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Electronic Supplementary Information for

Photoluminescence properties of TADF-emitting three-coordinate silver(I) halide complexes with diphosphine ligands: a comparison study with copper(I) complexes

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Contents

1. Crystal Structure determination

Table S1. Crystallographic data of **1**−**3**.

	1	**2**	**3**
Formula	$C_{68}H_6$ Ag_2Br P_4	$C_{38}H_{40}AgBrP_2$	$C_{42}H_{48}AgBrP_2$
formula weight	1380.64	764.42	802.52
cryst syst	triclinic	triclinic	orthorhombic
space group	$P\bar{1}$	$P\bar{1}$	$Pna2_1$
a / Å	13.6283 (14)	10.4800(10)	20.3555(14)
b / Å	14.8803 (15)	11.6374(9)	9.5582(6)
c / Å	16.1037 (17)	15.2140(16)	19.5813(12)
α / deg	102.969 (2)	80.148(6)	-
β / deg	95.674 (1)	87.232(6)	-
γ / deg	107.632 (2)	64.089(4)	-
V / Å^3	2983.6 (5)	1643.6(3)	3809.8(4)
Z	2	2	4
d_{calcd} / g cm^{-3}	1.537	1.508	1.399
T / K	90(2)	90(2)	90(2)
radiation	Mo Kα	Mo Kα	Mo Kα
	(λ = 0.71073 Å)	(λ = 0.71073 Å)	(λ = 0.71073 Å)
μ / cm^{-1}	2.144	1.952	1.690
Diffractometer	Rigaku AFC-8	Rigaku AFC-8	Rigaku AFC-8
max 2θ / deg	60	60	60
reflns collcd	80385	19809	18741
indep reflns	18806	9502	9221
	(Rint = 0.0295)	(Rint = 0.0245)	(Rint = 0.0262)
no. of param refined	685	379	415
$R1$,[a] $wR2$ ($I > 2\sigma I$)[b]	0.0345, 0.0868	0.0284, 0.0725	0.0222, 0.0395
S	0.880	1.051	0.902

2.

[a] $R1 = Ł||Fo| ï |Fc||/Ł|Fo|$. [b] $wR2 = [Łw(|Fo| ï |Fc|)^2/Łw|Fo|^2]^{1/2}$

2. NMR Experiments

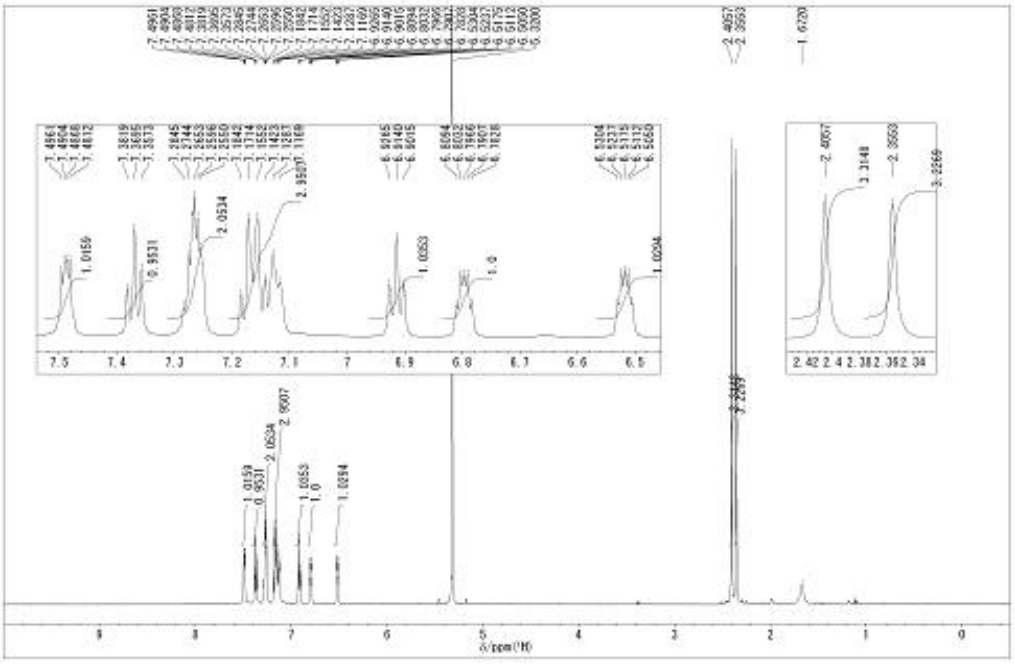


Fig. S1 ^{1}H NMR spectrum of **1** in CD_2Cl_2 at 220 K.

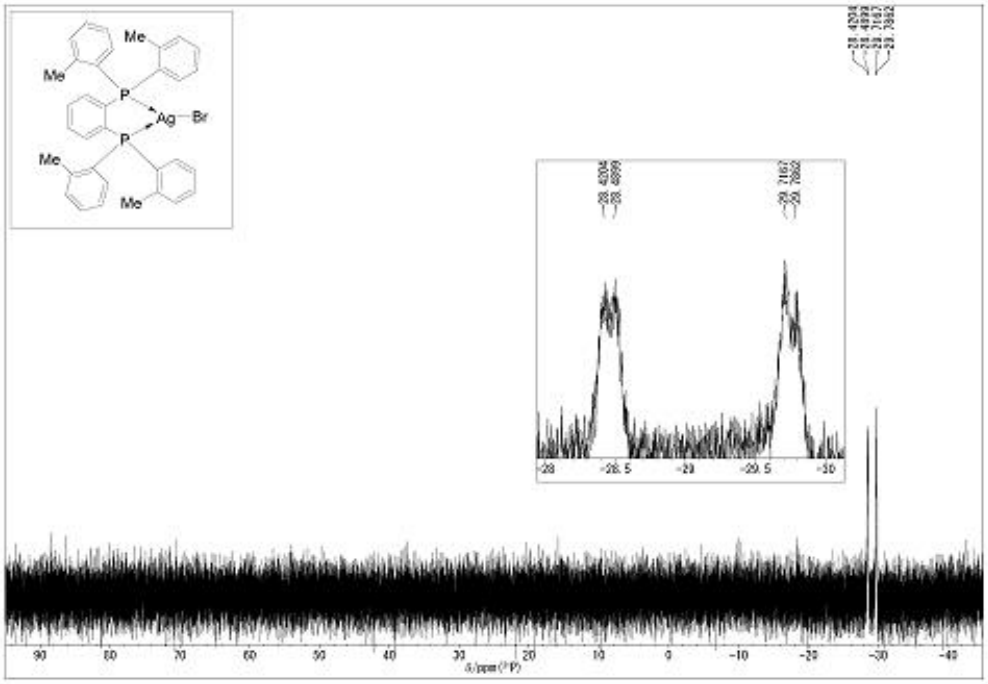


Fig. S2 $^{31}P\{^{1}H\}$ NMR spectrum of **1** in CD_2Cl_2 at 220 K.

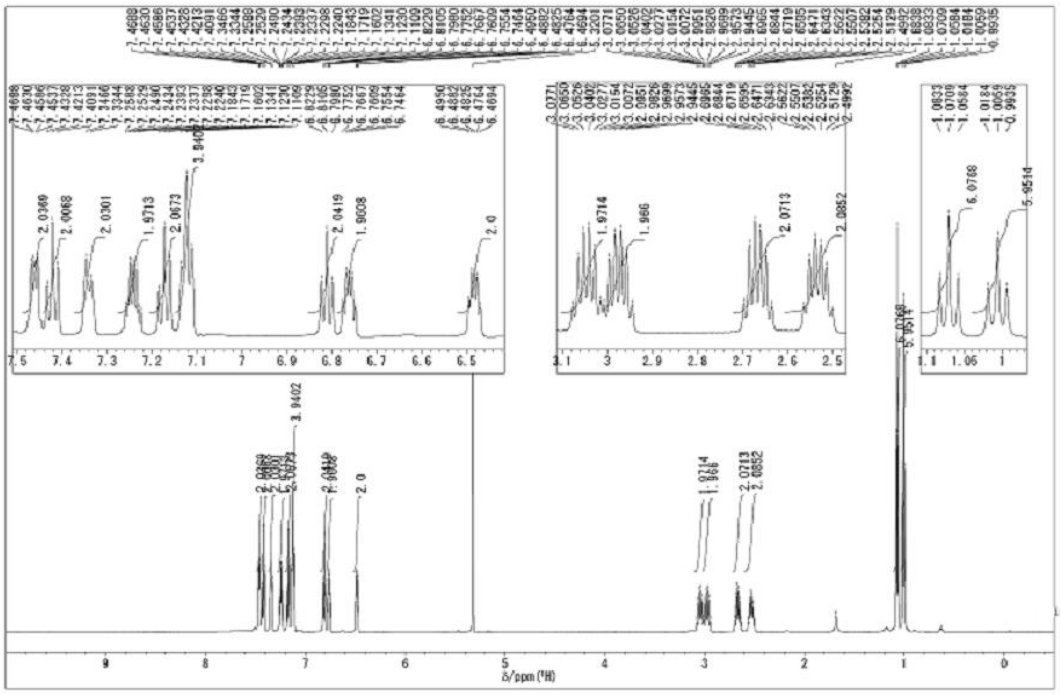


Fig. S3. ^{1}H NMR spectrum of **2** in CD_2Cl_2 at 220 K.

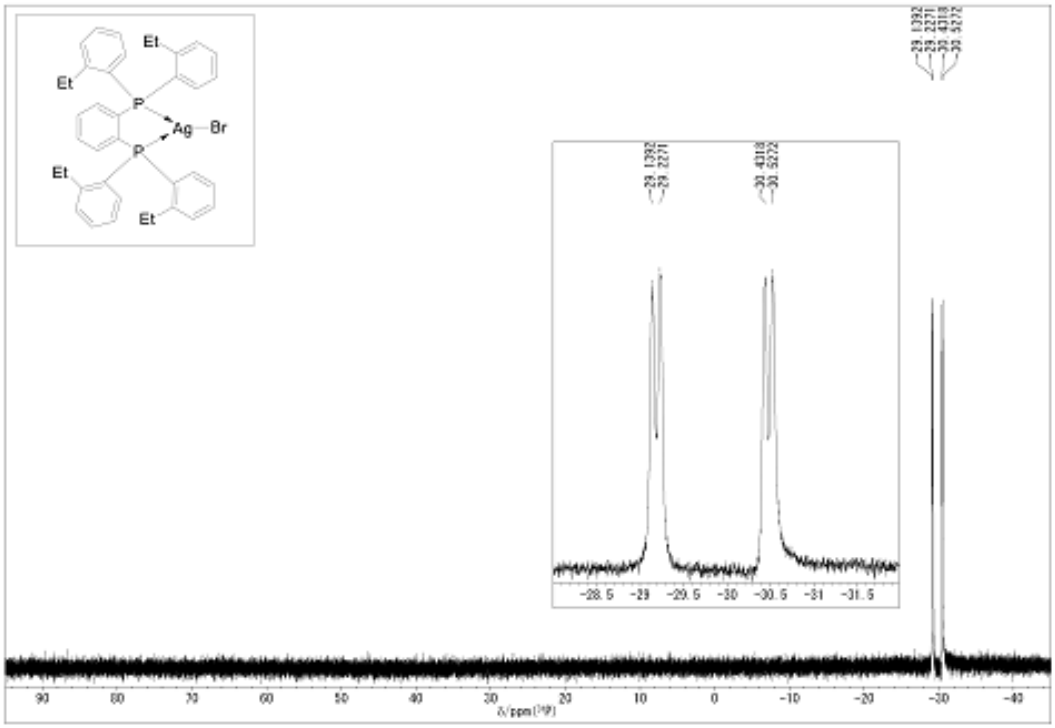


Fig. S4 $^{31}P\{^{1}H\}$ NMR spectrum of **2** in CD_2Cl_2 at 220 K.

