Electronic Supplementary Information

Copper(II) and silver(I) complexes with dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate: the influence of the metal ion on the antimicrobial potential of the complex

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Abstract

Dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate (py-2pz) was used as a ligand for the synthesis of new copper(II) and silver(I) complexes, $[CuCl_2(py\text{-}2pz)]_2$ (**1**), $[Cu(CF_3SO_3)(H_2O)(py\text{-}2pz)_2]CF_3SO_3\cdot 2H_2O$ (**2**), $[Ag(py\text{-}2pz)_2]PF_6$ (**3**) and $\{[Ag(NO_3)(py\text{-}2pz)]\cdot 0.5H_2O\}_n$ (**4**). The complexes were characterized by spectroscopic and electrochemical methods, while their structures were determined by single crystal X-ray diffraction analysis. The X-ray analysis revealed the bidentate coordination mode of py-2pz to the corresponding metal ion *via* its pyridine and pyrazine nitrogen atoms in all complexes, while in polynuclear complex **4**, the heterocyclic pyrazine ring of one py-2pz additionally behaves as a bridging ligand between two Ag(I) ions. DFT calculations were performed to elucidate the structures of the investigated complexes in solution. The antimicrobial potential of the complexes **1–4** was evaluated against two bacterial (*Pseudomonas aeruginosa* and *Staphylococcus aureus*) and two *Candida* (*C. albicans* and *C. parapsilosis*) species. Silver(I) complexes **3** and **4** have shown good antibacterial and antifungal properties with minimal inhibitory concentration (MIC) values ranging from 4.9 to 39.0 μM (3.9–31.2 μg mL^{-1}). All complexes inhibited the filamentation of *C. albicans* and hyphae formation, while silver(I) complexes **3** and **4** had also the ability to inhibit the biofilm formation process of this fungus. The binding affinity of the complexes **1–4** with calf thymus DNA (ct-DNA) and bovine serum albumin (BSA) was studied by fluorescence emission spectroscopy to clarify the mode of their antimicrobial activity. Catechol oxidase biomimetic catalytic activity of copper(II) complexes **1** and **2** was additionally investigated by using 3,5-di-*tert*-butylcatechol (3,5-DTBC) and *o*-aminophenol (OAP) as substrates.

Keywords: Copper(II) complexes; Silver(I) complexes; Nitrogen-containing heterocycles; Antimicrobial activity; DNA/BSA interaction; Catalytic activity

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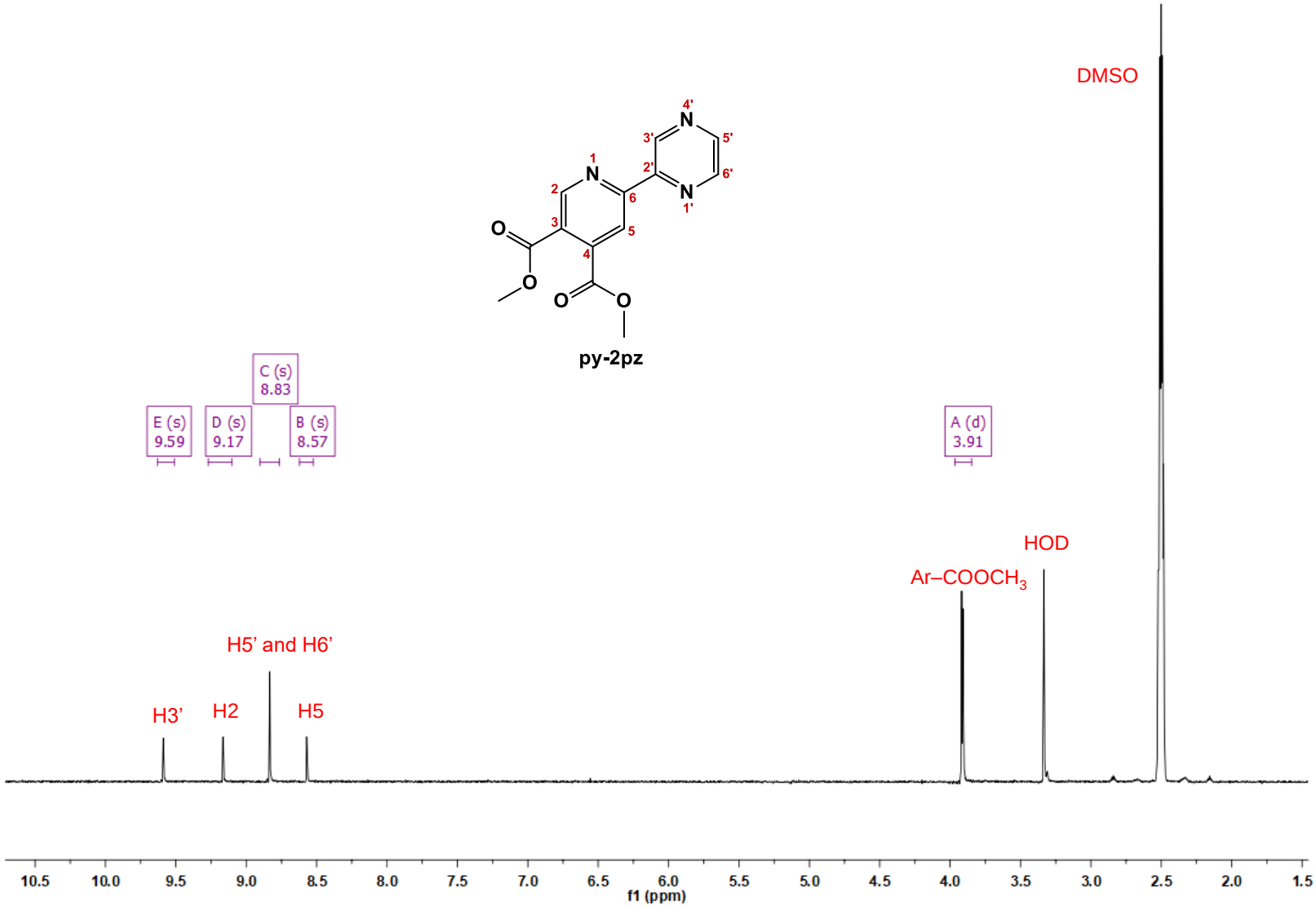
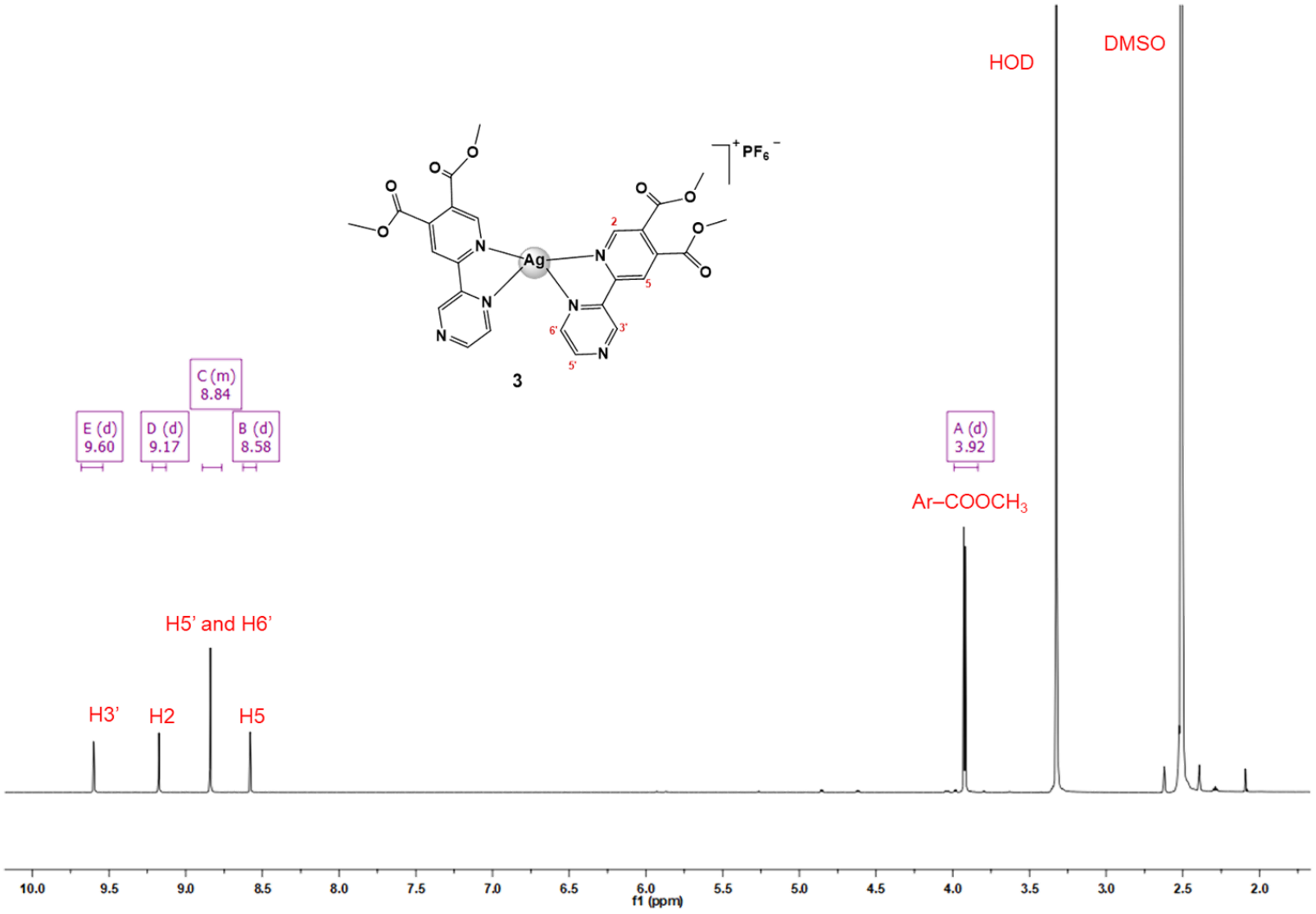
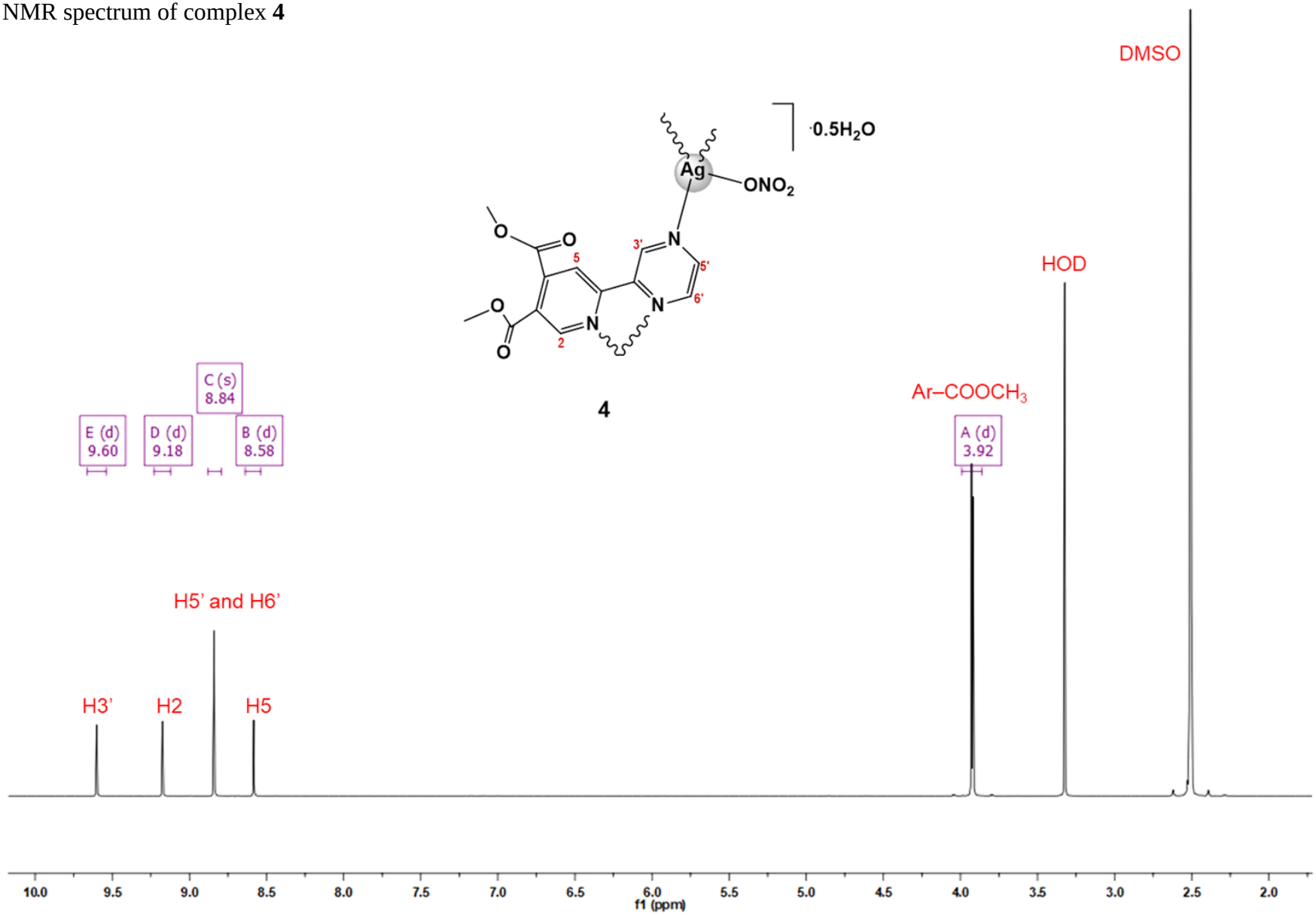
^{1}H NMR spectrum of py-2pz



