10.1071/CH13260_AC

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SUPPLEMENTARY MATERIAL

$Cu_3(\mu_2\text{-}Cl)_3$ and $Ag_3(\mu_2\text{-}Cl)_3$ complexes supported by tetradentate trisphosphino-stibine and -bismuthine ligands

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XYZ coordinates the optimized structures of 1, 2, 3 and 4.

Complex 1

Sb	0.000000	-0.000002	0.770708	1.031944
Cu	-1.251051	-0.910837	-1.565692	-0.107229
Cl	-2.041319	0.883024	-2.833892	-0.350312
P	-2.725665	-1.994849	-0.292392	0.096289
C	-0.992088	-1.628935	1.947408	-0.274787
Cu	-0.163281	1.538869	-1.565692	-0.104814
Cl	1.785387	1.326319	-2.833892	-0.350076
P	-0.364744	3.357908	-0.292392	0.092493
C	-2.110851	-2.331856	1.427108	-0.080761
Cu	1.414333	-0.628038	-1.565692	-0.106489
Cl	0.255934	-2.209349	-2.833892	-0.349994
P	3.090411	-1.363065	-0.292392	0.093736
C	-2.713360	-3.341728	2.215908	-0.121448
H	-3.570190	-3.899712	1.822108	0.163197
C	-2.223250	-3.663357	3.489908	-0.150151
H	-2.704230	-4.453692	4.077308	0.150574
C	-1.109396	-2.977779	3.995408	-0.124190
H	-0.704071	-3.229875	4.982308	0.146835
C	-0.503575	-1.969785	3.226308	-0.169196
H	0.376189	-1.455589	3.630108	0.161207
C	-0.914661	1.673630	1.947408	-0.274739
C	-0.963993	2.993964	1.427108	-0.080466
C	-1.537286	4.020673	2.215908	-0.121494
H	-1.592200	5.041727	1.822108	0.163212
C	-2.060973	3.756981	3.489908	-0.150269
H	-2.504937	4.568814	4.077308	0.150572
C	-2.024214	2.449699	3.995408	-0.124131
H	-2.445106	2.224706	4.982308	0.146860
C	-1.454183	1.420978	3.226308	-0.169269
H	-1.448716	0.402071	3.630108	0.161215
C	1.906750	-0.044701	1.947408	-0.274847
C	3.074845	-0.662115	1.427108	-0.080785
C	4.250720	-0.679020	2.215908	-0.121247
H	5.162392	-1.142021	1.822108	0.163266
C	4.284156	-0.093704	3.489908	-0.150191
H	5.209096	-0.115059	4.077308	0.150551
C	3.133539	0.528143	3.995408	-0.124250
H	3.149178	1.005163	4.982308	0.146840
C	1.957687	0.548869	3.226308	-0.169158
H	1.072524	1.053652	3.630108	0.161208
C	-4.104043	0.315264	0.525908	-0.530688
H	-5.041414	0.902191	0.535108	0.170162
H	-3.356260	0.876519	-0.060592	0.270490
H	-3.747102	0.236550	1.569008	0.207315
C	-4.363597	-1.073077	-0.085092	-0.252638