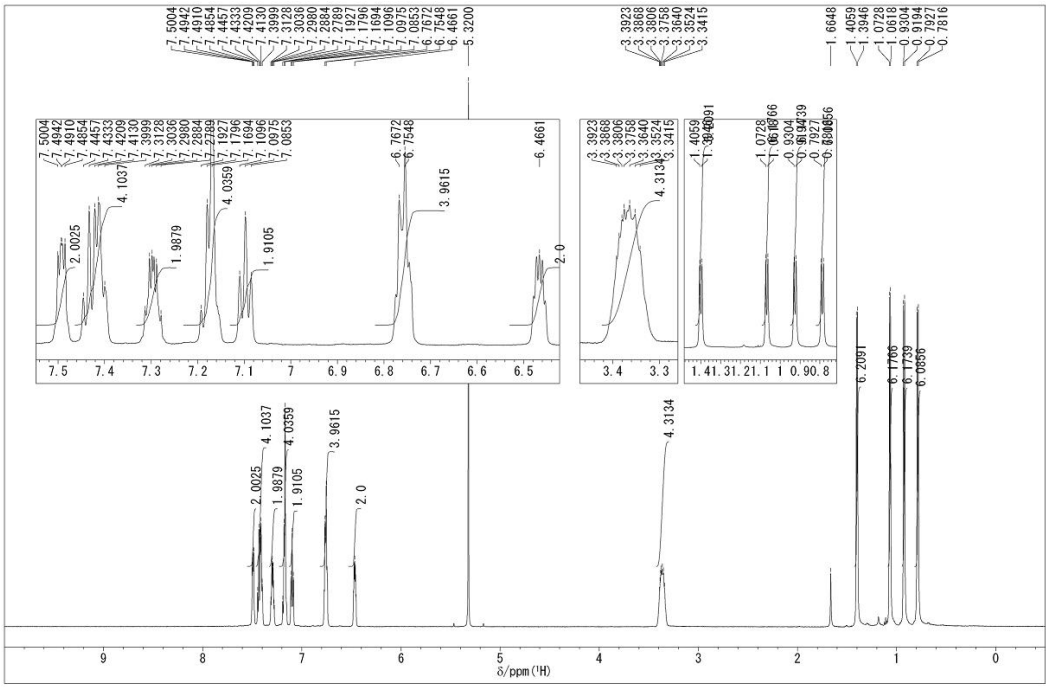


Fig. S5 ^{1}H NMR spectrum of **3** in CD_2Cl_2 at 220 K.

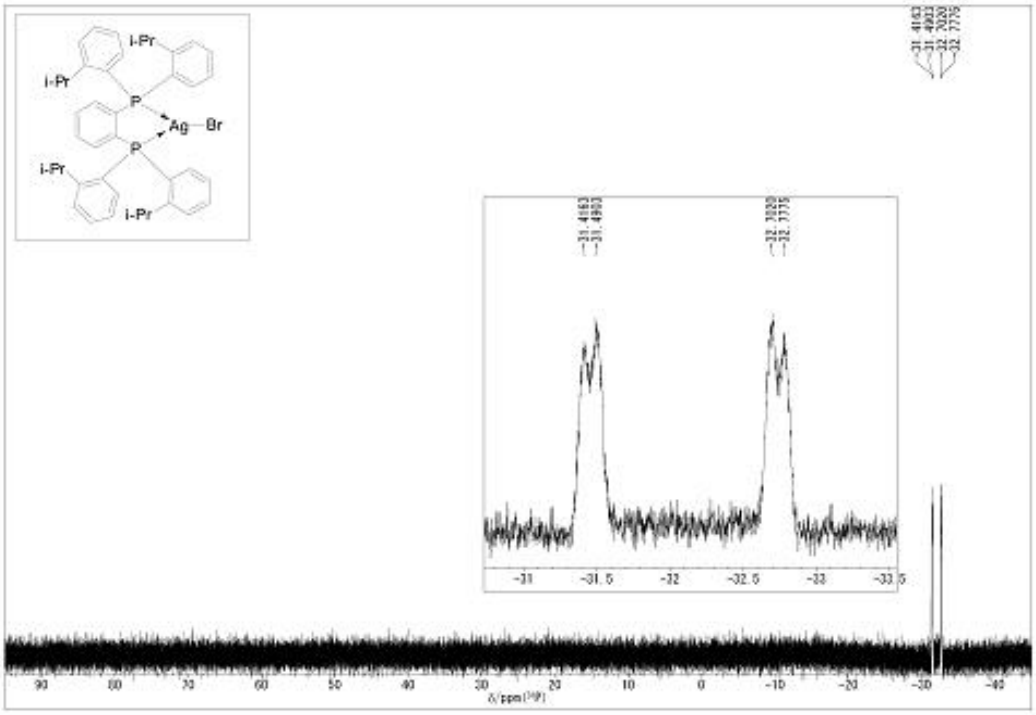


Fig. S6 $^{31}P\{^{1}H\}$ NMR spectrum of **3** in CD_2Cl_2 at 220 K.

3. Photophysical data

Table S2 k_r and k_{nr} values of **1**−**3** in the solid at 300 K and at 77 K.

	K_r at 293 K [a]	K_{nr} at 293 K [b]	K_r at 77 K [a]	K_{nr} at 77 K [b]
1	1.0×10^5	7.9×10^4	7.8×10^2	87
2	1.0×10^5	4.3×10^4	1.1×10^3	22
3	1.3×10^5	2.6×10^3	7.5×10^2	15

[a] Radiative rate constant. $k_r = \Phi / \tau$. The k_r values, tentatively estimated from the average lifetime $(\tau_1+\tau_2)/2$ and Φ_{PL}. [b] Non-radiative constant. $k_{nr} = (1 / \Phi - 1) \times k_r$.

4. Theoretical Studies

Table S3 Composition of hole and electron in S_1 and T_1 of (L_{Et})CuBr **2** (S_1-optimized geometry).

	percentage composition (%)	
	hole (S_1)	hole (T_1)
Cu	28	28
P	28	29
Br	18	19

Table S4 Composition of hole and electron in S_1 and T_1 of **2** (S_1-optimized geometry).

	percentage composition (%)	
	hole (S_1)	hole (T_1)
Ag	14	14
P	27	27
Br	35	36

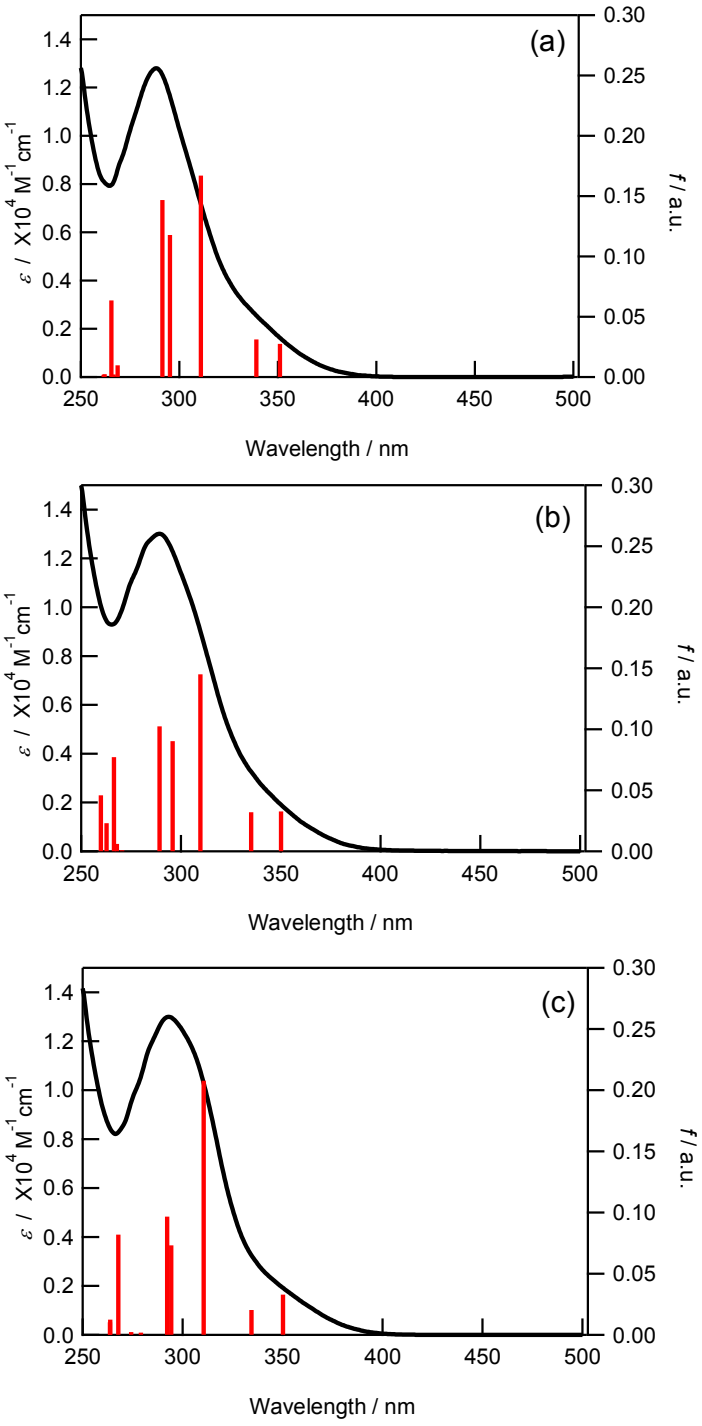
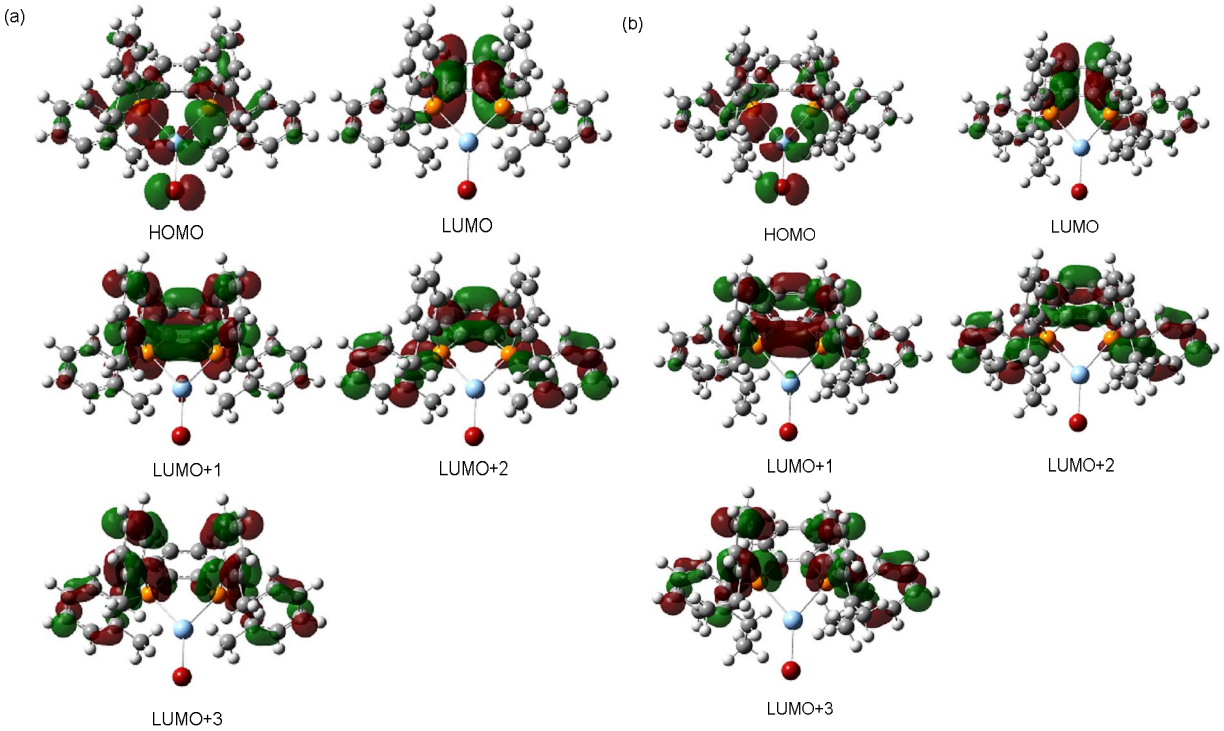


