Electronic Supplementary Information

Luminescent Zn(II) and Cd(II) complexes with chiral 2,2'-bipyridine ligands bearing natural monoterpene groups: synthesis, speciation in solution and photophysics

Tatyana E. Kokina,*[a,b] Marianna I. Rakhmanova,[a] Nikita A. Shekhovtsov,*[a,b] Ludmila A. Glinskaya,[a] Vladislav Y. Komarov,[a,b] Alexander M. Agafontsev,[c] Andrey Y. Baranov,[a] Pavel E. Plyusnin,[a,b] Liliya A. Sheludyakova,[a] Alexey V. Tkachev *[c] and Mark B. Bushuev *[a,b]

[a] *Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, 3, Acad. Lavrentiev Ave., Novosibirsk 630090, Russia*

[b] *Novosibirsk State University, 2, Pirogova Str., 630090 Novosibirsk, Russia*

[c] *N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Siberian Branch of Russian Academy of Sciences, 9, Acad. Lavrentiev Ave., Novosibirsk 630090, Russia*

E-mail addresses: kokina@niic.nsc.ru (T. E. Kokina), shna1998@mail.ru (N. A. Shekhovtsov), atkachev@nioch.nsc.ru (A.V. Tkachev), bushuev@niic.nsc.ru (M. B. Bushuev)

Table of Contents

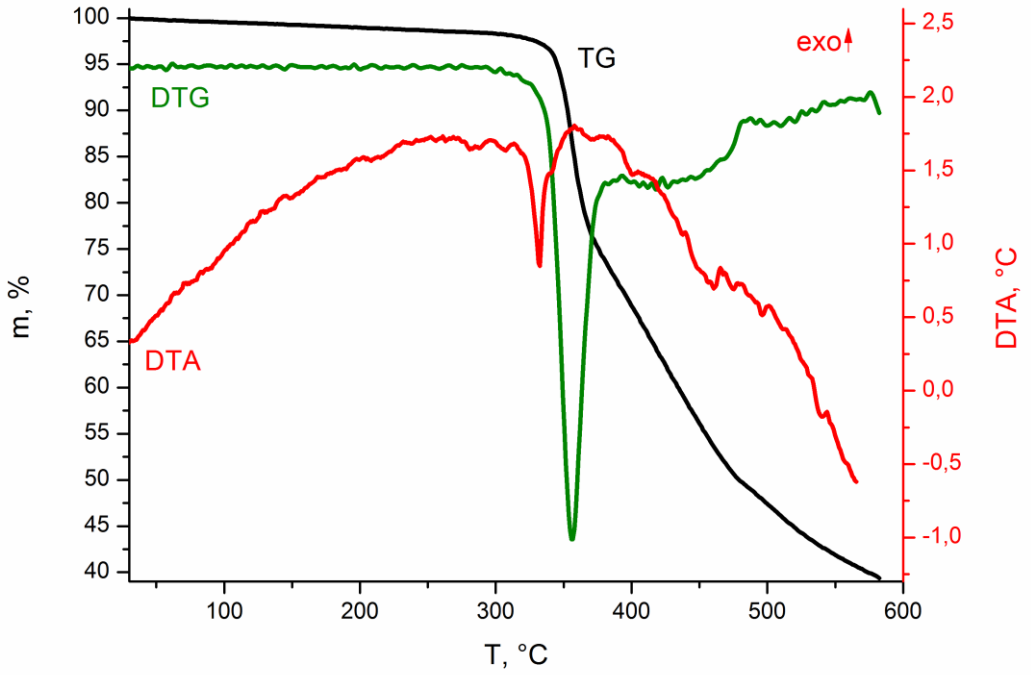


Figure S1. The TG-, DTG- and DTA-curves for the complex **1**.

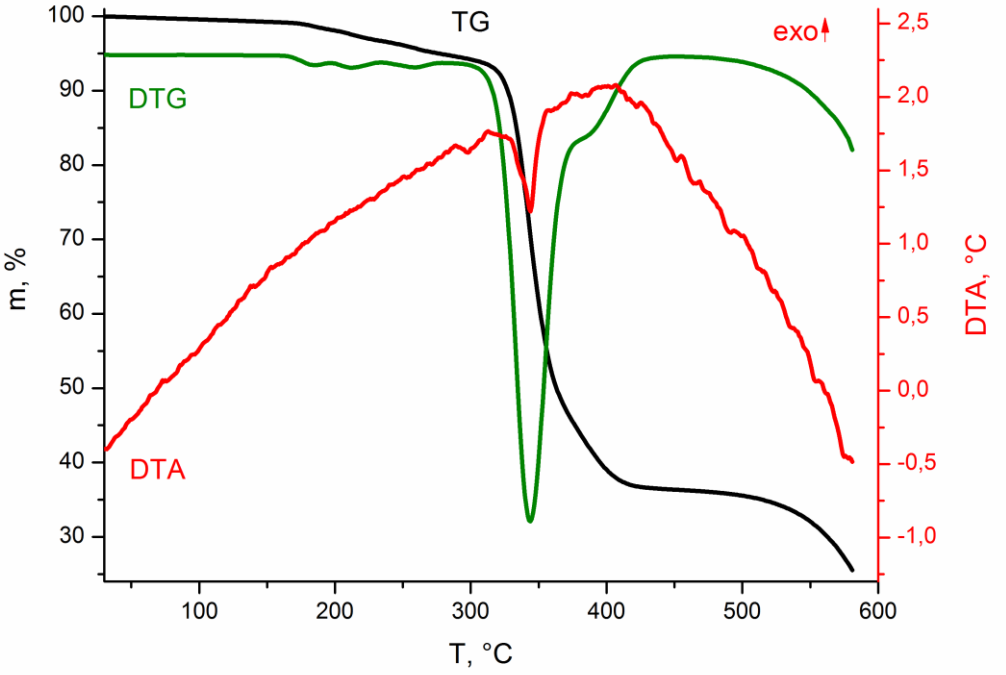


Figure S2. The TG-, DTG- and DTA-curves for the complex **2**.

