Supporting Information

Phosphorescent Dinuclear Copper(I) Complex Bridged by Bis(diphenylphosphino)methane and Lactate

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Contents

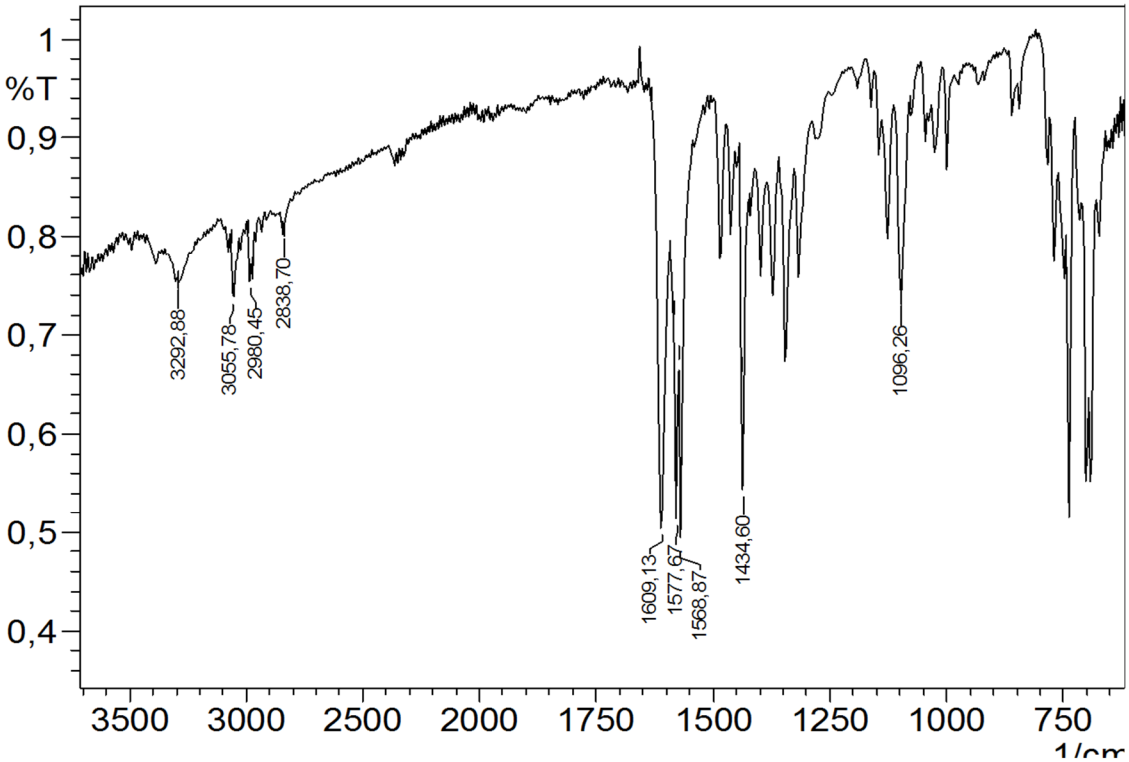


Figure S1. Infrared spectrum (ATR) of compound **1**.

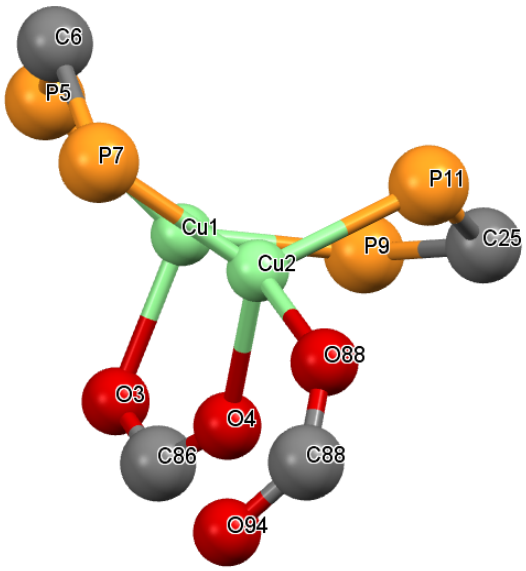


Figure S2. Central fragment of the crystal structure of compound **1** highlighting the octa-atomic distorted boat-chair conformation of the $\{Cu_2(\mu\text{-dppm})_2\}^{2+}$ unit and the two different coordination modes of the lactate anions.

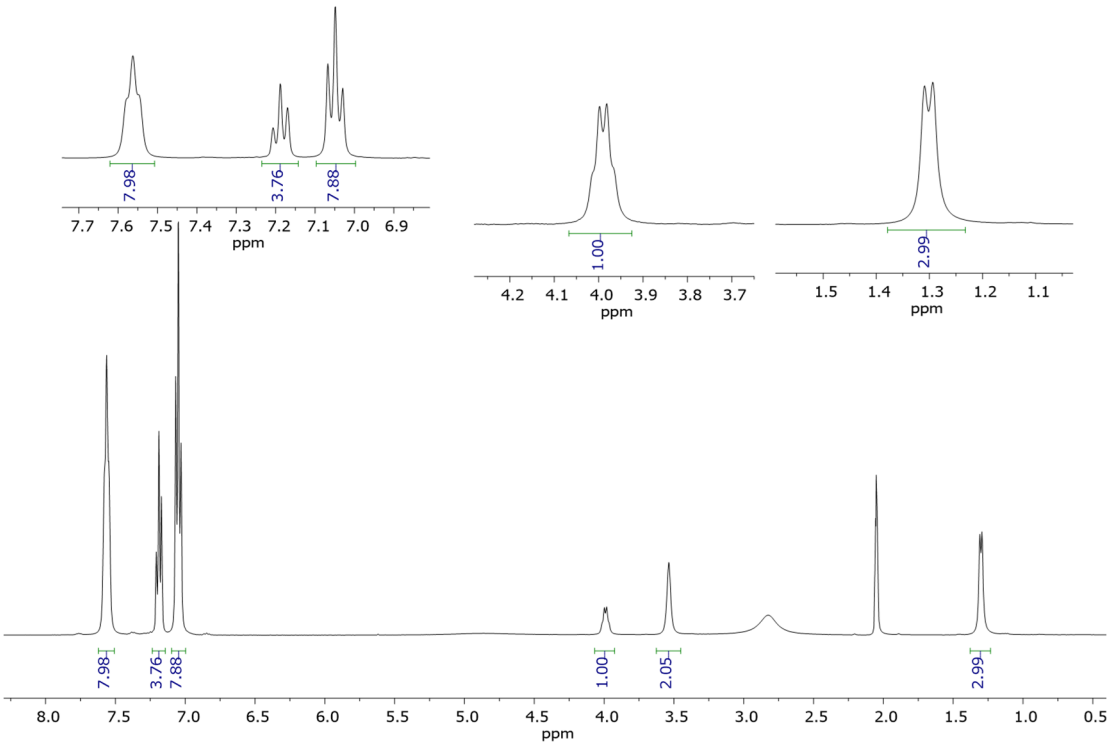


Figure S3. ^{1}H NMR spectrum (Acetone-d_6, 25°C) of compound **1**.

