BONDING SITUATION IN HETEROMULTIMETALLIC CARBONYL COMPLEXES

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SUPPORTING INFORMATION

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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	$ ho_{ m b}$	$ abla^2 oldsymbol{ ho}_{ extsf{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
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	Х	Y	Z
Au	12.876316	-3.577879	5.215368
Au	15.307734	-2.833860	6.658846
Fe	13.603400	-1.182571	5.699914
Р	12.525727	-5.803452	4.818543
Р	16.857438	-4.196523	7.636461
С	12.178487	-0.489329	4.902153
0	11.251457	-0.019506	4.382338
С	14.476653	0.268610	6.226753
0	15.037933	1.227820	6.566285
С	14.592492	-1.595288	4.270451
0	15.235178	-1.826573	3.321990
С	12.887370	-1.659994	7.266659
0	12.409205	-1.930396	8.298241
С	18.436575	-3.369177	8.022017
С	18.990146	-2.548512	7.026897
С	20.211487	-1.915784	7.244266
С	20.880570	-2.083492	8.460449
С	20.324673	-2.886076	9.457750
С	19.104398	-3.529916	9.242016
С	17.362893	-5.641827	6.644969
С	18.611810	-6.261499	6.802333
С	18.931658	-7.381941	6.035871
С	18.014363	-7.882650	5.106853
С	16.778606	-7.256527	4.936711
С	16.456211	-6.136565	5.700594
С	16.299211	-4.879533	9.233700
С	16.760513	-6.105472	9.730021
С	16.319350	-6.566371	10.970522
С	15.412858	-5.810577	11.717934
С	14.943217	-4.591601	11.220843
С	15.382292	-4.126862	9.981508
С	13.453234	-6.361517	3.347202
С	14.508085	-5.563449	2.881414
С	15.278852	-5.984648	1.798246
С	14.997774	-7.199619	1.170454
С	13.933296	-7.988431	1.616817
С	13.157860	-7.569922	2.697866
С	10.846889	-6.455393	4.538025
С	10.098596	-5.899350	3.488819
С	8.813545	-6.366370	3.225241
С	8.258373	-7.378039	4.015203

С		8.993002	-7.919326	5.069715
С		10.286369	-7.462227	5.332901
С		13.180522	-6.802444	6.200891
С		13.647247	-8.112446	6.028876
С		14.153416	-8.822463	7.116704
С		14.186898	-8.232782	8.381852
С		13.715330	-6.931417	8.559931
С		13.223407	-6.211862	7.472733
Н		18.452626	-2.402424	6.088468
Н		20.636342	-1.279215	6.468421
Н		21.831540	-1.579664	8.633176
Н		20.839376	-3.010664	10.410629
Н		18.670214	-4.152373	10.023509
Н		19.334833	-5.857426	7.511243
Н		19.903106	-7.861305	6.157742
Н		18.271440	-8.754738	4.505303
Н		16.067875	-7.628177	4.199607
Н		15.502575	-5.628020	5.567939
Н		17.449812	-6.707348	9.138776
Н		16.680008	-7.521815	11.352120
Н		15.064949	-6.175819	12.684295
Н		14.225774	-4.004773	11.793748
Н		15.002109	-3.187123	9.577589
н		14.716403	-4.608699	3.366734
Н		16.095908	-5.357239	1.443778
Н		15.598841	-7.527234	0.322118
Н		13.701083	-8.928318	1.115674
Н		12.311794	-8.172351	3.029708
Н		10.527788	-5.100333	2.882973
Н		8.238944	-5.935286	2.406220
Н		7.250208	-7.738067	3.810756
Н		8.561469	-8.703274	5.691969
Н		10.859664	-7.889320	6.154009
Н		13.634347	-8.571994	5.041566
Н		14.529977	-9.835253	6.973254
Н		14.590802	-8.783599	9.231031
н		13.749303	-6.466809	9.543697
Н		12.888041	-5.181238	7.598711
	Complex		2	
	Atom	Х	Y	Z
Au		13.129864	-3.923686	5.132894
Au		14.550039	0.864138	5.998365
Fe		13.765606	-1.526468	5.664367
Р		12.590043	-6.091465	4.707063
Р		15.424872	2.952486	6.226290
С		12.338028	-0.488414	5.916652

0	11.357373	0.126215	6.079128
С	15.548981	-1.498568	5.679394
0	16.718005	-1.552581	5.684285
С	13.552841	-1.705139	3.900687
0	13.427164	-1.738230	2.738709
С	13.574120	-2.411960	7.198732
0	13.457069	-2.937257	8.237259
С	14.409700	4.286422	5.511952
С	13.743077	4.021557	4.306324
С	12.978323	5.015902	3.700301
С	12.862324	6.273120	4.300244
С	13.513175	6.534550	5.507392
С	14.288852	5.545318	6.114206
С	17.046476	3.116851	5.411030
С	17.459813	4.314729	4.813097
С	18.720637	4.398024	4.221521
С	19.571845	3.290751	4.227237
С	19.158704	2.093724	4.817584
С	17.897432	2.001285	5.403185
С	15.710248	3.466515	7.950676
С	16.869365	4.140043	8.354240
С	17.021885	4.524048	9.687483
С	16.019755	4.243000	10.617514
С	14.864661	3.565504	10.217729
С	14.711660	3.170498	8.890830
С	13.419072	-6.782469	3.238346
С	14.746617	-6.398036	2.998033
С	15.436164	-6.918152	1.904946
С	14.802613	-7.814539	1.039841