^{1}H NMR spectrum of complex **3**



^{1}H NMR spectrum of complex **4**



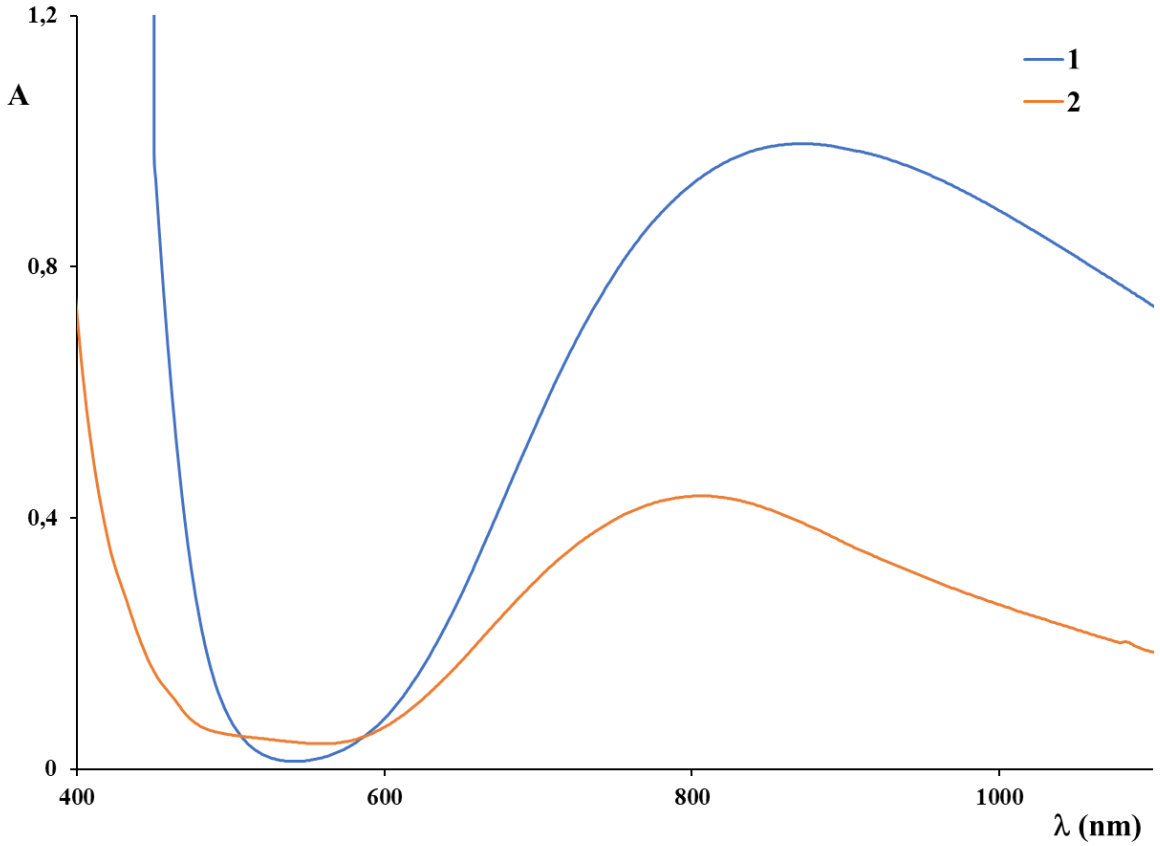


Fig. S1 UV-Vis spectra of copper(II) complexes **1** and **2** recorded in DMSO at room temperature.

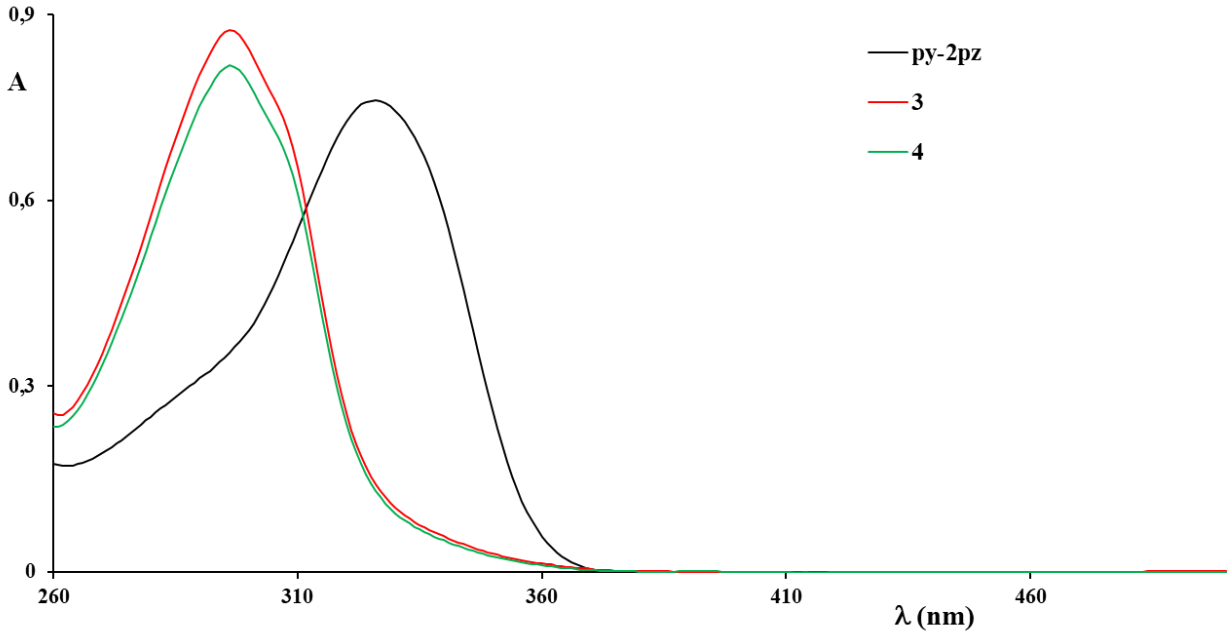


Fig. S2 UV-Vis spectra of silver(I) complexes **3** and **4** in respect to the spectrum of uncoordinated py-2pz recorded in DMSO at room temperature.