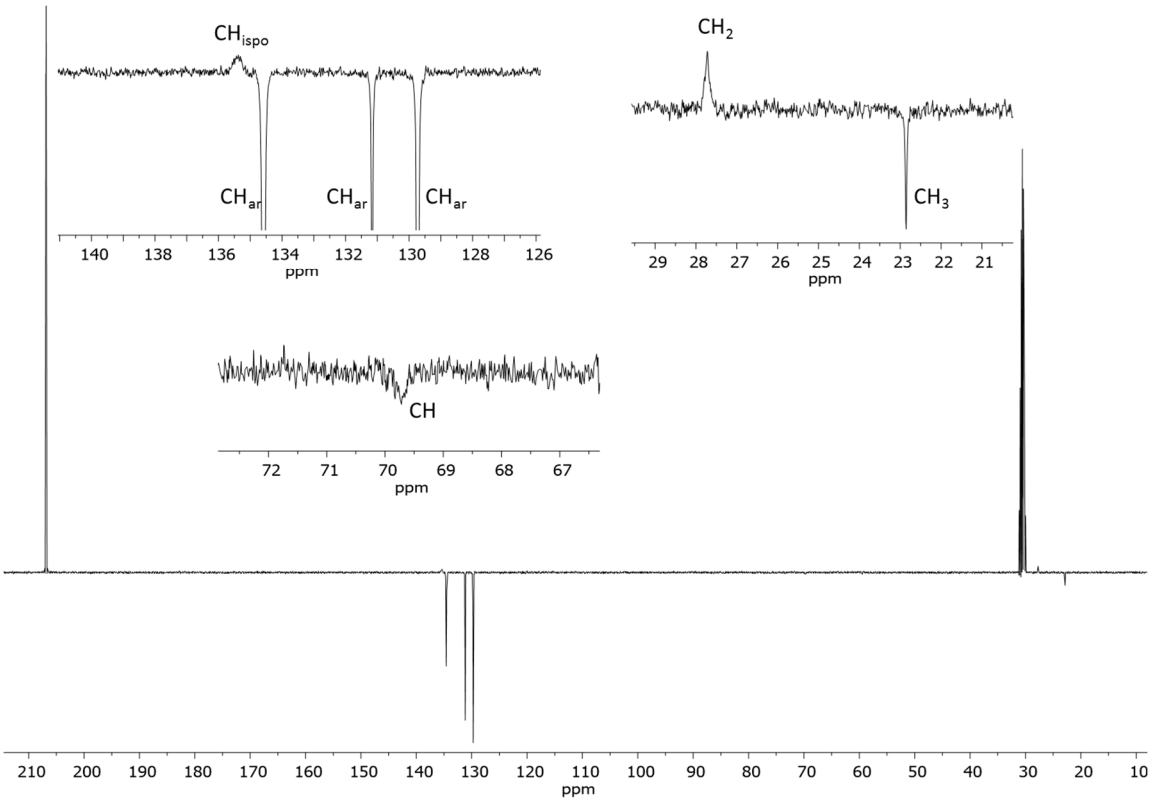


Figure S4. ^{13}C NMR spectrum (Acetone-d_6, 25°C) of compound **1**.

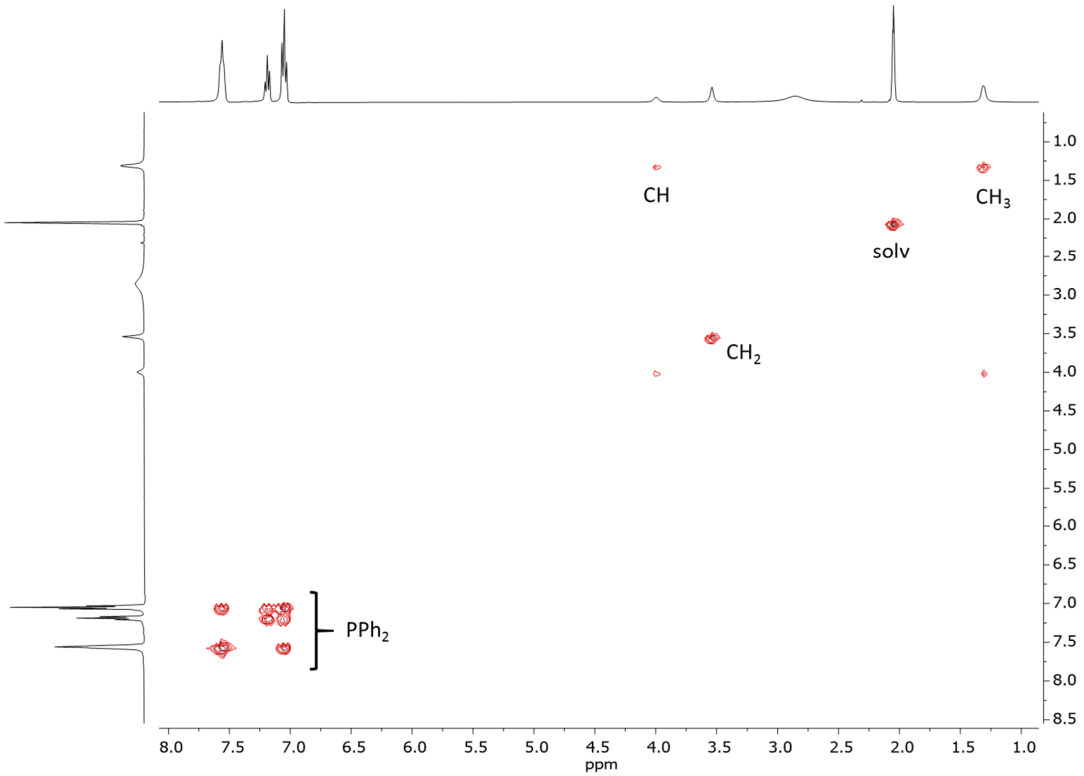


Figure S5. ^{1}H,^{1}H COSY spectrum (Acetone-d_6, 25°C) of compound **1**.