С	13.477131	-8.188644	1.269257
С	12.783545	-7.676266	2.366790
С	10.816314	-6.367969	4.396676
С	10.156387	-5.448997	3.565768
С	8.807456	-5.623689	3.266721
С	8.104440	-6.703769	3.808165
С	8.754578	-7.609172	4.648487
С	10.109453	-7.445502	4.943251
С	13.029443	-7.228488	6.060661
С	13.373923	-8.566068	5.822156
С	13.685669	-9.405233	6.891695
С	13.655080	-8.914234	8.199006
С	13.318766	-7.579598	8.438126
С	13.011947	-6.734250	7.372954
Н	13.819412	3.029933	3.857334
Н	12.461623	4.805385	2.764092
Н	12.254975	7.046776	3.830523

Н	13.415937	7.511571	5.980942
Н	14.793714	5.747082	7.058506
Н	16.792353	5.176112	4.802834
Н	19.036842	5.329622	3.751817
Н	20.554744	3.357422	3.760948
Н	19.814194	1.223179	4.811318
Н	17.562838	1.059300	5.840452
Н	17.652518	4.356943	7.628787
Н	17.927873	5.043367	9.999379
Н	16.142447	4.542660	11.658101
Н	14.086264	3.333816	10.944263
Н	13.823144	2.620888	8.576860
Н	15.225943	-5.679383	3.664693
Н	16.466084	-6.613361	1.720210
Н	15.340081	-8.212676	0.179235
Н	12.978506	-8.879744	0.589558
Н	11.746710	-7.962304	2.542170
Н	10.705062	-4.595537	3.164619
Н	8.299908	-4.908227	2.619961
Н	7.046156	-6.833428	3.581656
Н	8.205578	-8.446590	5.078931
Н	10.616201	-8.151361	5.600478
Н	13.408458	-8.945271	4.800964
Н	13.958648	-10.443513	6.702744
Н	13.904540	-9.570597	9.032511
Н	13.308300	-7.189467	9.455582
Н	12.774946	-5.684461	7.552746
Complex		3	
Atom	Х	Y	Z
Au	12.988983	-3.583143	5.243091
Au	15.355444	-2.712076	6.709452
Fe	13.605815	-1.166294	5.712399
Р	12.428149	-5.751211	4.808527
Р	16.929845	-4.096852	7.614364
P C	16.929845 12.190060	-4.096852 -0.503722	7.614364 4.869260
P C O	16.929845 12.190060 11.271097	-4.096852 -0.503722 -0.055156	7.614364 4.869260 4.321521
P C O C	16.929845 12.190060 11.271097 14.433643	-4.096852 -0.503722 -0.055156 0.302723	7.614364 4.869260 4.321521 6.269566
P C O C O	16.929845 12.190060 11.271097 14.433643 14.959979	-4.096852 -0.503722 -0.055156 0.302723 1.273178	7.614364 4.869260 4.321521 6.269566 6.625719
P C O C C	16.929845 12.190060 11.271097 14.433643 14.959979 14.618330	-4.096852 -0.503722 -0.055156 0.302723 1.273178 -1.503740	7.614364 4.869260 4.321521 6.269566 6.625719 4.271648
P C O C C O	16.929845 12.190060 11.271097 14.433643 14.959979 14.618330 15.269065	-4.096852 -0.503722 -0.055156 0.302723 1.273178 -1.503740 -1.678677	7.614364 4.869260 4.321521 6.269566 6.625719 4.271648 3.322938
P C O C O C C	16.929845 12.190060 11.271097 14.433643 14.959979 14.618330 15.269065 12.802030	-4.096852 -0.503722 -0.055156 0.302723 1.273178 -1.503740 -1.678677 -1.608931	7.614364 4.869260 4.321521 6.269566 6.625719 4.271648 3.322938 7.252625
P C O C O C O C O	16.929845 12.190060 11.271097 14.433643 14.959979 14.618330 15.269065 12.802030 12.267825	-4.096852 -0.503722 -0.055156 0.302723 1.273178 -1.503740 -1.678677 -1.608931 -1.854028	7.614364 4.869260 4.321521 6.269566 6.625719 4.271648 3.322938 7.252625 8.256767
P C O C O C O C O H	16.929845 12.190060 11.271097 14.433643 14.959979 14.618330 15.269065 12.802030 12.267825 18.279253	$\begin{array}{c} -4.096852 \\ -0.503722 \\ -0.055156 \\ 0.302723 \\ 1.273178 \\ -1.503740 \\ -1.678677 \\ -1.608931 \\ -1.854028 \\ -3.680983 \end{array}$	7.614364 4.869260 4.321521 6.269566 6.625719 4.271648 3.322938 7.252625 8.256767 7.761462
P C O C O C O C O H H	16.929845 12.190060 11.271097 14.433643 14.959979 14.618330 15.269065 12.802030 12.267825 18.279253 17.188204	$\begin{array}{c} -4.096852\\ -0.503722\\ -0.055156\\ 0.302723\\ 1.273178\\ -1.503740\\ -1.678677\\ -1.608931\\ -1.854028\\ -3.680983\\ -5.349342\end{array}$	7.614364 4.869260 4.321521 6.269566 6.625719 4.271648 3.322938 7.252625 8.256767 7.761462 6.995169
Р С О С О С О С О С О С О С О С О С О С	16.929845 12.190060 11.271097 14.433643 14.959979 14.618330 15.269065 12.802030 12.267825 18.279253 17.188204 16.737568	$\begin{array}{c} -4.096852\\ -0.503722\\ -0.055156\\ 0.302723\\ 1.273178\\ -1.503740\\ -1.678677\\ -1.608931\\ -1.854028\\ -3.680983\\ -5.349342\\ -4.580779\end{array}$	7.614364 4.869260 4.321521 6.269566 6.625719 4.271648 3.322938 7.252625 8.256767 7.761462 6.995169 8.934488

