Electronic Supplementary Information

Cationic-anionic complexes of Cu(II) and Co(II) with N-scorpionate ligand – structure, spectroscopy, and catecholase activity

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Table S1 Bond lengths and angles for **1.**

Bond lengths (Å)			
Cu1-Cl1	2.2604(5)	Cu2-N3	1.9572(16)
Cu1-Cl2	2.2338(5)	Cu2-N5	1.9813(16)
Cu2-Cl3	2.2258(5)	Cu2-N7	2.3583(16)
Cu2-N1	2.1503(15)		
Bond angles (°)			
Cl2-Cu1-Cl2^{i}	99.96(3)	N3-Cu2-Cl3	99.00(5)
Cl2-Cu1-Cl1^{i}	101.589(17)	N5-Cu2-Cl3	97.06(5)
Cl2-Cu1-Cl1	127.487(17)	N1-Cu2-Cl3	163.85(4)
Cl2^{i}-Cu1-Cl1	101.588(17)	N3-Cu2-N7	91.88(6)
Cl1^{i}-Cu1-Cl1	101.99(3)	N5-Cu2-N7	90.42(6)
Cl1^{i}-Cu1-Cl2^{i}	127.487(17)	N1-Cu2-N7	79.40(5)
N3-Cu2-N1	81.29(6)	Cl3-Cu2-N7	116.66(4)
N5-Cu2-N1	80.30(6)	N3-Cu2-N5	160.69(6)

Symmetry codes: (i) –x, y, 0.5-z.

Table S2 Relevant interatomic contacts for **1**.

D-H···A	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<DHA (°)
C18-H18c···Cl3^{i}	0.960	2.942	3.793	148.33
C6-H6b···Cl2^{ii}	0.960	2.707	3.634	162.43
C1-H1a···Cl1	0.970	2.649	3.510	128.60
C7-H7b···Cl1	0.970	2.780	3.652	149.84
C7-H7b···Cl2^{iii}	0.970	2.782	3.498	131.24
C1-H1b···Cl2^{iv}	0.970	2.706	3.637	160.99
C5-H5c···Cl2^{iv}	0.960	2.797	3.744	169.31
C7-H7a···Cl1^{iv}	0.970	2.833	3.759	160.00
C11-H11a···Cl1^{iv}	0.960	2.786	3.714	162.70
C13-H13b···Cl1^{iv}	0.970	2.852	3.797	164.99
C17-H17a···Cl2^{v}	0.960	2.789	3.707	160.24

Symmetry codes: (i) -0.5+x, -0.5-y, z; (ii) -x, -1+y, 0.5-z; (iii) -x, y, 0.5-z; (iv) -0.5+x, 0.5-y, z; (v) -0.5-x, 0.5-y, 05-z.

Tabel S3 Bond lengths and angles for **2.**

Bond lengths (Å)			
Co1-Cl1	2.2580(5)	Co2-Cl2	2.2409(5)
Co1-N1	2.067(1)	Co2-Cl3	2.2532(4)
Co1-N3	2.305(1)	Co2-Cl4	2.2971(4)
Co1-N5	2.068(1)	Co2-N8	2.033(1)
Co1-N7	2.089(1)		
Bond angles (°)			
N1-Co1-Cl1	105.11(4)	N7-Co1-N3	76.08(5)
N3-Co1-Cl1	177.72(3)	N7-Co1-N5	117.16(5)
N3-Co1-N1	76.32(5)	Cl3-Co2-Cl2	111.89(2)
N5-Co1-Cl1	104.76(4)	Cl4-Co2-Cl2	104.22(2)
N5-Co1-N1	112.42(5)	Cl4-Co2-Cl3	108.68(2)
N5-Co1-N3	76.14(5)	N8-Co2-Cl2	111.20(4)
N7-Co1-Cl1	101.67(4)	N8-Co2-Cl3	111.98(4)
N7-Co1-N1	113.83(5)	N8-Co2-Cl4	108.49(4)

Table S4 Relevant interatomic contacts and π···π interactions for **2**.

D-H···A	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<DHA (°)
C4-H4a···Cl1	0.98(1)	2.679	3.490	140.30
C10-H10b···Cl1	0.98(1)	2.602	3.411	139.98
C16-H16b···Cl1	0.980(5)	2.757	3.421	125.56
C10-H10a···Cl4^{i}	0.980(7)	2.703	3.557	145.93
C11-H11a···Cl3^{ii}	0.979(8)	2.876	3.832	165.55
C12-H12a···Cl3^{ii}	0.970(2)	2.806	3.690	148.99
C12-H12a···Cl4^{ii}	0.990(2)	2.785	3.405	121.19
C18-H18a···Cl2^{ii}	0.990(2)	2.924	3.593	125.70
C18-H18a···Cl4^{ii}	0.990(2)	2.929	3.814	149.32
N10-H10f···Cl4	0.91(2)	2.188	3.038	154.78
C20-H20···Cl2^{iii}	0.950(2)	2.795	3.549	136.96
π···π	d(Cg···Cg) (Å)		Offset (Å)	
Cg01-Cg01^{iv}	3.561		0.430	
Cg02-Cg02^{v}	3.821		0.977	

Symmetry codes: (i) x, -1+y, 1+z; (ii) 1-x, 1-y, 1-z; (iii) -x, 1-y, 1-z; (iv) 1-x, -y, 1-z; (v) 1-x, -y, 2-z.