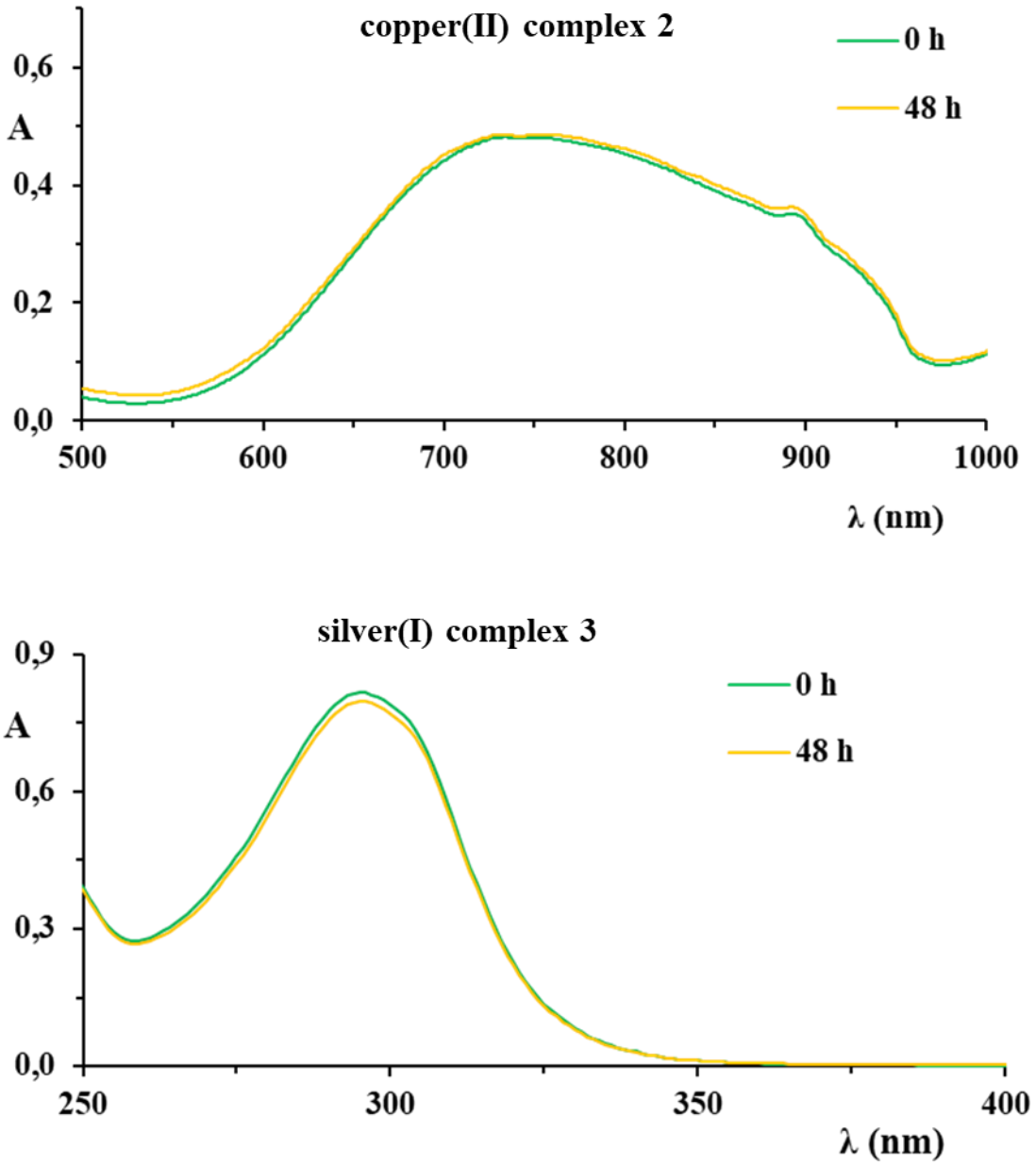


Fig. S3 Time-dependant UV-Vis spectra of copper(II) complex **2** and silver(I) complex **3** recorded in DMSO/PBS (*v/v* 2 : 1 and 1 : 42.9 for **2** and **3**, respectively) at room temperature.

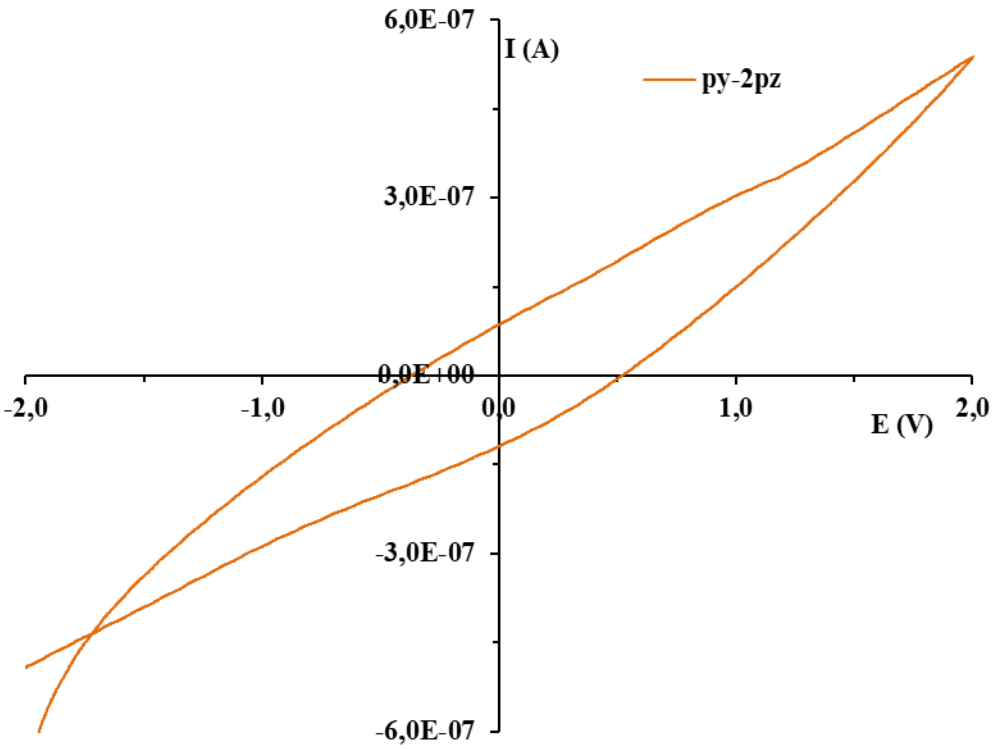


Fig. S4 Cyclic voltammogram of py-2pz ligand at GC electrode in DMSO (c = 1×10^{-3} M) and 0.1 M TBAHP as a supporting electrolyte with a scan rate of 50 mV s^{-1}.

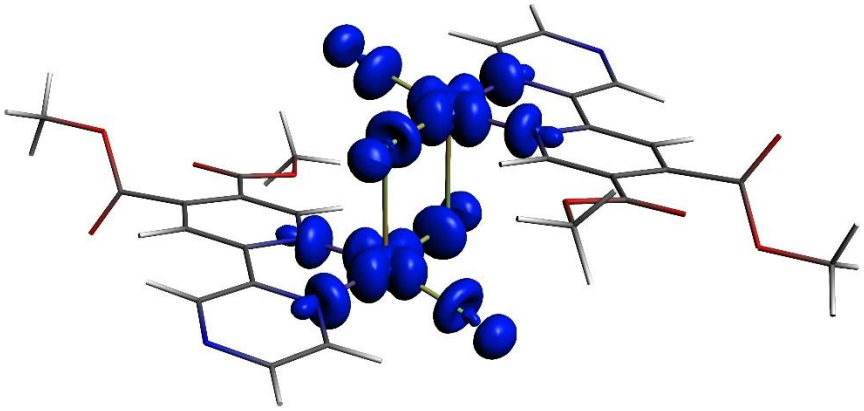


Fig. S5 Graphical representation of the spin density of the high-spin state of **1**. Isosurfaces were drawn at 0.003 a.u. with α-spin depicted by blue surfaces.