н		11.070817	-6.134602	4.648704
Н		12.796054	-6.768188	5.730370
Сс	omplex		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
Р		12.506632	-6.063617	4.755364
Р		15.348073	2.957161	6.293011
С		12.370596	-0.534478	5.816670
0		11.381422	0.067761	5.946073
С		15.622589	-1.575553	5.615223
0		16.784337	-1.665809	5.610836
С		13.655763	-1.715100	3.843022
0		13.552388	-1.760539	2.682999
С		13.659162	-2.337530	7.206028
0		13.552984	-2.800545	8.269849
Н		14.547896	4.034070	5.834663
Н		16.571796	3.357626	5.699704
Н		15.598112	3.445354	7.601245
Н		12.976274	-6.720870	3.589431
Н		11.131204	-6.385566	4.617640
Н		12.846915	-7.068399	5.697098
Co	omplex		5	
Co /	omplex Atom	X	5 Y Z	
Co Ag	omplex Atom	X 12.777340	5 Y Z -3.467317	5.239047
Ag Ag	omplex Atom	X 12.777340 15.292978	5 Y Z -3.467317 -2.812319	5.239047 6.594806
Ag Fe	omplex Atom	X 12.777340 15.292978 13.648418	5 Y Z -3.467317 -2.812319 -1.113741	5.239047 6.594806 5.651506
Ag Ag Fe P	omplex Atom	X 12.777340 15.292978 13.648418 12.444631	5 YZ -3.467317 -2.812319 -1.113741 -5.785042	5.239047 6.594806 5.651506 4.840967
Ag Ag Fe P P	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154	5.239047 6.594806 5.651506 4.840967 7.633734
Ag Ag Fe P P C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796
Ag Ag Fe P C O	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660
Ag Ag Fe P C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361
Co Ag Ag Fe P C C C C O C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501
Ag Ag Fe P C C C C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286 -1.637119	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653
Ag Ag Fe P C C C C C C C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552	5 Y Z -3.467317	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920
Ag Ag Fe P C C C C C C C C C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552 12.982382	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286 -1.637119 -1.921581 -1.567279	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920 7.243881
Ag Ag Fe P C C C C C C C C C C C C C C C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552 12.982382 12.529445	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286 -1.637119 -1.921581 -1.567279 -1.798501	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920 7.243881 8.302958
Co Ag Ag Fe P C C O C O C O C O C O C C O C C O C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552 12.982382 12.529445 18.450473	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286 -1.637119 -1.921581 -1.567279 -1.798501 -3.416032	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920 7.243881 8.302958 8.021870
Ag Ag Fe P C O C O C O C O C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552 12.982382 12.529445 18.450473 18.992465	5 Y Z -3.467317 - -2.812319 - -1.113741 - -5.785042 - -4.237154 - -0.383987 0.127483 0.300180 1.245286 -1.637119 - -1.921581 - -1.567279 - -3.416032 - -2.572076 -	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920 7.243881 8.302958 8.021870 7.039786
Ag Ag Fe P C O C O C O C O C C C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552 12.982382 12.529445 18.450473 18.992465 20.209403	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286 -1.637119 -1.921581 -1.567279 -1.798501 -3.416032 -2.572076 -1.932370	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920 7.243881 8.302958 8.021870 7.039786 7.262239
Ag Ag Fe P C O C O C O C O C C C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552 12.982382 12.529445 18.450473 18.992465 20.209403 20.885947	5 -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286 -1.637119 -1.921581 -1.567279 -1.798501 -3.416032 -2.572076 -1.932370 -2.116228	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920 7.243881 8.302958 8.021870 7.039786 7.262239 8.471713