H	-4.683408	-0.925509	-1.135592	0.235413
C	-5.465911	-1.827414	0.678408	-0.503379
H	-6.394789	-1.226924	0.675408	0.178245
H	-5.181922	-1.990170	1.734108	0.205023
H	-5.706229	-2.806892	0.228108	0.190613
C	-3.794471	-3.499527	-2.394992	-0.526298
H	-4.066867	-4.487144	-2.811492	0.172812
H	-3.046631	-3.040567	-3.066592	0.261903
H	-4.701339	-2.869632	-2.409892	0.198338
C	-3.218927	-3.681051	-0.973992	-0.255169
H	-4.011860	-4.095707	-0.320192	0.184572
C	-2.017997	-4.645794	-0.984892	-0.527124
H	-2.334179	-5.622175	-1.397892	0.167480
H	-1.615436	-4.820086	0.028108	0.205053
H	-1.204366	-4.250729	-1.618792	0.264164
C	2.325111	3.396618	0.525908	-0.530680
H	3.302023	3.914886	0.535108	0.170196
H	2.437215	2.468244	-0.060592	0.270404
H	2.078367	3.126793	1.569008	0.207250
C	1.252444	4.315602	-0.085092	-0.252454
H	1.540236	4.518714	-1.135592	0.235390
C	1.150341	5.647248	0.678408	-0.503259
H	2.134831	6.151530	0.675408	0.178242
H	0.867436	5.482772	1.734108	0.204955
H	0.422186	6.345219	0.228108	0.190602
C	-1.133452	5.035850	-2.394992	-0.526194
H	-1.852542	5.765512	-2.811492	0.172800
H	-1.109953	4.158779	-3.066592	0.261881
H	-0.134399	5.506273	-2.409892	0.198260
C	-1.578395	4.628157	-0.973992	-0.255005
H	-1.541015	5.522254	-0.320192	0.184563
C	-3.014423	4.070548	-0.984892	-0.526993
H	-3.701902	4.832530	-1.397892	0.167469
H	-3.366552	3.809060	0.028108	0.205073
H	-3.079075	3.168461	-1.618792	0.264256
C	1.779074	-3.711884	0.525908	-0.530700
H	1.739393	-4.817083	0.535108	0.170211
H	0.918978	-3.344842	-0.060592	0.270484
H	1.668737	-3.363348	1.569008	0.207292
C	3.111150	-3.242390	-0.085092	-0.252384
H	3.143246	-3.593279	-1.135592	0.235439
C	4.315572	-3.819840	0.678408	-0.503274
H	4.259960	-4.924613	0.675408	0.178203
H	4.314487	-3.492609	1.734108	0.205078
H	5.283972	-3.538264	0.228108	0.190677
C	5.032422	0.575239	-0.984892	-0.527218
H	6.036009	0.789707	-1.397892	0.167513
H	4.981990	1.011020	0.028108	0.205056
H	4.283438	1.082403	-1.618792	0.264181
C	4.797323	-0.947112	-0.973992	-0.254694
H	5.552949	-1.426622	-0.320192	0.184496
C	4.927924	-1.536330	-2.394992	-0.526303
H	5.919342	-1.278448	-2.811492	0.172812
H	4.156513	-1.118150	-3.066592	0.261849
H	4.835813	-2.636716	-2.409892	0.198329