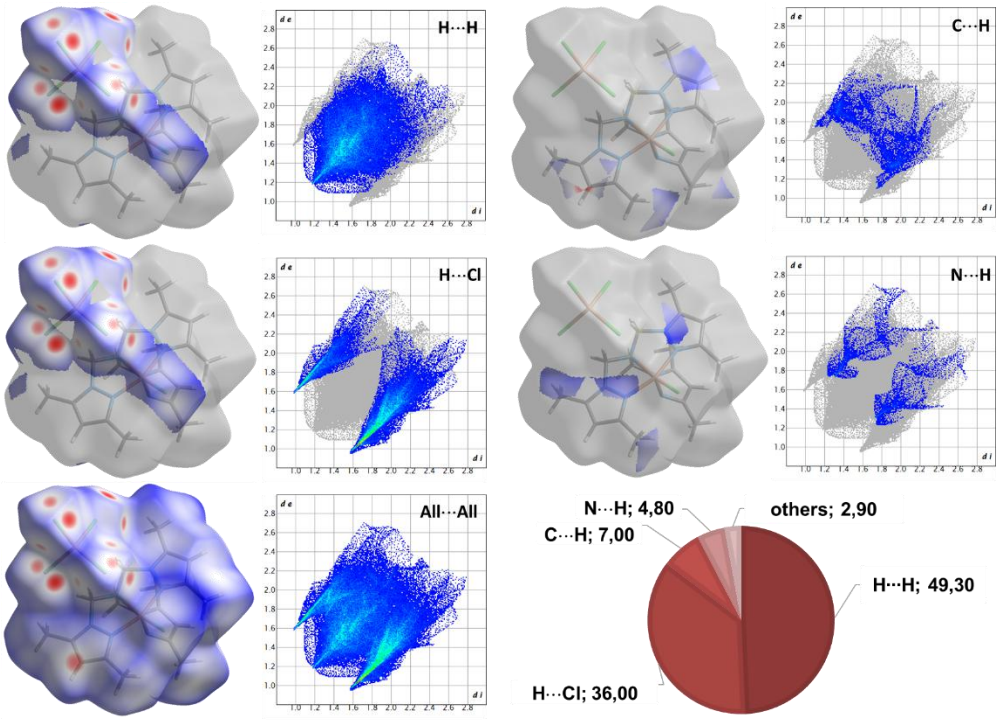

Fig. S1 3D Hirshfeld surfaces mapped with d_{norm} with corresponding 2D fingerprint plots and the percentage of non-covalent interactions in complex **1**.

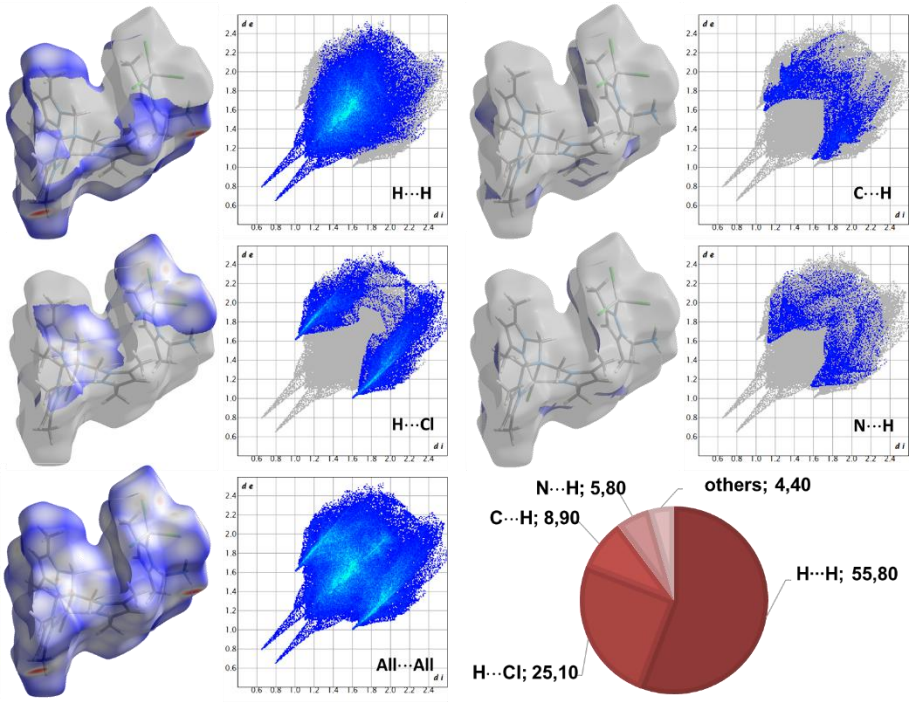

Fig. S2 3D Hirshfeld surfaces mapped with d_{norm} with corresponding 2D fingerprint plots and the percentage of non-covalent interactions in complex **2**.

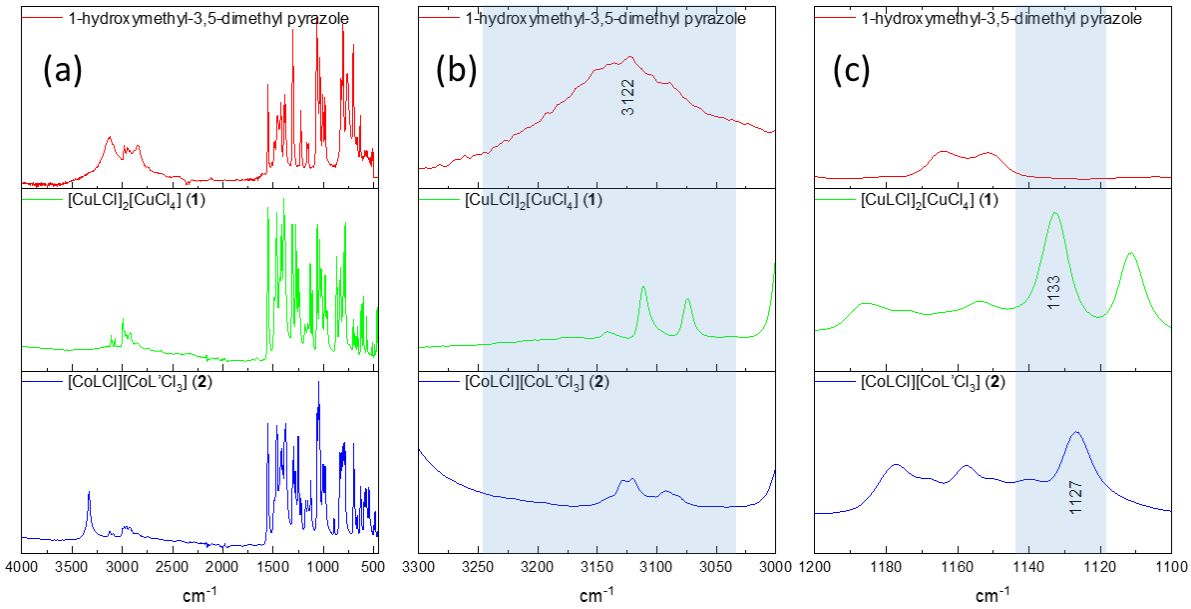

Fig. S3 The FTIR spectra of the scorpionate ligand's precursor (3,5-DMePzCH$_2$OH) and complexes **1** and **2** (a) with the separation of spectral ranges for the OH stretching band (b) and ν(C-N) stretching vibrations (c) showing changes in the spectra connected with the formation of poly pyrazole ligand.