Figure S7 Absorption spectra (black) and calculated singlet transitions (red) at the optimized ground state S_0 geometry in CH_2Cl_2. The oscillator strengths of $S_n \hat{Y} S_0$ (n Ò 10) transitions calculated are presented with bars; (a) complex **1**, (b) complex **2** and (c) complex **3**.

Table S5 Calculated energy levels, oscillator strengths (*f*), and orbital transitions for selected lower-lying transitions of **1**ī **3**

	states	λ_{cal} / nm (eV)	*f*	assignments
1	S1	351 (3.532)	0.0275	HOMOŸ LUMO (100%)
	S2	339 (3.656)	0.0312	HOMOŸ LUMO+1 (100%)
	S3	311 (3.987)	0.1670	HOMOŸ LUMO+2 (100%)
	S4	295 (4.200)	0.1177	HOMOŸ LUMO+3 (100%)
2	S1	350 (3.541)	0.0327	HOMOŸ LUMO (100%)
	S2	335 (3.699)	0.0320	HOMOŸ LUMO+1 (100%)
	S3	309 (4.003)	0.1450	HOMOŸ LUMO+2 (100%)
	S4	296 (4.191)	0.0902	HOMOŸ LUMO+3 (100%)
3	S1	350 (3.542)	0.0329	HOMOŸ LUMO (100%)
	S2	334 (3.707)	0.0203	HOMOŸ LUMO+1 (100%)
	S3	310 (3.993)	0.2077	HOMOŸ LUMO+2 (100%)
	S4	294 (4.213)	0.0732	HOMOŸ LUMO+3 (100%)



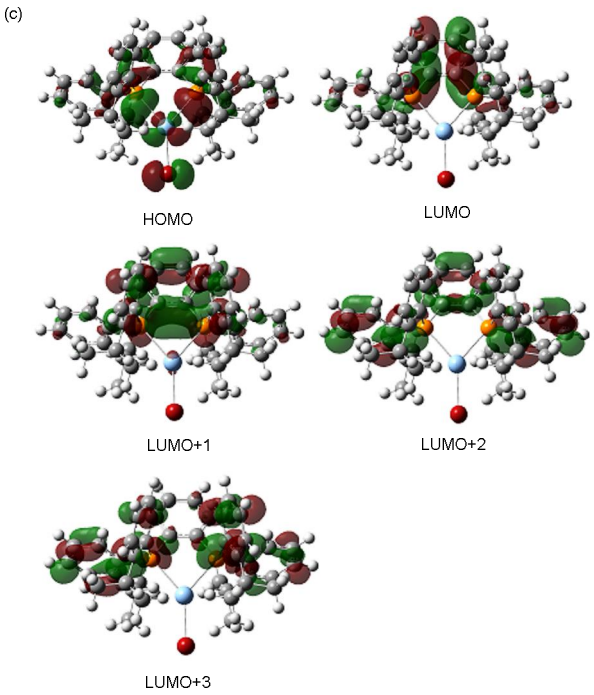


Figure S8 Frontier orbitals of HOMO, LUMO, LUMO+1, LUMO+2, and LUMO+3 obtained with the calculation of **1**ī **3** in the optimized S_0 structures.

Table S6 Geometry data of **1** (S_0 in CH_2Cl_2, S_0, S_1, and T_1)

S_0 optimization in CH_2Cl_2: unit Å

Br	-0.171312	-0.826560	-0.626067
Ag	-0.070635	-0.307177	1.965171
P	1.657723	-0.031194	3.858040
P	-1.698953	0.204814	3.898459
C	3.316976	0.749862	3.700324
C	3.473610	1.923789	2.924898
C	4.758429	2.461172	2.790734
C	5.869499	1.868163	3.388091
C	5.710523	0.711323	4.146032
C	4.439714	0.159980	4.299135
C	1.967338	-1.611532	4.744832
C	2.450169	-2.731307	4.024500
C	2.639252	-3.931557	4.718831
C	2.362177	-4.045334	6.080098
C	1.889776	-2.940756	6.783206
C	1.695961	-1.733206	6.114917
C	0.771038	1.037616	5.076977
C	1.515090	1.804642	5.986509
C	0.893840	2.656982	6.896106
C	-0.495361	2.757726	6.910237
C	-1.250822	2.004366	6.014997
C	-0.643189	1.139071	5.092424
C	-3.216028	1.234605	3.741545
C	-3.192507	2.404473	2.944985
C	-4.376610	3.137501	2.811122
C	-5.560912	2.739767	3.429411
C	-5.579683	1.585675	4.207808
C	-4.411348	0.841293	4.360642
C	-2.243397	-1.294800	4.811650

C	-2.902196	-2.334903	4.111703	H	3.557987	-1.921911	2.345953
C	-3.276634	-3.478124	4.826713	H	-1.144606	3.112870	2.965305
C	-3.012758	-3.613069	6.188644	H	-2.146013	3.792106	1.675213
C	-2.364676	-2.587539	6.871182	H	-1.554952	2.127510	1.559208
C	-1.985381	-1.436901	6.182325	H	-3.863546	-1.382553	2.416964
C	2.314417	2.611840	2.254963	H	-3.754351	-3.144723	2.310128
C	2.783931	-2.669662	2.557280	H	-2.321335	-2.144197	2.032135
C	-1.945625	2.884486	2.252072				
C	-3.226978	-2.246285	2.643886	S_0 optimization: unit Å			
H	4.886734	3.364606	2.198778	Ag	-2.00290169	-0.00058903	0.16391199
H	6.853997	2.310183	3.258958	Br	-0.14272717	-0.00635363	-2.00107675
H	6.566239	0.237569	4.619639	P	-3.98636690	1.70621040	0.18121194
H	4.320000	-0.741980	4.892404	P	-3.99006893	-1.70327619	0.18002785
H	3.012483	-4.795720	4.173979	C	-4.12583614	3.25757802	1.17386645
H	2.517184	-4.994473	6.586467	C	-3.72345476	3.26761583	2.53069806
H	1.672529	-3.012273	7.845497	C	-3.80159727	4.47326343	3.23735829
H	1.330816	-0.874158	6.669159	H	-3.49279184	4.48634976	4.28035261
H	2.599231	1.736113	5.977526	C	-4.25925177	5.64720280	2.64195737
H	1.495736	3.239927	7.587867	H	-4.30264809	6.56704934	3.21948670
H	-0.992905	3.420502	7.612954	C	-4.65989917	5.63169055	1.30882432
H	-2.333621	2.091945	6.028043	H	-5.02470990	6.53625979	0.82931760
H	-4.366241	4.038948	2.202572	C	-4.59290115	4.44220011	0.58554955
H	-6.463913	3.330660	3.300089	H	-4.90797374	4.43629814	-0.45399038
H	-6.494649	1.262789	4.697273	C	-4.45425833	2.22657069	-1.52264348
H	-4.429947	-0.058037	4.969501	C	-3.52545490	2.95318965	-2.30810320
H	-3.786774	-4.279942	4.297737	C	-3.88871447	3.29147054	-3.61674350
H	-3.314732	-4.516798	6.711513	H	-3.18190957	3.85258925	-4.22397858
H	-2.154551	-2.676145	7.933639	C	-5.12111007	2.92812029	-4.15697554
H	-1.484174	-0.638634	6.720844	H	-5.36699763	3.20338949	-5.17937050
H	2.652914	3.494921	1.705143	C	-6.03032232	2.21621113	-3.38023977
H	1.560268	2.940378	2.980002	H	-6.99742200	1.92843247	-3.78392719
H	1.809841	1.947851	1.541172	C	-5.69462857	1.87266579	-2.07156101
H	1.909073	-2.402183	1.950534	H	-6.41144667	1.32323584	-1.46978913
H	3.151175	-3.637504	2.203560	C	-5.43080466	0.71083313	0.77665817