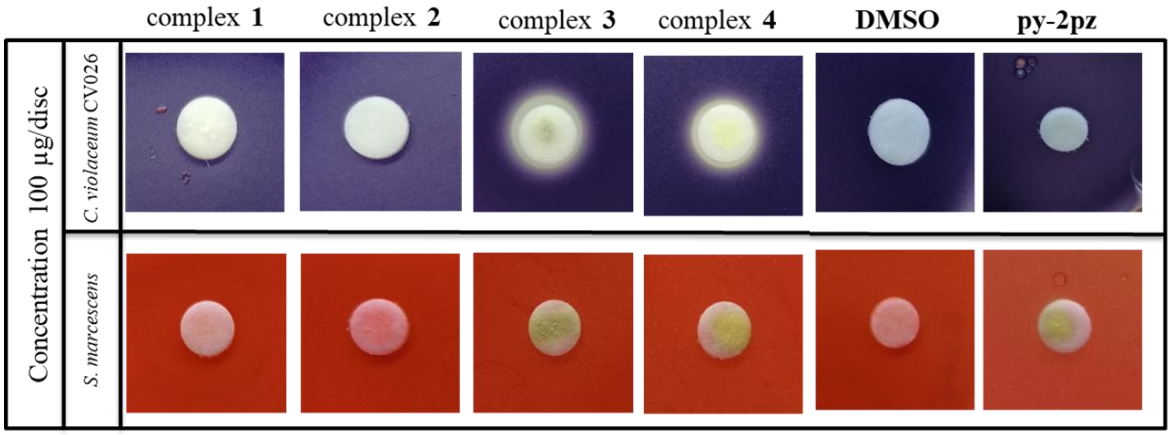
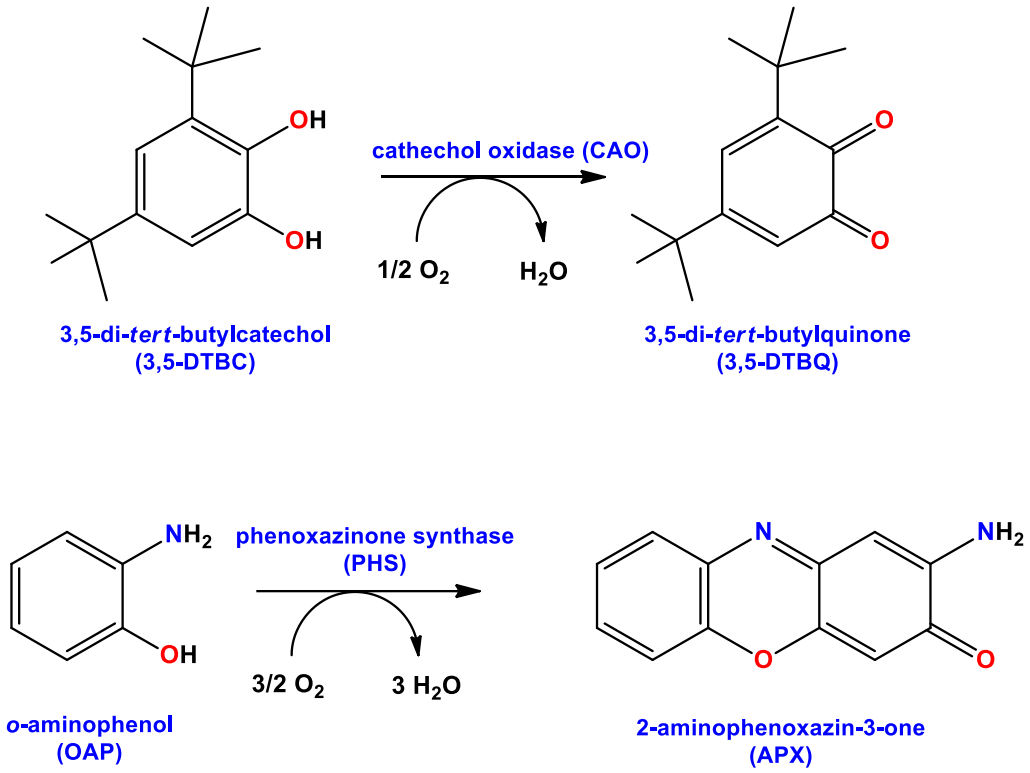


Fig. S6 Inhibition of violacein and prodigiosin production in the presence of complexes **1 – 4** and py-2pz ligand tested on *Chromobacterium violaceum* CV026 and *Serratia marcescens* at 100 µg per disc concentration. DMSO was used as a control.



Scheme S1 Catechol oxidase (CAO) and phenoxazinone synthase (PHS) activity.

Table S1 *C. albicans* ATCC10231 biofilm inhibition (%) in the presence of silver(I) complexes **3** and **4** in range of subinhibitory concentrations

Concentration (μg mL^{-1})	**3**	**4**
3.5	51 ± 5	62 ± 4
1.75	51 ± 7	nd[a]
0.87	36 ± 3	nd
0.44	32 ± 5	nd

[a]nd = not detected.

Table S2 Details of the crystal structure determination for copper(II) complexes **1** and **2**

Complex	**1**	**2 (solution 1; solvent mask)**	**2 (solution 2; constrained triflate)**
Empirical formula	$C_{26}H_{22}Cl_4Cu_2N_6O_8$	$C_{27}H_{26}CuF_3N_6O_{13}S$	$C_{28}H_{28}CuF_6N_6O_{17}S_2$
Formula weight	815.37	795.14	962.22
Temperature/K	149.5(8)	150.05(10)	150.05(10)
Crystal system	triclinic	triclinic	triclinic
Space group	*P*$\bar{1}$	*P*$\bar{1}$	*P*$\bar{1}$
a/Å	7.7916(6)	8.2856(3)	8.2856(3)
b/Å	8.9848(6)	12.1191(5)	12.1191(5)
c/Å	11.9955(7)	19.2393(6)	19.2393(6)
α/°	104.394(6)	82.105(3)	82.105(3)
β/°	106.396(6)	86.220(3)	86.220(3)
γ/°	104.368(6)	77.071(3)	77.071(3)
Volume/Å^3	733.10(9)	1863.83(12)	1863.83(12)
Z	1	2	2
ρ_{calc}/g cm^{-3}	1.847	1.417	1.715
μ/mm^{-1}	1.877	0.723	0.812
F(000)	410.0	812.0	978.0
Crystal size/mm^3	0.2 × 0.05 × 0.05	0.2 × 0.15 × 0.1	0.2 × 0.15 × 0.1
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.982 to 54.952	5.162 to 58.918	5.162 to 58.918
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 11, -15 ≤ l ≤ 11	-10 ≤ h ≤ 11, -15 ≤ k ≤ 15, -26 ≤ l ≤ 25	-10 ≤ h ≤ 11, -15 ≤ k ≤ 15, -26 ≤ l ≤ 25
Reflections collected	6360	14431	14431
Independent reflections	3355 [R_{int} = 0.0270, R_{sigma} = 0.0520]	8653 [R_{int} = 0.0272, R_{sigma} = 0.0516]	8653 [R_{int} = 0.0272, R_{sigma} = 0.0516]
Data/restraints/parameters	3355/0/210	8653/0/468	8653/0/534
Goodness-of-fit on F^2	1.070	1.026	1.026
Final R indexes [I ≥ 2σ (I)]	R_1 = 0.0339, wR_2 = 0.0676	R_1 = 0.0390, wR_2 = 0.0861	R_1 = 0.1091, wR_2 = 0.2941
Final R indexes [all data]	R_1 = 0.0457, wR_2 = 0.0748	R_1 = 0.0508, wR_2 = 0.0916	R_1 = 0.1249, wR_2 = 0.3109
Largest diff. peak/hole / e Å^{-3}	0.41/-0.42	0.40/-0.43	9.72/-2.38
Flack parameter	/	/	

Table S3 Details of the crystal structure determination for silver(I) complexes **3** and **4**

Complex	**3**	**4**
Empirical formula	$C_{26}H_{22}AgF_6N_6O_8P$	$C_{13}H_{12}AgN_4O_{7.5}$
Formula weight	799.33	452.14
Temperature/K	150.00(10)	150.00(10)
Crystal system	triclinic	monoclinic
Space group	$P\bar{1}$	$P2_1/n$
a/Å	7.4731(4)	11.0042(12)
b/Å	11.7049(4)	12.8657(8)
c/Å	17.6092(8)	12.5820(12)
α/°	97.285(4)	90
β/°	96.617(4)	115.436(13)
γ/°	102.781(4)	90
Volume/Å^3	1473.58(12)	1608.6(3)
Z	2	4
ρ_{calc} g cm^{-3}	1.801	1.867
μ/mm^{-1}	0.837	1.303
F(000)	800.0	900.0
Crystal size/mm^3	0.25 × 0.1 × 0.1	0.3 × 0.3 × 0.1
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.472 to 54.966	4.782 to 54.958
Index ranges	-8 ≤ h ≤ 9, -14 ≤ k ≤ 15, -19 ≤ l ≤ 22	-14 ≤ h ≤ 13, -16 ≤ k ≤ 12, -16 ≤ l ≤ 12
Reflections collected	11043	6610
Independent reflections	6475 [R_{int} = 0.0302, R_{sigma} = 0.0524]	3459 [R_{int} = 0.0168, R_{sigma} = 0.0263]
Data/restraints/parameters	6475/0/456	3459/0/240
Goodness-of-fit on F^2	1.027	1.022
Final R indexes [I ≥ 2σ (I)]	R_1 = 0.0370, wR_2 = 0.0779	R_1 = 0.0312, wR_2 = 0.0729
Final R indexes [all data]	R_1 = 0.0528, wR_2 = 0.0854	R_1 = 0.0409, wR_2 = 0.0788
Largest diff. peak/hole / e Å^{-3}	0.60/-0.60	0.93/-0.71
Flack parameter	/	/

Cartesian coordinates of all DFT optimized structures

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$C_{26}H_{22}Cl_4Cu_2N_6O_8$ optimized with ADF in AMS. Complex **1** - optimized Hs ZORA-BP86-D4/DZP

Cu	-1.09882700000000	2.27236000000000	5.36626300000000
Cl	-2.41871600000000	3.56749400000000	6.67850600000000
Cl	-0.60355600000000	3.97927100000000	4.02580500000000
O	-1.95250100000000	-3.59509000000000	9.06289900000000
O	0.16001800000000	-3.05798200000000	9.63021500000000
O	-2.60008200000000	0.85465100000000	10.44259700000000
N	0.14088400000000	0.98245100000000	4.40264700000000
N	-1.09632600000000	0.72272600000000	6.69050500000000
O	-2.08947400000000	-1.27301200000000	10.89694800000000
N	1.57892800000000	-1.06600300000000	3.17818200000000
C	-0.50182400000000	-1.57443600000000	6.97254200000000
C	-0.51575700000000	-0.41044800000000	6.22772300000000
C	0.16430600000000	-0.25656800000000	4.92618200000000
C	0.85584800000000	1.20707600000000	3.30790300000000
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C	-2.13185600000000	-0.34107600000000	10.13450800000000
C	-3.10631600000000	0.98971400000000	11.80143200000000
C	-1.84647500000000	-4.82532100000000	9.83182400000000
H	-1.63450311055476	-5.64783099581682	9.14051381633331
H	-2.82096639413989	-4.96723014268033	10.30490739658884
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Cu	-4.51676400000000	2.48582100000000	5.44387900000000
Cl	-3.19687600000000	1.19068700000000	4.13163600000000
Cl	-5.01203500000000	0.77891000000000	6.78433700000000
O	-3.66309100000000	8.35327100000000	1.74724300000000
O	-5.77561000000000	7.81616300000000	1.17992700000000
O	-3.01551000000000	3.90353000000000	0.36754500000000
N	-5.75647600000000	3.77573000000000	6.40749600000000
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O	-3.52611800000000	6.03119400000000	-0.08680500000000
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C	-6.47144000000000	3.55110600000000	7.50223900000000
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C	-6.46985200000000	6.03523300000000	6.53148800000000
C	-4.74283900000000	7.57533000000000	1.72529900000000
C	-3.97490700000000	4.04363100000000	2.90252300000000
C	-7.20483900000000	4.57081100000000	8.08274300000000
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H	-3.98108880978845	10.40601252264146	1.66962869971585
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H	-2.26583710511892	2.71006321452930	-1.09815170378976
H	-3.27842619615475	4.07542368443615	-1.70689429503271