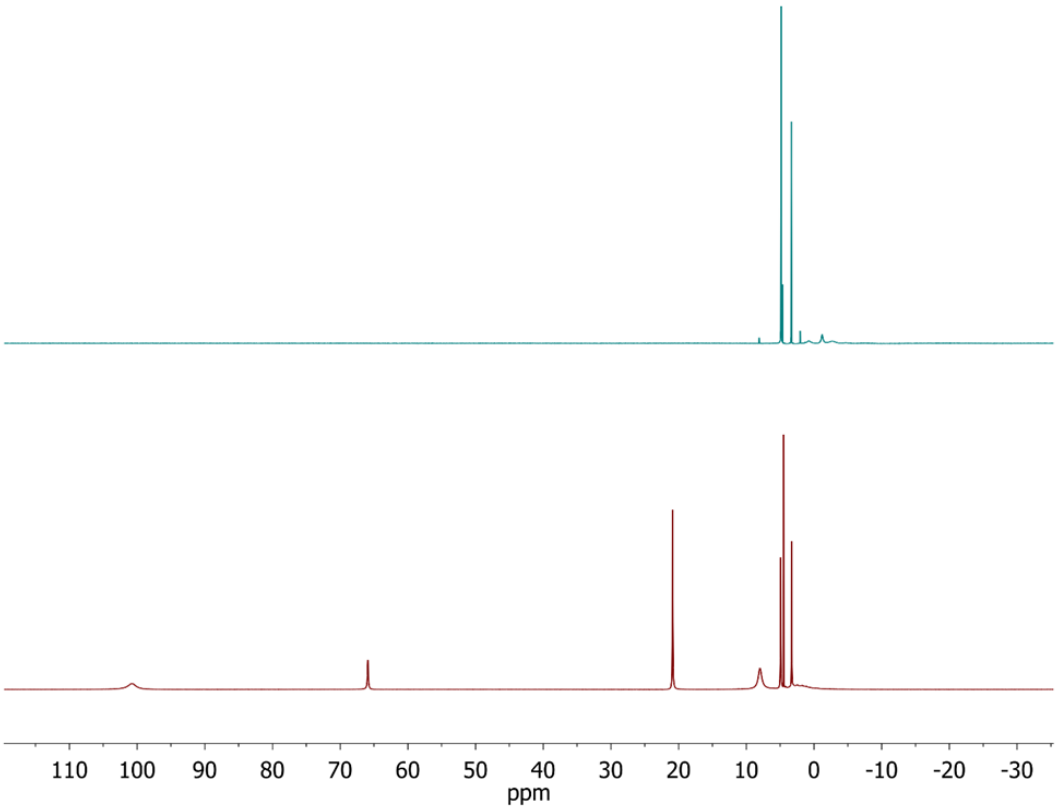

Fig. S4 The superposition of ^{1}HNMR spectra of complexes **1** - green and **2** - red ([D$_3$]MeOH, 298K).

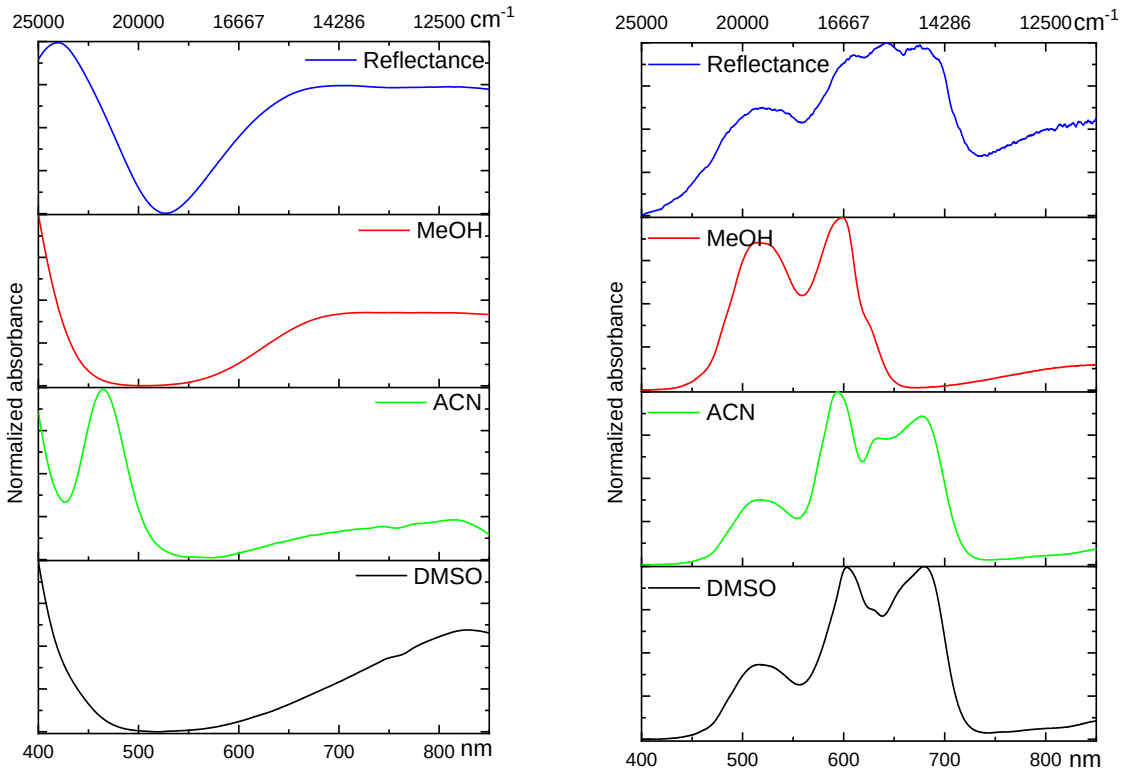

Fig. S5 Normalized UV-Vis spectra for complexes **1** (on the left) and **2** (on the right).

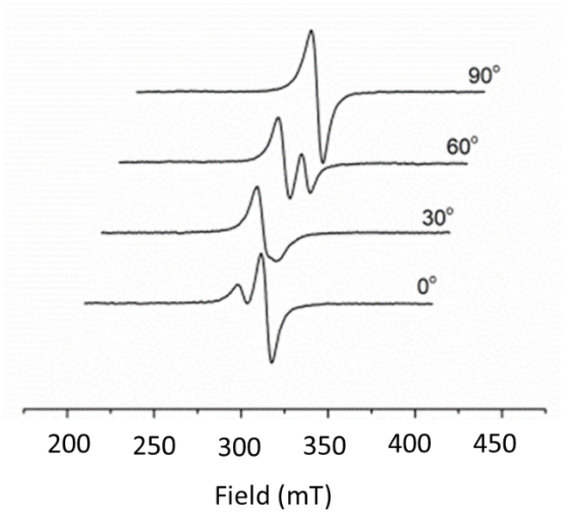

Fig. S6 The experimental EPR spectra of single crystal of complex **1** recorded at T = 5K at different angles of the external magnetic field with respect to the crystal.