C	-6.55486217	1.38724639	1.27809421	H	-1.57692930	2.52908484	-1.47113451
H	-6.56043203	2.47349614	1.28704068	H	-2.28421805	4.05190156	-0.91317359
C	-7.66058206	0.69981610	1.77060859	H	-1.62556849	3.92891245	-2.55073334
H	-8.51464180	1.25255688	2.15268763	C	-3.25625459	-1.99745866	3.23846653
C	-7.66130968	-0.69315406	1.77057628	H	-2.95155408	-2.21900374	4.26577086
H	-8.51606661	-1.24507221	2.15228643	H	-4.04668951	-1.23830422	3.28292114
C	-6.55594127	-1.38129023	1.27848539	H	-2.39981061	-1.54251161	2.72523691
H	-6.56180318	-2.46747185	1.28572184	C	-2.20261715	-3.39211259	-1.79416059
C	-5.43110512	-0.70590166	0.77756310	H	-1.65680227	-3.94584300	-2.56407551
C	-4.12414707	-3.24889154	1.18276662	H	-2.29359625	-4.04316546	-0.91643989
C	-3.72876261	-3.24383405	2.54170052	H	-1.58624916	-2.53170427	-1.50452273
C	-3.80513069	-4.44282262	3.25971217	Ag	2.00285155	0.00100863	-0.16398494
H	-3.50316527	-4.44390405	4.30479526	Br	0.14260473	0.00612638	2.00112159
C	-4.25293131	-5.62503901	2.67313285	P	3.98626253	-1.70619934	-0.18148950
H	-4.29525975	-6.53932309	3.25950152	P	3.99014419	1.70327625	-0.17977549
C	-4.64464813	-5.62479871	1.33733599	C	4.12579696	-3.25750246	-1.17425557
H	-5.00078748	-6.53610215	0.86408509	C	3.72361290	-3.26742430	-2.53114668
C	-4.57982646	-4.44204853	0.60270952	C	3.80184354	-4.47301219	-3.23790052
H	-4.88786473	-4.44953627	-0.43901248	C	4.25939998	-5.64700796	-2.64253742
C	-4.47075643	-2.22965232	-1.51854951	C	4.65986448	-5.63161144	-1.30934742
C	-3.54861853	-2.95793590	-2.31042793	C	4.59278255	-4.44218061	-0.58598492
C	-3.92270642	-3.29932317	-3.61537153	C	4.45407027	-2.22672865	1.52234062
H	-3.22035297	-3.86170053	-4.22668925	C	3.52522231	-2.95341514	2.30767985
C	-5.15974324	-2.93805516	-4.14630908	C	3.88842542	-3.29186114	3.61629364
H	-5.41385802	-3.21557108	-5.16607994	C	5.12080308	-2.92859105	4.15661887
C	-6.06262859	-2.22513775	-3.36325098	C	6.03004910	-2.21658300	3.38001130
H	-7.03345214	-1.93902458	-3.75916346	C	5.69441446	-1.87288156	2.07135878
C	-5.71611772	-1.87855251	-2.05831029	C	5.43076148	-0.71081300	-0.77677386
H	-6.43051086	-1.32925822	-1.45362998	C	6.55479745	-1.38719231	-1.27829788
C	-3.24412527	2.02975212	3.23800097	C	7.66053120	-0.69973374	-1.77074611
H	-4.03906855	1.27727442	3.30953199	C	7.66129623	0.69323510	-1.77055287
H	-2.91898682	2.26538761	4.25589471	C	6.55595466	1.38134336	-1.27835936
H	-2.40051435	1.56057037	2.71639608	C	5.43110893	0.70592520	-0.77750358
C	-2.18456027	3.38864957	-1.78074212	C	4.12422230	3.24900866	-1.18232825

C	3.72879911	3.24412798	-2.54125356	H	2.40083295	-1.56026983	-2.71687826
C	3.80520417	4.44320130	-3.25912074	H	4.30286856	-6.56680549	-3.22013998
C	4.25306473	5.62532857	-2.67240710	H	1.57684838	-2.52921654	1.47039085
C	4.64481076	5.62491259	-1.33661954	H	2.28406514	-4.05218213	0.91274164
C	4.57996251	4.44207515	-0.60213618	H	1.62519284	-3.92889738	2.55019041
C	4.47091240	2.22941413	1.51885954	H	3.49319355	-4.48600328	-4.28094204
C	3.54885842	2.95766602	2.31085774	H	2.95162750	2.21954560	-4.26548250
C	3.92300451	3.29883898	3.61584094	H	4.04656731	1.23862686	-3.28263224
C	5.16002156	2.93739044	4.14670193	H	2.39967924	1.54295967	-2.72506506
C	6.06283296	2.22451583	3.36351920	H	3.50321922	4.44442501	-4.30419798
C	5.71626181	1.87814351	2.05853748	H	1.65748074	3.94644145	2.56441868
C	3.24445267	-2.02948565	-3.23843198	H	2.29370153	4.04230061	0.91648172
C	2.18434939	-3.38879726	1.78020368	H	1.58607828	2.53151831	1.50596631
C	3.25621679	1.99786808	-3.23817406				
C	2.20283636	3.39194777	1.79472513	S_1 optimization: unit Å			
H	5.02460259	-6.53622360	-0.82986647	Ag	2.15851604	0.06873962	-0.15611278
H	4.29541806	6.53968140	-3.25866676	Br	0.27150938	0.68124343	1.79779386
H	4.90770654	-4.43637113	0.45360108	P	4.23620558	1.50743317	0.25627661
H	5.00099479	6.53614539	-0.86326675	P	3.90563090	-1.69109656	-0.67213201
H	3.18158544	-3.85303829	4.22343444	C	4.27624235	3.20189252	-0.44856644
H	4.88802884	4.44942117	0.43957912	C	3.58997236	3.56006817	-1.63231660
H	5.36664361	-3.20398635	5.17899120	C	3.77411438	4.84875598	-2.14319632
H	6.99712968	-1.92885068	3.78377747	H	3.24444877	5.12824980	-3.05133012
H	6.41125458	-1.32336694	1.46968848	C	4.61074302	5.77709550	-1.52328896
H	3.22071540	3.86119723	4.22725006	H	4.73073140	6.76959532	-1.94959042
H	6.56033826	-2.47344072	-1.28736989	C	5.28658676	5.42131323	-0.35885249
H	5.41418145	3.21474515	5.16650527	H	5.94258176	6.13005572	0.14001659
H	8.51457074	-1.25245458	-2.15289988	C	5.11500430	4.14583160	0.17334150
H	7.03364825	1.93827580	3.75935940	H	5.63472480	3.88039866	1.09015253
H	8.51605958	1.24517594	-2.15221548	C	4.56861516	1.73347757	2.05808453
H	6.43059527	1.32887471	1.45376405	C	3.78756050	2.56742338	2.89523305
H	6.56185213	2.46752550	-1.28545893	C	4.06912578	2.56836995	4.26685751
H	4.03946905	-1.27707072	-3.30985604	H	3.47324420	3.20363810	4.91894109
H	2.91938724	-2.26504160	-4.25636721	C	5.08166169	1.78315255	4.81505244

H	5.26745703	1.80956817	5.88578544	H	6.17057778	-2.30235086	0.98659331
C	5.84359874	0.96220577	3.98673745	C	2.67675073	2.61056858	-2.35458321
H	6.63512508	0.34159187	4.39828666	H	3.18280461	1.66713678	-2.58621067
C	5.57757467	0.93556942	2.62039893	H	2.32948021	3.04194519	-3.29844166
H	6.16150589	0.29171298	1.96904685	H	1.78662519	2.36919054	-1.75866073
C	5.56955842	0.58666278	-0.47932838	C	2.69961183	3.47372474	2.3826747
C	6.85664884	1.18261069	-0.61226332	H	2.10630312	3.00481062	1.59209118
H	6.99258870	2.21258337	-0.28899850	H	3.11872552	4.40167890	1.97469285
C	7.92548692	0.51481149	-1.16537092	H	2.01527263	3.74304472	3.19291763
H	8.88208640	1.02007871	-1.26950251	C	3.42653570	-0.92220209	-3.72505379
C	7.76933005	-0.83267346	-1.62485383	H	2.56051974	-0.45054189	-3.24442008
H	8.59987755	-1.35828863	-2.08682171	H	3.33205374	-0.77384175	-4.80500138
C	6.53937294	-1.44912804	-1.49829703	H	4.32550675	-0.39773640	-3.38034278
H	6.42064795	-2.47219783	-1.85186323	C	1.56594596	-3.30732592	0.87255404
C	5.41698218	-0.78993105	-0.94614042	H	1.11884013	-2.32100048	1.05445853
C	3.66934919	-2.85372255	-2.06497502	H	0.91771449	-4.05097629	1.3463372
C	3.48428022	-2.38446393	-3.38904737	H	1.53787875	-3.47584300	-0.20867735
C	3.35246198	-3.32945181	-4.41104635	Ag	-1.95237268	0.07834829	0.1226212
H	3.21233112	-2.97602227	-5.43000020	Br	0.02300499	-0.69560148	-1.79047283
C	3.39150353	-4.69998046	-4.15847613	P	-3.95987870	-1.47031484	0.76656579
H	3.28315506	-5.40515337	-4.97839449	P	-3.89850980	1.73777930	-0.37346702
C	3.57416143	-5.15623072	-2.85576725	C	-4.07139245	-2.60430900	2.21844114
H	3.61557718	-6.22081041	-2.64176104	C	-3.59718875	-2.18114953	3.48295033
C	3.71159588	-4.23665166	-1.81914953	C	-3.65600920	-3.08524374	4.54980018
H	3.86606983	-4.59883298	-0.80752941	C	-4.16261843	-4.37426313	4.39495761
C	4.06720757	-2.73632217	0.84004319	C	-4.63344332	-4.78424574	3.15061398
C	2.95948194	-3.38516919	1.43640289	C	-4.58696577	-3.90071581	2.07368657
C	3.17928863	-4.11553123	2.60977853	C	-4.53014291	-2.49503235	-0.65374886
H	2.33656699	-4.62475626	3.07217881	C	-3.66070130	-3.46566412	-1.20976513
C	4.44051511	-4.20307740	3.19744322	C	-4.10225889	-4.18879179	-2.32394489
H	4.57250401	-4.77718929	4.11089476	C	-5.35672413	-3.97400877	-2.89196104
C	5.52323922	-3.55109267	2.61248926	C	-6.20852805	-3.02208563	-2.33947981
H	6.51206258	-3.60966590	3.05939615	C	-5.79356958	-2.29203928	-1.22689321
C	5.33073666	-2.81671348	1.44458870	C	-5.34890141	-0.28231892	1.06339445

C	-6.45484328	-0.71125781	1.81495988	H	-7.15156360	0.80969330	-4.03125529
C	-7.51836620	0.14093174	2.09875907	H	-8.31554506	2.13082522	1.84441742
C	-7.49401595	1.45258155	1.63020654	H	-6.44266136	0.98599247	-1.68054953
C	-6.40611484	1.89619602	0.88356127	H	-6.39149293	2.92207771	0.52650338
C	-5.32427958	1.05140137	0.58697543	H	-3.84101880	-0.03566665	3.57990948
C	-3.93793820	3.53230880	0.05609752	H	-2.68380925	-0.69567843	4.74280275
C	-3.50303067	3.96365552	1.33214587	H	-2.24336472	-0.54842751	3.03453403
C	-3.49929194	5.33689057	1.60241119	H	-4.18934562	-5.05193082	5.24436421
C	-3.90769110	6.27455238	0.65576317	H	-1.67185967	-2.86601659	-0.59844580
C	-4.34054251	5.84535264	-0.59578854	H	-2.37548377	-4.15053951	0.39136420
C	-4.35472821	4.48256238	-0.88774706	H	-1.78273027	-4.51128030	-1.23642905
C	-4.44996096	1.67852177	-2.12951997	H	-3.29270999	-2.76540614	5.52394128
C	-3.54163947	2.02890399	-3.15869278	H	-2.67478382	3.53823963	3.27143635
C	-3.97441791	1.92706734	-4.4858809	H	-3.92674378	2.39896193	2.75945288
C	-5.25680969	1.48882131	-4.81111505	H	-2.31011356	2.30395224	2.05618516
C	-6.14620996	1.14871531	-3.79609246	H	-3.16574783	5.67379846	2.58148770
C	-5.74075033	1.24671779	-2.46612513	H	-1.55832207	1.77386684	-2.33191130
C	-3.06265520	-0.79546934	3.72122555	H	-1.62206203	2.74363341	-3.80972320
C	-2.30315648	-3.76248373	-0.63196223	H	-2.15368542	3.43722645	-2.27160279
C	-3.08003184	3.00170668	2.40829753				
C	-2.14793109	2.52221512	-2.87614972	T_1 optimization: unit Å			
H	-5.03714503	-5.78386378	3.01288401	Ag	2.15782399	0.10469055	-0.22141764
H	-3.88779112	7.33393655	0.8981701	Br	0.27584091	0.47073757	1.87193354
H	-4.95780569	-4.22545674	1.10566176	P	4.26019443	1.51151487	0.07685864
H	-4.66781507	6.56190505	-1.34453663	P	3.90169872	-1.77439724	-0.41746985
H	-3.44037792	-4.93735391	-2.75368338	C	4.37449894	3.09019385	-0.84955319
H	-4.69610854	4.15424132	-1.86527154	C	3.94460812	3.20137359	-2.19489569
H	-5.66430195	-4.55056732	-3.76051655	C	4.16357036	4.40836409	-2.86495286
H	-7.19195628	-2.84457557	-2.76646755	H	3.83084991	4.49743886	-3.89679870
H	-6.46658197	-1.55615963	-0.7988831	C	4.79669368	5.48999917	-2.25149746
H	-3.28312983	2.19820109	-5.28068273	H	4.95215855	6.41286053	-2.80405368
H	-6.47972038	-1.73119312	2.18780412	C	5.23287690	5.37282964	-0.93394787
H	-5.55692538	1.41707437	-5.85331676	H	5.73730904	6.20040883	-0.44181657
H	-8.35931648	-0.22053572	2.68440810	C	5.01901236	4.18407552	-0.24121491