Complex 2

Sb	0.000986	-0.002879	0.972877
Ag	-1.655339	-0.678572	-1.537467
Cl	-2.002903	1.370835	-2.911976
P	-0.174016	3.555714	0.043856
C	-0.851484	1.692595	2.159872
C	-0.809924	3.040910	1.716192
C	-1.298879	4.060840	2.569288
H	-1.264512	5.105682	2.236685
C	-1.845831	3.769654	3.825815
H	-2.221356	4.579276	4.461690
C	-1.917452	2.435123	4.250110
H	-2.355527	2.184432	5.223184
C	-1.420653	1.414447	3.423302
H	-1.478762	0.378925	3.776566
C	2.380315	3.696680	1.180809
H	3.244748	4.304897	1.506798
H	2.747959	2.941056	0.462541

H	1.986906	3.166158	2.064760
C	1.324556	4.605317	0.523783
H	0.964855	5.340673	1.272608
C	1.929324	5.358863	-0.675790
H	2.878149	5.836141	-0.366730
H	1.266392	6.155864	-1.051099
H	2.156389	4.668382	-1.508946
C	-1.254483	5.074690	-2.086285
H	-1.988021	5.834781	-2.415002
H	-1.409630	4.166081	-2.694408
H	-0.246911	5.462494	-2.303547
C	-1.486308	4.764472	-0.590439
H	-1.379318	5.698402	0.000632
C	-2.905230	4.187935	-0.404748
H	-3.641740	4.897437	-0.826038
H	-3.162966	4.016597	0.653530
H	-3.004427	3.234975	-0.956326
Ag	0.229980	1.778849	-1.525950
Cl	2.193325	1.079020	-2.891532
P	3.167848	-1.629732	0.033511
C	1.896944	-0.117586	2.157756
C	3.044589	-0.821852	1.706837
C	4.174844	-0.909787	2.556306
H	5.062270	-1.458475	2.217807
C	4.198234	-0.297617	3.816156
H	5.089395	-0.377956	4.448776
C	3.076957	0.425106	4.248199
H	3.079804	0.923659	5.224436
C	1.941984	0.506225	3.425189
H	1.072293	1.066765	3.785336
C	2.019853	-3.911651	1.178725
H	2.117476	-4.962936	1.508488
H	1.183399	-3.857385	0.458222
H	1.752674	-3.303214	2.059597
C	3.333322	-3.449459	0.521044
H	4.150028	-3.497393	1.270527
C	3.687975	-4.356581	-0.672112
H	3.644761	-5.414418	-0.351632
H	4.704008	-4.170204	-1.057442
H	2.968273	-4.227572	-1.501325
C	5.013352	-1.449162	-2.104615
H	6.032057	-1.180468	-2.442126
H	4.291194	-0.868345	-2.705306
H	4.857546	-2.517871	-2.321110
C	4.869231	-1.097839	-0.607160
H	5.627127	-1.660146	-0.021736
C	5.080190	0.418455	-0.415281
H	6.059387	0.704432	-0.842759
H	5.069122	0.720840	0.644919
H	4.300051	0.984053	-0.957318
Ag	1.425576	-1.085536	-1.533922
Cl	-0.169873	-2.419828	-2.902670
P	-2.996529	-1.923986	0.027624
C	-1.045983	-1.592569	2.150042
C	-2.234430	-2.225700	1.699767
C	-2.878184	-3.160561	2.547778
H	-3.800222	-3.650628	2.211073
C	-2.357798	-3.494153	3.804917
H	-2.875367	-4.224943	4.436519
C	-1.166011	-2.893681	4.235485
H	-0.733783	-3.152335	5.209081
C	-0.525285	-1.952110	3.413982
H	0.400001	-1.487284	3.771989
C	-4.413765	0.194579	1.192375
H	-5.376281	0.622904	1.529382
H	-3.955421	0.906796	0.482320
H	-3.752122	0.114128	2.071786
C	-4.659991	-1.167256	0.516575
H	-5.109739	-1.861077	1.256579
C	-5.617299	-1.013934	-0.680013
H	-6.512154	-0.447001	-0.361496
H	-5.964108	-1.984985	-1.070348
H	-5.140839	-0.453329	-1.505248
C	-3.759039	-3.611192	-2.113196
H	-4.046569	-4.625539	-2.448350
H	-2.890813	-3.287259	-2.713977
H	-4.598783	-2.933339	-2.333432
C	-3.385273	-3.662512	-0.614627
H	-4.253877	-4.034444	-0.031332
C	-2.182666	-4.609177	-0.421976
H	-2.429922	-5.598784	-0.849495
H	-1.916296	-4.752529	0.638239
H	-1.300350	-4.221461	-0.963566

Complex 3

Bi	0.001847	-0.003120	0.728696
Cu	0.293664	1.617906	-1.685760
Cu	1.250445	-1.064520	-1.688408
Cu	-1.551248	-0.548465	-1.683924
Cl	2.087308	0.744206	-2.880334
Cl	-0.409051	-2.181409	-2.876312
Cl	-1.696911	1.445695	-2.869662
P	0.688401	3.349966	-0.326016
P	2.561902	-2.267355	-0.333276
P	-3.247053	-1.078423	-0.327213
C	-0.294788	1.953183	1.965740
C	0.044649	3.213791	1.412943
C	-0.153875	4.379724	2.192956
H	0.092891	5.363697	1.778763
C	-0.682913	4.305478	3.489876
H	-0.832258	5.222453	4.071261
C	-1.030631	3.057587	4.027774
H	-1.461254	2.989156	5.033831
C	-0.836478	1.892183	3.265656
H	-1.135882	0.926176	3.690249
C	1.847912	-0.724270	1.962050
C	2.772052	-1.643033	1.403641
C	3.885003	-2.053018	2.178125
H	4.613767	-2.755811	1.758496
C	4.088150	-1.560714	3.475760
H	4.960058	-1.888554	4.053194
C	3.179371	-0.640943	4.019641
H	3.337458	-0.236189	5.026348
C	2.068653	-0.227985	3.262732
H	1.381553	0.511431	3.691661
C	-1.545030	-1.241742	1.964011
C	-2.808475	-1.571127	1.410830
C	-3.722709	-2.323379	2.189300
H	-4.699496	-2.595792	1.774127
C	-3.396691	-2.747116	3.485999
H	-4.119192	-3.331483	4.067088