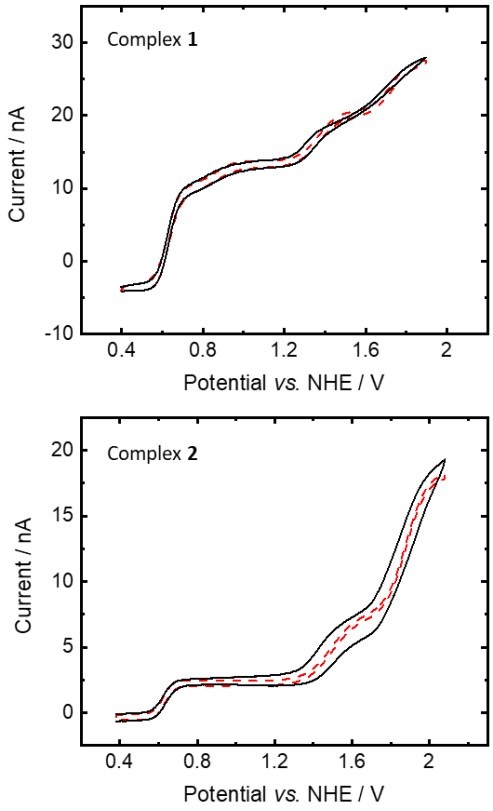

Fig. S7 Cyclic voltammograms of complexes **1** and **2** (each at a concentration of 1 mM) recorded under ambient air atmosphere in acetonitrile solution containing 0.1 M NBu_4PF_6 with the scan rate 25 mV/s. Lines (–) and (---) represent the experimental and simulated curves, respectively.

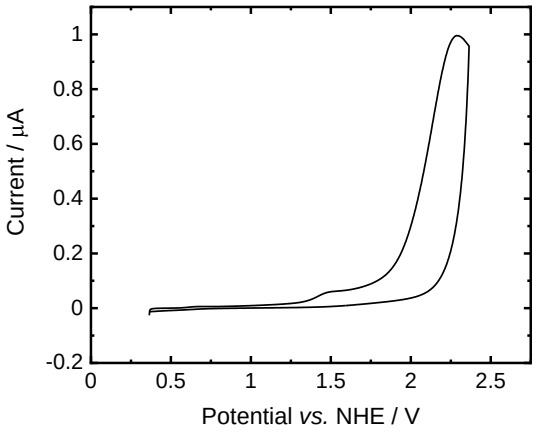

Fig. S8 Cyclic voltammogram of the scorpionate ligand recorded under ambient air atmosphere in acetonitrile solution containing 0.1 M NBu_4PF_6 with the scan rate 1 V/s.

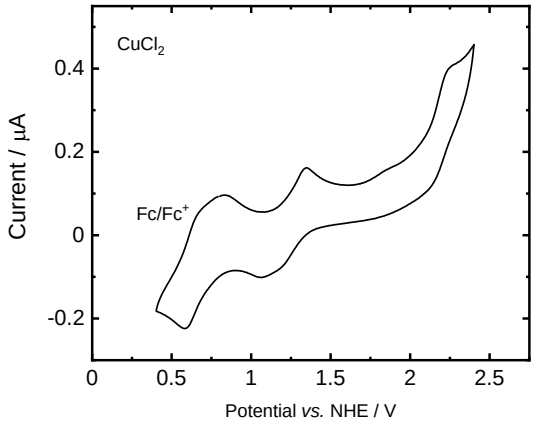

Fig. S9 Cyclic voltammogram of anhydrous $CuCl_2$ recorded under ambient air atmosphere in acetonitrile solution containing 0.1 M NBu_4PF_6 with the scan rate 1 V/s.

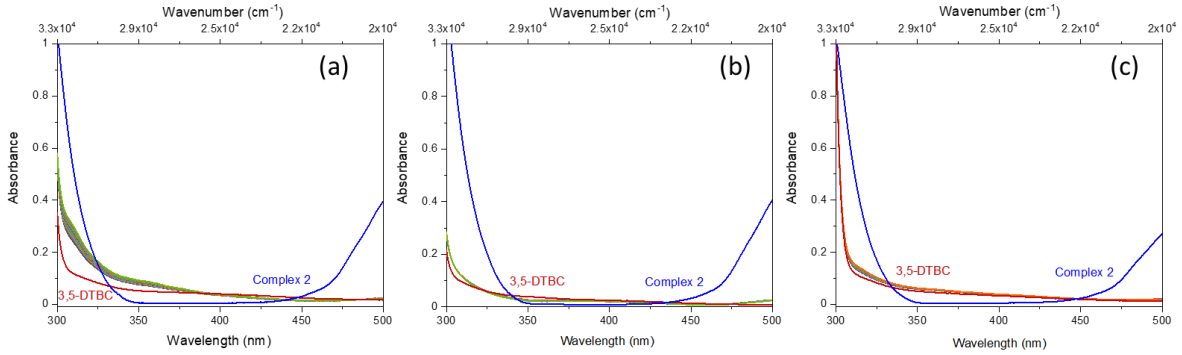

Fig. S10 Spectral changes observed during the oxidation of 3,5-DTBC ($1 \cdot 10^{-2}$ M) in the presence of **2** ($5 \cdot 10^{-5}$ M) in different solvents: (a) in MeOH, (b) CH_3CN and (c) DMSO. No changes in the absorbance at 400 nm indicate the lack of activity in the reaction.

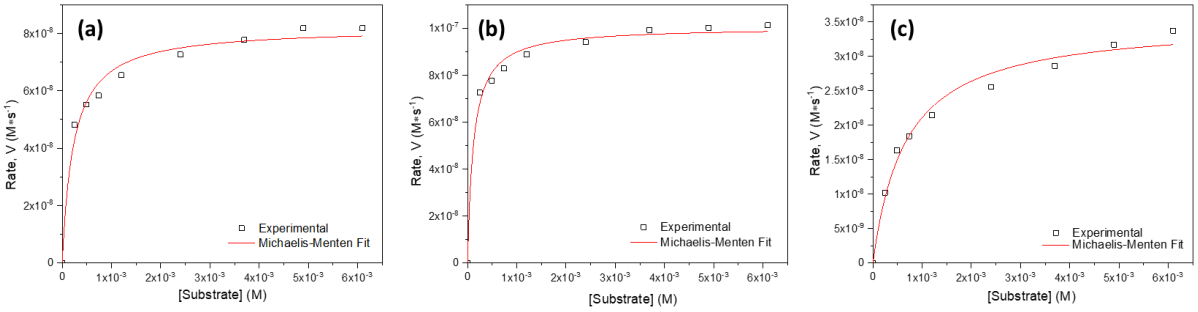

Fig. S11 Plots of rate vs substrate concentration for the catalytic oxidation of 3,5-DTBC in the presence of $(NH_4)_2[CuCl_4]$ in different solvents: (a) in MeOH, (b) in CH_3CN and (c) in DMSO.