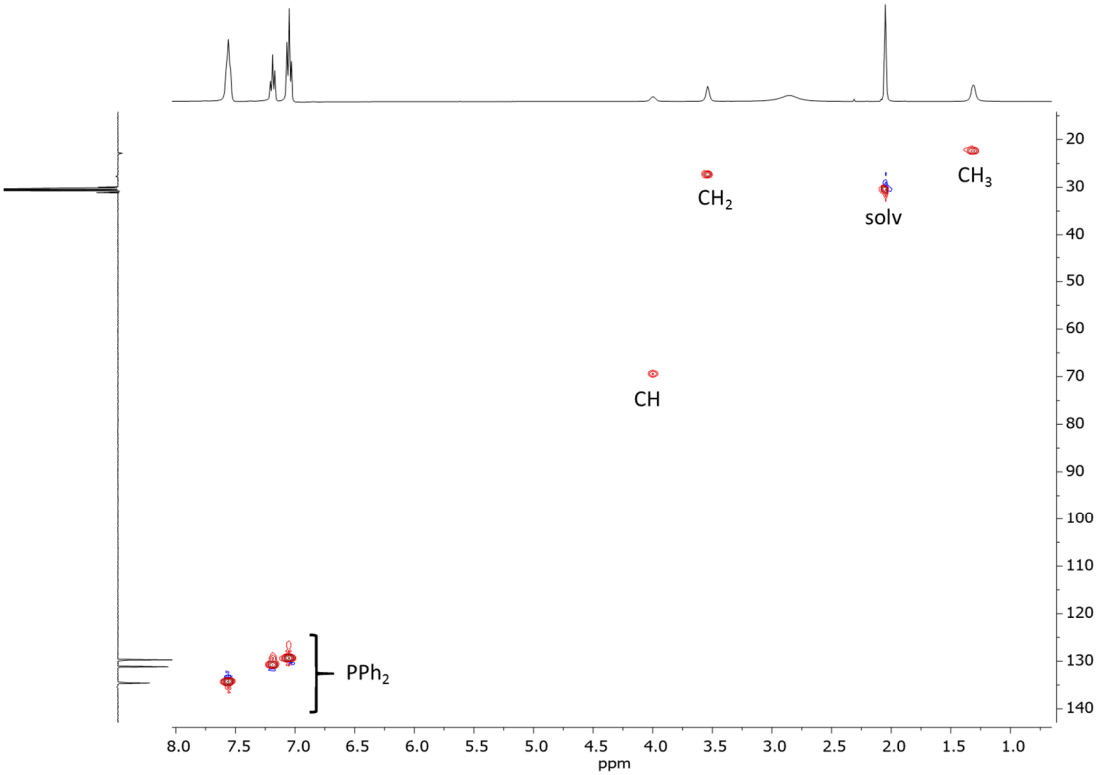


Figure S6. ^{1}H,^{13}C HSQC spectrum (Acetone-d_6, 25°C) of compound **1**.

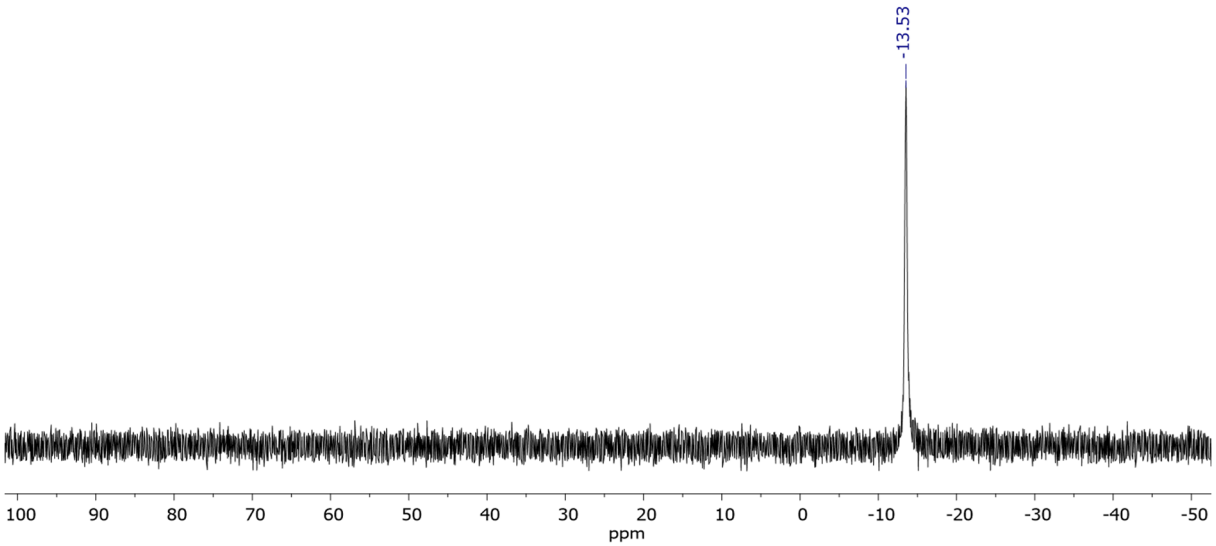


Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum (Acetone-d_6, 25°C) of compound **1**.

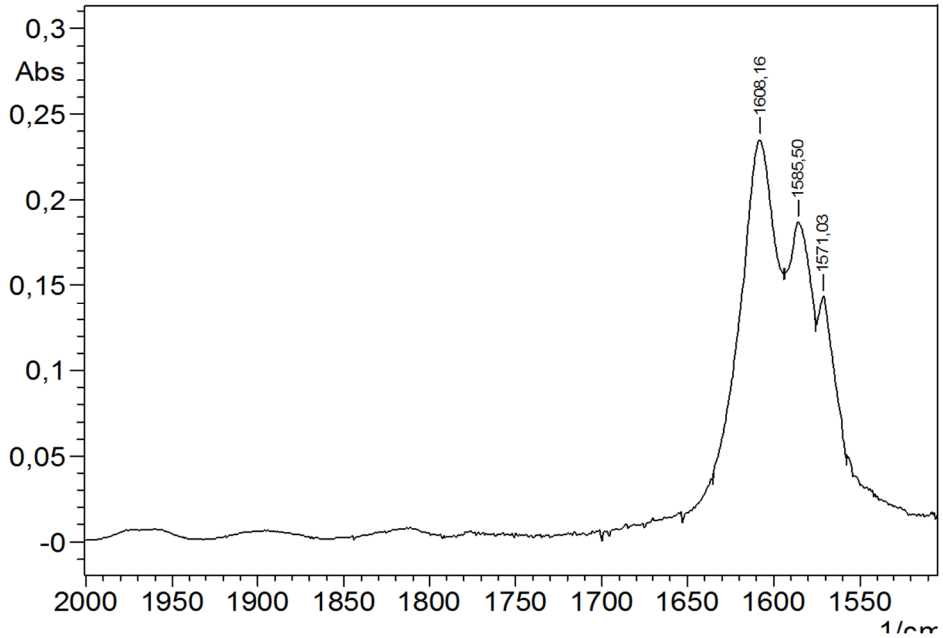


Figure S8. Infrared spectrum of compound **1** (solution, CH_2Cl_2, 25°C).