H	5.36004794	4.10183367	0.78690198	H	1.96429175	-4.03114634	3.61733755
C	4.46164324	1.98533415	1.84618688	C	3.99982567	-3.40944365	3.91832308
C	3.57214692	2.86285318	2.51435517	H	4.02853102	-3.76368460	4.94550272
C	3.77174539	3.08143874	3.88255011	C	5.11888220	-2.80351352	3.35150548
H	3.09186151	3.74978586	4.40659567	H	6.03373657	-2.68380299	3.92549599
C	4.80818038	2.47007576	4.58576613	C	5.05560231	-2.34506755	2.03859418
H	4.92874667	2.66375227	5.64858745	H	5.92190152	-1.87048511	1.58618359
C	5.67906864	1.60833519	3.92263355	C	3.28736697	2.06531992	-2.92452450
H	6.49238486	1.12419261	4.45662684	H	3.90695201	1.16257422	-2.88435137
C	5.49484188	1.36367142	2.56469606	H	3.12703480	2.31747465	-3.97737597
H	6.16378558	0.68727945	2.04083849	H	2.31062627	1.80629059	-2.49530371
C	5.60866118	0.46580585	-0.42594322	C	2.45377446	3.59478297	1.82118386
C	6.90193328	1.02802831	-0.62625745	H	1.91858398	2.95548088	1.11184342
H	7.05562366	2.08076861	-0.39596033	H	2.83109886	4.46147261	1.26470526
C	7.95341001	0.29316287	-1.12580183	H	1.72404754	3.95709207	2.55150057
H	8.92146502	0.76544647	-1.27216342	C	3.41386864	-1.59240326	-3.56113560
C	7.76390947	-1.08335333	-1.47492278	H	2.65468210	-0.98321056	-3.05709296
H	8.58190759	-1.66157945	-1.89562780	H	3.14877181	-1.65059982	-4.62103058
C	6.52862345	-1.66696450	-1.28801548	H	4.37160902	-1.06476578	-3.47735921
H	6.38802317	-2.71287456	-1.55467808	C	1.46826546	-3.33867840	1.07958504
C	5.42753551	-0.94626865	-0.75714920	H	0.64053258	-3.54084896	1.76529568
C	3.72195765	-3.17329899	-1.57371887	H	1.55828630	-4.19649677	0.40162182
C	3.50669946	-2.96427201	-2.95815174	H	1.18667546	-2.47408886	0.46831912
C	3.40763135	-4.08653467	-3.78650534	Ag	-1.92869346	0.10293500	0.14999862
H	3.23737887	-3.93458734	-4.84974541	Br	0.01383634	-0.41121142	-1.91445538
C	3.52374267	-5.38324491	-3.28800576	P	-3.93791357	-1.54422720	0.49517083
H	3.44067647	-6.23168781	-3.96216316	P	-3.88364845	1.79478319	-0.17604953
C	3.75340353	-5.58367232	-1.92882658	C	-4.06675857	-2.86313347	1.78047702
H	3.86082555	-6.58740361	-1.52677552	C	-3.62709269	-2.60467274	3.10061438
C	3.84727174	-4.48442027	-1.08033826	C	-3.69464905	-3.64187447	4.03800416
H	4.03457458	-4.64482827	-0.02296861	C	-4.17751594	-4.90549176	3.70315393
C	3.88741969	-2.49837592	1.27547371	C	-4.61412792	-5.15394895	2.40473599
C	2.74509136	-3.11194957	1.84382220	C	-4.55796280	-4.13591975	1.45432737
C	2.83428239	-3.55803861	3.16722998	C	-4.45954151	-2.37816963	-1.06225073

C	-3.56165833	-3.25657579	-1.71727521	H	-7.06212196	-2.48122671	-3.27304309
C	-3.96252712	-3.83101230	-2.92901779	H	-6.40906389	-1.45577921	-1.13394878
C	-5.20546056	-3.55888914	-3.49757518	H	-3.10543359	2.98447625	-4.93512791
C	-6.08662111	-2.70025241	-2.84703524	H	-6.49279884	-2.02758849	1.78565458
C	-5.71207284	-2.11835914	-1.63696942	H	-5.33446053	2.24591938	-5.70505828
C	-5.35213113	-0.42374907	0.91091370	H	-8.41362197	-0.62224592	2.42134025
C	-6.47413719	-0.96559611	1.55823923	H	-6.97597476	1.34125698	-4.05615862
C	-7.56037811	-0.17366569	1.91973709	H	-8.38281523	1.82214570	1.91064965
C	-7.54307296	1.18990637	1.63502476	H	-6.35566970	1.18671000	-1.67668823
C	-6.43884382	1.74541635	0.99466543	H	-6.43066623	2.81068298	0.78197876
C	-5.33320458	0.96305615	0.62355860	H	-3.91536952	-0.50025839	3.49480176
C	-3.97641813	3.51051693	0.49944935	H	-2.74352554	-1.29063585	4.55744369
C	-3.56033696	3.76995188	1.82693117	H	-2.30726343	-0.89891463	2.88625874
C	-3.60846196	5.08936291	2.29108226	H	-4.21238444	-5.68947819	4.45525560
C	-4.04737858	6.13765634	1.48424683	H	-1.60431525	-2.71733794	-0.96942309
C	-4.45859857	5.87724335	0.18001127	H	-2.31170082	-4.13574309	-0.18638129
C	-4.42267141	4.57037227	-0.30335177	H	-1.66399558	-4.26122967	-1.82895991
C	-4.36964406	1.98096528	-1.94269761	H	-3.35759435	-3.44840007	5.05403763
C	-3.43458409	2.49882936	-2.87262076	H	-2.77623120	3.09587580	3.71331060
C	-3.81660341	2.58392005	-4.21622292	H	-3.89595457	1.95683018	2.95471311
C	-5.07400079	2.16995263	-4.65252155	H	-2.25166412	2.11814553	2.33340254
C	-5.98951460	1.66427972	-3.73434957	H	-3.29091710	5.29448267	3.31108381
C	-5.63470051	1.57454592	-2.38923759	H	-1.52018867	3.36367999	-3.32963904
C	-3.12055000	-1.25546646	3.53095940	H	-2.11238995	3.76577681	-1.71192132
C	-2.21618777	-3.61050135	-1.14444454	H	-1.46922463	2.15158949	-2.04270609
C	-3.09603032	2.67964982	2.75322352				
C	-2.06453757	2.97072837	-2.46553845	**Table S7** Geometry data of **2** (S_0 in CH_2Cl_2, S_0, S_1, and T_1)			
H	-4.99865561	-6.13189916	2.12729813	S_0 optimization in CH_2Cl_2: unit Å			
H	-4.06774377	7.15140903	1.87587112	Ag	-0.299609	-0.078970	0.056479
H	-4.90086054	-4.33588615	0.44311195	Br	-0.013009	0.377841	2.641733
H	-4.80841511	6.68165193	-0.46166972	P	1.168780	-0.013031	-2.087232
H	-3.27787798	-4.50770096	-3.43542635	P	-2.064647	-0.879589	-1.638718
H	-4.74771917	4.37212031	-1.32065651	C	2.395787	1.284941	-2.542471
H	-5.48158953	-4.01872765	-4.44295124	C	2.130298	2.647722	-2.260933

C	3.113025	3.591318	-2.598297	C	-2.635978	-2.857629	0.723990
C	4.319750	3.219918	-3.202593	C	-2.898648	-3.798864	1.896332
C	4.570783	1.881296	-3.482959	H	2.937266	4.640785	-2.384886
C	3.610619	0.921298	-3.149229	H	5.056503	3.980651	-3.448397
C	2.060110	-1.606685	-2.340372	H	5.500566	1.577689	-3.956902
C	2.934605	-2.102411	-1.341307	H	3.807236	-0.123992	-3.369561
C	3.523735	-3.360425	-1.543087	H	4.194373	-3.748605	-0.778818
C	3.268140	-4.124118	-2.681964	H	3.737335	-5.097607	-2.800105
C	2.400691	-3.634023	-3.659074	H	2.187403	-4.215334	-4.552237
C	1.800706	-2.388130	-3.481447	H	1.126286	-2.015127	-4.245864
C	-0.071128	0.068626	-3.459286	H	1.369584	0.826539	-4.873115
C	0.331713	0.545269	-4.718474	H	-0.230646	1.048243	-6.734712
C	-0.572202	0.674178	-5.773228	H	-2.626005	0.423534	-6.394750
C	-1.909612	0.325855	-5.583472	H	-3.372152	-0.415583	-4.199073
C	-2.328337	-0.149628	-4.341371	H	-6.042793	2.107115	-1.059020
C	-1.431133	-0.289617	-3.268663	H	-7.686231	0.305061	-1.460834
C	-3.859516	-0.449083	-1.643475	H	-6.885585	-2.005812	-2.011576
C	-4.308419	0.872139	-1.353408	H	-4.466637	-2.468669	-2.114198
C	-5.693152	1.103645	-1.295112	H	-2.345765	-5.519790	0.151806
C	-6.622346	0.090102	-1.523090	H	-1.801175	-6.599710	-1.991669
C	-6.175643	-1.204029	-1.825203	H	-1.421369	-5.206417	-4.026582
C	-4.806392	-1.462443	-1.884481	H	-1.570196	-2.747800	-3.864043
C	-2.033637	-2.718038	-1.755330	H	0.714645	2.511701	-0.669400
C	-2.263904	-3.502384	-0.596464	H	-0.005737	2.741675	-2.246009
C	-2.172113	-4.897776	-0.720371	H	0.701214	5.161894	-2.233441
C	-1.866323	-5.515819	-1.938037	H	1.435196	4.927644	-0.634365
C	-1.652764	-4.741404	-3.071913	H	-0.308325	4.737072	-0.845669
C	-1.736495	-3.348569	-2.975350	H	3.160764	-2.018318	0.777349
C	0.828530	3.070182	-1.610198	H	2.620768	-0.505753	0.081798
C	0.662907	4.559308	-1.318892	H	4.911145	-0.098532	-0.866901
C	3.301635	-1.348298	-0.081065	H	5.461208	-1.653759	-0.220212
C	4.747520	-0.835138	-0.073796	H	4.974991	-0.358034	0.885921
C	-3.394286	2.054980	-1.122193	H	-2.380324	1.716588	-0.881920
C	-3.342201	3.010195	-2.321778	H	-3.747868	2.606773	-0.241742

