	7.244266
C	20.880570	–2.083492	8.460449
C	20.324673	–2.886076	9.457750
C	19.104398	–3.529916	9.242016
C	17.362893	–5.641827	6.644969
C	18.611810	–6.261499	6.802333
C	18.931658	–7.381941	6.035871
C	18.014363	–7.882650	5.106853
C	16.778606	–7.256527	4.936711
C	16.456211	–6.136565	5.700594
C	16.299211	–4.879533	9.233700
C	16.760513	–6.105472	9.730021
C	16.319350	–6.566371	10.970522
C	15.412858	–5.810577	11.717934
C	14.943217	–4.591601	11.220843
C	15.382292	–4.126862	9.981508
C	13.453234	–6.361517	3.347202
C	14.508085	–5.563449	2.881414
C	15.278852	–5.984648	1.798246
C	14.997774	–7.199619	1.170454
C	13.933296	–7.988431	1.616817
C	13.157860	–7.569922	2.697866
C	10.846889	–6.455393	4.538025
C	10.098596	–5.899350	3.488819
C	8.813545	–6.366370	3.225241
C	8.258373	–7.378039	4.015203

C	8.993002	–7.919326	5.069715
C	10.286369	–7.462227	5.332901
C	13.180522	–6.802444	6.200891
C	13.647247	–8.112446	6.028876
C	14.153416	–8.822463	7.116704
C	14.186898	–8.232782	8.381852
C	13.715330	–6.931417	8.559931
C	13.223407	–6.211862	7.472733
H	18.452626	–2.402424	6.088468
H	20.636342	–1.279215	6.468421
H	21.831540	–1.579664	8.633176
H	20.839376	–3.010664	10.410629
H	18.670214	–4.152373	10.023509
H	19.334833	–5.857426	7.511243
H	19.903106	–7.861305	6.157742
H	18.271440	–8.754738	4.505303
H	16.067875	–7.628177	4.199607
H	15.502575	–5.628020	5.567939
H	17.449812	–6.707348	9.138776
H	16.680008	–7.521815	11.352120
H	15.064949	–6.175819	12.684295
H	14.225774	–4.004773	11.793748
H	15.002109	–3.187123	9.577589
H	14.716403	–4.608699	3.366734
H	16.095908	–5.357239	1.443778
H	15.598841	–7.527234	0.322118
H	13.701083	–8.928318	1.115674
H	12.311794	–8.172351	3.029708
H	10.527788	–5.100333	2.882973
H	8.238944	–5.935286	2.406220
H	7.250208	–7.738067	3.810756
H	8.561469	–8.703274	5.691969
H	10.859664	–7.889320	6.154009
H	13.634347	–8.571994	5.041566
H	14.529977	–9.835253	6.973254
H	14.590802	–8.783599	9.231031
H	13.749303	–6.466809	9.543697
H	12.888041	–5.181238	7.598711

Complex		**2**	
Atom	X	Y	Z
Au	13.129864	–3.923686	5.132894
Au	14.550039	0.864138	5.998365
Fe	13.765606	–1.526468	5.664367
P	12.590043	–6.091465	4.707063
P	15.424872	2.952486	6.226290
C	12.338028	–0.488414	5.916652

O	11.357373	0.126215	6.079128
C	15.548981	–1.498568	5.679394
O	16.718005	–1.552581	5.684285
C	13.552841	–1.705139	3.900687
O	13.427164	–1.738230	2.738709
C	13.574120	–2.411960	7.198732
O	13.457069	–2.937257	8.237259
C	14.409700	4.286422	5.511952
C	13.743077	4.021557	4.306324
C	12.978323	5.015902	3.700301
C	12.862324	6.273120	4.300244
C	13.513175	6.534550	5.507392
C	14.288852	5.545318	6.114206
C	17.046476	3.116851	5.411030
C	17.459813	4.314729	4.813097
C	18.720637	4.398024	4.221521
C	19.571845	3.290751	4.227237
C	19.158704	2.093724	4.817584
C	17.897432	2.001285	5.403185
C	15.710248	3.466515	7.950676
C	16.869365	4.140043	8.354240
C	17.021885	4.524048	9.687483
C	16.019755	4.243000	10.617514
C	14.864661	3.565504	10.217729
C	14.711660	3.170498	8.890830
C	13.419072	–6.782469	3.238346
C	14.746617	–6.398036	2.998033
C	15.436164	–6.918152	1.904946
C	14.802613	–7.814539	1.039841
C	13.477131	–8.188644	1.269257
C	12.783545	–7.676266	2.366790
C	10.816314	–6.367969	4.396676
C	10.156387	–5.448997	3.565768
C	8.807456	–5.623689	3.266721
C	8.104440	–6.703769	3.808165
C	8.754578	–7.609172	4.648487
C	10.109453	–7.445502	4.943251
C	13.029443	–7.228488	6.060661
C	13.373923	–8.566068	5.822156
C	13.685669	–9.405233	6.891695
C	13.655080	–8.914234	8.199006
C	13.318766	–7.579598	8.438126
C	13.011947	–6.734250	7.372954
H	13.819412	3.029933	3.857334
H	12.461623	4.805385	2.764092
H	12.254975	7.046776	3.830523