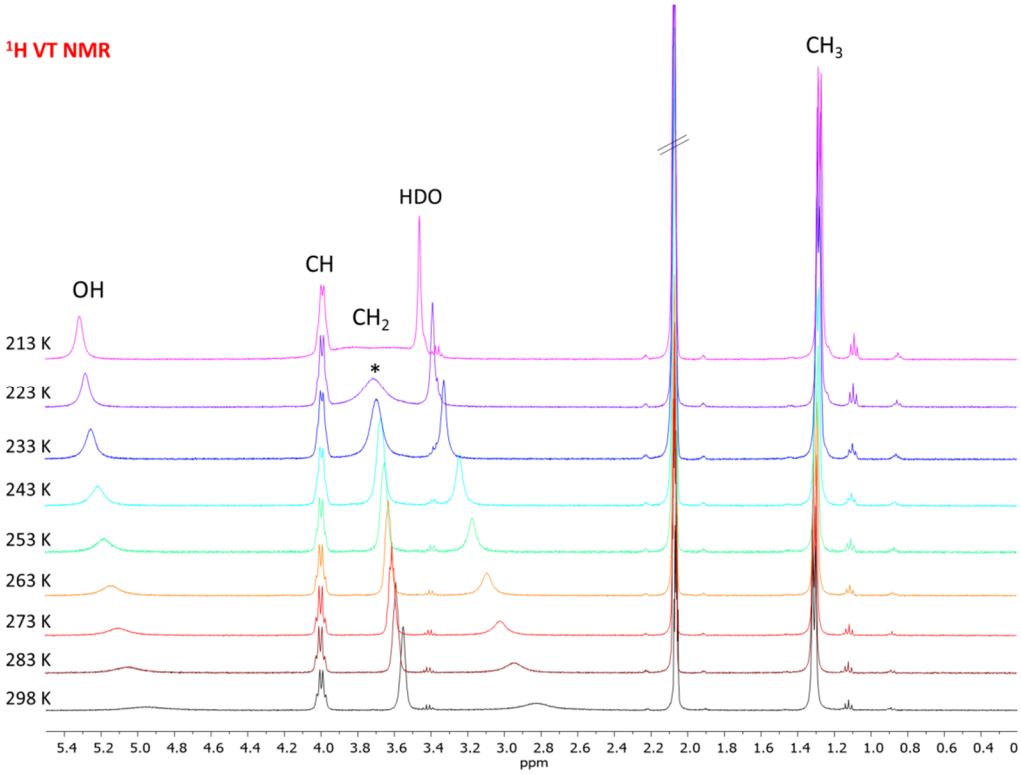


Figure S9. VT ^{1}H NMR spectra (Acetone-d_6, 25°C) of compound **1**.

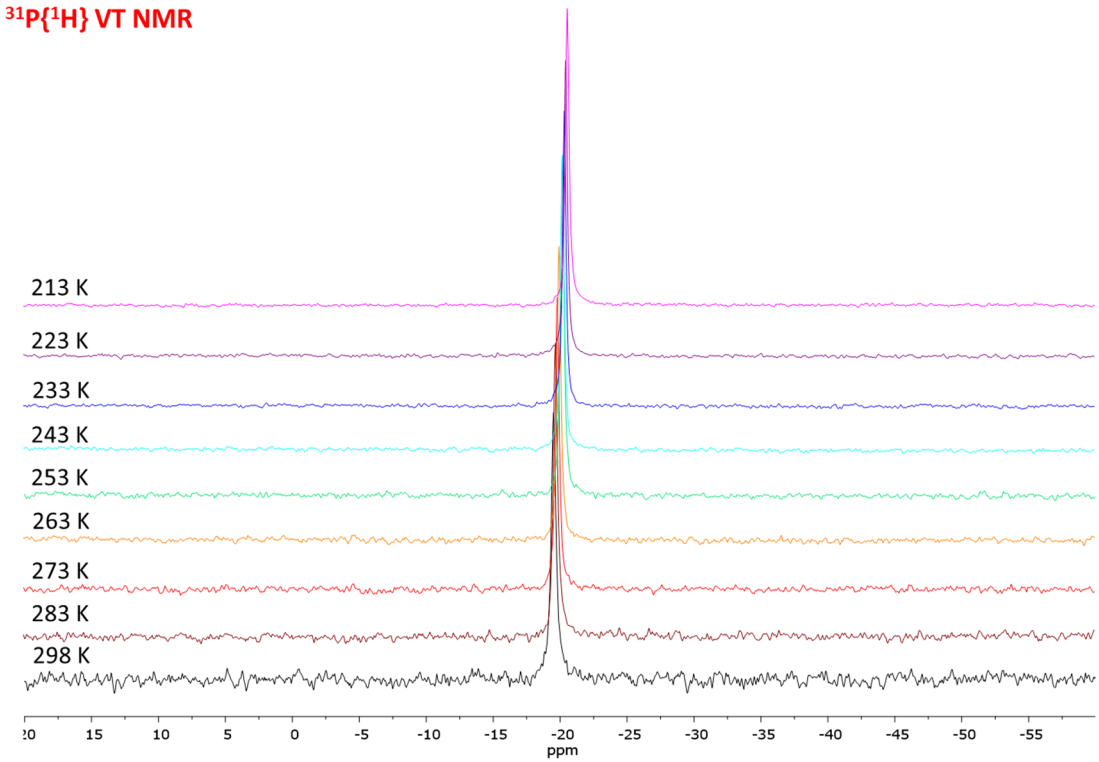


Figure S10. VT ^{31}P NMR spectra (Acetone-d_6, 25°C) of compound **1**.

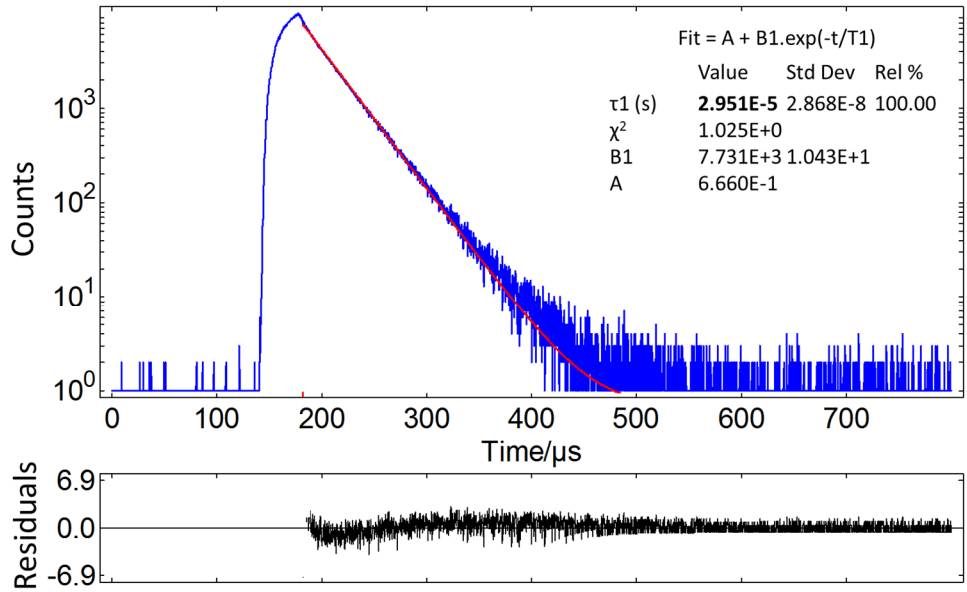


Figure S11. Fitting of the lifetime decay for compound **1** in the solid state.