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$C_{26}H_{22}Cl_4Cu_2N_6O_8$ optimized with ADF in AMS. Complex **1** - optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

Cu	1.69169526792667	0.06663691998131	-0.28996263357283
Cl	0.50450949816236	1.47212266030495	1.07026567589232
Cl	1.94868472420777	1.67633980432282	-1.85927564876745
O	0.90326877929972	-5.77328394787722	3.12016579842339
O	2.55645494311177	-5.04808732180215	4.52082631209871
O	0.25568409719570	-1.09638080206521	4.84873659669983
N	2.81268395620469	-1.29166800828031	-1.29181675328885
N	1.86858171153743	-1.36195041414669	1.14077122624091
O	0.02466082388054	-3.35954117582281	5.03167267956160
N	4.28998292083620	-3.35195777450874	-2.44785002704143
C	2.41342929111539	-3.67017638326029	1.49500086357414
C	2.43908008950680	-2.51612085449950	0.71548398363292
C	3.03133810726006	-2.44495723498136	-0.62111253109655
C	3.31127425913528	-1.16601155007186	-2.52449062968252
C	1.78637902024023	-3.63603836329252	2.73889287501903
C	3.78390555660179	-3.46504125156589	-1.21586852787887
C	1.78630327069986	-4.87792008771235	3.58753847315084
C	1.28543497641607	-1.32133273649997	2.33838039834071
C	4.04706881442850	-2.20503818819005	-3.09801085003332
C	1.21802904976656	-2.43541713247143	3.17717162287249
C	0.44551831777754	-2.36761135814320	4.44708728120192
C	-0.56953591510785	-0.94480068617823	6.04029964312863
C	0.84657142501853	-7.03173091837223	3.86458444382964
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H	-0.09871088190696	-1.45183792260690	6.88954663742462
Cu	-1.69169526792667	-0.06663691998131	0.28996263357283
Cl	-0.50450949816236	-1.47212266030495	-1.07026567589232
Cl	-1.94868472420777	-1.67633980432282	1.85927564876745
O	-0.90326877929972	5.77328394787722	-3.12016579842339
O	-2.55645494311177	5.04808732180215	-4.52082631209871
O	-0.25568409719570	1.09638080206521	-4.84873659669983
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C	-3.78390555660179	3.46504125156589	1.21586852787887
C	-1.78630327069986	4.87792008771235	-3.58753847315084
C	-1.28543497641607	1.32133273649997	-2.33838039834071
C	-4.04706881442850	2.20503818819005	3.09801085003332
C	-1.21802904976656	2.43541713247143	-3.17717162287249
C	-0.44551831777754	2.36761135814320	-4.44708728120192
C	0.56953591510785	0.94480068617823	-6.04029964312863
C	-0.84657142501853	7.03173091837223	-3.86458444382964
H	-1.82521819922605	7.52206398503384	-3.83735118434247
H	-0.09297682820691	7.63126292590676	-3.35071367247309
H	-0.55082625919636	6.83033277614849	-4.89973429968171
H	-2.85819908727319	4.59289233280181	-1.13164424408509
H	-3.11407841196027	0.22388153182369	3.03430817022971
H	-3.98419490333949	4.39295686146135	0.68144237809653
H	-0.82541910214921	0.37627477121198	-2.61562502535641
H	-4.44928812977018	2.10006113925289	4.10544099946262
H	1.56488711467934	1.36501824845537	-5.85718398316668
H	0.62530328638142	-0.13197754939085	-6.21279621242686
H	0.09871088190696	1.45183792260690	-6.88954663742462

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$C_{13}H_{11}Cl_2CuN_3O_4$ optimized with ADF in AMS. $[CuCl_2(py\text{-}2pz)]$ optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

Cu	2.01524422081029	-0.03977526118906	0.15004757278396
Cl	0.28889569866991	1.05996375711591	1.08190983727625
Cl	2.90041536527344	1.75632963785443	-0.86867315721953
O	0.86147696706201	-5.85219233869379	3.69270946987489
O	3.06684285142075	-5.61020403330232	4.24156557717497
O	0.04782514211418	-1.62039884984689	4.98106944454335
N	2.95717735201806	-1.39106741604332	-0.99840036060720
N	1.92442828735795	-1.62562820740219	1.37930064564904
O	0.98312803381237	-3.60150867410016	5.61574393074544
N	4.15015546889004	-3.47470491997635	-2.40538054263916
C	2.55682237428097	-3.91955085060276	1.65921534123774
C	2.51533218770760	-2.75057813502671	0.90368016234134
C	3.07490252965560	-2.61856272700346	-0.44316931339814
C	3.42115274079171	-1.19844809787455	-2.23587816576598
C	1.97441028146307	-3.93250885973317	2.92334948646067
C	3.68462231059305	-3.65118937371614	-1.16414829128616
C	2.03619561626450	-5.20680926642631	3.72237111575076
C	1.37263740429684	-1.62938359535399	2.59488347229693
C	4.01182714019754	-2.25273782151248	-2.93721780325593
C	1.37286946108308	-2.76350865183693	3.41016061841228
C	0.78974493652085	-2.72513200356295	4.78104136497460
C	-0.53024118303054	-1.50269412114927	6.31631244790073
C	0.82802231252543	-7.10300050799232	4.45178003432508
H	1.57535011645677	-7.79822233954084	4.05613105692788
H	-0.18186275639545	-7.49194609899882	4.31192923769937
H	1.02564151943506	-6.89216459287810	5.50802960900484
H	3.03222246385467	-4.81533687523336	1.26787314181570
H	3.32533654299206	-0.19699118560155	-2.65114687261366
H	3.79486797534401	-4.64488325670191	-0.73115494578563
H	0.91082791128119	-0.69811741718764	2.91568265937899
H	4.38226433431247	-2.09525237571888	-3.94997511550995
H	-1.17332767381950	-2.36516910712199	6.51967139831103
H	-1.11038556919361	-0.57864632764788	6.29382413194396

H	0.27010713595365	-1.44518510599424	7.06184831125152

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$C_{27}H_{24}CuF_3N_6O_{12}S$ optimized with ADF in AMS. Complex **2** - optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

Cu	7.57762545208314	9.50421070649117	13.57688246295078
S	4.10440494380832	8.35929566492817	12.59102399655067
O	6.25424550125495	11.07495120284678	14.27721717931177
H	6.34407431050657	11.29611981122932	15.22537343068375
H	5.45089765814027	10.49141124969528	14.21432734786140
O	5.40594220339384	13.61823829477737	10.90341969431786
O	5.38903129529990	13.26050663280336	8.64689099961499
O	6.91563131280888	11.21694544870495	6.88552218607629
O	4.97315071032565	8.85342968520385	13.70403531611169
O	9.04130987373445	5.64864610575634	18.97259006525080
O	6.13483100149199	6.15111038444258	19.01690554952227
O	8.87247912603928	7.57401403030935	20.19923346763283
N	7.22666928317369	10.10084549140275	11.72963556258175
O	5.25732785122930	5.97330950588740	16.91430910301123
N	7.79735039796456	8.76895255408397	15.40193814810039
O	4.81397415981297	8.08294239981971	11.33336942710774
N	7.93732227128728	7.74821011093435	12.61891990845794
N	9.37695774230176	10.46794340174535	14.13632285077621
F	2.87085996689758	5.98923887232416	12.33748675284216
F	4.76794750221613	5.91149851901368	13.45522458708234
O	2.82006859351140	9.06847932917124	12.47290986294002
O	4.79554994660810	10.51265205058884	7.38204388662157
N	11.76894251961102	11.44025934512181	15.20098617318224
F	2.96194066883020	6.74243986404039	14.40555055882256
C	9.81869188389904	10.05217323887614	15.34647294777655
C	8.95385126249949	9.08776106732035	16.04370295214892
C	7.37503375829329	9.14524558691177	10.77485534395287
C	6.27633157748576	11.58562493572840	10.10895848018853
C	6.70235522717627	11.28915368020701	11.40504888869176
H	6.59774625558257	12.01190768271855	12.21027768211201
C	8.37956069808277	7.59533560016600	17.84705377103480
C	7.02164511021723	9.39094238810119	9.45009547998388
H	7.14541270293608	8.61703763152509	8.69671216113887
N	8.53694268755831	5.57329091174357	10.97484731836587
C	5.64944280934492	12.90306270752626	9.78967910413941
C	6.92278076541977	7.92218656339508	15.96415320352133
H	6.00255177846135	7.73881228501313	15.41122059054472
C	6.44844553569797	10.61363560358729	9.11138402081320
C	8.32053405642328	6.57791813563087	13.14039350935969
H	8.39903999908263	6.49869220425046	14.22228666105008
C	7.17075135847050	7.30698689521459	17.19290199591697
C	5.93831243531878	10.80241697463855	7.70381830324345
C	7.84608370594807	7.85137466747278	11.27193926353871
C	10.11739619313441	11.35283130362282	13.46456194866100
H	9.75769705440971	11.67959363847387	12.48947625292081
C	11.02156362017324	10.54824188422724	15.86496886168869
H	11.39172851234991	10.22547528895526	16.83793816763395
C	9.26193291641635	8.50828514785621	17.27530764939377
H	10.19348123968456	8.74993613911708	17.78093434708047
C	6.14683659351125	6.41592472148747	17.82119558851763
C	11.31363727192444	11.83912025631443	14.00407772679762
H	11.91024322264024	12.56624689754973	13.45260866682368
C	8.76588067029265	6.94848614689912	19.15446751683214
C	8.16148165819485	6.75140768722886	10.46371529613499
H	8.11010899033711	6.82596701619937	9.37768463578830