Co Ag Ag Fe P C O C O C O C O C O C C C C C C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552 12.982382 12.529445 18.450473 18.992465 20.209403 20.885947 20.342120	5 Y Z -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286 -1.637119 -1.921581 -1.567279 -1.798501 -3.416032 -2.572076 -1.932370 -2.116228 -2.941930	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920 7.243881 8.302958 8.021870 7.039786 7.262239 8.471713 9.456873
Cc Ag Ag Fe P C O C O C O C O C O C C C C C C C C C	omplex Atom	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552 12.982382 12.529445 18.450473 18.992465 20.209403 20.885947 20.342120 19.126843	5 -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286 -1.637119 -1.921581 -1.567279 -1.798501 -3.416032 -2.572076 -1.932370 -2.116228 -2.941930 -3.592720	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920 7.243881 8.302958 8.021870 7.039786 7.262239 8.471713 9.456873 9.235384
Co Ag Ag Fe P C O C O C O C O C O C O C O C C C C C	Atom 2	X 12.777340 15.292978 13.648418 12.444631 16.867476 12.232168 11.313359 14.600511 15.211508 14.585360 15.199552 12.982382 12.529445 18.450473 18.992465 20.209403 20.885947 20.342120 19.126843 17.359916	5 -3.467317 -2.812319 -1.113741 -5.785042 -4.237154 -0.383987 0.127483 0.300180 1.245286 -1.637119 -1.567279 -1.798501 -3.416032 -2.572076 -1.932370 -2.116228 -2.941930 -3.592720 -5.686459	5.239047 6.594806 5.651506 4.840967 7.633734 4.882796 4.381660 6.119361 6.419501 4.228653 3.267920 7.243881 8.302958 8.021870 7.039786 7.262239 8.471713 9.456873 9.235384 6.641730

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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 4.328438 C 14.424615 0.346628 6.620720 C 14.595499 -1.60309 7.241400 O 15.244909 -1.60309 7.24140 O 12.276892 -1.865203 8.250356 H 16.797042 -4.625788 8.938615 H 12.299674 -6.471738 3.697933 H 12.2668954 -6.792168 5.769956 Complex 8 2 2 4.625788 8.938615 H 12.2668954 -6.1792168	н		12.558148	-5.426502	7.323047
Atom X Y Z Ag 12.975922 -3.529879 5.240655 Ag 15.341629 -2.655083 6.703985 Fe 13.588880 -1.110604 5.709748 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 14.4948532 1.332368 6.600720 C 14.595499 -1.601641 4.283079 O 15.244909 -1.695109 7.792853 H 18.343431 -3.726449 7.792853 H 11.606655 -6.195378 4.52275 H 12.2699674 -6.471738 3.698994 H 11.2668954 -6.792168 5.769956 Complex 8 3 4.52275 H 12.668954 -6.195378 4.52275 H 12.668954		Complex		7	
Ag 12 975922 -3 529879 5 240655 Ag 15.341629 -2.655083 6.703985 Fe 13.588880 -1.110604 5.709750 P 12.396904 -5.797750 4.792789 P 12.173646 -0.455039 4.81146 O 11.253234 0.001107 4.326338 C 14.424615 0.346628 6.6267656 O 14.2984532 1.323268 6.620720 C 14.598499 -1.603909 7.241400 O 15.244909 -1.603909 7.241400 O 12.276892 -1.865203 8.250356 H 17.243290 -5.359213 6.99984 H 12.699674 -6.471738 3.697893 H 12.698954 -6.195378 4.52275 Ag 13.617665		Atom	X	Y	Z
Ag 15.341629 −2.655083 6.703985 Fe 13.588880 −1.10604 5.709750 P 12.396904 −5.797750 4.722789 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 14.595499 −1.501641 4.283079 O 15.244909 −1.603909 7.241400 O 12.276892 −1.865203 8.250356 H 18.343431 −3.726449 7.722853 H 17.243290 −5.359213 6.99984 H 12.69954 −6.671738 3.697893 H 12.69954 −6.792168 5.759955 Complex 8 3.117665 −3.919659 5.153274 Ag 13.117665 −3.919659 5.615337 Fe 13.827976 −1.53945 5.615337 Fe 13.827976 −1.539455 5.615337 Fe	Ag		12.975922	-3.529879	5.240655
Fe 13.58880 -1.110604 5.709548 P 12.396904 -5.797750 4.792789 P 16.986971 -4.112234 7.628388 C 12.173646 -0.455039 4.871946 O 11.253234 0.001107 4.326438 C 14.424615 0.346528 6.620720 O 14.595499 -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 12.999674 -6.471738 3.697893 H 12.668954 -6.792168 5.769756 Complex 8 - - Atom X Y Z Ag 13.117665 -3.919659 5.152924 Ag 14.621668 0.831248 5.90937 Fe 13.827976 -1.539645 5.615387 P 12.486169 -6.16118	Ag		15.341629	-2.655083	6.703985