Table S5 Kinetic parameters for catecholase activity of $(NH_4)_2[CuCl_4]$.

Solvent	V_{max} (M·s^{-1}) (·10^{-8})	Std. error (·10^{-9})	K_M (M) (·10^{-4})	Std. error (·10^{-5})	K_{cat} (h^{-1})
MeOH	8.21	2.22	2.27	3.51	2.95
CH_3CN	9.98	1.80	1.19	1.72	3.62
DMSO	3.52	1.26	6.66	8.88	1.27

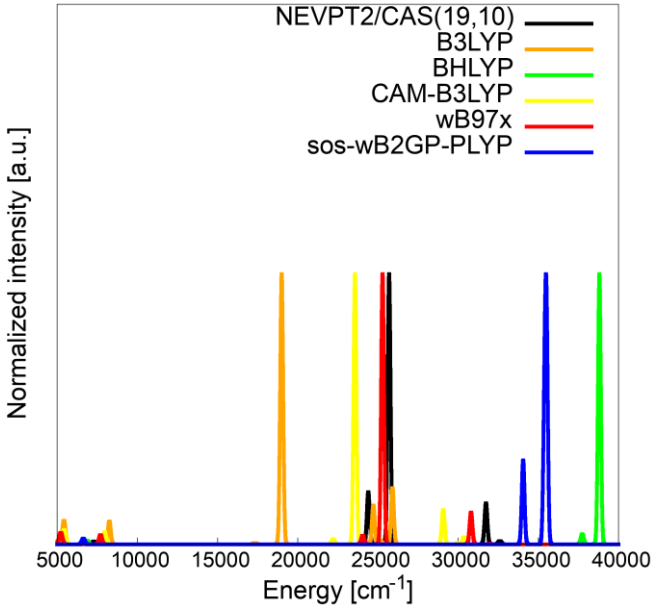

Fig. S12 Comparison of computed reference spectrum of $[CuCl_4]^{2-}$ (black) with those obtained from TD-DFT calculations with various functionals. Reference calculations were performed at a multireference level using CASSCF(19,10) wavefunction augmented with NEVPT2 dynamic correlation treatment. The averaging was performed over 10 states, and active space covered five 3d orbitals of Cu and five ligand-based orbitals. We show that ωB97x (red) provides a spectra profile close to reference NEVPT2 (black).

XYZ coordinates of key structures discussed in the main manuscript (fully optimized structures if not stated otherwise)

1 anion

Cu	-1.40647302439797	3.52729091136835	7.19744103222713
Cl	-0.87108521216340	2.05037563857723	5.52672483178254
Cl	-0.15363793951266	5.01703694863571	8.40559338651244
Cl	-1.94186079511489	2.05037558768867	8.86815716498594
Cl	-2.65930802881106	5.01703691373004	5.98928858449193

1 cation

C	-3.67467230354865	0.68651246631254	6.26694247264088
H	-2.72631628526721	1.25129534385057	6.28046328800222
H	-4.27568191636484	0.96257746663236	7.15096138581995
C	-3.57737058623010	-1.63515925542426	7.33929044522721
C	-3.17383589624704	-2.87380526110569	6.82555294798749
H	-3.16418870203667	-3.82416482648236	7.36308896679686
C	-2.79440101822991	-2.65388397883010	5.47664947928489
C	-4.06766900100223	-1.25171520511895	8.69559642294511
H	-3.34948545467871	-0.59217422695205	9.21707656645195
H	-4.20662343920763	-2.15848100006194	9.30554151308016
H	-5.03486362297011	-0.71867772235288	8.64232687576770

C	-2.39201811008604	-3.65293393492073	4.44237063523761
H	-3.28474120278705	-4.01641313433728	3.89770231229284
H	-1.90593388038482	-4.52430047581408	4.91178600490361
H	-1.71528614394726	-3.19412496873708	3.70223067222263
C	-4.12594278725519	2.32744598545300	4.47054975174932
H	-4.85430797008843	3.06027136766882	4.86017322919893
H	-3.10345683172763	2.64073104162451	4.74714133622550
C	-4.86627146289811	3.14359558459798	2.16433012069264
C	-4.65203679591264	2.61857513127330	0.88510368404346
H	-4.99549185510331	3.04957592499338	-0.05734728731339
C	-3.90932835727787	1.42139550244751	1.05154469766123
C	-5.55964398107317	4.38949830079508	2.60581107579516
H	-6.27286964993819	4.19151628799464	3.42619571070448
H	-6.11645001702892	4.82013845673531	1.75840999499073
H	-4.83916134068464	5.14813862265877	2.96482390511734
C	-3.47740801039712	0.44950059973847	0.00446780473540
H	-2.67576039758034	-0.20231487793627	0.38918517896294
H	-3.11910452765146	0.98545804609058	-0.89162140277225
H	-4.32937432011067	-0.18266326970130	-0.30703150178234
C	-5.75383103678134	0.50314246443662	4.92127399994446
H	-5.90271268198323	-0.24098142554102	5.72141062444881
H	-6.46306006633603	1.33636571303550	5.05892622158319
C	-6.98592041939239	0.15843757213890	2.70411908949145
C	-6.76131827653202	-0.73923992995332	1.64968742292763
H	-7.34288855140485	-0.80989251313432	0.72799862458510
C	-5.62839270595448	-1.51006235326923	2.01962446473723
C	-8.01316108693563	1.22653906060902	2.87798086434709
H	-8.71076987408735	0.99481343021940	3.70418017648808
H	-8.60087196171802	1.32759645195413	1.95162592769374
H	-7.54570287489533	2.20356334066700	3.09675371315723
C	-4.91356943873381	-2.59408560370299	1.27513140882687
H	-3.82197013274066	-2.49536813407216	1.41669318869913
H	-5.14013369000777	-2.54986805223729	0.19729407268756
H	-5.21219399527326	-3.59453475571736	1.64172531312368
N	-4.35084578409340	0.97385682853051	4.99176488552484
N	-3.42008749267530	-0.73989132024852	6.31696525576878
N	-2.92663143956541	-1.34097814002603	5.19381373683426
N	-4.26396105161677	2.27172745098619	3.02818369074886
N	-3.66626048259847	1.23468595651568	2.36742198761021
N	-6.02109615696961	-0.12012953743350	3.63611429942267
N	-5.19025544552834	-1.12061897550277	3.23566467589673
Cu	-3.19510158309827	-0.29484875277257	3.54688611696463
Cl	-1.36076590336199	-1.00770576657379	2.41008995181730