C	8.60946211407525	5.49014674186540	12.31157867542118
H	8.90782537920016	4.53638766870497	12.74685904604647
C	6.51115200592110	11.41026450360539	5.48867995136336
H	6.14464830876406	10.46462253983554	5.07591904035364
H	7.41729609983879	11.73818790503346	4.97655846274343
H	5.73050809077389	12.17691257873906	5.43989812674372
C	4.78234386298482	14.92192721657072	10.68167975039717
H	3.82014489232548	14.78913624103896	10.17548774541658
H	5.44609667914621	15.55067998994452	10.07814591671426
H	4.64457832649724	15.34216234583240	11.67979174712197
C	9.40211423455994	4.91221565741183	20.18768412832201
H	9.59653206092005	3.89241913805137	19.85088912457229
H	8.56253240659517	4.94169957064962	20.89055981554749
H	10.29577419951430	5.35539783211517	20.63944913850006
C	3.64588701513855	6.64949677107692	13.23508980537727
C	4.19571858725098	5.12357108551964	17.45292112310279
H	3.58969322133736	4.84628417035547	16.58864949455459
H	3.60552802404169	5.68848696737564	18.18262108000012
H	4.63494427285124	4.23791653471916	17.92432746356618

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$C_{27}H_{22}CuF_3N_6O_{11}S$ optimized with ADF in AMS. $[Cu(CF_3SO_3)(py\text{-}2pz)_2]^+$ optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

Cu	7.54552571843897	8.95166850607592	13.33401220372621
S	4.22679692542082	8.52440056414214	13.02576425875856
O	6.35595327058178	13.65312670735941	10.93475629079591
O	5.30545184903444	13.24281087638219	8.94699398910341
O	7.04829657615980	11.75479133142947	7.08449841153130
O	5.40583535919790	8.98579225478864	13.83506570648744
O	9.04719007185680	6.34205160522411	19.54024711219585
O	6.18565927299323	5.86559453723862	18.91685213546695
O	8.02388502052489	8.27627051453650	20.21130831541110
N	7.14693245057541	9.71345312515459	11.55982765812741
O	5.89829309729519	5.11915093373450	16.77530958641077
N	7.82159318785368	8.31499097962855	15.18090084288835
O	4.52995975765832	8.17543024202683	11.63113288840570
N	7.69390440084584	7.23720424377444	12.22240452309265
N	8.95034991457768	10.29372198350683	13.90991659040323
F	2.71193186625927	6.32795646339541	13.24866834395359
F	4.84954849793406	5.98927250403807	13.65208925851715
O	3.02572487890707	9.33792746705732	13.26174025257271
O	5.08031856320111	10.58557733409767	7.04329098542273
N	11.03249651893089	11.83046778270202	14.96237657670904
F	3.59220614258020	7.00448986252688	15.15048632592480
C	9.37979882727493	10.10542198521087	15.18190432123565
C	8.69615356889550	9.04371532670495	15.92222326178874
C	7.13823715618637	8.82800741546706	10.53107978823352
C	6.41818225135309	11.46081485185889	10.09541442980144
C	6.77719868987562	10.98321144584276	11.35781753071427
H	6.75563128892410	11.63853110719900	12.22685668483846
C	8.16582522072578	7.74438218259300	17.87653214962304
C	6.79705183865201	9.23567944633649	9.24280718249286
H	6.79726568284067	8.52561428236818	8.41947042677077
N	7.79335971378817	5.12479977097983	10.40109086296904
C	5.96264953142859	12.87283071983348	9.91155132436976
C	7.12151778483232	7.33048631047646	15.75352039285734
H	6.41294643947030	6.79841052624563	15.12486098394607
C	6.44672885518407	10.56397916891782	9.01535573945516
C	7.98192352489762	5.99617538961285	12.62577963989192
H	8.18558666740408	5.83702990715529	13.68342400028430

C	7.26172718946242	7.00060292828824	17.10262154837798
C	6.08795432732623	10.98136508717599	7.61051853260212
C	7.46481511168203	7.44697636168569	10.90388147080314
C	9.56303715020950	11.22271935428908	13.16799580817596
H	9.23594637247647	11.35748784205870	12.13944181191571
C	10.42476564137992	10.88662729712636	15.69057558142593
H	10.78366113765533	10.73847775274604	16.70888440280879
C	8.88265408263648	8.77722504407496	17.27733455967532
H	9.57578272354112	9.37309966934951	17.86629052246651
C	6.40400075419843	5.94074300305391	17.71445962238563
C	10.60059088149780	11.99193851266516	13.70369008392739
H	11.08772121415419	12.75050497493321	13.09084968854773
C	8.37502318403564	7.48551087969651	19.34749212829912
C	7.52430837415027	6.37504172511883	10.00495235432801
H	7.34675286340618	6.52763990246025	8.94061984548150
C	8.02377597840976	4.94074540524092	11.70937801036292
H	8.24795657048126	3.92926671258653	12.04834728751930
C	6.77879850176189	12.24395743124935	5.72872739974593
H	6.64894978691786	11.39684644344126	5.04738547090208
H	7.65859867899265	12.83194954462071	5.46158452458250
H	5.87790074080416	12.86653364591145	5.74239052765503
C	5.92142463494297	15.04775949181961	10.85075556500263
H	4.82704744454062	15.09307239430288	10.83773304237786
H	6.33138744710466	15.50682393294472	9.94469175688809
H	6.32296641704395	15.52316989126611	11.74779057505637
C	9.28711480419664	5.99177705617096	20.94371741139625
H	9.84385300464731	5.05372759342595	20.90823904378649
H	8.32635021897125	5.86146144684949	21.45320122446123
H	9.87339199575833	6.77985760388959	21.42721181961030
C	3.81454411754517	6.86542770308091	13.81958907091544
C	4.98562866753903	4.09081628383749	17.27470823623734
H	4.69049070345953	3.52197679276484	16.39104446670434
H	4.11740727570895	4.56646678614848	17.74395450209349
H	5.50535977593383	3.45332259405827	17.99733965951810

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$C_{26}H_{24}CuN_6O_9$ optimized with ADF in AMS. $[Cu(H_2O)(py\text{-}2pz)_2]^{2+}$ optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

Cu	7.50343770306860	9.20146294529396	13.48609863638251
O	5.79491579135874	10.47466569499444	14.17643242061880
H	5.77336935477793	10.69235303245756	15.12913480723067
H	4.90403244441310	10.11502769086539	13.99433508286449
O	6.39194311826005	13.78552655205151	10.89864142811426
O	5.68524361351384	13.39832548035636	8.76118304068277
O	7.11566649823836	11.45207140810126	7.01423216183780
O	9.37519463171625	6.12729624842566	19.30420184234701
O	6.45089465976791	5.81590972405871	19.01054658342359
O	8.51108689473709	8.00149556026232	20.29525697711486
N	7.05763014677220	9.87570393626651	11.68450571903197
O	5.76593396925198	5.38263770311979	16.87354576576162
N	7.78009835635526	8.54302622321482	15.32774063652519
N	7.48170492728158	7.43492857172961	12.49929594825532
N	8.99961585835625	10.48315022727757	14.05381929318348
O	4.95301669532152	10.72121958939244	7.18432468889773
N	11.07309176544555	12.00141078613557	15.14525682567878
C	9.44657142814970	10.24600598667837	15.31155972988783
C	8.76619143521549	9.16327949474037	16.03047976398955
C	6.97753588779551	8.93036306482018	10.71163126614351
C	6.46273576160097	11.57633048156743	10.10786227952715
C	6.78881566964081	11.15484329725477	11.39898580737142

H	6.81739944315954	11.86112202747970	12.22589779736102
C	8.35674675357231	7.72279945812576	17.91655063135904
C	6.65195442853515	9.27758198856052	9.40244297080892
H	6.58728215580147	8.51512208514753	8.63001773684805
N	7.54207826373210	5.21357785651843	10.80482207196487
C	6.13802261711005	13.00838318606111	9.83030605715648
C	7.06096915203228	7.56871998873937	15.89969939917621
H	6.25179639571035	7.13847835452309	15.31249618630693
C	6.40705816939311	10.61292884515684	9.08926855557850
C	7.76617663943351	6.21602993992406	12.97073002533959
H	7.98510183528161	6.11107665459335	14.03089624141895
C	7.31904955834994	7.11305302669602	17.19427158780197
C	6.05188307104352	10.95899163133074	7.66353473739118
C	7.24605480715540	7.56653979402147	11.17003599800265
C	9.58853624963988	11.45134097055481	13.34567426816272
H	9.24195872316709	11.62575879189162	12.32884700712905
C	10.48884804576961	11.01778577472576	15.84025479562058
H	10.85935109572830	10.83938471562056	16.84936488406316
C	9.06614116962239	8.77060774269445	17.33400843617603
H	9.85581107374791	9.26810633757620	17.89167126948874
C	6.47794726154883	6.03943057960221	17.80718790483902
C	10.62354666554757	12.21234115319816	13.90050947699943
H	11.08712104331017	13.01183851106665	13.32162925520740
C	8.72634855021535	7.29961046544756	19.31799585696693
C	7.28200603833927	6.44021754828571	10.33845540011197
H	7.09541334225894	6.53395560732399	9.26892952658053
C	7.78822082547256	5.10817641151390	12.11775156583999
H	8.01288967218743	4.11908779527626	12.51685415967435
C	6.87250256669330	11.81819748776662	5.61478741987791
H	6.54868608486934	10.93646902361411	5.05257322810649
H	7.83301026941281	12.18660471651275	5.24983890079612
H	6.10803443656909	12.60143695159817	5.57330268539560
C	6.06612286014952	15.20078333715822	10.73088968916553
H	5.00015114073727	15.30999664518967	10.50453760585348
H	6.67189515387996	15.62627431284496	9.92386438512597
H	6.31256437143496	15.65808945016783	11.69042738438367
C	9.76778945472332	5.61907639906883	20.62325161409728
H	10.27312661180160	4.67308664125676	20.42029496153133
H	8.87113057853625	5.46475557132967	21.23311232687884
H	10.44294864538380	6.33149010790243	21.10810400751818
C	4.88159647949004	4.33786956686235	17.39061607706747
H	4.38081318670332	3.93107940315852	16.51005995995250
H	4.15934350073411	4.77803812147365	18.08626344470525
H	5.47642706547052	3.56949122552275	17.89585798353583