H	-4.338485	3.401411	-2.556985
H	-2.960302	2.505231	-3.214928
H	-2.688855	3.862627	-2.106002
H	-3.525870	-2.231433	0.570663
H	-1.839255	-2.154664	1.010939
H	-3.161680	-3.213807	2.783567
H	-2.015076	-4.397227	2.145434
H	-3.729226	-4.484410	1.692609

S_0 optimization: unit Å

Ag	-0.01419800	-0.87833800	-1.24387000
Br	-0.05907300	-2.22539700	-3.36801300
P	1.67138600	0.21800300	0.39690200
P	-1.65278100	0.05391100	0.51949800
C	3.34161100	-0.47493400	0.75516400
C	3.53949500	-1.87964600	0.76956600
C	4.83278000	-2.35498300	1.00811600
C	5.90903500	-1.49399900	1.21740000
C	5.71080800	-0.11847900	1.19215900
C	4.43132600	0.38278100	0.96117100
C	1.96155100	2.02651700	0.18525600
C	2.17001000	2.58350000	-1.09858300
C	2.37401300	3.96805600	-1.18829400
C	2.38616800	4.79009000	-0.06720300
C	2.18562800	4.23558700	1.19476600
C	1.97139800	2.86631800	1.31135100
C	0.77773300	0.08349200	2.01157200
C	1.50656900	-0.03355800	3.20421200
C	0.86935600	-0.17149100	4.43493800
C	-0.52127000	-0.19652300	4.49082200
C	-1.26285900	-0.09160800	3.31651100
C	-0.64067400	0.04639200	2.06690500
C	-3.29464900	-0.62497800	1.02183600
C	-3.63073000	-1.98313300	0.81310100
C	-4.91136300	-2.40818500	1.19522900
C	-5.84165100	-1.54291900	1.76078400
C	-5.50953000	-0.20354700	1.95278200
C	-4.24720900	0.24574200	1.57902100
C	-2.01809600	1.82293800	0.17678900
C	-2.66444400	2.17449100	-1.03646900
C	-2.90423600	3.53068100	-1.27679200
C	-2.52312700	4.51951900	-0.37037900
C	-1.88666400	4.16702300	0.81383100
C	-1.63860800	2.82193700	1.08123400
C	2.39089300	-2.83722500	0.53069200
C	2.72113300	-4.32601300	0.58609100
C	2.23054200	1.78193500	-2.37833200
C	3.65412100	1.35368300	-2.75751900
C	-2.69359200	-3.00613800	0.21542700
C	-1.76615600	-3.65703800	1.24845100
C	-3.09782700	1.11609000	-2.02989400
C	-3.70012000	1.61423500	-3.34046000
H	5.00809900	-3.42594100	1.02494800
H	6.90024000	-1.90378000	1.39509700
H	6.54066200	0.56558100	1.34952200
H	4.27954700	1.45769100	0.93754300
H	2.52500200	4.40449800	-2.17362500
H	2.54637800	5.85952000	-0.17967200
H	2.19049600	4.86216200	2.08304300
H	1.80707300	2.43932700	2.29645800
H	2.59249300	-0.02431500	3.16309100
H	1.46017500	-0.26253900	5.34279200
H	-1.03302000	-0.30668500	5.44345700
H	-2.34669000	-0.13223500	3.36858000
H	-5.18057600	-3.44939200	1.02983700
H	-6.82633200	-1.91081600	2.03829100
H	-6.22772100	0.48993700	2.38260200
H	-3.99633700	1.29497900	1.71033300

H	-3.39896600	3.82490500	-2.19715600
H	-2.72468000	5.56377200	-0.59613200
H	-1.58000200	4.92711500	1.52725200
H	-1.13972100	2.54661800	2.00561400
H	1.95303900	-2.61563100	-0.45489600
H	1.59541100	-2.62663000	1.25940000
H	3.10873400	-4.62549900	1.56701700
H	3.45747300	-4.60585400	-0.17545100
H	1.81604500	-4.91025400	0.39249600
H	1.81219200	2.39078000	-3.18940400
H	1.59804100	0.88893900	-2.31380900
H	4.09741000	0.71515900	-1.98645900
H	4.30714900	2.22468500	-2.88841500
H	3.64115400	0.78873900	-3.69561900
H	-2.09279600	-2.56042800	-0.58627600
H	-3.29601800	-3.78849700	-0.26183400
H	-2.34061400	-4.15511700	2.03834900
H	-1.11668000	-2.91646500	1.72830400
H	-1.12784500	-4.40489800	0.76551200
H	-3.82088500	0.44770300	-1.54104100
H	-2.23532100	0.47540000	-2.26715500
H	-3.93973900	0.75905800	-3.98017000
H	-2.99947200	2.25100800	-3.89256000
H	-4.62579300	2.17979500	-3.18101000

S_1 optimization: unit Å

Ag	0.02625200	-0.24748900	1.26502600
Br	-0.45868800	-0.60699900	3.75219600
P	-1.57719200	0.10184100	-0.64600600
P	1.74509700	-0.06387000	-0.52710700
C	-3.16427700	-0.81281500	-0.66945600
C	-3.27038200	-2.16516900	-0.25946200
C	-4.51684800	-2.78641700	-0.36563300
C	-5.63528700	-2.11704100	-0.86265600
C	-5.52513600	-0.79201200	-1.26810300
C	-4.29608300	-0.14451200	-1.16442800
C	-2.03925000	1.88659000	-0.72148400
C	-2.65777600	2.55801500	0.35323600
C	-2.84961300	3.94081400	0.24055800
C	-2.46388100	4.64848600	-0.89404400
C	-1.85792900	3.97875600	-1.95518800
C	-1.63589700	2.60896800	-1.86155700
C	-0.61280600	-0.35663900	-2.07724300
C	-1.24106100	-0.50626200	-3.33571300
C	-0.52857500	-0.74603300	-4.49392600
C	0.89981300	-0.82652500	-4.43992600
C	1.54867800	-0.65357700	-3.23496700
C	0.85102100	-0.41941600	-2.02311700
C	3.20240200	-1.17721300	-0.40947300
C	3.07157400	-2.56419400	-0.17171500
C	4.23692800	-3.33275400	-0.07319700
C	5.50398700	-2.77636300	-0.22242300
C	5.62801900	-1.41415400	-0.48158000
C	4.48565500	-0.62434900	-0.56847100
C	2.44577400	1.64568000	-0.58200700
C	2.99982300	2.27616500	0.56239400
C	3.42249900	3.60275500	0.43362000
C	3.30841900	4.29972000	-0.76919900
C	2.75392500	3.67798600	-1.88237700
C	2.31560200	2.35987600	-1.77976400
C	-2.06650800	-2.90970200	0.26707500
C	-2.27010800	-4.38048200	0.61772000
C	-3.11135500	1.87103400	1.62409700
C	-4.62367600	1.94890500	1.86359800
C	1.74528800	-3.27597500	-0.06395100
C	1.40541100	-4.07619400	-1.32189500
C	3.13327200	1.54169200	1.88106400
C	3.78327500	2.30836200	3.02927000

H	-4.62052000	-3.82071100	-0.05323400
H	-6.58790600	-2.63608000	-0.93156000
H	-6.38546200	-0.25859100	-1.66387500
H	-4.21315400	0.89116900	-1.47775800
H	-3.30950400	4.41401200	1.01018100
H	-2.62790000	5.72208100	-0.94409800
H	-1.54836200	4.51929800	-2.84514400
H	-1.14503700	2.08179400	-2.61449100
H	-2.32803800	-0.46551200	-3.38375000
H	-1.05271600	-0.90656300	-5.43132800
H	1.47073700	-1.04567900	-5.33760900
H	2.63489700	-0.72816000	-3.20326800
H	4.13983000	-4.39814200	0.12688400
H	6.38721600	-3.40435300	-0.13822000
H	6.60181900	-0.96218800	-0.61261800
H	4.58942500	0.43832100	-0.16586800
H	3.85172500	4.10871100	1.29288600
H	3.64903300	5.33058500	-0.82781900
H	2.65576700	4.21131700	-2.82430500
H	1.86537300	1.87041000	-2.63858500
H	-1.69715800	-2.38732600	1.16277300
H	-1.26723700	-2.82532800	-0.48288300
H	-2.59450100	-4.96602400	-0.25024000
H	-3.01074800	-4.50893500	1.41494300
H	-1.32911700	-4.80977000	0.91681200
H	-2.58901700	2.32885800	2.41514500
H	-2.80977800	0.81923900	1.62826000
H	-5.17585400	1.44932400	1.06099500
H	-4.97323100	2.98596300	1.91933900
H	-4.88142100	1.45776600	2.80825800
H	0.94173900	-2.55730300	0.13479500
H	1.77329100	-3.95043900	0.80205300
H	2.18451600	-4.81574800	-1.54488300
H	1.31161200	-3.41498100	-2.19456100
H	0.45901000	-4.61407900	-1.20314200
H	3.69466400	0.61243500	1.71667000
H	2.13377000	1.21619500	2.20795000
H	3.82202500	1.67235100	3.91941300
H	3.21626000	3.20808400	3.29369100
H	4.81011400	2.60866200	2.78993500

T_1 optimization: unit Å

Ag	0.00369900	-0.30374300	1.24796100
Br	0.43051100	-0.79264200	3.65763400
P	-1.63711800	0.05698400	-0.58493800
P	1.63127100	-0.00747700	-0.68390200
C	-3.21529200	-0.85492400	-0.47388500
C	-3.27629100	-2.21209000	-0.06289000
C	-4.52122700	-2.84361900	-0.07683400
C	-5.68162800	-2.18316100	-0.48418500
C	-5.61615700	-0.85486000	-0.89047600
C	-4.38966300	-0.19565300	-0.87815900
C	-2.10655200	1.84264400	-0.60647300
C	-2.58526100	2.51685200	0.53964800
C	-2.83380100	3.89130100	0.43361400
C	-2.63665000	4.58602200	-0.75610400
C	-2.16989400	3.91190500	-1.88281100
C	-1.89522000	2.55091300	-1.79916300
C	-0.78215300	-0.39023500	-2.07393500
C	-1.48758200	-0.71746800	-3.25869600
C	-0.83858000	-1.08354900	-4.41924600
C	0.59055000	-1.15330600	-4.44277200
C	1.31265800	-0.85159000	-3.31090500
C	0.67975500	-0.45874400	-2.09749600
C	3.17874500	-0.97190100	-0.62558800
C	3.20014100	-2.35027400	-0.30924100
C	4.43841400	-3.00236000	-0.29508500
C	5.62574600	-2.34238300	-0.59943900