P 12.396904 -5.797750 4.792789 P 16.986971 -4.112234 7.62838 C 12.173646 -0.455039 4.871946 O 11.253234 0.001107 4.326438 C 14.424615 0.346628 6.620720 C 14.4946532 1.323268 6.620720 C 14.595499 -1.603009 7.241400 O 12.276892 -1.865203 8.250356 H 18.34331 -3.726449 7.792853 H 17.243290 -5.359213 6.999994 H 12.666954 -6.792168 5.769956 H 12.666954 -6.792168 5.769956 Complex 8 - 4.52275 H 12.666954 -6.195378 4.52275 H 12.666954 -6.195178 5.152924 Ag 13.117665 -3.919659 5.152924 Ag 13.617605 -1.539645 5.615387 P 12.466169 </td <td>Fe</td> <td></td> <td>13.588880</td> <td>-1.110604</td> <td>5.709548</td>	Fe		13.588880	-1.110604	5.709548
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 14.4948532 1.323268 6.620720 C 14.4595499 -1.501641 4.283079 O 15.244909 -1.694169 3.329274 C 12.076892 -1.865203 8.250356 H 18.343431 -3.726449 7.792853 H 17.243290 -5.359213 6.998994 H 12.999674 -6.471738 3.697933 H 12.999674 -6.471738 3.697833 H 11.060655 -6.195378 4.52275 H 12.668954 -6.792168 5.769956 Complex 8 - - Atom X Y Z Ag 13.117665 -3.919659 5.152924 Ag 13.627219 -1.5396	Ρ		12.396904	-5.797750	4.792789
C 12.173646 -0.455039 4.871946 O 11.252324 0.001107 4.326438 C 14.424615 0.346628 6.620720 O 14.948532 1.323268 6.620720 C 14.595499 -1.501641 4.283079 O 15.244909 -1.603909 7.241400 O 12.276892 -1.865203 8.250356 H 18.34341 -3.726449 7.792853 H 17.243290 -5.359213 6.998984 H 16.797042 -4.625788 8.938615 H 12.2999674 -6.471738 3.697893 H 11.060655 -6.195378 4.52275 H 12.686954 -6.792168 5.769956 Complex 8	Р		16.986971	-4.112234	7.628838
0 11.253234 0.001107 4.326438 C 14.424615 0.346628 6.267656 0 14.948532 1.323268 6.620720 C 14.595499 -1.501641 4.283079 O 15.244909 -1.603909 7.241400 O 12.276892 -1.865203 8.250356 H 18.343431 -3.726449 7.792853 H 16.797042 -4.625788 8.938615 H 12.999674 -6.471738 3.697893 H 11.06655 -6.195378 4.52275 Complex 8 9.305078 4.52275 Complex 8 11.4621668 0.831248 5.990937 Fe 13.117665 -3.919659 5.152924 Ag 14.621668 0.831248 5.990937 Fe 13.827976 -1.539645 5.613387 P 12.486169 -6.161186 4.739823 P 15.344189 3.0505855 6.305396 <t< td=""><td>С</td><td></td><td>12.173646</td><td>-0.455039</td><td>4.871946</td></t<>	С		12.173646	-0.455039	4.871946
C 14.424615 0.346628 6.267656 O 14.948522 1.323268 6.620720 C 14.595499 -1.601641 4.283079 O 15.244909 -1.603909 7.241400 O 12.276892 -1.865203 8.250356 H 18.343431 -3.726449 7.722853 H 16.797042 -4.625788 8.938615 H 12.299674 -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 13.17665 -3.919659 5.152924 Ag 13.4621668 0.831248 5.90037 Fe 13.827976 -1.539645 5.615387 P 12.466169 -6.161186 4.739823 C 13.827976 -1.539645 5.615387 P 15.613405 -1.514	0		11.253234	0.001107	4.326438
0 14.948532 1.323268 6.620720 C 14.595499 -1.501641 4.283079 0 15.244909 -1.603809 7.241400 0 12.276892 -1.865203 8.250356 H 18.343431 -3.726449 7.792853 H 17.243290 -5.359213 6.989844 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 - - Adom X Y Z Ag 13.117665 -3.919659 5.152924 Ag 13.137665 -3.61186 4.739823 P 12.486169 -6.161186 4.739823 P 15.384189 3.050585 6.305396 C 12.491397 -0.476205 5.831616 O 16.782191 -1.88742	С		14.424615	0.346628	6.267656
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 16.797042 -4.625788 8.938615 H 12.668954 -6.792168 5.697893 H 12.668954 -6.792168 5.769956 Complex 8 5.769956 -5.759178 4.52275 Adom X Y Z - -6.792168 5.769956 Complex 8 13.117665 -3.919659 5.152924 Ag 14.621668 0.831248 5.90937 Fe 13.827976 -1.539645 5.615387 P 12.486169 -6.161186 4.739823 P 15.384189 3.050585 6.305396 G.305396 G.305396 G.305396 C 12.411397 -0.476205 5.831616 G.94933	0		14.948532	1.323268	6.620720
0 15.244909 -1.694169 3.329274 C 12.807459 -1.603909 7.241400 0 12.276892 -1.865203 8.250356 H 18.343431 -3.726449 7.792853 H 17.243290 -5.559213 6.998984 H 16.797042 -4.625788 8.338615 H 12.999674 -6.471738 3.697893 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 12.486169 -6.161186 4.739823 P 12.486169 -1.514099 5.631344 C 13.627219 -1.7170731 3.855778 O 13.513806 -1.8	С		14.595499	-1.501641	4.283079
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 12.668954 -6.792168 5.769956 Complex 8 - - - Atom X Y Z - - Ag 13.117665 -3.919659 5.152924 - - - Ag 13.117665 -1.539645 5.615387 - <td< td=""><td>0</td><td></td><td>15.244909</td><td>-1.694169</td><td>3.329274</td></td<>	0		15.244909	-1.694169	3.329274