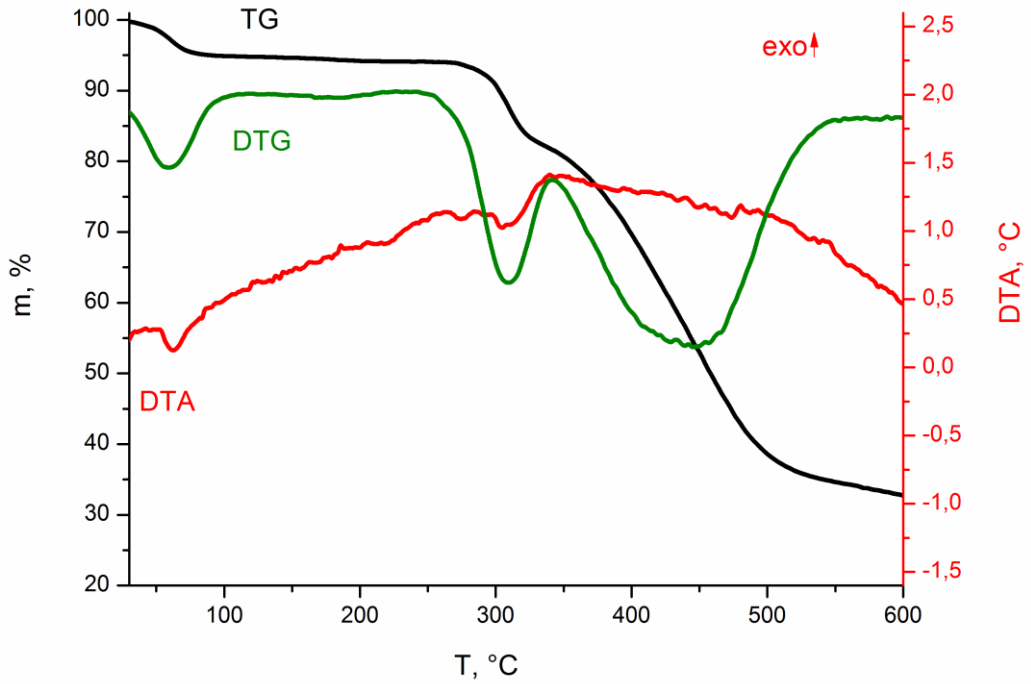


Figure S3. The TG-, DTG- and DTA-curves for the complex **3**.

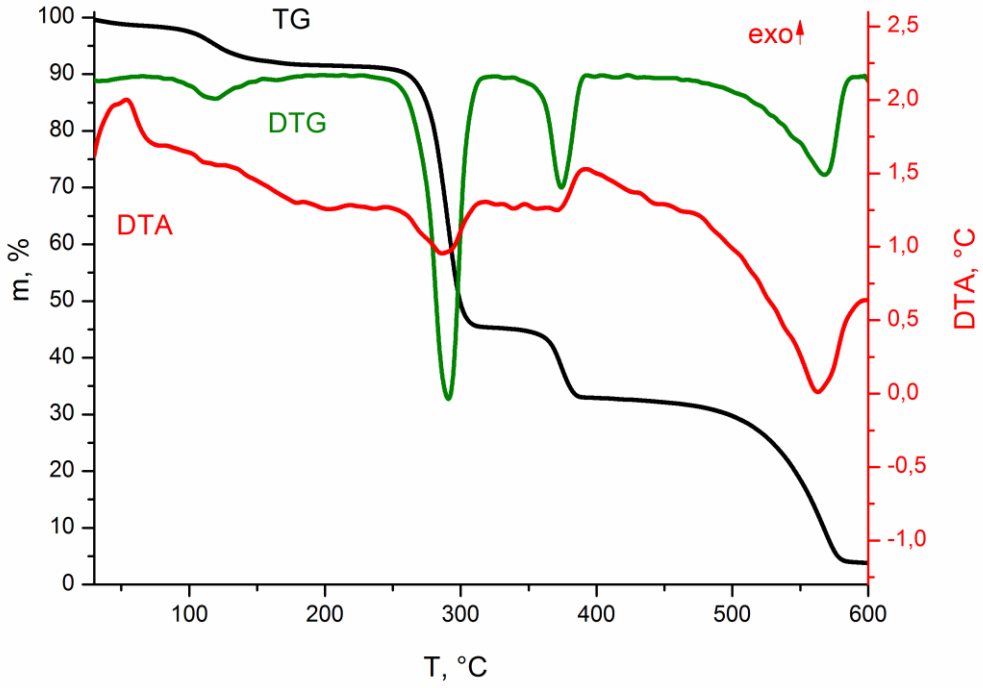


Figure S4. The TG-, DTG- and DTA-curves for the complex **4**.

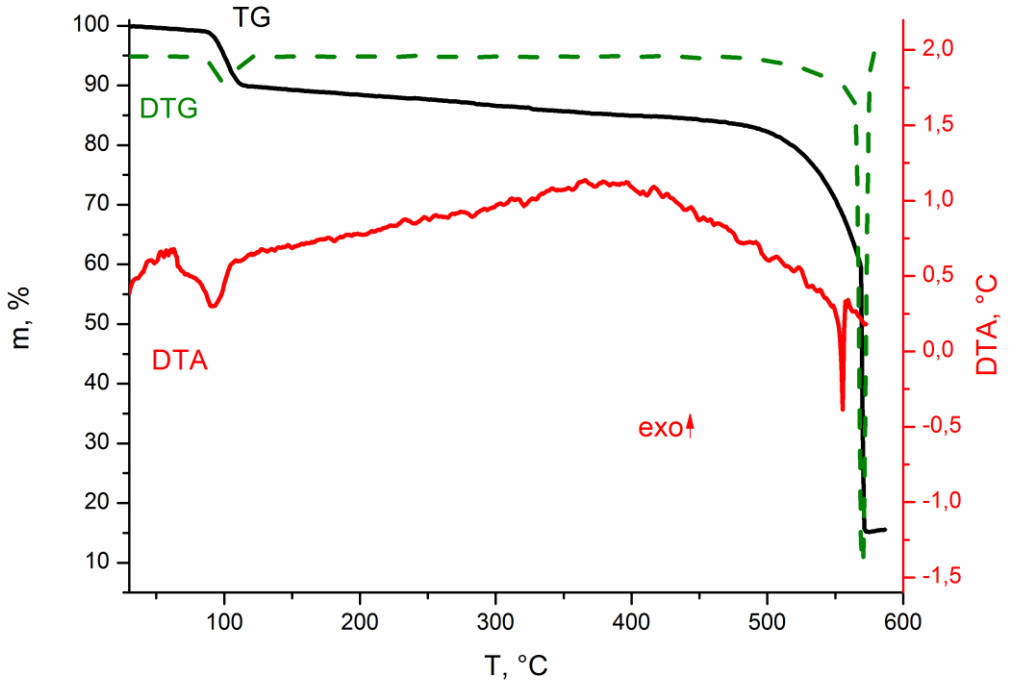


Figure S5. The TG-, DTG- and DTA-curves for $CdCl_2 \cdot 2.5H_2O$.