C	5.59723400	-0.98919900	-0.92948200
C	4.38381100	-0.31076200	-0.93290300
C	2.13352600	1.76633700	-0.70739300
C	2.72554300	2.42679600	0.40098200
C	2.98505400	3.79466100	0.27111400
C	2.68100200	4.49811100	-0.89473700
C	2.09614900	3.84239900	-1.97301200
C	1.81380200	2.48330100	-1.86940600
C	-2.03089300	-2.94908400	0.37407000
C	-2.19601500	-4.42529200	0.72341000
C	-2.84595000	1.84384000	1.87045000
C	-4.32563400	1.82563200	2.27177600
C	1.96734200	-3.17212800	-0.02087600
C	1.56743300	-4.06422300	-1.20293800
C	3.08855600	1.68216700	1.66820200
C	3.55637200	2.53033700	2.84736100
H	-4.59190500	-3.87998500	0.23786700
H	-6.63138000	-2.71187000	-0.48272500
H	-6.51020400	-0.32852800	-1.21464100
H	-4.34104900	0.84345700	-1.19009400
H	-3.18729400	4.42727900	1.31239800
H	-2.84004900	5.65315000	-0.79966900
H	-2.01088000	4.44241700	-2.81799500
H	-1.51154300	2.01765700	-2.66502000
H	-2.57582600	-0.69510200	-3.24126600
H	-1.41342300	-1.34081800	-5.30432500
H	1.10666000	-1.46726700	-5.34590500
H	2.39833800	-0.92747900	-3.33384300
H	4.46456200	-4.05843700	-0.03412800
H	6.56833000	-2.88329700	-0.57736500
H	6.51345800	-0.46039400	-1.17855500
H	4.36492700	0.74613300	-1.18200100
H	3.43677500	4.32848100	1.10148100
H	2.89951900	5.56165700	-0.95224500
H	1.85429300	4.38075000	-2.88554300
H	1.34396100	1.95835400	-2.69702100
H	-1.60845500	-2.43356700	1.25157200
H	-1.27912800	-2.84916200	-0.42201600
H	-2.56956100	-5.00645500	-0.12758700
H	-2.88142600	-4.56986600	1.56601300
H	-1.22882700	-4.84602900	1.01691200
H	-2.26859400	2.36439400	2.64638000
H	-2.47224900	0.81369500	1.86676800
H	-4.92370100	1.26576300	1.54554400
H	-4.73718100	2.83916400	2.33884700
H	-4.44604100	1.34873900	3.25065800
H	1.12563100	-2.52342700	0.24754600
H	2.15941300	-3.79437500	0.86265000
H	2.38358600	-4.74186000	-1.47864600
H	1.31513700	-3.46163000	-2.08118200
H	0.69639800	-4.67711000	-0.94570300
H	3.86629100	0.94271800	1.43187700
H	2.22624800	1.08629400	2.00002600
H	3.72884900	1.88428100	3.71372300
H	2.80366500	3.27301700	3.13540700
H	4.49430200	3.05652300	2.63408200

Table S8 Geometry data of **3** (S_0 in CH_2Cl_2, S_0, S_1, and T_1)

S_0 optimization in CH_2Cl_2: unit Å

Ag	-0.071214	-0.047293	0.110328
Br	0.208721	-0.329779	2.731119
P	1.473113	-0.011071	-1.981557
P	-1.896189	0.177546	-1.698552
C	3.025277	-0.983556	-2.242642
C	3.154596	-2.306901	-1.761749
C	4.380832	-2.960138	-1.950031
C	5.453059	-2.350815	-2.594086

C	5.317772	-1.050660	-3.075228	C	-2.559524	-4.072839	-1.483843
C	4.112268	-0.378127	-2.896619	C	-3.041867	2.406815	0.300431
C	1.945592	1.697173	-2.498856	C	-2.154470	3.121731	1.328007
C	2.644200	2.547924	-1.609416	C	-4.529316	2.615464	0.621110
C	2.957796	3.841964	-2.047226	H	4.497106	-3.976866	-1.582932
C	2.609560	4.298310	-3.315189	H	6.387839	-2.890886	-2.720568
C	1.930763	3.453046	-4.189555	H	6.141524	-0.559349	-3.586219
C	1.604566	2.163612	-3.778672	H	4.014729	0.635501	-3.272299
C	0.340292	-0.610153	-3.315354	H	3.494235	4.508941	-1.376740
C	0.889120	-1.209205	-4.459960	H	2.871760	5.308661	-3.618470
C	0.082939	-1.709563	-5.479388	H	1.656026	3.790514	-5.185314
C	-1.302139	-1.619968	-5.368303	H	1.080821	1.508114	-4.467121
C	-1.866328	-1.033644	-4.238027	H	1.968546	-1.287031	-4.552363
C	-1.071380	-0.522252	-3.200207	H	0.538531	-2.167612	-6.353090
C	-3.577060	-0.593871	-1.717604	H	-1.945275	-2.006681	-6.154143
C	-3.798164	-1.892188	-1.203767	H	-2.947750	-0.975507	-4.157066
C	-5.109914	-2.387702	-1.207532	H	-5.297804	-3.382504	-0.811143
C	-6.178648	-1.649287	-1.705723	H	-7.181146	-2.069147	-1.691928
C	-5.953742	-0.375416	-2.222788	H	-6.774455	0.214149	-2.622625
C	-4.661940	0.142677	-2.223813	H	-4.493593	1.137313	-2.624886
C	-2.224790	1.945895	-2.110647	H	-3.269471	4.873565	-0.732646
C	-2.705741	2.835576	-1.120369	H	-2.804156	5.689251	-3.006336
C	-2.900003	4.175944	-1.480285	H	-1.974804	4.103910	-4.748819
C	-2.640425	4.641886	-2.766117	H	-1.618249	1.737872	-4.170732
C	-2.177178	3.759159	-3.738384	H	1.154932	-2.403463	-1.018874
C	-1.973868	2.422223	-3.407087	H	3.266016	-4.102644	0.408382
C	2.032422	-3.061402	-1.067697	H	1.566987	-3.922595	0.872879
C	2.406505	-3.422701	0.376400	H	2.659043	-2.528394	0.955865
C	1.620496	-4.307670	-1.864438	H	0.781072	-4.811583	-1.372451
C	3.087379	2.122317	-0.217844	H	2.444015	-5.027958	-1.934377
C	2.433792	2.987624	0.867742	H	1.313050	-4.046492	-2.882916
C	4.616754	2.128888	-0.078779	H	2.753641	1.090453	-0.050356
C	-2.689982	-2.781332	-0.663791	H	2.763244	4.031317	0.801024
C	-2.890099	-3.086075	0.827225	H	2.699687	2.612981	1.862458

H	1.342165	2.972730	0.781894
H	4.904911	1.764913	0.914280
H	5.025143	3.139867	-0.194830
H	5.088891	1.483949	-0.827291
H	-1.739332	-2.240701	-0.758330
H	-2.939171	-2.164411	1.417033
H	-2.056985	-3.688075	1.207630
H	-3.815024	-3.649169	0.999152
H	-2.375350	-3.856424	-2.541836
H	-3.467560	-4.683400	-1.416987
H	-1.726245	-4.677208	-1.108329
H	-2.841446	1.332131	0.394221
H	-2.376276	2.759404	2.338096
H	-2.320184	4.205517	1.315262
H	-1.092915	2.939489	1.130378
H	-4.800996	3.677254	0.590376
H	-4.751658	2.243913	1.628169
H	-5.169867	2.080448	-0.087736

S_0 optimization: unit Å

Ag	-0.00052100	-0.32092500	1.33610700
Br	0.02505200	-0.86363100	3.79441100
P	1.68917700	0.04891300	-0.59335900
P	-1.66932500	0.06680400	-0.60327100
C	3.29427200	-0.83982900	-0.81652000
C	3.42648000	-2.20449900	-0.47199500
C	4.69021600	-2.79592300	-0.60465400
C	5.79406000	-2.08868800	-1.06854700
C	5.65544800	-0.74828100	-1.41923500
C	4.41353100	-0.13414200	-1.28983800
C	2.13956200	1.82245400	-0.81897900
C	2.72241300	2.54961600	0.24614400
C	3.02050800	3.90133100	0.02887600
C	2.76071100	4.53172400	-1.18378600
C	2.18795500	3.80976400	-2.22721400
C	1.88326000	2.46507600	-2.04023800
C	0.72172200	-0.39849200	-2.10529300
C	1.40058900	-0.81877300	-3.25943000
C	0.71383400	-1.22365000	-4.40091100
C	-0.67857900	-1.21956300	-4.40482800
C	-1.37051700	-0.80981900	-3.26816300
C	-0.69705000	-0.39295300	-2.10954100
C	-3.29867100	-0.77052100	-0.85399300
C	-3.50946500	-2.10706300	-0.44526000
C	-4.78922000	-2.65286000	-0.61985900
C	-5.83294900	-1.92885500	-1.18503500
C	-5.61734500	-0.61558000	-1.59543000
C	-4.35955700	-0.04600400	-1.42511300
C	-2.06884000	1.85383800	-0.81629100
C	-2.66697300	2.57915200	0.24160200
C	-2.92227500	3.94150200	0.03759000
C	-2.60588900	4.58398500	-1.15529200
C	-2.01861100	3.86370700	-2.19162500
C	-1.75592700	2.50830400	-2.01774400
C	2.27261100	-3.06244400	0.02119200
C	2.49372200	-3.53244200	1.46531000
C	2.01474800	-4.24540100	-0.92339500
C	3.05378300	1.93818600	1.59970000
C	2.28715200	2.63118700	2.73410800
C	4.56523500	1.94572200	1.87156600
C	-2.42815300	-2.98272200	0.16694500
C	-2.76211700	-3.35895500	1.61703100
C	-2.16381100	-4.22865500	-0.69017800
C	-3.06312800	1.95290300	1.57090300
C	-2.33438700	2.61203000	2.74944400
C	-4.58467500	1.98314900	1.77747200
H	4.81101500	-3.84249500	-0.33580200
H	6.75786200	-2.58407900	-1.15595300