1 dimer (cut from crystal structure; position of H atoms were optimized)

Cu	-1.69250642245164	3.96654454324681	7.16453706151711
Cl	-0.77261570796267	2.45151591230311	5.64203582630027
Cl	-0.72135107941821	5.54876199618799	8.46010408686284
Cl	-2.40551582041467	2.52202244834147	8.80847380962730
Cl	-2.81255006631998	5.33633206895527	5.69485412751388
C	-3.71819711945927	0.59812738331898	6.16317805609733
H	-2.74761011628909	1.13576224451537	6.15985624610351
H	-4.27788238861846	0.90907307971303	7.06331123820937
C	-3.49465312216192	-1.66782892706062	7.32077539756167
C	-3.11910808291165	-2.92940726430896	6.84024045975086
H	-3.01082959293507	-3.84198834758047	7.43065573246666
C	-2.91363139270102	-2.78936021700816	5.44389482119817
C	-3.82219832521072	-1.19875206579680	8.70235739395785
H	-3.23616765988225	-0.30029107928656	8.97525748336191
H	-3.60310472782065	-1.99988485852497	9.42679776816145
H	-4.89331846826551	-0.93636896165417	8.79771149824853
C	-2.57069701719135	-3.84420518456450	4.43910377899294
H	-3.48634091296380	-4.24891187444049	3.96612768353222
H	-2.04501702897117	-4.68378092271047	4.92447506414569
H	-1.93786115296644	-3.42228469955639	3.63885478760971
C	-4.15016947126913	2.26713132560214	4.41666223090375
H	-4.92877794511257	2.98534115961636	4.72886469465760
H	-3.17520640722225	2.60805230857626	4.81966040870680
C	-4.41648899991305	3.28040573761571	2.09805137549917
C	-3.99548308483493	2.85645374416666	0.83192933101754
H	-4.09260719026875	3.41112647062225	-0.10407411141505

C	-3.42580481323822	1.56930895534077	1.00263575451982
C	-5.04366960338649	4.56100251988243	2.54768055639490
H	-6.04653917582790	4.39195375845285	2.98346241901839
H	-5.15328196407321	5.24192973051473	1.68818992338795
H	-4.42402853932373	5.05842534689539	3.31932410335236
C	-2.88993708231775	0.65331648214847	-0.05294567125315
H	-2.18312353858000	-0.07198336282623	0.38467321755673
H	-2.38176202683622	1.23490046318040	-0.84187161853574
H	-3.70958354924890	0.08903250838232	-0.53767374549336
C	-5.82317732378594	0.47502518559075	4.87623321176625
H	-5.96545844980009	-0.27464825444970	5.67492125851492
H	-6.51105845525453	1.32051905387240	5.05320717279665
C	-7.39308485061667	-0.12637029380374	2.95310266404349
C	-7.25965674163974	-1.01292602824585	1.87674829271039
H	-8.02859229812960	-1.25487684582792	1.13920382600579
C	-5.92960945924303	-1.50965929073944	1.93537788674667
C	-8.56637769412244	0.68021110170028	3.41150887029154
H	-8.96188505689576	0.32077525328252	4.38038491320285
H	-9.37657400741885	0.60645174182059	2.66772207407948
H	-8.30844749190764	1.74851233360001	3.53258817345826
C	-5.22887648611922	-2.47829483370223	1.03110654790605
H	-4.14065564275341	-2.45160271212690	1.21322280757351
H	-5.41754843501309	-2.24417968936065	-0.03153632893661
H	-5.58114721120284	-3.51316122088234	1.20455751346947
N	-4.41547654812198	0.90801205677897	4.90227457303139
N	-3.50443136378107	-0.84153639870465	6.23086052342194
N	-3.13047393100380	-1.50212594479281	5.09590369900501
N	-4.10401474800287	2.26287426118441	2.95655957042252
N	-3.47739369204502	1.23330996009267	2.31261388495072
N	-6.17654783070052	-0.12628942681451	3.58832855375575
N	-5.29427617714186	-0.96808944930620	2.99273263690055
Cu	-3.26045614150365	-0.41887082227303	3.43030200511269
Cl	-1.31072336742695	-1.17447915915272	2.49275548023295

2 anion

Co	4.39761264361949	7.69060473184899	3.96495262263983
Cl	5.96874460314143	6.52925356791096	5.10808008766081
Cl	4.33187990001814	9.83217237951590	4.68358887071264
Cl	4.79271584588502	7.72477683606703	1.72090746188607
N	2.69195455552192	6.68807652879863	4.22168852974812
N	2.53134832745453	5.39973666642555	3.78948997183116
N	3.30806701812902	4.81422114510868	1.59190193888885
H	3.80150398001497	4.05765990189486	1.10735349548682
H	3.70315810553622	5.70835747358885	1.25540398485946
C	1.51240252348095	7.05128309170430	4.78252965092690
C	0.59038578481606	5.97853835699955	4.68194892838958
H	-0.44144453225171	5.96188272930848	5.04000771725712
C	1.26846425965714	4.93951211378956	4.03495778968356
C	1.30892918069841	8.38602338099620	5.42586913084789
H	1.69308901934219	8.38971846908773	6.46443240883589
H	1.85970896551556	9.17695621434121	4.88825649034745
H	0.23404437258206	8.63202854733130	5.46370736952807
C	0.82386422998443	3.57493303775974	3.62199091894680
H	0.96243841418855	3.42998160810082	2.53461733901837
H	1.40227251160310	2.78399588167782	4.13618314611180
H	-0.24168250241999	3.43520714354839	3.86570356804115
C	3.57873881304560	4.72680640939375	3.01514009378546
H	4.52811231676718	5.19340780961873	3.35048863654010
H	3.58803766366968	3.66961197518285	3.33050184802603

2 cation

Co	4.94148771141369	2.19857556132603	9.65088613658370
Cl	3.09130035858919	0.93719448414490	10.01940956622740
N	5.12880661437107	2.23482560377238	7.64863228632031
N	6.31026402551761	2.67953053330375	7.12417292371185
N	6.87644040796317	3.51143517219177	9.25265856579924
N	5.32955569401226	5.04175811895451	10.14925314676732
N	4.51767300579082	3.98809259415615	10.46508927844664
N	7.60934041489657	1.87403950058232	10.77577229505167
N	6.42103941301344	1.22166018721246	10.59977510694849
C	4.29823461919157	2.03839300463206	6.59467635477835