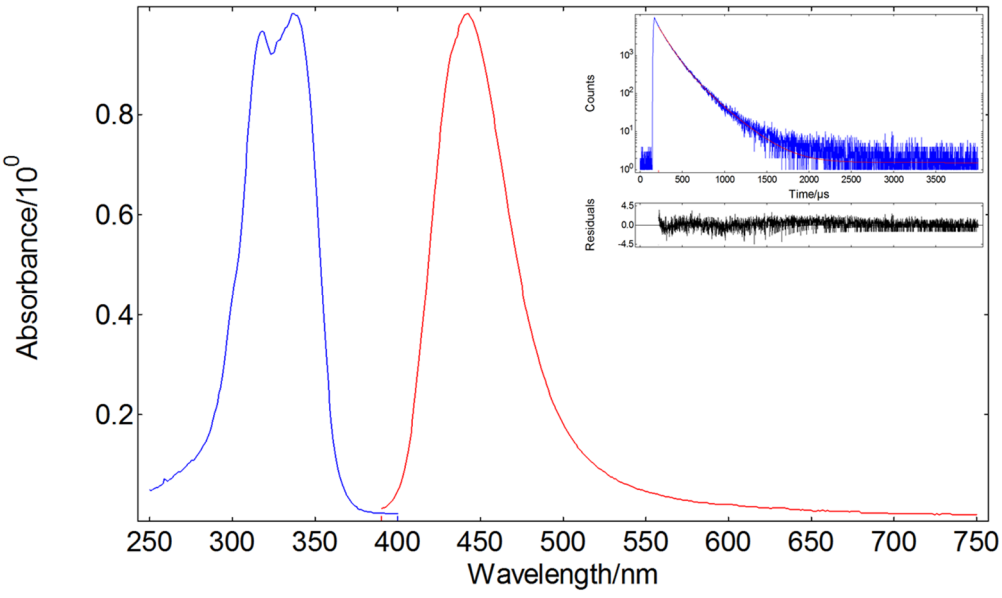
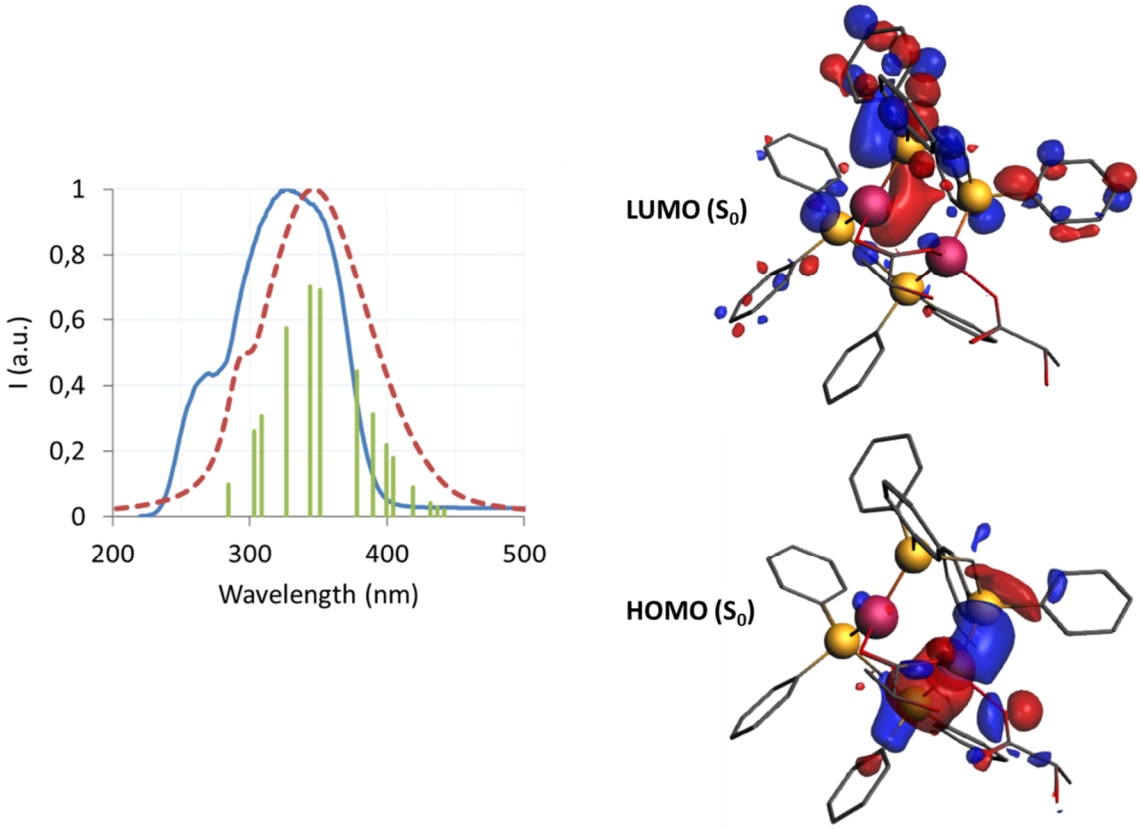
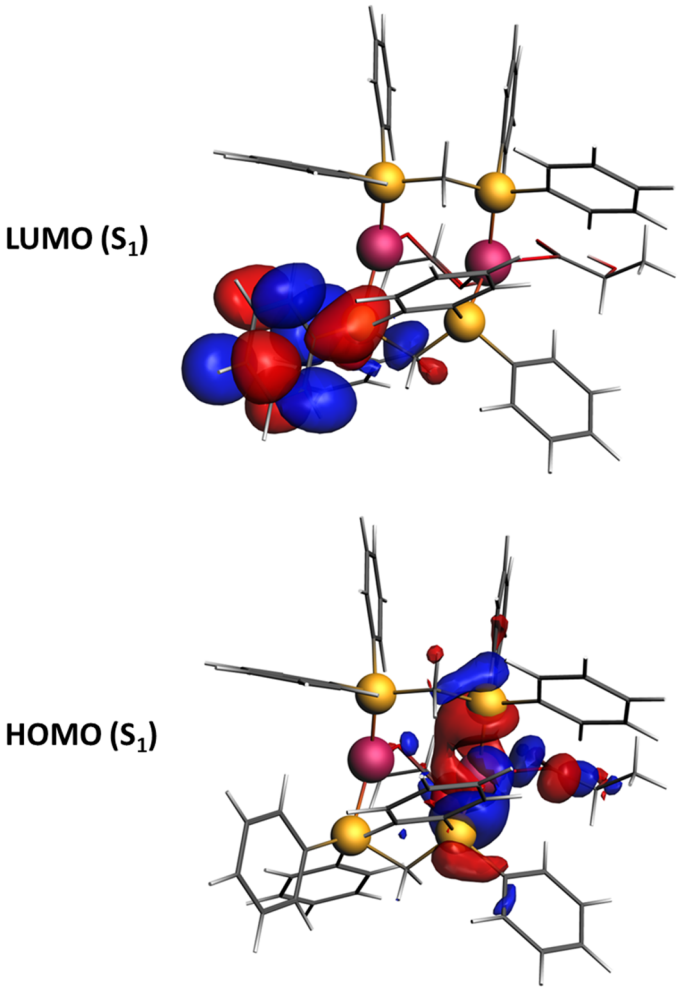