H	6.50549500	-0.18036700	-1.78855600	H	-1.94810400	-3.94782500	2.05357100
H	4.31114300	0.91344400	-1.55654200	H	-3.68083300	-3.95559400	1.67406100
H	3.47052800	4.47425800	0.83595100	H	-1.87971000	-3.95872200	-1.71340500
H	3.00660000	5.58299600	-1.31182000	H	-3.04765400	-4.87519900	-0.74570400
H	1.97940300	4.28590800	-3.18176000	H	-1.35155500	-4.82065800	-0.25374700
H	1.44172400	1.90365800	-2.85788900	H	-2.75986800	0.89826500	1.56297400
H	2.48695000	-0.83549800	-3.25698500	H	-2.57358600	2.08901500	3.68118600
H	1.26735800	-1.54507500	-5.27951200	H	-2.62317100	3.66402400	2.86446200
H	-1.22877600	-1.53837900	-5.28646500	H	-1.24872000	2.56877200	2.61951200
H	-2.45670100	-0.82023400	-3.27446500	H	-4.95968000	3.01223900	1.83613700
H	-4.97034900	-3.67685800	-0.30254000	H	-4.84559600	1.47957900	2.71537200
H	-6.81074400	-2.38923400	-1.30122300	H	-5.11088500	1.47650700	0.96170800
H	-6.42037900	-0.03444900	-2.04147900				
H	-4.19796600	0.98224800	-1.73521100	S_1 optimization: unit Å			
H	-3.38405800	4.51334700	0.83876300	Ag	-0.00827500	-0.29242100	-1.13368900
H	-2.81938900	5.64344500	-1.27343100	Br	0.47283800	-0.92978400	-3.56451700
H	-1.76600800	4.34934500	-3.13056800	P	-1.66896900	0.13539100	0.66750500
H	-1.30343400	1.94793600	-2.83009100	P	1.65918500	0.06220900	0.73318400
H	1.36315000	-2.44704100	0.02117200	C	-3.31279000	-0.69149600	0.71892000
H	3.39288500	-4.15487100	1.54943200	C	-3.55297000	-2.00678900	0.26260900
H	1.63901600	-4.12746300	1.80591100	C	-4.85582200	-2.50998900	0.36745300
H	2.59437200	-2.68384000	2.14902000	C	-5.89563900	-1.77142900	0.92447200
H	1.14552300	-4.81924400	-0.58335000	C	-5.64921400	-0.48508900	1.39448000
H	2.86993500	-4.93095300	-0.95280900	C	-4.36971000	0.04949600	1.28091600
H	1.82015800	-3.90568200	-1.94666700	C	-2.07893100	1.94366400	0.68192600
H	2.73320300	0.88874900	1.59662300	C	-2.66530700	2.60196200	-0.42380700
H	2.59498800	3.67811100	2.84630600	C	-2.86811600	3.98422900	-0.32911700
H	2.47004200	2.11701800	3.68322700	C	-2.50708900	4.70703000	0.80504000
H	1.20804000	2.61182800	2.55281800	C	-1.92207900	4.05231700	1.88560200
H	4.77535600	1.45312800	2.82781300	C	-1.70540300	2.67931700	1.81630800
H	4.95717400	2.96853600	1.93040700	C	-0.77708800	-0.28019300	2.16127000
H	5.11717000	1.41550600	1.08834300	C	-1.46245000	-0.45388100	3.38264300
H	-1.49408600	-2.40647000	0.19500700	C	-0.80402200	-0.64915400	4.58264900
H	-2.89000800	-2.46792200	2.23927400	C	0.62666800	-0.65241900	4.60663300

C	1.33144400	-0.46683700	3.43677300	H	-2.55082100	-0.45969300	3.37237100
C	0.68826400	-0.29227800	2.18293500	H	-1.37012200	-0.82591100	5.49218300
C	3.14277500	-1.02172500	0.72888200	H	1.15876700	-0.83242100	5.53652800
C	3.06094900	-2.42274600	0.55366400	H	2.41984900	-0.49377500	3.46481300
C	4.24872800	-3.16138500	0.60619100	H	4.20099700	-4.23890700	0.47078000
C	5.48558800	-2.56436900	0.83200100	H	6.38456900	-3.17455900	0.86589800
C	5.55858400	-1.18788100	1.02240300	H	6.51213200	-0.70350900	1.21599700
C	4.39539400	-0.42690100	0.96748300	H	4.45873200	0.64451500	1.12440900
C	2.32662900	1.78749200	0.80064800	H	3.86741700	4.24734700	-0.96589800
C	2.96094200	2.41792500	-0.29624200	H	3.52644200	5.47027900	1.14123100
C	3.37876700	3.74519700	-0.13437600	H	2.38156400	4.35107300	3.05758000
C	3.18560300	4.44144000	1.05494200	H	1.59967100	2.01815500	2.81309500
C	2.54616000	3.81875900	2.12441200	H	-1.51439200	-2.38923600	-0.21487600
C	2.11082400	2.50516100	1.98816200	H	-3.65607300	-3.59744900	-2.04646900
C	-2.48146600	-2.89316600	-0.34696000	H	-1.90059300	-3.67257100	-2.29593200
C	-2.70869200	-3.07956700	-1.85370500	H	-2.73652500	-2.11772500	-2.37610700
C	-2.38051400	-4.24447600	0.37269700	H	-1.55592500	-4.83339400	-0.04439100
C	-3.08657500	1.88309800	-1.69780500	H	-3.29496300	-4.83664800	0.25215800
C	-2.31767100	2.40276300	-2.92068100	H	-2.20227600	-4.11166400	1.44489800
C	-4.60249200	1.97001000	-1.92507600	H	-2.83990300	0.81892100	-1.59042000
C	1.75309700	-3.16851600	0.35884700	H	-2.54693400	3.45638100	-3.12004700
C	1.74625000	-3.99206800	-0.93568300	H	-2.58551400	1.82588900	-3.81288700
C	1.44204300	-4.03657000	1.58685500	H	-1.23503000	2.31519300	-2.78167600
C	3.18297200	1.74144400	-1.64071400	H	-4.88389800	1.40451200	-2.82112400
C	2.36850500	2.43862400	-2.74045900	H	-4.92496800	3.00775600	-2.07237500
C	4.66706000	1.67359700	-2.02715400	H	-5.15746700	1.55938200	-1.07558700
H	-5.06104800	-3.51350600	0.00343200	H	0.94719200	-2.42562400	0.28128300
H	-6.89139900	-2.20230700	0.99168200	H	1.92949100	-3.36324700	-1.81265100
H	-6.44441500	0.10537000	1.84214800	H	0.77345900	-4.47918900	-1.06853200
H	-4.18626200	1.05963200	1.63377200	H	2.50673200	-4.78136600	-0.91461600
H	-3.32213800	4.50936300	-1.16627100	H	1.38553700	-3.42780200	2.49450000
H	-2.67964800	5.77993200	0.83995600	H	2.21298000	-4.80259800	1.73459100
H	-1.63175200	4.60390200	2.77593900	H	0.48238800	-4.54913500	1.45943200
H	-1.24676800	2.15936900	2.65255200	H	2.82245600	0.70758500	-1 57437000

H	2.45130600	1.88904300	-3.68366800
H	2.72330500	3.46313800	-2.90618800
H	1.30666000	2.49098800	-2.47188600
H	5.09841100	2.67446700	-2.14925700
H	4.78048100	1.14523000	-2.98062800
H	5.25538500	1.13942500	-1.27445400

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Ag	-0.03246700	-0.25501800	-1.14826900
Br	0.62151000	-0.76303300	-3.50386000
P	-1.66519400	0.07461500	0.69029800
P	1.62099300	0.04600100	0.78866400
C	-3.29314900	-0.77015800	0.65538600
C	-3.48962400	-2.07697900	0.15260600
C	-4.77996200	-2.61653500	0.21753700
C	-5.84904900	-1.92303800	0.77860800
C	-5.64607600	-0.64524800	1.29213900
C	-4.38048800	-0.07269200	1.21840300
C	-2.08899300	1.87691700	0.73732700
C	-2.66751100	2.55872100	-0.35803400
C	-2.90368900	3.93210200	-0.21840100
C	-2.58324900	4.62181400	0.94809700
C	-2.00846500	3.94262800	2.01925700
C	-1.76012200	2.57821100	1.90660400
C	-0.79724200	-0.40459900	2.16402500
C	-1.49338100	-0.76755600	3.34224900
C	-0.83849100	-1.15560600	4.49337200
C	0.59102600	-1.20874300	4.51162800
C	1.30614500	-0.87086800	3.38639900
C	0.66553800	-0.45570300	2.18229100
C	3.17282600	-0.91560500	0.71862700
C	3.19703800	-2.30046400	0.42470800
C	4.43695800	-2.94980600	0.44355700
C	5.62045200	-2.28422000	0.75011700
C	5.58855500	-0.92619700	1.05591400
C	4.37434400	-0.25006100	1.03283400
C	2.14421600	1.81698000	0.90190800
C	2.72911300	2.54068900	-0.16343000
C	3.06650400	3.87996900	0.07143700
C	2.83749200	4.49666300	1.29825700
C	2.24704300	3.77914100	2.33663100
C	1.89462600	2.45021500	2.13096800
C	-2.38359100	-2.92053600	-0.45619700
C	-2.61656500	-3.15422400	-1.95537200
C	-2.20737400	-4.24628000	0.29630800
C	-3.05424800	1.87562100	-1.66252400
C	-2.29085600	2.45910100	-2.85933000
C	-4.56998500	1.92900700	-1.90152400
C	1.95468800	-3.12259000	0.12954700
C	2.03180300	-3.81203200	-1.23903100
C	1.69905800	-4.13073900	1.25997700
C	2.99339900	1.94746500	-1.53855000
C	2.18733700	2.68309400	-2.61954600
C	4.48717800	1.93895400	-1.89268400
H	-4.95137600	-3.61325800	-0.18143200
H	-6.83382300	-2.38191300	0.81472500
H	-6.46555100	-0.09066200	1.74199800
H	-4.23056100	0.93136600	1.60349300
H	-3.35239900	4.47667400	-1.04592000
H	-2.78124000	5.68869900	1.01647400
H	-1.75257200	4.46859100	2.93527400
H	-1.31159600	2.03529300	2.73442800
H	-2.58148500	-0.75603800	3.32938900
H	-1.40898100	-1.44329300	5.37178200
H	1.11383300	-1.53960700	5.40496900
H	2.39267300	-0.93382400	3.40546600
H	4.47466600	-4.01159000	0.21418800
H	6.56184800	-2.82775300	0.75513100

H	6.50020200	-0.39294500	1.31223900	H	-4.82699900	1.38699100	-2.81909600
H	4.35370500	0.80756700	1.27377500	H	-4.91851200	2.96240900	-2.01723100
H	3.52070900	4.45561000	-0.73149700	H	-5.12191400	1.47518400	-1.07237500
H	3.11509100	5.53840000	1.43926600	H	1.09305400	-2.44146400	0.10499200
H	2.06089300	4.24876500	3.29895100	H	2.14963300	-3.08319200	-2.04708500
H	1.43099700	1.87937200	2.93110800	H	1.10942100	-4.37343000	-1.42788700
H	-1.43999700	-2.36749800	-0.35069800	H	2.86431200	-4.52394800	-1.28646200
H	-3.53779800	-3.72363900	-2.12826300	H	1.57691500	-3.62348300	2.22240800
H	-1.78359500	-3.71823100	-2.38913600	H	2.52822200	-4.84288700	1.35028300
H	-2.69376000	-2.20792900	-2.50071600	H	0.78792900	-4.70463100	1.05922700
H	-1.37994100	-4.81867800	-0.13804900	H	2.65550400	0.90352800	-1.54149400
H	-3.10620800	-4.87048300	0.23083500	H	2.28687300	2.16870700	-3.57950500
H	-1.99033700	-4.07515500	1.35591100	H	2.53510900	3.71635000	-2.74031900
H	-2.77761500	0.81521700	-1.59171000	H	1.12237700	2.71431500	-2.36759400
H	-2.54217300	3.51427800	-3.02056300	H	4.89421300	2.95633100	-1.94265900
H	-2.54172200	1.90976200	-3.77348400	H	4.63383900	1.47297400	-2.87368600
H	-1.20783900	2.38713000	-2.71802600	H	5.07273700	1.37390400	-1.16066700