Table S1. Crystallographic characteristics, experimental data and structure refinement for the complexes **1** and **2**.

Compound	**1**	**2**
Empirical formula	$C_{26}H_{27}Cl_2N_3OZn$	$C_{26}H_{27}CdCl_2N_3O$
Molecular mass	533.77	580.80
Crystal system	orthorhombic	orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$
a (Å) *b* (Å) *c* (Å)	8.1145(2) 11.1511(3) 26.8325(7)	8.2814(4) 11.3343(5) 26.1739(10)
V E^3	2428.0(1)	2456.8(2)
Z	4	4
ρ_{calc} (g/cm^{-3})	1.460	1.570
μ (mm^{-1})	1.256	1.130
Crystal size, mm	0.47 x 0.36 x 0.31	0.2 x 0.2 x 0.1
Scan range, θ, degree	3.04 – 61.08	3.92 – 59.38
Number of measured reflections Number of independent reflections R_{int}	28237 7387 0.0349	17884 6906 0.0241
Number of reflections with [$I>2\sigma(I)$]	6695	6551
Number of refined parameters	304	304
Goodness-of-fit (GOF) on F^2	1.035	1.026
R-factor, [$I>2\sigma(I)$] R_1 wR_2	 0.0293 0.0614	 0.0243 0.0507
R-factor (for all I_{hkl}) R_1 wR_2	 0.0351 0.0634	 0.0270 0.0518
Residual electron density (max / min) e/ $Å^3$	0.27 / -0.31	0.54 /-0.59

Table S2. Selected bond lengths (Å) and angles (°) for the complexes **1** and **2**.

1		**2**	
Bond	*d,* Å	Bond	*d,* Å
Zn(1)–Cl(1)	2.2392(6)	Cd(1)–Cl(1)	2.2440(8)
Zn(1)–Cl(2)	2.2344(6)	Cd(1)–Cl(2)	2.2427(6)
Zn(1)–N(1)	2.095(2)	Cd(1)–N(1)	2.308(2)
Zn(1)–N(2)	2.108(2)	Cd(1)–N(2)	2.338(2)
Zn(1)–N(3)	2.713(2)	Cd(1)–N(3)	2.637(2)
O(1)–C(11)	1.219(3)	O(1)–C(11)	1.212(3)
N(1)–C(2)	1.347(3)	N(1)–C(2)	1.344(3)
N(1)–C(13)	1.351(3)	N(1)–C(13)	1.348(3)
N(2)–C(22)	1.343(3)	N(2)–C(22)	1.346(3)
N(2)–C(26)	1.332(3)	N(2)–C(26)	1.338(4)
N(3)–C(1)	1.481(3)	N(3)–C(1)	1.490(3)
N(3)–C(11)	1.378(3)	N(3)–C(11)	1.398(4)
Angle	ω (°)	Angle	ω (°)
Cl2Zn1Cl1	114.67(2)	Cl2Cd1Cl1	112.72(2)
NlZn1Cl1	123.83(5)	NlCd1Cl1	127.19(6)
N1Zn1Cl2	119.97(5)	N1Cd1Cl2	120.08(6)
N1Zn1N2	79.00(7)	N1Cd1N2	71.59(8)
N2Zn1Cl1	97.58(5)	N2Cd1Cl1	92.27(6)
N2Zn1Cl2	106.74(5)	N2Cd1Cl2	109.97(6)
Cl1Zn1N3	95.4(4)	Cl1Cd1N3	104.35(5)
Cl2Zn1N3	93.0(4)	Cl2Cd1N3	96.74(5)
N1Zn1N3	70.4(3)	N1Cd1N3	69.51(7)
N2Zn1N3	149.0(6)	N2Cd1N3	140.16(7)

Table S3. Selected intermolecular interactions in the structures of **1** and **2**.

	1			**2**		
D–H...A	H...A	D...A	D-H...A	H...A	D...A	D-H...A
N(3)–H(3)...Cl(1)	3.16(3)	3.853(2)	144(2)	2.865(3)	3.612(2)	149(3)
C(10)–H(10a)...Cl(2)‘	2.755(1)	3.633(2)	150(1)	2.928(1)	3.812(2)	151(1)
C(10)–H(10b)...Cl(2)	2.764(1)	3.721(2)	165(1)	2.783(1)	3.758(3)	173(1)
C(10)–H(10c)...Cl(1)	2.804(1)	3.727(2)	150(1)	2.797(1)	3.673(3)	149(1)
C(18)–H(18)...O(1)	2.408(2)	3.180(3)	138(1)	2.517(2)	3.207(4)	130(1)

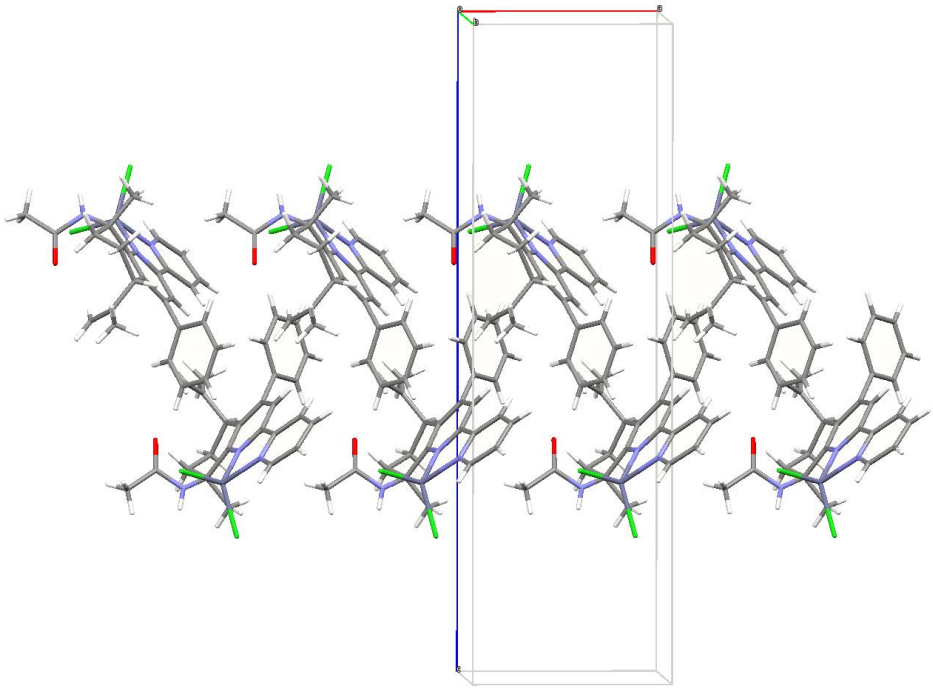


Figure S6. A 1D helical chain in the structure of **1** (view along the *b* axis).