Figure S12. Normalized excitation and emission spectra of compound **1** recorded in acetone (77 K). Inset: fitting of the lifetime decay for compound **1** in acetone (77 K).



 # Figure S13. Left**:** calculated (dotted red) vs. experimental (full blue) UV traces for compound **1** in the solid state. Right: HOMO and LUMO for S_0.



 # Figure S14. Frontier molecular orbitals for the excited singlet state (S_1).

 # Table S1. Photophysical data for compound **1** recorded in acetone at 77 K.

		Stokes shift			
λ_{exc} (nm)	λ_{em} (nm)	(nm)	(cm^{-1})	(eV)	τ (μs)[a]
337	441	104	6997.8	0.87	106.1 (0.65) 237.6 (0.35)

[a] Pre-exponential factor given in bracket.

 # Table S2. Crystallographic and structure refinement parameters for compound **1**.

	1
Chemical formula	$C_{56}H_{54}Cu_2O_6P_4$
Formula weight	1073.95
Crystal system	Triclinic
Space group	*P* 1 (no. 1)
Crystal color and shape	Colorless block
Crystal size	0.17 x 0.18 x 0.15
a (Å)	10.5507(7)
b (Å)	12.4800(9)
c (Å)	21.6816(14)
α (°)	100.391(5)
β (°)	97.054(5)
γ (°)	113.523(5)
V (Å^3)	2513.9(3)
Z	2
T (K)	293(2)
D_c (g·cm^{-3})	1.419
μ (mm^{-1})	1.024
Scan range (°)	1.84 < θ < 27.50
Unique reflections	22011
Observed refls [I>2σ(I)]	17270
R_{int}	0.0875
Final *R* indices [I>2σ(I)]*	0.0603, wR_2 0.1580
R indices (all data)	0.0756, wR_2 0.1698
Goodness-of-fit	0.969
Max, Min Δρ/e (Å^{-3})	0.648, - 0.559

 # Table S3. Optimized molecular geometries for compound **1**

S_0				**S_1**				**T_1**			
Cu	0.930009	-0.63918	-0.9367	Cu	1.012377	-0.82265	-0.92756	Cu	0.842368	-0.7203	-0.75359
Cu	-0.38636	-0.20576	1.642272	Cu	-0.39102	-0.17111	1.826507	Cu	-0.35674	-0.26398	1.628239
P	-1.1635	-0.90255	-1.7502	P	-1.13801	-0.80417	-1.83404	P	-1.18551	-0.61928	-1.8245
P	-2.47184	-0.02497	0.86598	P	-2.42687	-0.04262	0.912903	P	-2.43712	-0.06367	0.895138
P	1.15128	1.24802	2.401042	P	1.155405	1.296959	2.590809	P	1.084804	1.25884	2.443586
P	1.653542	1.497646	-0.65022	P	1.557779	1.440264	-0.54207	P	1.551084	1.470876	-0.62148
O	2.237493	-1.56277	-2.32125	O	1.769233	-2.00672	-2.32766	O	1.675564	-1.80629	-2.2912
C	-2.45743	0.166165	-0.97072	C	-2.33567	0.261248	-0.92022	C	-2.40258	0.407342	-0.90233
C	-3.4759	1.400614	1.448561	C	-3.53636	1.303653	1.487848	C	-3.54794	1.229217	1.600889