H	13.415937	7.511571	5.980942
H	14.793714	5.747082	7.058506
H	16.792353	5.176112	4.802834
H	19.036842	5.329622	3.751817
H	20.554744	3.357422	3.760948
H	19.814194	1.223179	4.811318
H	17.562838	1.059300	5.840452
H	17.652518	4.356943	7.628787
H	17.927873	5.043367	9.999379
H	16.142447	4.542660	11.658101
H	14.086264	3.333816	10.944263
H	13.823144	2.620888	8.576860
H	15.225943	–5.679383	3.664693
H	16.466084	–6.613361	1.720210
H	15.340081	–8.212676	0.179235
H	12.978506	–8.879744	0.589558
H	11.746710	–7.962304	2.542170
H	10.705062	–4.595537	3.164619
H	8.299908	–4.908227	2.619961
H	7.046156	–6.833428	3.581656
H	8.205578	–8.446590	5.078931
H	10.616201	–8.151361	5.600478
H	13.408458	–8.945271	4.800964
H	13.958648	–10.443513	6.702744
H	13.904540	–9.570597	9.032511
H	13.308300	–7.189467	9.455582
H	12.774946	–5.684461	7.552746

Complex		**3**	
Atom	X	Y	Z
Au	12.988983	–3.583143	5.243091
Au	15.355444	–2.712076	6.709452
Fe	13.605815	–1.166294	5.712399
P	12.428149	–5.751211	4.808527
P	16.929845	–4.096852	7.614364
C	12.190060	–0.503722	4.869260
O	11.271097	–0.055156	4.321521
C	14.433643	0.302723	6.269566
O	14.959979	1.273178	6.625719
C	14.618330	–1.503740	4.271648
O	15.269065	–1.678677	3.322938
C	12.802030	–1.608931	7.252625
O	12.267825	–1.854028	8.256767
H	18.279253	–3.680983	7.761462
H	17.188204	–5.349342	6.995169
H	16.737568	–4.580779	8.934488
H	12.935980	–6.373417	3.639186

H	11.070817	–6.134602	4.648704
H	12.796054	–6.768188	5.730370
Complex		**4**	
Atom	X	Y	Z
Au	13.125969	–3.914148	5.157169
Au	14.620264	0.823551	5.990061
Fe	13.833856	–1.541427	5.615223
P	12.506632	–6.063617	4.755364
P	15.348073	2.957161	6.293011
C	12.370596	–0.534478	5.816670
O	11.381422	0.067761	5.946073
C	15.622589	–1.575553	5.615223
O	16.784337	–1.665809	5.610836
C	13.655763	–1.715100	3.843022
O	13.552388	–1.760539	2.682999
C	13.659162	–2.337530	7.206028
O	13.552984	–2.800545	8.269849
H	14.547896	4.034070	5.834663
H	16.571796	3.357626	5.699704
H	15.598112	3.445354	7.601245
H	12.976274	–6.720870	3.589431
H	11.131204	–6.385566	4.617640
H	12.846915	–7.068399	5.697098
Complex		**5**	
Atom	X	Y	Z
Ag	12.777340	–3.467317	5.239047
Ag	15.292978	–2.812319	6.594806
Fe	13.648418	–1.113741	5.651506
P	12.444631	–5.785042	4.840967
P	16.867476	–4.237154	7.633734
C	12.232168	–0.383987	4.882796
O	11.313359	0.127483	4.381660
C	14.600511	0.300180	6.119361
O	15.211508	1.245286	6.419501
C	14.585360	–1.637119	4.228653
O	15.199552	–1.921581	3.267920
C	12.982382	–1.567279	7.243881
O	12.529445	–1.798501	8.302958
C	18.450473	–3.416032	8.021870
C	18.992465	–2.572076	7.039786
C	20.209403	–1.932370	7.262239
C	20.885947	–2.116228	8.471713
C	20.342120	–2.941930	9.456873
C	19.126843	–3.592720	9.235384
C	17.359916	–5.686459	6.641730
C	18.605325	–6.316811	6.783929