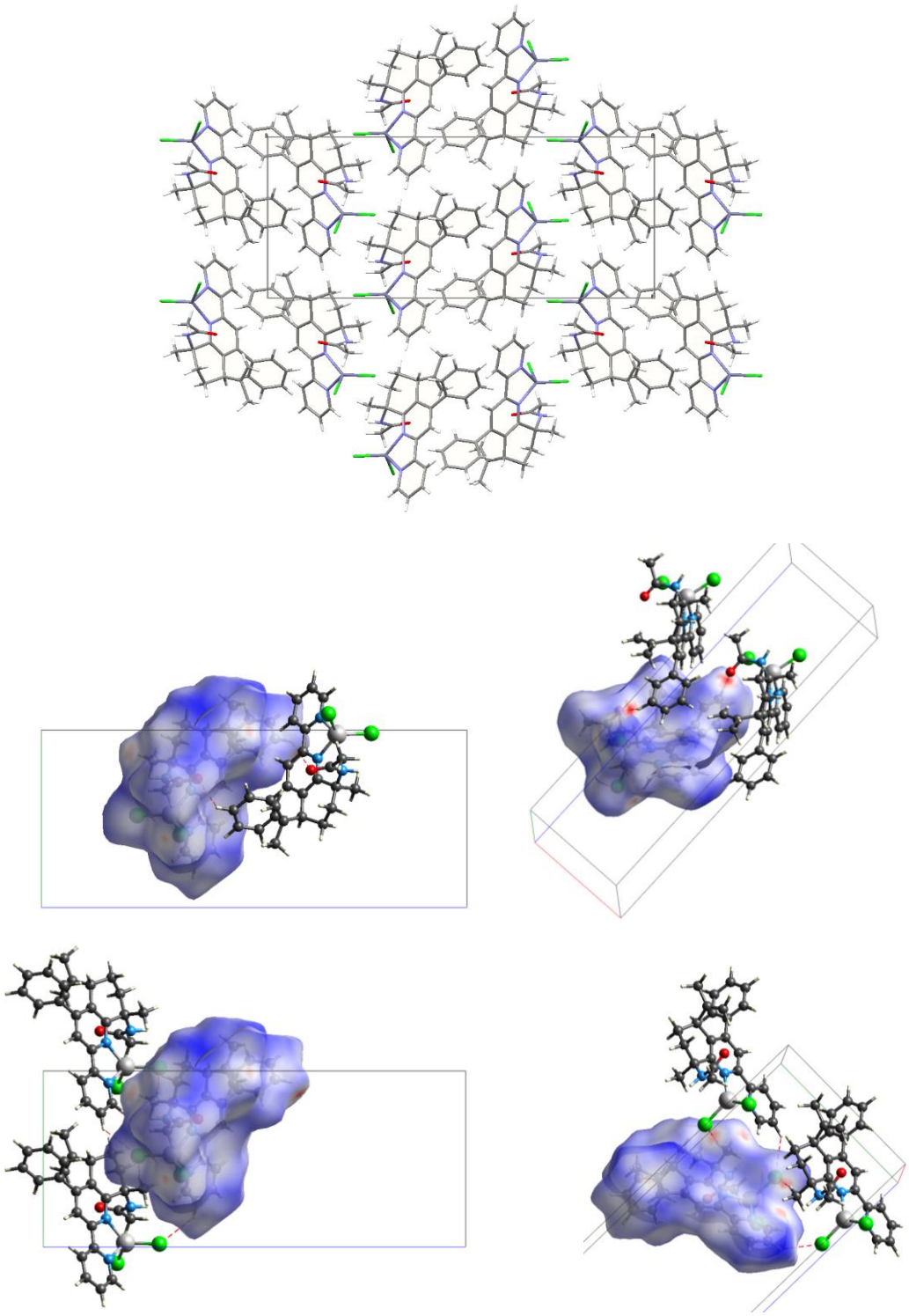


Figure S7. 3D supramolecular structure of **1**. (Top) The crystal packing along the 1D helical chains (view along the *a* axis), (middle) three unit of the helical chain. (Middle-left) the same and (middle-right) arbitrary view on three units of the helical chain, (bottom) Ar···Cl and Ar···H_3C contacts. Orientations of top, middle-left and bottom left figures are the same. For middle and bottom figures the "central" molecules are shown with Hirshfeld surface. [M. J. Turner, J. J. McKinnon, S. K. Wolff, D. J. Grimwood, P. R. Spackman, D. Jayatilaka and M. A. Spackman, CrystalExplorer17 (2017). University of Western Australia. http://hirshfeldsurface.net]

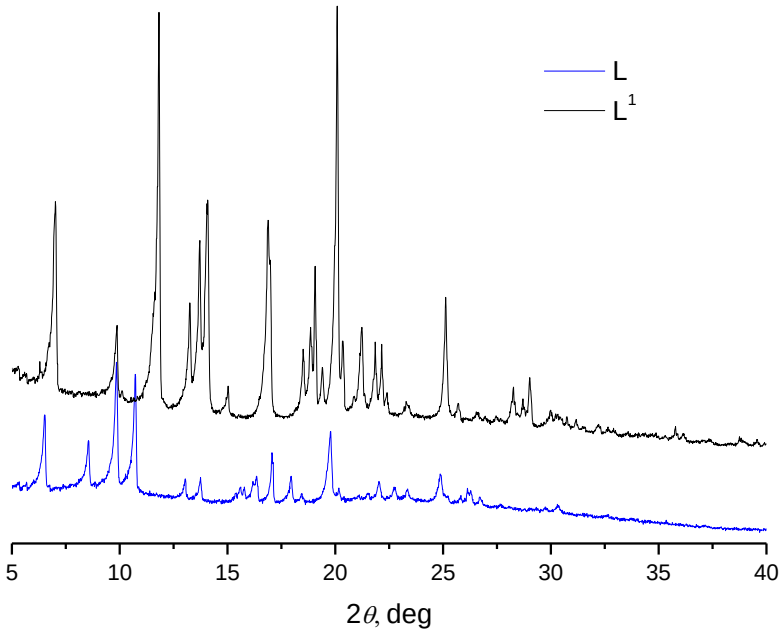


Figure S8. X-ray powder diffraction patterns of the ligands **L** and **L**[1].