0 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 12.668954 -6.792168 5.769956 H 12.668954 -6.792168 5.769956 Complex 8 5.769956 5.152924 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 12.486169 -6.161186 4.739823 P 12.486169 -1.611469 5.615387 P 12.486169 -1.611468 4.739823 P 12.486169 -1.611468 4.739823 C 13.617219 -1.7170731 3.85778 O <t< td=""><td>С</td><td></td><td>12.807459</td><td>-1.603909</td><td>7.241400</td></t<>	С		12.807459	-1.603909	7.241400
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 2 Atom X Y Z Ag 13.117665 -3.919659 5.152924 Ag 13.827976 -1.539645 5.615387 P 12.486169 -6.161186 4.739823 P 12.486169 -6.161186 4.739823 C 11.429520 0.146980 5.969133 C 15.613405 -1.514099 5.633444 C 13.627219 -1.770731 3.855778 O 13.513806 -1.832184 2.691513 C 13.626051 -2.837213 8.828518 H 16.605488 3.461249 5.711809 H 15.644207 3.549709 7.608060 <td>0</td> <td></td> <td>12.276892</td> <td>-1.865203</td> <td>8.250356</td>	0		12.276892	-1.865203	8.250356
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 2 2 Atom X Y Z Ag 13.117665 -3.919659 5.152924 Ag 13.827976 -1.539645 5.615387 P 12.486169 -6.161186 4.739823 P 12.486169 -6.161186 4.739823 C 12.411397 -0.476205 5.831616 O 11.429520 0.146980 5.969133 C 13.627219 -1.707731 3.855778 O 13.513806 -1.832184 2.691513 C 13.627219 -1.707731 3.855778 O 13.513806 -2.837235 7.168922 O 13.505656	Н		18.343431	-3.726449	7.792853
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 7 Z Atom X Y Z 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 13.613405 -1.514099 5.63344 C 13.627219 -1.770731 3.855778 O 13.513806 -1.832184 2.691513 C 13.626051 -2.393935 7.168922 O 13.505656	Н		17.243290	-5.359213	6.998984
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 5.90937 Fe 13.827976 -1.539645 5.615387 P 12.486169 -6.161186 4.739823 P 12.481619 -6.161186 4.739823 C 12.411397 -0.476205 5.831616 O 11.429520 0.146980 5.969133 C 15.613405 -1.514099 5.63344 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 12.953493 -6.826391 3.577333 H 12.2953493 -6.826391 3.577333 H 12.2827262	н		16.797042	-4.625788	8.938615
H 11.060655 6.195378 4.522275 H 12.668954 6.792168 5.769956 Complex 8 2 Atom X Y Z Ag 13.117665 3.919659 5.152924 Ag 13.827976 -1.539645 5.615387 P 12.486169 -6.161186 4.739823 P 12.486169 -6.161186 4.739823 C 12.441397 -0.476205 5.831616 O 11.429520 0.146980 5.969133 C 15.613405 -1.514099 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 14.5924393 -6.826391 3.577333 H 15.644207 3.549709 7.608060 H 12.82762 -7.172460 <	Н		12.999674	-6.471738	3.697893
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 16.605488 3.461249 5.711809 H 12.953493 -6.826391 3.57733 <td>н</td> <td></td> <td>11.060655</td> <td>-6.195378</td> <td>4.522275</td>	н		11.060655	-6.195378	4.522275
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 15.644207 3.549709 7.608600 H 12.953493 -6.826391 3.577333 <td>Н</td> <td></td> <td>12.668954</td> <td>-6.792168</td> <td>5.769956</td>	Н		12.668954	-6.792168	5.769956
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 15.644207 3.549709 7.608060 H 12.953493 -6.826391 3.57733 H 11.116230		Complex		8	
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Ag 14.621668 0.831248 5.90937 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 5.633944 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 12.953493 -6.826391 3.577333 H 12.827262 -7.172460 5.674390 Complex 9 2 5.674390 Cu 12.997194 -3.640712 5.311106		Atom	Λ	I	2
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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 12.953493 -6.826391 3.57733 H 12.827262 -7.172460 5.674390 Cumplex 9 2 2 2 Atom X Y Z 2 Cu 12.997194 -3.640712 5.311106	Ag Ag	Aom	13.117665 14.621668	-3.919659 0.831248	5.152924 5.990937