C	18.915597	–7.425073	5.996075
C	17.992378	–7.903767	5.060989
C	16.758558	–7.269468	4.907667
C	16.446661	–6.161786	5.693262
C	16.309145	–4.906579	9.236246
C	16.747677	–6.139905	9.734832
C	16.306920	–6.585176	10.981196
C	15.424358	–5.805591	11.732896
C	14.977855	–4.578513	11.234461
C	15.415400	–4.130361	9.988370
C	13.419325	–6.300884	3.382603
C	14.447658	–5.456513	2.939007
C	15.252251	–5.835405	1.864762
C	15.030956	–7.055136	1.222492
C	13.992824	–7.890932	1.645658
C	13.184916	–7.515078	2.718556
C	10.805809	–6.526836	4.536252
C	10.046946	–6.008896	3.474110
C	8.789907	–6.536658	3.190797
C	8.271312	–7.573229	3.973513
C	9.014917	–8.077702	5.040653
C	10.280392	–7.558816	5.323792
C	13.129570	–6.757835	6.227772
C	13.617124	–8.061659	6.064730
C	14.131214	–8.757982	7.157266
C	14.152264	–8.160809	8.419228
C	13.663624	–6.864819	8.588868
C	13.163464	–6.158988	7.495819
H	18.451173	–2.412042	6.105388
H	20.623633	–1.276944	6.496500
H	21.832516	–1.605979	8.649417
H	20.862334	–3.078654	10.405070
H	18.701472	–4.231613	10.008406
H	19.333620	–5.928223	7.496179
H	19.885003	–7.911683	6.104774
H	18.243576	–8.764632	4.441184
H	16.042534	–7.623020	4.166489
H	15.493049	–5.649958	5.570675
H	17.419539	–6.758445	9.140469
H	16.650216	–7.546095	11.365184
H	15.077351	–6.158107	12.704278
H	14.279346	–3.972835	11.811078
H	15.050151	–3.182902	9.587824
H	14.613678	–4.495037	3.428102
H	16.046171	–5.169625	1.528329
H	15.657006	–7.349491	0.380092

H	13.806519	–8.834724	1.132632
H	12.359154	–8.154501	3.031694
H	10.446350	–5.192853	2.869874
H	8.208652	–6.133818	2.361640
H	7.285172	–7.981651	3.753409
H	8.612094	–8.881298	5.657282
H	10.859607	–7.958209	6.155040
H	13.611961	–8.526507	5.079845
H	14.522632	–9.766046	7.020725
H	14.560280	–8.701289	9.272833
H	13.689771	–6.394576	9.570172
H	12.808865	–5.134056	7.620137

Complex		**6**	
Atom	X	Y	Z
Ag	12.611700	–3.696991	4.902433
Ag	13.990957	0.986447	6.014084
Fe	12.918415	–1.274514	5.579855
P	12.553286	–6.014435	4.499677
P	15.238167	2.961139	6.328549
C	11.695507	–0.074723	6.062754
O	10.813261	0.634801	6.371535
C	14.691108	–1.348249	5.396551
O	15.851287	–1.494007	5.257319
C	12.377443	–1.360748	3.883627
O	12.016922	–1.318911	2.767607
C	12.697431	–2.274586	7.034050
O	12.554582	–2.858979	8.043222
C	14.377328	4.513990	5.912255
C	13.474369	4.491631	4.839453
C	12.823184	5.660599	4.450645
C	13.059964	6.854284	5.136962
C	13.947605	6.876966	6.214499
C	14.606883	5.710539	6.603910
C	16.750802	2.991124	5.308949
C	17.309128	4.185980	4.834182
C	18.485211	4.155422	4.084815
C	19.106385	2.936286	3.805234
C	18.547023	1.743745	4.269751
C	17.368458	1.766773	5.014520
C	15.823477	3.217512	8.036701
C	17.131133	3.615589	8.340079
C	17.509782	3.805150	9.670317
C	16.588189	3.601837	10.698688
C	15.283822	3.198314	10.398809
C	14.904003	2.997062	9.074002
C	13.553244	–6.594021	3.088515