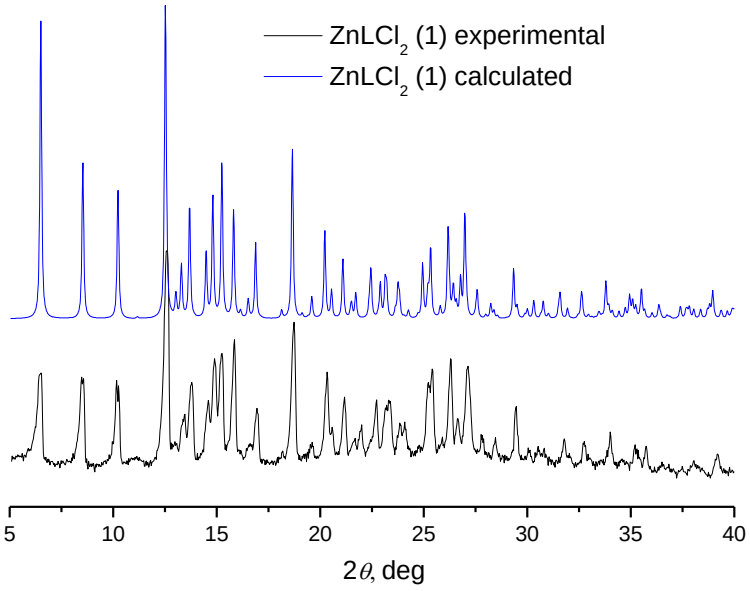


Figure S9. X-ray powder diffraction pattern of the complex **1**.

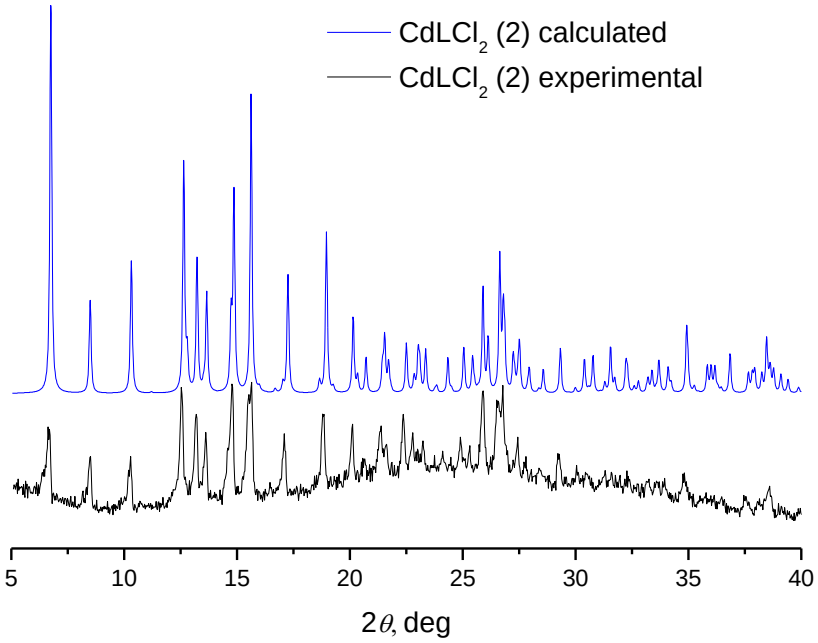


Figure S10. X-ray powder diffraction pattern of the complex **2**.

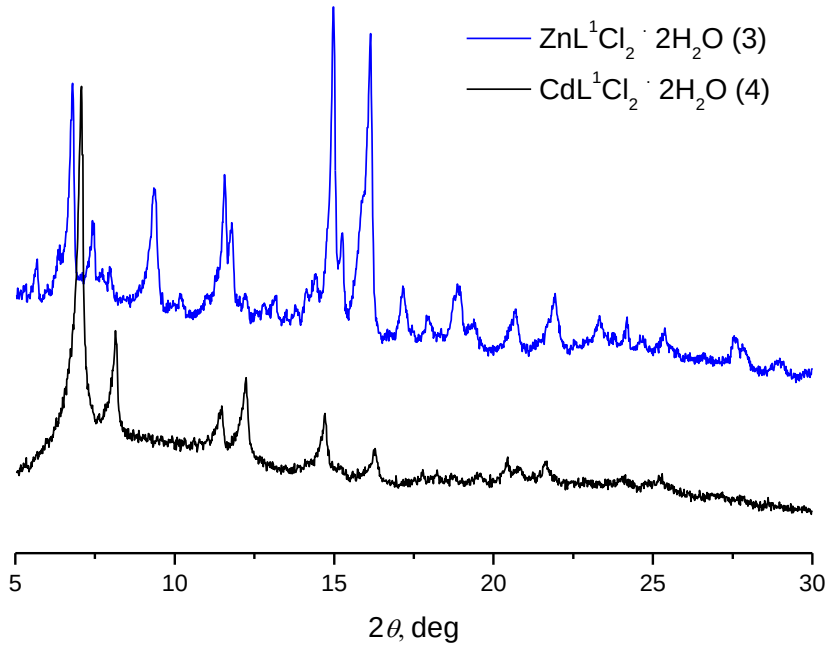
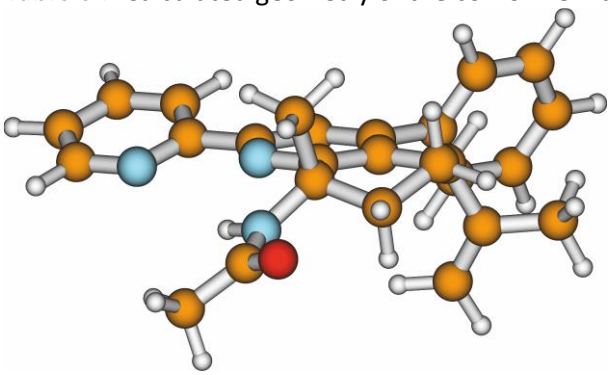


Figure S11. X-ray powder diffraction pattern of the complexes **3** and **4**.

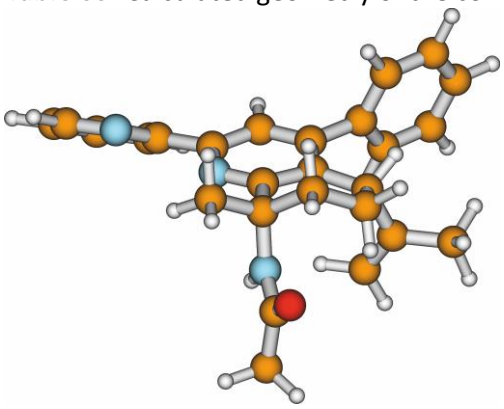
Table S4. Calculated geometry of the conformer **La** in cartesian (XYZ) coordinates.