C	-4.12204	1.298501	2.694627	C	-4.02717	1.191435	2.801286	C	-4.1152	0.96909	2.863235
C	3.211606	-0.47864	3.202693	C	3.411721	-0.34028	3.297616	C	3.408691	-0.1161	3.295431
C	-1.29475	-0.44315	-3.5327	C	-1.21763	-0.15214	-3.55112	C	-1.34489	-0.06806	-3.55578
C	2.30786	0.511067	3.628456	C	2.43818	0.57879	3.725708	C	2.325021	0.693403	3.683191
C	-1.86105	-2.60349	-1.70782	C	-1.88984	-2.46983	-1.94507	C	-1.84619	-2.32746	-1.89437
C	0.568049	2.786801	3.207883	C	0.575386	2.783357	3.322905	C	0.421757	2.789821	3.210655
C	-4.96485	-1.3668	0.795478	C	-4.89495	-1.4249	0.707555	C	-4.85474	-1.51459	0.61388
C	-4.81411	2.388942	3.223609	C	-4.82615	2.194675	3.345912	C	-4.87468	1.939449	3.515931
C	-3.90546	-3.78025	1.730325	C	-3.77746	-3.89773	1.37677	C	-3.71	-3.92357	1.461085
C	2.2949	1.839256	1.055077	C	2.267572	1.738069	1.12721	C	2.180276	1.896037	1.065294
C	-4.21681	3.709277	1.289494	C	-4.6547	3.448402	1.287001	C	-4.49909	3.467662	1.680044
C	3.077153	2.093185	-1.66265	C	2.917961	1.893763	-1.69437	C	3.061732	1.671932	-1.63743
C	-3.52246	2.619865	0.757143	C	-3.85522	2.441907	0.735717	C	-3.74906	2.489897	1.016369
C	-3.60095	-1.45252	1.123217	C	-3.52564	-1.51561	1.01086	C	-3.49222	-1.56016	0.958616
C	1.450432	3.822026	3.565001	C	1.469932	3.892569	3.616741	C	1.250518	3.882697	3.524938
C	-4.86619	3.598505	2.5212	C	-5.1427	3.327893	2.588535	C	-5.0654	3.197566	2.927019
C	-5.78987	-2.48285	0.935536	C	-5.69605	-2.56614	0.737791	C	-5.63776	-2.66706	0.70134
C	-3.07564	-2.66296	1.59735	C	-2.97006	-2.75674	1.35486	C	-2.92629	-2.76998	1.386914
C	-5.25983	-3.69228	1.401041	C	-5.13614	-3.80554	1.068508	C	-5.06668	-3.87308	1.122079
O	1.643943	-1.96222	0.510336	O	2.123388	-1.71812	0.506784	O	2.095496	-1.68519	0.562822
O	2.358734	-3.80662	-1.91013	O	2.203852	-4.06842	-1.46177	O	2.175924	-3.92386	-1.61422
O	0.112295	-2.10758	2.16762	O	0.230873	-2.09168	1.693384	O	0.43727	-2.10284	2.058849
C	-0.80469	2.93933	3.443565	C	-0.83436	3.02107	3.490724	C	-0.94664	2.8586	3.505621
C	2.705049	-2.73	-2.48959	C	2.384745	-3.14874	-2.28489	C	2.29827	-2.9162	-2.36837
C	0.060011	3.829819	-0.09694	C	-0.22375	3.57894	0.080447	C	-0.27534	3.578053	-0.18651
C	1.042321	-2.58401	1.43685	C	1.411357	-2.4008	1.319324	C	1.520321	-2.39392	1.459403
O	4.258342	-4.23394	-3.59112	O	3.910243	-4.68472	-3.38592	O	3.898125	-4.34691	-3.49047
C	-0.41826	5.147579	4.353402	C	-0.43194	5.355069	4.092577	C	-0.65933	5.088519	4.40256
C	-0.25767	2.730377	-2.2284	C	-0.10262	2.889081	-2.24313	C	0.154376	2.983024	-2.50039
C	5.012144	1.55915	-3.02877	C	4.579027	1.244788	-3.34127	C	5.11298	0.649398	-2.45344
C	3.83337	-2.85966	-3.53958	C	3.449653	-3.34024	-3.39231	C	3.318418	-3.03228	-3.52489
C	0.395635	2.796352	-0.98349	C	0.314501	2.744431	-0.90747	C	0.416658	2.797162	-1.13043
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C	2.231415	0.825815	4.994581	C	2.374729	0.91355	5.087881	C	2.145365	0.975112	5.050124
C	4.48181	3.870443	-2.5368	C	4.426661	3.551839	-2.6231	C	4.58332	2.936743	-3.0469
C	3.977153	-0.78562	5.48137	C	4.247255	-0.5521	5.562291	C	4.134892	-0.29754	5.602512
C	-0.22238	-0.81492	-4.36236	C	-0.16832	-0.5095	-4.41505	C	-0.59899	-0.78207	-4.52086
C	3.3927	-2.36642	-4.91403	C	2.948515	-2.96142	-4.78465	C	2.700035	-2.74036	-4.88692
C	-1.56159	4.695497	-1.67846	C	-1.59567	4.680289	-1.58814	C	-1.44377	4.72825	-1.9723
C	-2.37505	0.262245	-4.08621	C	-2.24892	0.672866	-4.02616	C	-2.083	1.061222	-3.96385
C	3.063305	0.179587	5.913989	C	3.274102	0.352264	5.997913	C	3.043846	0.485059	5.999672
C	3.371817	3.461074	-1.79509	C	3.372456	3.222121	-1.77163	C	3.402865	2.864708	-2.30408
C	-0.23889	-0.50251	-5.72268	C	-0.15528	-0.04949	-5.73238	C	-0.60067	-0.38284	-5.85349
C	-1.3177	0.201517	-6.26844	C	-1.18467	0.771904	-6.20135	C	-1.33878	0.742895	-6.25293
C	-0.91607	4.770106	-0.44241	C	-1.17333	4.546166	-0.26352	C	-1.1999	4.537764	-0.61015
C	0.956604	4.99805	4.130342	C	0.960277	5.124295	3.98079	C	0.710172	5.024937	4.117847
C	-1.45137	-4.96711	-1.33201	C	-1.67169	-4.86695	-1.67046	C	-1.60749	-4.71281	-1.53512