C	-2.141101	-2.430197	4.024705
H	-1.868860	-2.770810	5.030768
C	-1.224801	-1.682622	3.264158
H	-0.238468	-1.463334	3.691097
C	3.262529	2.531195	0.459599
H	4.352295	2.720181	0.472017
H	3.084790	1.617294	-0.132869
H	2.942921	2.346345	1.501573
C	2.531551	3.741404	-0.149468
H	2.857127	3.835413	-1.204326
C	2.870785	5.039544	0.602223
H	3.965689	5.197037	0.592099
H	2.555255	4.984022	1.659778
H	2.406771	5.932037	0.146526
C	0.475286	5.206602	-2.416872
H	0.007248	6.120947	-2.826799
H	0.238572	4.369230	-3.098261
H	1.569139	5.358051	-2.427296
C	-0.075171	4.935711	-1.000984
H	0.225240	5.771953	-0.338818
C	-1.612088	4.833013	-1.016160
H	-2.041571	5.773854	-1.408668
H	-2.025926	4.664764	-0.006651
H	-1.943205	4.005283	-1.668653
C	0.567974	-4.077423	0.471804
H	0.182164	-5.113851	0.489446
H	-0.137803	-3.463607	-0.114351
H	0.580412	-3.706680	1.513138
C	1.975644	-4.056157	-0.150703
H	1.884428	-4.385851	-1.204533
C	2.936558	-4.998065	0.594631
H	2.522939	-6.024101	0.595348
H	3.059539	-4.690522	1.648996
H	3.936460	-5.047068	0.127701
C	4.260605	-3.003255	-2.437744
H	5.285214	-3.071556	-2.848366
H	3.666319	-2.360809	-3.112773
H	3.824416	-4.017568	-2.458263
C	4.313180	-2.407598	-1.015428
H	4.882335	-3.099496	-0.362798
C	5.005857	-1.031267	-1.017354
H	6.030704	-1.134017	-1.420832
H	5.080668	-0.603068	-0.002689
H	4.455472	-0.316610	-1.655280
C	-3.827696	1.556662	0.468486
H	-4.535055	2.406860	0.479230
H	-2.941703	1.862772	-0.114168
H	-3.516995	1.365974	1.512029
C	-4.507073	0.322559	-0.152735
H	-4.742021	0.563369	-1.208428
C	-5.806826	-0.036508	0.586833
H	-6.487669	0.835496	0.581904
H	-5.608722	-0.293859	1.643135
H	-6.347745	-0.878062	0.118775
C	-4.732965	-2.187037	-2.428130
H	-5.302888	-3.041133	-2.838905
H	-3.879874	-1.991879	-3.103337
H	-5.394829	-1.303208	-2.448426
C	-4.241306	-2.529055	-1.006076
H	-5.123658	-2.675018	-0.351785
C	-3.396651	-3.817118	-1.005315
H	-4.000693	-4.654727	-1.401990
H	-3.060615	-4.090932	0.009893
H	-2.504309	-3.703143	-1.646499