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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 2 2 Cu 12.997194 -3.640712 5.311106	Ag Ag Fe P P	AUIII	x 13.117665 14.621668 13.827976 12.486169 15.384189	-3.919659 0.831248 -1.539645 -6.161186 3.050585	5.152924 5.990937 5.615387 4.739823 6.305396
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 7 7 Cu 12.997194 -3.640712 5.311106	Ag Ag Fe P P C	AUT	X 13.117665 14.621668 13.827976 12.486169 15.384189 12.411397	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616
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 2 2 Atom X Y Z Cu 12.997194 -3.640712 5.311106	Ag Ag Fe P C O	AUT	x 13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133
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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 7 2 Cu 12.997194 -3.640712 5.311106	Ag Ag Fe P C C C C O	AUT	x 13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429	2 5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344
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 2 Cu 12.997194 -3.640712 5.311106	Ag Ag Fe P C C C C C	AUT	x 13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.627219	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731	2 5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778
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 9 7 Cu 12.997194 -3.640712 5.311106	Ag Ag Fe P C O C O C O C	AUT	X 13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.627219 13.513806	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184	2 5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513
H14.5926394.1381575.854595H16.6054883.4612495.711809H15.6442073.5497097.608060H12.953493-6.8263913.577333H11.116230-6.5048494.600738H12.827262-7.1724605.674390Complex9-2AtomXYZCu12.997194-3.6407125.311106	Ag Ag P P C O C O C O C	AUT	13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.513806 13.626051	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922
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 2 Atom X Y Z Cu 12.997194 -3.640712 5.311106	Ag Ag Fe P C O C O C O C O C O C		13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.627219 13.513806 13.505656	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935 -2.877213	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922 8.228518
H15.6442073.5497097.608060H12.953493-6.8263913.577333H11.116230-6.5048494.600738H12.827262-7.1724605.674390Complex9AtomXYZCu12.997194-3.6407125.311106	Ag Ag Fe P C O C O C O C O H		13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.513806 13.505656 14.592639	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935 -2.877213 4.138157	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922 8.228518 5.854595
H 12.953493 -6.826391 3.577333 H 11.116230 -6.504849 4.600738 H 12.827262 -7.172460 5.674390 Complex 9 Z Atom X Y Z Cu 12.997194 -3.640712 5.311106	Ag Ag Fe P C O C O C O C O C O H H		13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.627219 13.513806 13.505656 14.592639 16.605488	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935 -2.877213 4.138157 3.461249	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922 8.228518 5.854595 5.711809
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	Ag Ag Fe P C O C O C O C O H H H		13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.513806 13.505656 14.592639 16.605488 15.644207	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935 -2.877213 4.138157 3.461249 3.549709	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922 8.228518 5.854595 5.711809 7.608060
H 12.827262 -7.172460 5.674390 Complex 9 Z Atom X Y Z Cu 12.997194 -3.640712 5.311106	Ag Fe P C O C O C O C O H H H H		13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.627219 13.513806 13.505656 14.592639 16.605488 15.644207 12.953493	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935 -2.877213 4.138157 3.461249 3.549709 -6.826391	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922 8.228518 5.854595 5.711809 7.608060 3.577333