C	4.98305322367789	2.34998408235530	5.39476054800248
H	4.58523165286035	2.29412993663868	4.37947141615352
C	6.27077140106135	2.76087177481253	5.76158234510533
C	2.87916034214396	1.59630906509733	6.74873381725456
H	2.81053709783541	0.67021337170833	7.34419162581571
H	2.28132990329634	2.35602661512271	7.28459901195177
H	2.42944162926401	1.43228149576822	5.75586816672149
C	7.43172208072712	3.20243409203159	4.93339506963741
H	7.80396451526961	4.19374243813665	5.25197269965475
H	8.27511651401622	2.49049136650775	5.00218429736335
H	7.12611192547607	3.27139643487305	3.87720664378379
C	7.41992144304702	2.93744575713802	8.02674811009966
H	7.93054409093788	1.99352772319476	8.28995261286449
H	8.13888166073198	3.59968144748016	7.51002546796411
C	6.62196516983964	-0.05011269544811	11.02535642481096
C	7.95343821190587	-0.18373630925686	11.48932621404345
H	8.42036883231983	-1.08479533929005	11.89210456684558
C	8.56643626202601	1.06368583473009	11.31570402375702
C	5.56704130284776	-1.10604236905933	10.95368776837428
H	4.64106407189447	-0.78136262339234	11.45797171433917
H	5.29053236028744	-1.32219483232147	9.90572161076298
H	5.93505430123652	-2.03482203570445	11.41930047514857
C	9.95296601020131	1.52560789444730	11.61995590379231
H	10.44917586383058	1.93846875528477	10.72198038325057
H	9.96036989265413	2.31171839514079	12.39756786070237
H	10.55233769301729	0.67620458015664	11.98466870151865
C	7.68325191469587	3.28788732155186	10.44683788182488
H	8.74802406411942	3.55689059348620	10.31956804165370
H	7.25808298713427	3.89580067600159	11.26531196106483
C	3.66039405073643	4.44236595752487	11.41226951484543
C	3.93345289467525	5.80708413238110	11.67492994377239
H	3.41767693236137	6.45401970634960	12.38742045376212
C	5.00979323501507	6.16688621911877	10.85421586592408
C	2.64152091283323	3.56990985432296	12.07077321147270
H	2.06342569619042	2.99704620971035	11.32651498597927
H	3.12525794721916	2.82709755563399	12.73211626514891
H	1.95961981768735	4.18447958895122	12.68097751970728
C	5.72777036192061	7.46580670887774	10.69544820371804
H	6.81597288859624	7.34942708775300	10.85393081462401
H	5.58057063669000	7.89427765279692	9.68661851617130
H	5.34707480038292	8.18938792359458	11.43385801024221
C	6.33443706449466	4.85900472243468	9.11523391895519
H	7.09344298822581	5.65536533315588	9.22513328356911
H	5.87507708985607	4.93938713992614	8.11364146721058

2 dimer isomer 1 (cut from crystal structure; position of H atoms were optimized)

Co	4.46617029848888	2.87570177426771	9.51448081537163
Cl	2.54841226842788	1.89922569516166	10.23907404970594
N	4.53252517184542	2.52332944370336	7.54300373095150
N	5.65438587530215	2.88010094042453	6.84647337209874
N	6.41192298125837	4.00418993519819	8.79537809708076
N	5.12894278932998	5.69088172229135	9.79854044708688
N	4.24741352145513	4.75061478077363	10.25291536204331
N	7.21694203887085	2.45023541430573	10.36895418431974
N	5.97587389795932	1.88047474534675	10.39704878580033
C	3.69963886663191	1.93980034778717	6.64273266312586
C	4.32744381544921	1.90988330920841	5.37569451055819
H	3.91190923483319	1.51233844124454	4.44855652438096
C	5.57935942201857	2.51439387622088	5.53310948247517
C	2.34154175803194	1.42918671935599	6.99517243055363
H	2.40086068406634	0.61649492696158	7.74029196356477
H	1.71883704945469	2.21809955451518	7.44917225544366
H	1.84092241298091	1.05380856029977	6.08819203949759
C	6.68788780719448	2.73602568996438	4.56086232964818
H	6.99099644984429	3.80063550032386	4.54950487061569
H	7.57894630124395	2.13168996970880	4.81696015007209
H	6.35735715557943	2.44661597530154	3.55084600807790
C	6.83323130163455	3.35250701103577	7.56345020174255
H	7.47749138791513	2.49478575266175	7.82847701689711
H	7.37926581108827	4.03882694433050	6.88857382234405
C	6.14197716249974	0.63395528924690	10.90139777828277

C	7.51000345730769	0.43279462437545	11.21082323761556
H	7.96323894031977	-0.46760254188315	11.63045470090153
C	8.17826765538377	1.61209644672575	10.85733413064563
C	5.01602591989297	-0.34098475615297	11.02467663586413
H	4.10312337409833	0.14905866074710	11.40211065773859
H	4.75988036357101	-0.77146415220154	10.03783173631511
H	5.30311688107288	-1.16884881931447	11.69371597177129
C	9.61964234355744	1.98918648616282	10.95376237642396
H	10.02385783930541	2.30142282825653	9.97293032657898
H	9.77733939208943	2.82434330972504	11.66120410046354
H	10.20358668530986	1.12454875898707	11.30763258745677
C	7.33538505412761	3.82498824947917	9.91192953454918
H	8.39203870898381	4.01018489073354	9.64588977213884
H	7.04321963180073	4.52248650075475	10.71623931116328
C	3.63277593489093	5.30181058653467	11.32993894343127
C	4.14513831438769	6.60478330718683	11.54398568531957
H	3.85758372694926	7.29908576758275	12.33612721420573
C	5.11316693193669	6.82605048858544	10.55575231807509
C	2.59877557014258	4.59094876214023	12.14132706155490
H	1.71335722355785	4.33819160779130	11.53301705484308
H	2.98495053624290	3.63532884920662	12.53671375602083
H	2.28553927174025	5.22903262365417	12.98407346320750
C	6.00853324325166	7.99167351412632	10.30285528435817
H	7.07377777042828	7.69722652397868	10.34538225261604
H	5.81047770950580	8.41815615591406	9.30156005296195
H	5.83282507679525	8.76707426930072	11.06561895215317
C	5.91306166531818	5.36866894566964	8.62710320675440
H	6.70621532751397	6.12740275915145	8.50775029210005
H	5.28436735190987	5.39872853748067	7.72010791205162
Co	4.81988379115876	6.84285545720201	5.39567569865321
Cl	6.99693228013008	6.18571886080494	5.46808240869266
Cl	4.35132012489738	8.08686805756376	7.23290660652131
Cl	4.52254683562216	8.24263981039321	3.63588117239435
N	3.53679671336519	5.34014895079226	5.15423716751518
N	3.41560191117994	4.71049523985574	3.94457787319296
N	3.81978203638540	5.68707229686899	1.78759086564508
H	4.35819188779155	5.52368268058688	0.93120686049512
H	3.90297169342951	6.68717392149803	2.03210300117631
C	2.46360583127818	4.95239437461294	5.89338416024473
C	1.64282290621374	4.10018967252477	5.11623224042151
H	0.71346395121560	3.62169276592498	5.42991863699307
C	2.27878099319034	3.95924321387946	3.87875975973744
C	2.27903794885345	5.33170231949070	7.32635651566579
H	2.85079002222127	4.64742559445652	7.98257665967655
H	2.63989649329962	6.35532477267468	7.52666724733189
H	1.21653181345879	5.24757905805962	7.61032144300153
C	1.92816224064255	3.15215882203384	2.67445500523165
H	1.90535670600667	3.78863712587092	1.77143885132496
H	2.67822670205483	2.35734884454078	2.49746852402274
H	0.94524178404007	2.67331477738325	2.81097919450452
C	4.39332486432352	4.91994861915361	2.87252773017878
H	5.26964483946038	5.38481043651916	3.37244159696308
H	4.70143026498309	3.92492882296921	2.50636435939447