C	14.779273	–5.953626	2.853228
C	15.600585	–6.380081	1.811345
C	15.198588	–7.437973	0.990888
C	13.972532	–8.067700	1.213496
C	13.149663	–7.650175	2.260892
C	10.893496	–6.703020	4.190336
C	10.041146	–5.979929	3.341149
C	8.767888	–6.465527	3.051092
C	8.329987	–7.665029	3.619667
C	9.169445	–8.378261	4.477387
C	10.450309	–7.901937	4.762577
C	13.196470	–6.954188	5.924718
C	13.833873	–8.194117	5.776784
C	14.282050	–8.884808	6.902926
C	14.097614	–8.342712	8.177637
C	13.471445	–7.103187	8.326817
C	13.025803	–6.405481	7.204728
H	13.279196	3.552897	4.317963
H	12.121021	5.636994	3.617796
H	12.544035	7.766153	4.837183
H	14.126773	7.805702	6.756286
H	15.294856	5.725704	7.448726
H	16.819785	5.136547	5.044426
H	18.914713	5.086333	3.714508
H	20.022751	2.915285	3.215608
H	19.020058	0.789029	4.042427
H	16.922759	0.831163	5.356401
H	17.851729	3.772008	7.538071
H	18.529979	4.110697	9.902364
H	16.887859	3.748281	11.736260
H	14.564807	3.027016	11.199721
H	13.892466	2.662171	8.837869
H	15.081712	–5.116329	3.485049
H	16.551506	–5.878696	1.632535
H	15.838110	–7.765045	0.171107
H	13.653304	–8.887372	0.569500
H	12.190886	–8.138835	2.432484
H	10.377684	–5.032901	2.915442
H	8.110848	–5.899834	2.390669
H	7.329348	–8.037901	3.401396
H	8.826747	–9.308808	4.930055
H	11.103520	–8.456963	5.435110
H	13.986694	–8.611913	4.781649
H	14.780543	–9.846995	6.784004
H	14.453082	–8.882729	9.055256
H	13.339394	–6.668457	9.317336

H	12.558148	–5.426502	7.323047
Complex		**7**	
Atom	X	Y	Z
Ag	12.975922	–3.529879	5.240655
Ag	15.341629	–2.655083	6.703985
Fe	13.588880	–1.110604	5.709548
P	12.396904	–5.797750	4.792789
P	16.986971	–4.112234	7.628838
C	12.173646	–0.455039	4.871946
O	11.253234	0.001107	4.326438
C	14.424615	0.346628	6.267656
O	14.948532	1.323268	6.620720
C	14.595499	–1.501641	4.283079
O	15.244909	–1.694169	3.329274
C	12.807459	–1.603909	7.241400
O	12.276892	–1.865203	8.250356
H	18.343431	–3.726449	7.792853
H	17.243290	–5.359213	6.998984
H	16.797042	–4.625788	8.938615
H	12.999674	–6.471738	3.697893
H	11.060655	–6.195378	4.522275
H	12.668954	–6.792168	5.769956
Complex		**8**	
Atom	X	Y	Z
Ag	13.117665	–3.919659	5.152924
Ag	14.621668	0.831248	5.990937
Fe	13.827976	–1.539645	5.615387
P	12.486169	–6.161186	4.739823
P	15.384189	3.050585	6.305396
C	12.411397	–0.476205	5.831616
O	11.429520	0.146980	5.969133
C	15.613405	–1.514099	5.631094
O	16.782191	–1.587429	5.633344
C	13.627219	–1.770731	3.855778
O	13.513806	–1.832184	2.691513
C	13.626051	–2.393935	7.168922
O	13.505656	–2.877213	8.228518
H	14.592639	4.138157	5.854595
H	16.605488	3.461249	5.711809
H	15.644207	3.549709	7.608060
H	12.953493	–6.826391	3.577333
H	11.116230	–6.504849	4.600738
H	12.827262	–7.172460	5.674390
Complex		**9**	
Atom	X	Y	Z
Cu	12.997194	–3.640712	5.311106