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$C_{26}H_{22}CuN_6O_8$ optimized with ADF in AMS. $[Cu(py\text{-}2pz)_2]^{2+}$ optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

Cu	8.20229383996006	8.88303938742404	13.22537702325915
O	6.78713941642581	13.68652519183885	11.17704980668513
O	5.82301441823789	13.45935520883061	9.11912925987975
O	6.42931379705636	11.34121279037146	7.04031480788071
O	8.82583403846876	6.67362315107765	19.71488439916211
O	6.19188321211776	5.78942604236884	18.66455257428208
O	7.40575116874218	8.42773010436875	20.09653009282862
N	7.46934136681478	9.71622830772516	11.60032293753622
O	6.17954328948619	5.04664355922992	16.50317729411830
N	8.12956437075882	8.32028852384322	15.11324961353062
N	7.89330894644585	7.21428817305296	12.20614590584901
N	9.36627282865719	10.30491731185257	13.95995963410906
O	4.33324060811823	11.00045058432477	7.89431689842349

N	11.10638574873041	12.04045507120848	15.26465183349029
C	9.54738579346926	10.21873470732169	15.29947065804434
C	8.80454914295477	9.14419783440338	15.96146741026215
C	7.10919925913558	8.82668474277279	10.63517747565419
C	6.61156583734942	11.52056134690268	10.27917047169207
C	7.21491362776765	11.01909628160656	11.43586121231489
H	7.49512829899208	11.68873428292232	12.24599336544386
C	8.04153136089877	7.87183984701215	17.85318092783471
C	6.50104791894719	9.25399959766087	9.45911903488151
H	6.21428875835048	8.53437429476369	8.69600497299349
N	7.51005765601587	5.08698184398280	10.45194324096949
C	6.35762831116689	12.98382458613479	10.11372791221856
C	7.41053459417722	7.30526199666612	15.60427745643111
H	6.86053065052357	6.69270946674586	14.89333849148761
C	6.25484108314266	10.61390944521444	9.27025373896252
C	8.21480536400576	5.96700378517018	12.56738854771634
H	8.63738408140127	5.81116858008721	13.55811307311890
C	7.34560265922599	7.03059354129266	16.97327387105063
C	5.54993918851549	11.03961559456893	8.00480095319418
C	7.39813274718894	7.42789667743000	10.96237166971168
C	10.05444367680634	11.22299462013478	13.27216340547725
H	9.92068432167322	11.26281999236832	12.19292409194290
C	10.42437920457760	11.10599632009052	15.93629577426096
H	10.58645708998482	11.05012374078605	17.01246195500186
C	8.76440134156167	8.94681652433175	17.33783767339982
H	9.29508225011612	9.61962892540453	18.00724100633651
C	6.51609461208604	5.89926143814986	17.48867604883024
C	10.92625059386607	12.09172994451995	13.93788311527092
H	11.48444528466219	12.83963918437284	13.37480727769996
C	8.02138928168477	7.68068660800633	19.34982849082084
C	7.21302418917928	6.34249738982790	10.09704206322361
H	6.82044459386176	6.49464035755316	9.09195240951938
C	8.01401884604961	4.90401937008473	11.67988133823633
H	8.27074118039423	3.88818353030944	11.98056558669689
C	5.83197102428457	11.73914154663396	5.75993123728879
H	5.21193657472471	10.92379149001555	5.37373242329659
H	6.68149563941943	11.93303225425840	5.10267742790442
H	5.23014051195517	12.64271729253706	5.90474130225998
C	6.58353673719472	15.13234552938466	11.08713306833172
H	5.51461007311940	15.34876540840155	10.98805678025049
H	7.13321513681426	15.52804638182716	10.22642142448615
H	6.98022552484520	15.52973666466430	12.02325204954082
C	8.87555631219832	6.41087953519437	21.15724693301539
H	9.58966569650507	5.59300875252549	21.26904985233294
H	7.88004528991857	6.11623793326532	21.50611717141287
H	9.21620483824426	7.30748742133621	21.68509667918541
C	5.34287352214423	3.92060759628860	16.91828712946126
H	5.17114344409369	3.34535233039946	16.00636464913505
H	4.40004128877766	4.29492304389163	17.33154598446184
H	5.87489313059965	3.32285465163606	17.66622731028123

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$C_{26}H_{22}AgN_6O_8$ optimized with ADF in AMS. Complex **3** - optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

Ag	-0.04644999348884	2.13464263453469	12.80319806916697
O	-1.86724854463389	3.92678501766659	6.20833893957570
O	0.34853452348842	7.82964233018184	16.71901369299164
O	0.33655896421684	4.36852875508959	5.79496791341041
O	-1.00398220918316	6.51719004374759	7.58409371985575
O	2.91126009909936	6.49516359459771	16.99093520650584
O	-0.15622578753157	6.58858511188149	18.56948464715105

O	-0.46869074479428	6.93096469403874	9.76191261447698
N	0.02572428722517	2.99309052249687	10.65689854417279
O	3.35027161463614	6.36666391782560	14.75392470044491
N	0.33133352683728	3.39812148286169	14.63278432067810
N	-1.93785640421087	1.93863580745848	14.14082291558168
N	0.52587463981893	0.43407603232007	11.41857205089823
N	0.97027304547720	-1.59547741953015	9.54715789321171
N	-3.79425347445667	1.51700965520729	16.19110063288601
C	-0.36932364323689	3.73585568316513	8.00319363954662
C	-0.73127872774236	3.56395636453753	15.45836867081032
C	0.14601245809405	6.68061014140139	17.38837273898119
C	-0.09251576856579	2.41374316140757	8.33515547036865
C	-0.57867648565803	4.08147198035937	6.55287905350017
C	-0.40681880925763	4.69976946961708	9.02048502689275
C	-0.78425422589383	4.61198294537316	16.38064544317001
C	0.28088191858568	5.50156406500826	16.47047868556230
C	0.11485073503934	2.06944257860638	9.67452915058945
C	-0.66506931116666	6.12886930365843	8.69701617312156
C	-0.21135969805139	4.26704339522425	10.33530345642970
C	-1.84750093586791	2.60902698913055	15.30803170874249
C	1.40502658950213	5.29267284441135	15.65629015636556
C	0.43866444660426	0.68587125287983	10.09320651885517
C	2.64835986437507	6.11335733162473	15.72463796746157
C	1.37147684882057	4.23486322780024	14.74645877961897
C	0.67185884542117	-0.34656196007495	9.17237822398785
C	-2.77669158136343	2.37435005490136	16.33159679508511
C	1.04350455101718	-1.82539211763272	10.86648445219010
C	4.09157806656084	7.33879130664971	17.15273989199243
C	-2.94995335085404	1.07493233449936	13.99583067271347
C	0.82624231043147	-0.81362155661436	11.80194396979699
C	-2.17525026897897	4.23137875609942	4.81080349363995
C	-3.88300017710865	0.87708831471612	15.01475131950294
C	0.25176343119543	9.04280948058421	17.52814700371369
C	-0.70113741266296	8.34984022082220	9.51422333675009
H	-0.04302871122459	8.69983653583936	8.71205422626016
H	-0.46225161421761	8.84533380028851	10.45664545135382
H	-1.74883479645057	8.51255080261846	9.23974454150624
H	1.28511453598645	-2.83773510491290	11.19170168734508
H	-0.05502278446163	1.66155746531182	7.55167314330639
H	-1.66905526786515	4.76978389664084	16.99276386756589
H	-0.26650197708958	4.97857045241590	11.15728711164487
H	2.22416253774282	4.05721274196728	14.09240214570100
H	0.62242880014485	-0.16417634108424	8.09968752695356
H	-2.68364830737628	2.87194917226096	17.29712059703195
H	3.97226786324774	8.25777254612010	16.56892294695984
H	4.98416436409941	6.79704450621958	16.82367217042220
H	4.14069186804215	7.55665671817734	18.22110908326816
H	-3.02358807524066	0.54002448548165	13.04933277973920
H	0.89355506961651	-1.00812943963799	12.87132060277689
H	-1.60300718807161	3.57167300112624	4.15074422448971
H	-1.93338026328761	5.27911390219129	4.60407742675870
H	-3.24674241869392	4.05023645299504	4.71136433180504
H	-4.71472518087035	0.18524091916628	14.87773490066568
H	0.46268052271150	9.86149924324820	16.83829713226001
H	0.99128299102858	9.00744355333938	18.33505034635443
H	-0.75666210564435	9.13177403247689	17.94476737027073

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$C_{26}H_{22}AgN_7O_{11}$ optimized with ADF in AMS. Model complex **4** [Ag(NO_3)(py-2pz-*N,N'*)(py-2pz-*N*)] optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