E(h) = -1245.5964

C	-7.22804981729179	0.92378965205594	0.60509591532949
C	-7.10906007345899	-0.39438023043460	1.33629323857885
C	-6.14344946171049	-1.34585866234851	0.62894146433751
C	-4.87465599846764	-0.64393316692507	0.22959049795223
C	-4.76044531317378	0.74771100774397	0.18093765418161
C	-5.89918858167332	1.67797407082626	0.60146274490278
C	-3.75497738049488	-1.39078425637538	-0.16187217388090
C	-2.61537798525015	-0.72671508472375	-0.57625754927150
C	-2.59337388135299	0.66505806557969	-0.58972031263783
N	-3.65265193711378	1.37079459557424	-0.21115281388254
C	-3.76113199282361	-2.87390298447792	-0.16377736448026
C	-1.38175823120653	1.40181188719188	-1.03049188044944
C	-6.82221551596705	-2.04688210195910	-0.53144595883660
C	-7.62456767870001	-3.24641744710846	-0.13796527460093
C	-6.72366081142887	-1.63908404051311	-1.79320900712113
C	-3.76245407683730	-3.58567020847805	1.03338053452739
C	-3.76787846536378	-4.97348302864939	1.02725499738111
C	-3.76982885160585	-5.66510511749317	-0.17654011901984
C	-3.74844709358118	-4.96166862687877	-1.37375936430439
C	-3.73913998595479	-3.57440741807832	-1.36711943116240
C	-0.13662082190719	0.77293139676511	-1.05186239014913
C	0.97347460509107	1.48344506155024	-1.47007597412866
C	0.81357033111472	2.80503388886947	-1.85110178472804
C	-0.46133033324678	3.34935269850782	-1.79229225888605
N	-1.53565066993303	2.67562956605867	-1.39974810417269
N	-5.91037057296087	2.76932647240481	-0.37164813396344
C	-5.59776206873799	2.25167018926015	1.99192972928293
C	-6.83274769711427	3.74511104458118	-0.44998911611594
C	-6.55291491554760	4.81278667117112	-1.47573286401016
O	-7.85772027658676	3.78050671308272	0.22482417225197
H	-7.53733061065732	0.74550013099199	-0.42989199263619
H	-7.98607040939083	1.55520872865345	1.06462275989701
H	-8.09209124473503	-0.86267941243088	1.41695296050096
H	-6.75790376234532	-0.22838951101665	2.35836103176036
H	-5.87579983969437	-2.13224750235111	1.34081116784924
H	-1.76026931812482	-1.30398375818778	-0.90098554570577
H	-8.36357038567731	-2.99708245930978	0.62965108483013
H	-6.96682683105965	-4.00666080090657	0.29686347674353
H	-8.14830835220294	-3.67982854955746	-0.99092169720631
H	-7.24899520319595	-2.15830245529243	-2.58791421784421
H	-6.11328893078065	-0.78811030972876	-2.07597490830928
H	-3.74852397485847	-3.04663464778725	1.97423144616701
H	-3.77007073150775	-5.51584463869843	1.96578967524415
H	-3.78354520854375	-6.74900232276564	-0.18196699290592
H	-3.74338305592461	-5.49533896313249	-2.31740941464434
H	-3.73461126253574	-3.02499436851082	-2.30144393975564
H	-0.02732128007344	-0.25182005034350	-0.72304636198832
H	1.94863303916064	1.01058434972922	-1.49011905940378
H	1.65305713465783	3.40227626343295	-2.18408175241751
H	-0.62615192626901	4.38218290474469	-2.08678540438425
H	-5.02497428991050	2.90732069438585	-0.83928214696493
H	-4.60808481505574	2.71167743549543	2.00523269247280
H	-6.34651179184401	3.00759497840022	2.23385125035923
H	-5.62975836796409	1.47334090900589	2.75485551585803
H	-5.52036976169961	4.81858746792755	-1.82754081586989
H	-7.21064369061633	4.65081618863258	-2.33284306425508
H	-6.80194657586578	5.78119909184002	-1.04081582031511

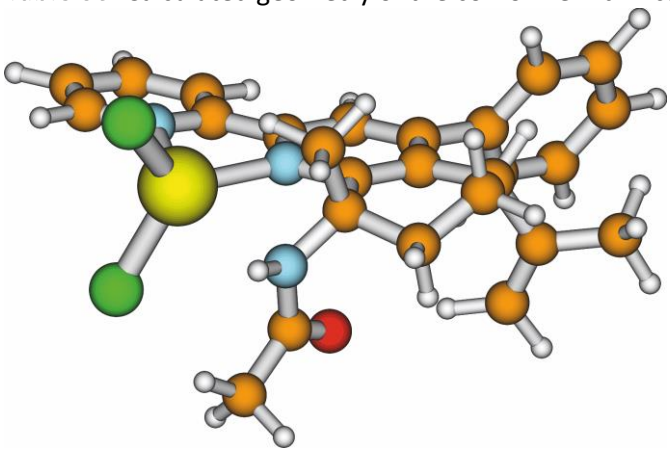
Table S5. Calculated geometry of the conformer **Lb** in cartesian (XYZ) coordinates.