2 dimer isomer 2 (cut from crystal structure; position of H atoms were optimized)

Co	9.84296131182642	11.07889209433022	2.97204153985834
Cl	11.81565444770722	12.13679131632745	2.55963481255943
N	9.72208276412201	10.96615827114078	4.98015948792977
N	8.50066572015480	10.68330737304716	5.52356179779054
N	7.78177983406011	10.02277386760718	3.38789693707607
N	9.09116247072253	8.32679067010002	2.41564405892481
N	10.01177239937780	9.27966801224487	2.08277943979706
N	7.21746355283193	11.80812014037873	1.96950801713598
N	8.47340123423019	12.30965120062679	2.16049162041367
C	10.59968024552835	10.98476991466184	6.01370578723906
C	9.90595133557121	10.72840848529644	7.22183172140724
H	10.33258575095262	10.67635266114964	8.22561483304783
C	8.56061919663590	10.53543451112768	6.87850331736282
C	12.06644199547703	11.19749858719699	5.82094696089912
H	12.25889242826756	12.03203697140591	5.12616639770162
H	12.54033865638185	10.30181954706067	5.37631282627662

H	12.55059903686109	11.39580742038935	6.79129732346310
C	7.35992002179631	10.23603177355897	7.71300707206646
H	6.81644216952115	9.35374235570123	7.32310736414543
H	6.65125838446219	11.08528526862822	7.72379865356140
H	7.66966340170998	10.03259904367579	8.75063645662085
C	7.34335139643555	10.61782008621808	4.64739146430626
H	6.96131510312983	11.63113371717689	4.43140323731473
H	6.54860350164647	10.03616569803820	5.14851804837478
C	8.40564407041823	13.62702084316828	1.84557667982933
C	7.08670481679012	13.94295220879362	1.43702720906849
H	6.71330506902903	14.92029935238107	1.12457219123514
C	6.34296331593162	12.75793254263134	1.52868146735828
C	9.57690013007199	14.54861162933967	1.96013298546619
H	10.38757029390959	14.25537217936975	1.27053665474911
H	10.00912213198348	14.51946871205112	2.97571329600861
H	9.26418017474909	15.58074678065602	1.73184587072689
C	4.91028146557308	12.46479154173810	1.22859403083703
H	4.42061031275346	11.93754613297100	2.07023276361147
H	4.80838049066829	11.82194595803741	0.33388043477269
H	4.37075914075635	13.40627111059002	1.03730447017346
C	6.98275310968935	10.39836141475224	2.22380423513515
H	5.89930193712937	10.24272373303630	2.37238848492106
H	7.31605639641726	9.78413658046272	1.36932789821573
C	10.78922933937171	8.73022288076124	1.11652011131765
C	10.35542344606464	7.40582094750851	0.86295086788460
H	10.77956420104078	6.70359237523008	0.14229077069975
C	9.26330129053393	7.17191722630409	1.71028777724178
C	11.88555908812683	9.48447185810226	0.43630292058043
H	12.51075743534530	10.02494348231540	1.16682017727737
H	11.47299457530524	10.24711567353903	-0.25100029619545
H	12.51010840824644	8.79284152671647	-0.15266993968825
C	8.40648599562718	5.96542121172084	1.90923792003479
H	7.33219439152928	6.21537030791178	1.81550530072674
H	8.55636790684208	5.52279937478913	2.91198084503266
H	8.65936360038556	5.20227079894864	1.15588811741633
C	8.13163505428857	8.60830393468116	3.46863797951741
H	7.26451702294353	7.93778679010855	3.33771711615176
H	8.57411366112907	8.41953999276168	4.46226260654592
Co	4.40531227724013	8.03055772663871	3.94923159589470
Cl	5.82254484324852	7.49391806464163	5.64693968449350
Cl	3.93589700626260	10.23746509531222	4.14544319023194
Cl	5.12279309963603	7.66200086144170	1.80830795452961
N	2.86864275632769	6.78726679556038	4.10483339554691
N	2.99995683953591	5.43398462392734	3.95908870141873
N	4.38933097073613	4.48259542658526	2.24465554247550
H	5.11518219807491	3.77238018331100	2.10853626705262
H	4.66677267425739	5.32475905576757	1.71912526182134
C	1.54669069174465	7.03073431703561	4.27984954244768
C	0.83372812048618	5.80807604903818	4.22648083093695
H	-0.24446432349017	5.67004023390725	4.33233774707139
C	1.78863329529287	4.80585231001181	4.01421123928049
C	1.01509830963614	8.40930504417711	4.51216834267252
H	1.25332199186868	8.76402295947057	5.53252876380219
H	1.46224811283774	9.13611497455720	3.81262774023669
H	-0.08139399472251	8.41694093973979	4.39568601959948
C	1.65361569161649	3.32859149650050	3.84838939961917
H	2.13351529051498	3.00130370079009	2.90798790005723
H	2.14091954390946	2.77975928126146	4.67665742894508
H	0.58897336136843	3.04564764345940	3.82807281448507
C	4.29819024929883	4.82421922703258	3.64952724569370
H	5.05125511231057	5.54941002860024	4.02109429136705
H	4.38644124994673	3.90929487276443	4.25979397839478