Cu	15.166592	–3.105025	6.670461
Fe	13.590377	–1.498159	6.011113
P	12.645043	–5.716308	4.842026
P	16.720750	–4.317784	7.545837
C	12.202434	–0.789780	5.164304
O	11.291635	–0.320074	4.610951
C	14.373069	–0.076573	6.729184
O	14.890547	0.852577	7.202015
C	14.722939	–1.925305	4.709521
O	15.470704	–2.157504	3.823727
C	12.884281	–2.272199	7.442616
O	12.415427	–2.762390	8.405271
C	18.262373	–3.370207	7.792297
C	18.715082	–2.599145	6.710344
C	19.909396	–1.889711	6.811674
C	20.650397	–1.932352	7.996366
C	20.193104	–2.684546	9.079541
C	19.000339	–3.404173	8.981134
C	17.299431	–5.789724	6.637451
C	18.530443	–6.409358	6.904158
C	18.910844	–7.535742	6.176277
C	18.078280	–8.038098	5.169793
C	16.866539	–7.408087	4.885355
C	16.482171	–6.286767	5.618749
C	16.261756	–4.894598	9.214688
C	16.703700	–6.103738	9.764217
C	16.296705	–6.476340	11.045882
C	15.445488	–5.648463	11.781339
C	14.998383	–4.442995	11.233386
C	15.402418	–4.067596	9.953639
C	13.578015	–6.299055	3.382031
C	14.628200	–5.504358	2.900480
C	15.395740	–5.938907	1.819551
C	15.114594	–7.162450	1.209097
C	14.052501	–7.946826	1.669428
C	13.280983	–7.515285	2.747843
C	10.945867	–6.288626	4.502166
C	10.244958	–5.652949	3.464918
C	8.945039	–6.045759	3.158005
C	8.328906	–7.063734	3.892804
C	9.018301	–7.687040	4.933310
C	10.325730	–7.303304	5.240060
C	13.214452	–6.748724	6.240024
C	13.688983	–8.057246	6.083630
C	14.144788	–8.771827	7.191027
C	14.122154	–8.187808	8.459195

C	13.640821	–6.888027	8.622252
C	13.196009	–6.165046	7.516780
H	18.126102	–2.554755	5.792273
H	20.257162	–1.292792	5.968777
H	21.580868	–1.370429	8.076920
H	20.764704	–2.710368	10.007419
H	18.640949	–3.987378	9.828696
H	19.194825	–5.998638	7.664911
H	19.866044	–8.017875	6.385168
H	18.386042	–8.913827	4.598142
H	16.222841	–7.776755	4.087160
H	15.545581	–5.778270	5.402170
H	17.346123	–6.764326	9.183462
H	16.640007	–7.420566	11.469029
H	15.123858	–5.945617	12.779638
H	14.323578	–3.798650	11.796031
H	15.034401	–3.138845	9.514368
H	14.843927	–4.541890	3.367108
H	16.210563	–5.314951	1.453893
H	15.713651	–7.500650	0.363513
H	13.819557	–8.893146	1.180882
H	12.435195	–8.113002	3.088934
H	10.722244	–4.849755	2.900956
H	8.406974	–5.550990	2.349568
H	7.308581	–7.365150	3.656395
H	8.538680	–8.476725	5.511830
H	10.863127	–7.790485	6.052798
H	13.727643	–8.510281	5.094149
H	14.528730	–9.783521	7.060237
H	14.489949	–8.741926	9.322440
H	13.631886	–6.424468	9.607567
H	12.842396	–5.141049	7.645447

Complex		**10**	
Atom	X	Y	Z
Cu	13.070613	–3.436437	5.308810
Cu	15.205176	–2.671514	6.588346
Fe	13.619146	–1.212011	5.714346
P	12.596098	–5.514013	4.995643
P	16.671848	–4.033150	7.382041
C	12.219364	–0.550888	4.841977
O	11.304532	–0.115753	4.272169
C	14.425029	0.252268	6.316789
O	14.947872	1.214063	6.707263
C	14.679203	–1.678514	4.359141
O	15.370339	–1.949853	3.451456
C	12.858551	–1.826902	7.204695

O	12.343808	–2.193088	8.192506
H	18.027292	–3.647010	7.560397
H	16.925899	–5.257522	6.706176
H	16.470964	–4.585156	8.675113
H	13.358571	–6.263582	4.059994
H	11.312052	–5.942183	4.562252
H	12.721783	–6.413996	6.088147

Complex		**11**	
Atom	X	Y	Z
Cu	13.214907	–3.724144	5.209928
Cu	14.530582	0.637020	5.927422
Fe	13.725513	–1.524482	5.716539
P	12.765637	–5.772958	4.757874
P	15.308995	2.632387	6.072309
C	12.455489	–0.308331	5.995478
O	11.558521	0.427559	6.173070
C	15.499072	–1.402926	5.840648
O	16.671479	–1.414786	5.913590
C	13.477517	–1.836326	3.979462
O	13.333765	–1.955708	2.819904
C	13.392968	–2.542490	7.139335
O	13.193517	–3.138438	8.130832
H	14.482769	3.732236	5.726552
H	16.439782	2.990495	5.294325
H	15.774396	3.130694	7.317265
H	13.271476	–6.350612	3.564350
H	11.414722	–6.183837	4.607424
H	13.175127	–6.793413	5.655002