C	-0.98387	-3.65093	-1.39189	C	-1.13195	-3.58318	-1.55604	C	-1.09452	-3.41765	-1.43815
C	-1.29701	4.115638	4.015892	C	-1.31758	4.257353	3.859651	C	-1.4872	4.00474	4.096168
C	3.901119	1.144092	-2.28714	C	3.525986	0.907662	-2.48552	C	3.930661	0.565476	-1.71974
O	2.429607	-4.50543	0.772084	O	3.260172	-4.03815	1.354464	O	3.231761	-4.09787	0.947781
C	1.875756	-4.30472	3.104316	C	1.964561	-3.81205	3.358906	C	2.592963	-3.8381	3.250888
C	-1.22771	3.671535	-2.57361	C	-1.05857	3.849913	-2.57816	C	-0.76189	3.950451	-2.91639
C	1.415994	-4.0544	1.673121	C	1.958642	-3.74378	1.835383	C	2.136103	-3.76362	1.799877
C	-2.79789	-5.24233	-1.58148	C	-2.9661	-5.04264	-2.16188	C	-2.88158	-4.92504	-2.07149
C	-3.2087	-2.88785	-1.98045	C	-3.18935	-2.64974	-2.44737	C	-3.12584	-2.54278	-2.43744
C	-3.67469	-4.20063	-1.90845	C	-3.72616	-3.93194	-2.54787	C	-3.64055	-3.83789	-2.51693
C	-2.38141	0.585588	-5.44643	C	-2.23004	1.130776	-5.34619	C	-2.07766	1.456987	-5.3029
C	5.305157	2.920017	-3.15338	C	5.031333	2.564032	-3.40973	C	5.440947	1.833496	-3.1263
H	-4.09036	0.35663	3.253482	H	-3.77484	0.311383	3.403935	H	-3.9586	-0.0069	3.337711
H	3.250782	-0.77545	2.149492	H	3.46394	-0.65688	2.252202	H	3.551978	-0.38885	2.245498
H	-5.38672	-0.42274	0.432766	H	-5.33981	-0.4532	0.465527	H	-5.30852	-0.57257	0.286091
H	-5.31632	2.292716	4.192938	H	-5.19351	2.097011	4.372985	H	-5.31689	1.715889	4.493556
H	-3.4857	-4.72797	2.086284	H	-3.33535	-4.86635	1.633657	H	-3.25622	-4.86885	1.779664
H	-4.2424	4.652958	0.732977	H	-4.88859	4.337894	0.691403	H	-4.64063	4.448837	1.211748
H	-3.01276	2.745108	-0.20064	H	-3.46905	2.575015	-0.27786	H	-3.32281	2.731164	0.039919
H	2.528428	3.712366	3.403364	H	2.555379	3.74845	3.564489	H	2.325256	3.840837	3.316493
H	-5.41127	4.453588	2.936386	H	-5.76079	4.122335	3.020557	H	-5.65444	3.963979	3.443351
H	-6.85246	-2.40994	0.676711	H	-6.76426	-2.48793	0.505947	H	-6.70036	-2.62445	0.43463
H	-2.01187	-2.73243	1.842136	H	-1.90411	-2.83053	1.589169	H	-1.86322	-2.80482	1.646067
H	-5.90822	-4.57024	1.502521	H	-5.76541	-4.70234	1.08925	H	-5.68134	-4.77873	1.181587
H	-1.49333	2.140756	3.156662	H	-1.53414	2.202709	3.301294	H	-1.59266	2.012363	3.258658
H	0.54596	3.91405	0.8765	H	0.074167	3.481443	1.12637	H	-0.10196	3.450234	0.882706
H	2.573122	2.896286	1.19602	H	2.605588	2.784081	1.213034	H	2.380896	2.977351	1.143451
H	3.65124	-4.64083	-2.90152	H	3.500703	-5.06155	-2.56092	H	3.452011	-4.74062	-2.68376
H	-0.80235	6.075161	4.793042	H	-0.8162	6.33669	4.382427	H	-1.08059	5.988672	4.864733
H	-0.01172	1.9271	-2.93143	H	0.322932	2.255089	-3.02773	H	0.662808	2.364683	-3.2468
H	5.647613	0.812188	-3.51896	H	5.045447	0.467752	-3.95711	H	5.77954	-0.21873	-2.5082
H	4.678239	-2.23439	-3.18175	H	4.285633	-2.65535	-3.11608	H	4.107771	-2.28018	-3.3181
H	4.754276	-1.87547	3.77584	H	5.060193	-1.6152	3.855076	H	5.157496	-1.21308	3.92659
H	1.525193	1.584261	5.346513	H	1.622332	1.635221	5.422818	H	1.302725	1.59347	5.375815
H	4.632324	-1.28609	6.203263	H	4.953047	-0.99118	6.276479	H	4.843857	-0.67552	6.347704
H	0.641374	-1.32586	-3.92794	H	0.642478	-1.14221	-4.04496	H	-0.01098	-1.64983	-4.20942
H	4.211055	-2.49046	-5.64325	H	3.727987	-3.20011	-5.52653	H	3.456895	-2.87766	-5.6772
H	3.125805	-1.29888	-4.86463	H	2.727383	-1.88386	-4.84296	H	2.340323	-1.70097	-4.92523
H	2.516743	-2.93706	-5.26922	H	2.040908	-3.53256	-5.04281	H	1.854934	-3.42146	-5.08819
H	-2.33175	5.428651	-1.9431	H	-2.341	5.438778	-1.85414	H	-2.16912	5.480522	-2.30147
H	-3.21804	0.579119	-3.46525	H	-3.06724	0.983491	-3.37007	H	-2.67325	1.633089	-3.2435
H	2.997667	0.439312	6.976868	H	3.217418	0.631897	7.056269	H	2.893981	0.724302	7.058917
H	2.727067	4.212337	-1.32587	H	2.890573	4.003291	-1.17357	H	2.750808	3.740739	-2.23984
H	0.604359	-0.79913	-6.35701	H	0.669958	-0.33351	-6.39465	H	-0.02029	-0.95027	-6.59043
H	-1.17603	5.560952	0.270095	H	-1.58037	5.183599	0.527554	H	-1.73287	5.13661	0.13674
H	1.648664	5.80415	4.398854	H	1.661029	5.941146	4.198171	H	1.362458	5.871578	4.360677
H	-0.75776	-5.77921	-1.08361	H	-1.06612	-5.73039	-1.37519	H	-1.00521	-5.56006	-1.18763

H	0.072729	-3.43501	-1.20951	H	-0.11222	-3.4632	-1.18333	H	-0.09454	-3.26697	-1.0272
H	-2.37363	4.225577	4.180744	H	-2.39899	4.389986	3.978638	H	-2.56053	4.047502	4.306668
H	3.64648	0.082801	-2.21674	H	3.1746	-0.12717	-2.44294	H	3.671368	-0.37029	-1.21539
H	2.285509	-4.04899	-0.10635	H	3.190715	-3.96665	0.371425	H	2.905013	-3.93551	0.018676
H	2.108478	-5.37387	3.24269	H	2.276049	-4.82028	3.675931	H	2.947994	-4.857	3.478358
H	1.082414	-4.02131	3.812722	H	0.9594	-3.60253	3.753821	H	1.758047	-3.59377	3.925255
H	2.777566	-3.71295	3.330186	H	2.668537	-3.07781	3.776884	H	3.411615	-3.12564	3.435041
H	-1.73257	3.59734	-3.54325	H	-1.37832	3.948973	-3.62111	H	-0.95416	4.084943	-3.98551
H	0.473583	-4.62104	1.497886	H	1.223737	-4.48893	1.450682	H	1.303875	-4.48735	1.650575
H	-3.17	-6.27142	-1.51967	H	-3.38836	-6.04979	-2.25128	H	-3.28807	-5.9407	-2.13946
H	-3.90829	-2.08496	-2.23569	H	-3.78461	-1.78869	-2.77017	H	-3.72084	-1.69915	-2.80347
H	-4.73295	-4.41179	-2.09872	H	-4.74263	-4.0671	-2.93307	H	-4.64299	-3.99776	-2.93005
H	4.704624	4.938896	-2.63782	H	4.776304	4.588589	-2.67856	H	4.839029	3.86956	-3.5627
H	-1.32677	0.457147	-7.33419	H	-1.17171	1.135563	-7.23467	H	-1.33827	1.05876	-7.30207
H	-3.22644	1.144733	-5.86432	H	-3.03937	1.775431	-5.70702	H	-2.66359	2.331926	-5.60774
H	6.173067	3.245046	-3.73853	H	5.856909	2.828035	-4.08008	H	6.36485	1.895623	-3.71193
H	3.224458	1.25184	1.121971	H	3.164505	1.098757	1.148052	H	3.150113	1.380206	1.135807
H	-3.47009	0.01935	-1.37904	H	-3.34793	0.182093	-1.3488	H	-3.40464	0.369508	-1.3624
H	-2.13505	1.194737	-1.19774	H	-1.9659	1.289454	-1.0662	H	-2.02132	1.441192	-0.96194