E(h) = -1245.5891

C	-6.75592497986778	0.69651092570503	1.38129333365700
C	-7.10445092703784	-0.77145918328420	1.31999631705291
C	-5.89437367944774	-1.67327467302010	0.97316539277002
C	-4.67627901119102	-0.92351614796618	0.49859839768983
C	-4.73420262217726	0.39041806638153	0.02537413348977
C	-6.04058248622032	1.16467030497710	0.11268736160518
C	-3.42020102394550	-1.54165752422296	0.48856039810088
C	-2.34202438572191	-0.86900749632056	-0.06859205282743
C	-2.52887238094909	0.40311877241552	-0.59947345141066
N	-3.70282217399366	1.02105437659053	-0.51885006111274
C	-3.20511261426369	-2.87777729532395	1.09792005212310
C	-1.42944239724855	1.13866609399302	-1.27152187762110
C	-6.35484104359734	-2.73596746371815	-0.00570127984388
C	-7.22529028847155	-3.78781626182677	0.60288675797374
C	-6.05865611017446	-2.72660785003850	-1.30158620217429
C	-3.06251890600092	-2.98217148382586	2.47996890038295
C	-2.85447630007628	-4.21857139730386	3.07341713008452
C	-2.78663187633675	-5.36319195829684	2.29047021345659
C	-2.91485625162935	-5.26407983859707	0.91180210376546
C	-3.11978200261617	-4.02653181709866	0.31715298117182
C	-0.46009993623777	0.46085964422900	-2.00952285812850
C	0.52664748203344	1.19100388217120	-2.65084294539209
C	0.51788311399150	2.57166370169476	-2.53969128816470
C	-0.48549672186467	3.15751660333394	-1.77985792979320
N	-1.43540991506930	2.46926013935326	-1.15955111581048
N	-6.76482853219267	0.81822694945878	-1.11459617805095
C	-5.80946784832212	2.66716762341168	0.17283840907143
C	-8.05735653989871	1.05457664106037	-1.40402092275836
C	-8.42894614013738	0.76452218575109	-2.83703462306545
O	-8.87215955642523	1.48439945294658	-0.59537652395849
H	-7.65745434092453	1.28712236469620	1.53875071362490
H	-6.07290793088244	0.90077796639139	2.21268352307038
H	-7.54001102178706	-1.08964533955289	2.26900885307977
H	-7.87818899355779	-0.90847088415352	0.56124582506435
H	-5.59865407159863	-2.20466308516999	1.88425097517112
H	-1.36198812328725	-1.33015938161123	-0.06143413604995
H	-8.04514336411994	-3.34248524071224	1.17389408873682
H	-6.63924452920943	-4.38843611307973	1.30787507569716
H	-7.64891091027725	-4.45112533545158	-0.15240123120200
H	-6.46187631824343	-3.48263232809594	-1.96680771544979
H	-5.40807936040897	-1.97771595028196	-1.73873175940052
H	-3.10989810681889	-2.08617899115738	3.08973344348357
H	-2.73670252866977	-4.28623565636741	4.14901132930410
H	-2.62488043703549	-6.32941035033072	2.75441921453481
H	-2.85292069893865	-6.15264779995662	0.29396910365390
H	-3.22768002704691	-3.95067138276756	-0.75841038746457
H	-0.49243834791479	-0.61757604060169	-2.10190925217693
H	1.28386729048301	0.68710282533625	-3.23959154382655
H	1.26289797311193	3.18535724804618	-3.03017497199084
H	-0.52336127294902	4.23730101147139	-1.66117976361655
H	-6.19024587472022	0.50884010534015	-1.88057127715475
H	-5.24314711415659	3.00950412179371	-0.69091394006994
H	-6.77716706238887	3.17079805111055	0.20029358710738
H	-5.25131285842242	2.93043842381183	1.07347612598471
H	-8.41089322366564	1.70671382420593	-3.39045963368531
H	-9.44036780757518	0.36135119064059	-2.87825028036437
H	-7.74218388390564	0.06999077381658	-3.32073253834379

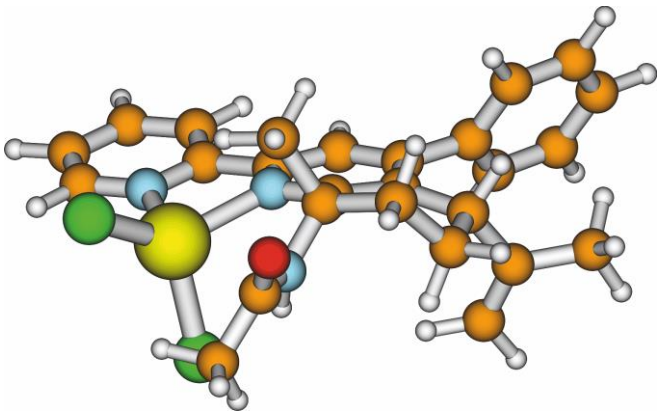
Table S6. Calculated geometry of the conformer **1a** in cartesian (XYZ) coordinates.



E(h) = -3945.0696

Zn	2.20234696771196	5.93154321934660	7.94227858176708
Cl	0.56579642918611	4.50751484748501	8.58073403248813
Cl	2.76235743720367	5.92542632051422	5.76285006283458
O	-0.08119106182063	8.03183219140371	10.13684042105288
N	2.86392126646892	7.45532174962567	9.24543522184991
N	3.72694297287456	4.93548853105634	8.98052787783053
N	0.50812799501949	8.10987522683825	7.96312264892888
C	1.51993972343261	9.15266728462828	8.15076027527839
C	2.46435770296820	8.73041264729302	9.26751969699236
C	2.90861848270091	9.63681395795505	10.23822858174768
C	2.50857704596805	11.09429640956166	10.24807474305097
C	1.86357552523828	11.51624047593554	8.92497597020959
C	0.84951948535148	10.48948286261746	8.47714689887156
C	1.62206122960070	11.49471751720866	11.41203189844673
C	0.74403285989218	10.67335047135211	11.97721143366266
C	1.77583191613588	12.91988032310515	11.84142292705294
C	2.29831598496553	9.28381408709187	6.84245328521906
C	-0.34937069044369	7.77650622285604	8.97481749066695
C	-1.63543901339507	7.11238032473714	8.59166672070488
C	3.69258664301296	6.98985234300969	10.18843193386867
C	4.12748375336078	7.80727209826725	11.21242272133473
C	3.74122009828012	9.13925458815215	11.24691682800505
C	4.20284513267398	9.94719190198522	12.39847180566593
C	3.76058582605740	9.58947398739201	13.66989932443164
C	4.20940407398154	10.27208470644316	14.78846568706129
C	5.11633771686970	11.31504847919234	14.64913179163211
C	5.56395975091947	11.67343507190286	13.38606044739942
C	5.10525864416214	10.99733272122894	12.26269815940876
C	4.12212403056517	5.57865825849850	10.08008453292088
C	4.88511831257825	4.93571526740454	11.04741586261668
C	5.24324460146978	3.61387801196140	10.84532355586633
C	4.84681579161867	2.96735590465810	9.68437980901240
C	4.07261407508483	3.66968808753663	8.77912571766873
H	0.15915828643648	8.00928259562713	7.02113106558148
H	3.43200539181140	11.66996602046589	10.35717943234797
H	1.38446688690845	12.48962400880571	9.04710500113071
H	2.64140720524108	11.64773997745550	8.16891218214294
H	0.31603933931951	10.82604853246965	7.58519278177699
H	0.11418519193992	10.34151571923512	9.27010235694616
H	0.10290110551503	11.02090657809269	12.78039825824182
H	0.63426738361045	9.64354510408705	11.65867973625272
H	2.79227398457438	13.10046509126795	12.20780651309172
H	1.07162035310344	13.17583956489456	12.63312298062455
H	1.61165821671382	13.60712853316598	11.00482795214100
H	2.76134066322619	8.34240573919977	6.54976000300448
H	3.08149392266112	10.03374570179743	6.93884855967482
H	1.61708134971472	9.59783770654659	6.04727910456964
H	-1.79583763383446	6.25573743433512	9.24301847050511
H	-1.66615303873101	6.78984763902194	7.55181509475074
H	-2.43514700914265	7.83655450883708	8.77240635925912
H	4.78321781336483	7.42908596049466	11.98357510257126
H	3.05072811839396	8.77662273554457	13.77484139520766
H	3.84999973831281	9.98291621900510	15.76970869227576
H	5.47916057240993	11.84240856856584	15.52384603378268
H	6.28039441558466	12.47861776346883	13.27188316524253
H	5.47211148689580	11.27368983559104	11.28038458788385
H	5.19129842120989	5.44768167464511	11.94861546790447
H	5.82776127568796	3.09200478515344	11.59312288821913
H	5.11780301041684	1.93896746177694	9.48483271158358
H	3.70444283896152	3.21090844220464	7.86857715773871