Ag	3.35378785458920	10.87384163401827	8.33887809589934
O	8.61892877363527	3.76744071710793	10.19350444631218
O	11.08713933459881	5.28836259063386	10.05929882820567
O	11.33204576108089	5.43260775209889	12.32359486703181
O	8.06983186339064	4.92683151193221	8.30454982202584
O	1.99534977323143	12.61016843792490	9.54622783603062
N	4.23883527361445	10.02792473933773	10.16253014948035
N	5.60682598667129	9.37055776327388	12.51998587799469
N	8.16338597425387	8.26011710480970	12.16093611596252
N	2.83451690840716	13.55516427673789	9.80307064376240
O	4.05591473459376	13.40982484109222	9.49312274154223
C	5.98754957474797	8.88066671689903	11.32572742272621
C	8.34645249344633	6.08861925506768	10.39125638454642
O	2.42372129057941	14.61442481464004	10.36687338702115
C	7.17286391013190	7.98968791161469	11.28639201464695
C	5.30714462726619	9.21283603167663	10.14755407091184
O	5.58760073462161	15.28999874451625	3.17270971107133
O	7.87321495153387	14.01380815158842	4.41503832957500
O	7.35982983911994	14.81682256062555	6.49026653399257
O	5.56729603156279	13.46436885127619	1.80013293136212
N	0.69058631367683	9.61349958884059	4.18716201417271
N	2.06721903576948	10.31381458673219	6.51907448821934
N	4.28377908197725	11.88381021970094	6.44882209727303
C	2.45883203944557	10.78833076719566	5.31711667713006
C	5.12122457059147	13.21220230180372	4.14976990089331
C	3.62909749146043	11.69735558002998	5.28333408351174
C	1.76049561334201	10.41606313511903	4.15828936695519
C	4.02389691060045	12.35820475318335	4.11512165763634
C	5.82546737122655	13.36402416999228	5.35419287381033
C	5.34730730722294	12.68908711919842	6.47969693595706
C	5.46389825483815	13.97656088530862	2.90611173935487
C	0.99576524815434	9.51217888170047	6.55626576973576
C	0.30564396877226	9.16987041130104	5.39314213513563
C	7.07852469283739	14.15895472145788	5.49637828763918
C	9.11409008631311	14.78140031589657	4.45066585682807
C	5.95075883295525	16.12230269322939	2.02849851579868
C	7.22731069211025	6.91709430168756	10.38943486544751
C	9.40017832475517	6.38664211706405	11.26790318724376
C	9.24430989708178	7.47779196101873	12.13378684470121
C	8.34102487177486	4.88567293861809	9.49689324094337
C	4.53165707510591	10.16698549866937	12.52400474107533
C	3.84056491543355	10.49780334763476	11.35993782073725
C	10.69230106989593	5.64649183618577	11.30039091312884
C	12.33221134736057	4.52940303473637	10.00328904594367
C	8.65942161353631	2.54048058066291	9.40232500353552
H	2.96711736557248	11.14784580742369	11.37334794153889
H	12.49207412664348	4.32175838707022	8.94367306874959
H	13.15278523702737	5.12857159349981	10.41108446958416
H	12.22653260332000	3.60041181940370	10.57390306532680
H	7.68532575669720	2.36673784191305	8.93392202249054
H	9.43667296146507	2.62224445715434	8.63509593658220
H	8.89585165306262	1.74945303395791	10.11613214632353
H	9.62079357259086	14.54689551079947	3.51284694684566
H	9.71909587100023	14.47207157898728	5.30916326276070
H	8.88650199526127	15.85066779564070	4.51738786430408
H	5.17763355597534	16.05168253841385	1.25666439611204
H	6.91541502146379	15.79497901924362	1.62630659216946
H	6.01556351981046	17.13723038126601	2.42446142868344
H	5.63687506304614	8.84491423343325	9.17772240076727
H	4.20273846057096	10.56059231654059	13.48681528715674

H	10.05142263716503	7.72691745607049	12.82514434010726
H	6.39009479115568	6.69428435398493	9.73067864089058
H	-0.56947632534007	8.52078790038079	5.43808817610427
H	0.68420159022637	9.13527723734077	7.52959151882698
H	2.07348421352277	10.76677900295045	3.17560250822912
H	3.47316547652907	12.24450428663012	3.18522937808673
H	5.85207976479383	12.80300157646419	7.43855373067284

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$C_{26}H_{22}AgN_6O_8$ optimized with ADF in AMS. [Ag(py-2pz-*N,N'*)(py-2pz-*N*)]$^+$ optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

Ag	1.98643609574607	10.23638347005036	8.46787241288405
O	9.51511915848342	5.89163204487576	9.05625542967563
O	10.93824759580936	8.35121071198602	8.52934417390204
O	11.55829704240733	8.98987936456271	10.62879915558388
O	8.23678082465953	6.72795076321680	7.35671121044465
N	2.91589618993144	9.49130496074181	10.25329090106503
N	4.82090754226183	9.60319502207109	12.30458882408974
N	7.47609058380221	9.72889680305522	11.39666236172118
C	5.15206906710369	9.20417686496572	11.06195504276878
C	8.29939233311560	7.85366078851801	9.47530277872621
C	6.58072131919784	8.96105631746280	10.74364711222789
C	4.19296758307035	9.11115235458158	10.05126662560734
O	7.40947470503083	12.56161632714393	4.10097136540632
O	8.06896662632563	10.12818056391789	5.51321586975353
O	7.94754222094174	10.86398873209301	7.67138229632645
O	6.35132414301897	11.10085175254879	2.69867543950118
N	-0.03693323114252	12.27969881459850	4.41416805191474
N	1.05797881656893	10.99634069301483	6.64247993648868
N	3.78653363798043	11.12589921932761	7.07857688789983
C	1.85968641362235	11.51824381626518	5.68342275619692
C	5.56989796666444	11.39119121965469	4.95416594390273
C	3.32792212737651	11.39325567040513	5.83885603827055
C	1.28512096370834	12.16716317791046	4.58100987737769
C	4.19981765052130	11.54287359999496	4.75529062165525
C	6.03622990099474	11.04928950193633	6.23320081164843
C	5.09504634031146	10.95852090812442	7.26105416819296
C	6.48355235304247	11.63790517179706	3.78917323702817
C	-0.26903079629454	11.10775796111169	6.48499501200231
C	-0.81067570882267	11.74143148192576	5.36633017618866
C	7.44829957915783	10.70136112403000	6.56546870760084
C	9.46403191666154	9.76809485193976	5.74107215052674
C	8.36825275100170	12.85951546321885	3.03883706076010
C	6.95108380254284	8.01267158652705	9.78413561906542
C	9.23587733795783	8.67693224947554	10.11735771243732
C	8.76300580588525	9.58401240392493	11.07616697548228
C	8.67888738852654	6.78368496312097	8.49520503928206
C	3.53558825615468	9.90221215780084	12.51553482967588
C	2.57885095456537	9.88007371360129	11.49735093572610
C	10.69439694547106	8.68271619299120	9.81608188536400
C	12.34743480659109	8.30893271696070	8.15457888698959
C	9.97380955581058	4.83006405581327	8.16313344269046
H	1.54939493607426	10.18397779831163	11.67255983351811
H	12.35468957045834	8.02264453343463	7.10102739824533
H	12.79965520891452	9.29624827176561	8.29337280595476
H	12.87208088561849	7.56611224216963	8.76428382245868
H	9.11971585893522	4.24184160860137	7.81218356931387
H	10.50342373404666	5.26965260711932	7.31127487835176
H	10.64584770369969	4.21984804824094	8.76912766446765
H	9.79491364237127	9.30854336782085	4.80775143166348

H	9.53312825855532	9.06316318032007	6.57445881090879
H	10.04586738721017	10.66970643442159	5.96119412403328
H	7.84195996550043	13.23525977371421	2.15560219030737
H	8.92951220087273	11.95347116627850	2.78642701392326
H	9.02573918952077	13.62366341943607	3.45683571860546
H	4.45165621243373	8.77264032867478	9.05037433140958
H	3.24755467556111	10.19470008454625	13.52588547133057
H	9.47639729430449	10.22952415426222	11.59128677250042
H	6.20915913269976	7.37274492987697	9.30999896571136
H	-1.89143853616185	11.81379316405313	5.24446830114611
H	-0.90532968767562	10.68002827860688	7.25670101102343
H	1.91397109112578	12.62802874024249	3.82011330159794
H	3.83000369714342	11.76756970650394	3.75787232325724
H	5.43649606589552	10.73943653081532	8.27384143875239

3

H_2O optimized with ADF in AMS. H_2O optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

O	6.17600128241422	11.10011763805232	14.37769484530109
H	6.54599938194425	11.36663424129698	15.24141320021151
H	5.27218273085021	10.80964452559959	14.60794858639334

8

CF_3O_3S optimized with ADF in AMS. $CF_3SO_3^-$ optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

S	4.12255230728017	8.36890026322970	12.60901814532217
O	4.97986740175963	8.89268656302250	13.69422881576414
O	4.82048529350875	8.08306792392918	11.33714838019341
F	2.85810930037675	6.00095297854726	12.33471362544881
F	4.75544940645539	5.88738436514326	13.44816466185805
O	2.81104189888241	9.03905770654579	12.46721085447276
F	2.96295426016022	6.73365953280419	14.40952679402945
C	3.64777369211749	6.65111177235623	13.23467902974564

4

NO_3 optimized with ADF in AMS. NO_3^- optimized ZORA-BP86-D4/TZP-COSMO(DMSO)

O	1.99868828150519	12.61214081964479	9.54622759583418
N	2.82728534449254	13.54745227582335	9.80236837652916
O	4.05738139459525	13.41187181425917	9.49315977972803
O	2.42614768621878	14.61811746066775	10.36753885626502