Complex 4

Bi	-0.005713	-0.010734	0.872212
Ag	-1.538094	-0.964946	-1.719326
Cl	-2.140854	1.166605	-3.010766
P	-3.106500	-1.787954	-0.056743
C	-1.960470	-0.292630	2.123172
Ag	-0.040808	1.813780	-1.727314
Cl	2.086573	1.246038	-3.036878
P	-0.012430	3.569907	-0.054306
C	-3.080498	-1.019324	1.637892
Ag	1.603519	-0.870915	-1.718165
Cl	0.057833	-2.505529	-2.958726
P	3.116932	-1.754869	-0.041490
C	-4.232300	-1.127697	2.457649
H	-5.109234	-1.676074	2.096370
C	-4.288028	-0.532900	3.725954
H	-5.193906	-0.630670	4.334930
C	-3.185396	0.192817	4.197969
H	-3.218382	0.675632	5.181778
C	-2.035738	0.308384	3.397881
H	-1.189411	0.894126	3.776313
C	0.721142	1.829190	2.118665
C	0.639226	3.164238	1.639964
C	1.104855	4.217653	2.466753
H	1.052072	5.252486	2.111558
C	1.649552	3.968569	3.734215
H	2.005937	4.803133	4.348638
C	1.742169	2.649287	4.199032
H	2.177837	2.436348	5.182378
C	1.279866	1.594554	3.393292
H	1.374095	0.568410	3.767957
C	1.231553	-1.549399	2.124874
C	2.439292	-2.127303	1.650309
C	3.125717	-3.052628	2.476538
H	4.055294	-3.513213	2.124546
C	2.634532	-3.411663	3.739562
H	3.184382	-4.133888	4.353640
C	1.435141	-2.850491	4.199960
H	1.030164	-3.132280	5.179067
C	0.745562	-1.927950	3.394507
H	-0.196963	-1.507833	3.765152
C	-5.180781	-0.015254	-0.750196
H	-6.213281	0.129096	-1.119815
H	-4.492434	0.494084	-1.449500
H	-5.101026	0.476527	0.234689
C	-4.867216	-1.522349	-0.673342
H	-5.560922	-2.005444	0.042972
C	-5.044706	-2.191364	-2.052212
H	-6.073885	-2.014357	-2.415654
H	-4.885534	-3.283490	-2.020928
H	-4.347126	-1.761329	-2.794118
C	-3.998823	-4.273822	1.156927
H	-3.870840	-5.372215	1.179413
H	-5.036484	-4.069892	0.837237
H	-3.874937	-3.903480	2.190460
C	-2.955019	-3.652537	0.213495
H	-3.107870	-4.052298	-0.808813

C	-1.517670	-4.001253	0.641758
H	-1.407946	-5.098831	0.723424
H	-1.272687	-3.566585	1.628184
H	-0.780650	-3.641589	-0.097847
C	2.541549	4.525900	-0.750276
H	3.168264	5.358476	-1.121008
H	2.647456	3.678393	-1.452265
H	2.938114	4.213252	0.231231
C	1.073029	4.985926	-0.662634
H	0.994012	5.820548	0.061677
C	0.566390	5.477820	-2.034284
H	1.220217	6.292621	-2.396640
H	-0.464576	5.871059	-1.993061
H	0.596088	4.664703	-2.782750
C	-1.758301	5.547579	1.166455
H	-2.781901	5.965797	1.191236
H	-1.078662	6.359811	0.852355
H	-1.494177	5.253684	2.198221
C	-1.718457	4.338274	0.216990
H	-1.993477	4.668339	-0.804406
C	-2.720338	3.248785	0.640866
H	-3.735882	3.681848	0.708620
H	-2.469088	2.830383	1.632601
H	-2.751850	2.424974	-0.093717
C	2.706719	-4.451829	-0.738646
H	3.131455	-5.406756	-1.100988
H	1.921269	-4.134389	-1.448871
H	2.231720	-4.640414	0.239749
C	3.823889	-3.393488	-0.646924
H	4.588114	-3.730157	0.081305
C	4.506297	-3.193362	-2.016325
H	4.899209	-4.162777	-2.374961
H	5.352807	-2.485731	-1.973717
H	3.785077	-2.824226	-2.768428
C	5.703066	-1.205981	1.167335
H	6.568580	-0.517698	1.190057
H	6.076838	-2.193723	0.842969
H	5.326274	-1.300199	2.201569
C	4.621019	-0.643013	0.230126
H	5.036960	-0.557699	-0.793240
C	4.162535	0.760078	0.667664
H	5.036942	1.434175	0.734991
H	3.681026	0.737985	1.662539
H	3.453532	1.195920	-0.058212