Complex 9 Atom X Y Z Cu 12.997194 -3.640712 5.311106	Ag Ag Fe P C O C O C O C O H H H H		13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.627219 13.513806 13.505656 14.592639 16.605488 15.644207 12.953493 11.116230	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935 -2.877213 4.138157 3.461249 3.549709 -6.826391 -6.504849	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922 8.228518 5.854595 5.711809 7.608060 3.577333 4.600738
Atom X Y Z Cu 12.997194 -3.640712 5.311106	Ag Ag P C O C O C O C O C O H H H H H		13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.627219 13.513806 13.505656 14.592639 16.605488 15.644207 12.953493 11.116230	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935 -2.877213 4.138157 3.461249 3.549709 -6.826391 -6.504849 -7.172460	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922 8.228518 5.854595 5.711809 7.608060 3.577333 4.600738 5.674390
Cu 12.997194 –3.640712 5.311106	Ag Ag P C O C O C O C O C O C O H H H H H	Complex	13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.627219 13.513806 13.505656 14.592639 16.605488 15.644207 12.953493 11.116230	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935 -2.877213 4.138157 3.461249 3.549709 -6.826391 -6.504849 -7.172460 9	5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922 8.228518 5.854595 5.711809 7.608060 3.577333 4.600738 5.674390
	Ag Ag Fe P C O C O C O C O C O H H H H H	Complex	X 13.117665 14.621668 13.827976 12.486169 15.384189 12.411397 11.429520 15.613405 16.782191 13.627219 13.513806 13.626051 13.505656 14.592639 16.605488 15.644207 12.953493 11.116230 12.827262 X	-3.919659 0.831248 -1.539645 -6.161186 3.050585 -0.476205 0.146980 -1.514099 -1.587429 -1.770731 -1.832184 -2.393935 -2.877213 4.138157 3.461249 3.549709 -6.826391 -6.504849 -7.172460 9 Y	Z 5.152924 5.990937 5.615387 4.739823 6.305396 5.831616 5.969133 5.631094 5.633344 3.855778 2.691513 7.168922 8.228518 5.854595 5.711809 7.608060 3.577333 4.600738 5.674390

Cu	15.166592	-3.105025	6.670461
Fe	13.590377	-1.498159	6.011113
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н		16.222841	-7.776755	4.087160
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н		15.034401	-3.138845	9.514368
н		14.843927	-4.541890	3.367108
н		16.210563	-5.314951	1.453893
н		15.713651	-7.500650	0.363513
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н		12.435195	-8.113002	3.088934
н		10.722244	-4.849755	2.900956
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н		13.727643	-8.510281	5.094149
н		14.528730	-9.783521	7.060237
н		14.489949	-8.741926	9.322440
н		13.631886	-6.424468	9.607567
Н		12.842396	-5.141049	7.645447
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	Atom	Х	Y	Z
Cu		13.070613	-3.436437	5.308810
Cu		15.205176	-2.671514	6.588346
Fe		13.619146	-1.212011	5.714346
Ρ		12.596098	-5.514013	4.995643
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53 4.272169	-0.115753	11.304532
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63 6.707263	1.214063	14.947872
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02 7.204695	-1.826902	12.858551

0	12.343808	-2.193088	8.192506			
Н	18.027292	-3.647010	7.560397			
Н	16.925899	-5.257522	6.706176			
Н	16.470964	-4.585156	8.675113			
Н	13.358571	-6.263582	4.059994			
Н	11.312052	-5.942183	4.562252			
Н	12.721783	-6.413996	6.088147			
Complex		11				
Atom	Х	Y	Z			
Cu	13.214907	-3.724144	5.209928			
Cu	14.530582	0.637020	5.927422			
Fe	13.725513	-1.524482	5.716539			
Р	12.765637	-5.772958	4.757874			
Р	15.308995	2.632387	6.072309			
С	12.455489	-0.308331	5.995478			
0	11.558521	0.427559	6.173070			
С	15.499072	-1.402926	5.840648			
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С	13.477517	-1.836326	3.979462			
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С	13.392968	-2.542490	7.139335			
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Н	14.482769	3.732236	5.726552			
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Н	15.774396	3.130694	7.317265			
Н	13.271476	-6.350612	3.564350			
Н	11.414722	-6.183837	4.607424			
Н	13.175127	-6.793413	5.655002			