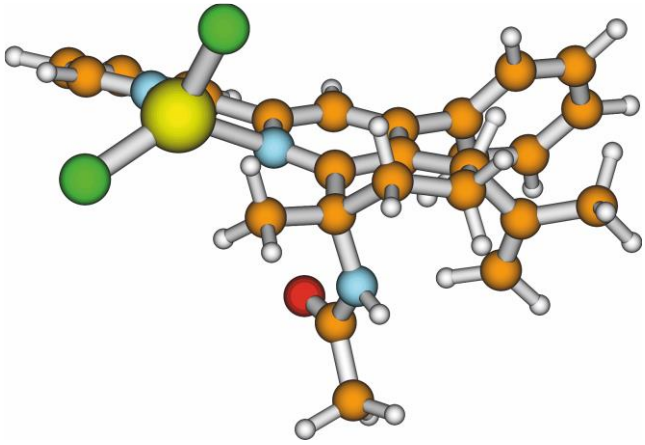
Table S7. Calculated geometry of the conformer **1c** in cartesian (XYZ) coordinates.



E(h) = -3945.0653

C	-6.35413597772300	0.55609776123800	2.48009920262634
C	-6.96412387014061	-0.68154496052779	1.87313320176494
C	-5.86504990111974	-1.66935585892604	1.48561494978909
C	-4.73690979627773	-0.97287450959829	0.76210054845996
C	-4.72574129189432	0.40893094584903	0.57818361176704
C	-5.56307329298233	1.34733293098758	1.43588931706135
C	-3.66844502719577	-1.70086811588251	0.21095067235878
C	-2.77475112510001	-1.05735669757352	-0.62703440302332
C	-2.93937981978410	0.29025884531504	-0.89862367832387
N	-3.88696069121450	0.99889474237506	-0.28221632450986
C	-3.43069354931819	-3.12148509795606	0.54344036030242
C	-2.05796660501428	1.02518930309675	-1.82721271989712
C	-6.45863820612152	-2.80771385131527	0.67179595017277
C	-6.71531049832102	-4.07742382142690	1.41458619257126
C	-6.78454828528200	-2.65001919098125	-0.60655917125417
C	-3.15846097809369	-3.47771905387348	1.86266604573657
C	-2.88015951509256	-4.79527660330317	2.19217994316583
C	-2.87720202931305	-5.77115957065572	1.20499565047923
C	-3.13773098792593	-5.41952558593214	-0.11292932023120
C	-3.40532238032831	-4.10071404972789	-0.44555848605352
C	-0.88993167280827	0.48641340574646	-2.34830180118311
C	-0.11366826119016	1.26224187931750	-3.19199985521810
C	-0.51524499443786	2.55386409047441	-3.48970428430622
C	-1.69124128635278	3.02145570426932	-2.93228237436985
N	-2.44048919806865	2.26950516556139	-2.13315223936623
N	-6.44739852769208	2.09049301217494	0.53939857117353
C	-4.58857428817221	2.28487309076962	2.15809828344843
C	-7.24161102952587	3.12119318605939	0.92338711142872
C	-7.98412500269640	3.79340965781618	-0.19645373146116
O	-7.31785581202274	3.50261594893196	2.08271701491211
H	-7.10597319827822	1.22009950712489	2.90551621472535
H	-5.67504808399021	0.27662693123233	3.29148360482251
H	-7.65709092303275	-1.16529470192245	2.56413725218461
H	-7.53956449499904	-0.41291385908227	0.98235115215240
H	-5.46377410973664	-2.09303200815706	2.41255329765077
H	-1.96155759967492	-1.61768661896247	-1.06653760299427
H	-7.33069424100052	-3.89090383938563	2.30074463520766
H	-5.77355926705758	-4.50824083138768	1.76888145473325
H	-7.22301772310362	-4.81132182336998	0.78838963642217
H	-7.25081627316689	-3.45108700493392	-1.16848328318786
H	-6.59594624162382	-1.72165304672663	-1.13656891008278
H	-3.14560885593838	-2.71397778626891	2.63226560414827
H	-2.66145903319937	-5.05892855427066	3.22050311999492
H	-2.66407490927982	-6.80239541104853	1.46176514798587
H	-3.13000547342468	-6.17723332680480	-0.88775788733218
H	-3.61679434643312	-3.82823129165341	-1.47298510200832
H	-0.57164836271058	-0.51173501595099	-2.08203709298149
H	0.80215658057487	0.85927618890058	-3.60724403417439
H	0.07097180576921	3.19494666813998	-4.13415863617086
H	-2.05379808885690	4.02365609491465	-3.12941382147542
H	-6.56346005849453	1.75670396994016	-0.40811262996625
H	-4.05512078913638	2.92787060848883	1.45878898854886
H	-5.14082002147500	2.91254201491971	2.85451823431858
H	-3.86281204291307	1.68655214203646	2.71263004016291
H	-8.26870412425089	3.09797689342306	-0.98599340562459
H	-7.32093759451168	4.54332665196179	-0.63698449072115
H	-8.86257459901662	4.29410899424552	0.20650044784934
Zn	-4.28071539406558	2.79774778816537	-1.33280041653898
Cl	-4.23471319739176	4.91574273425604	-0.66725552236965
Cl	-5.84280750837169	2.10424825987340	-2.81915637329994

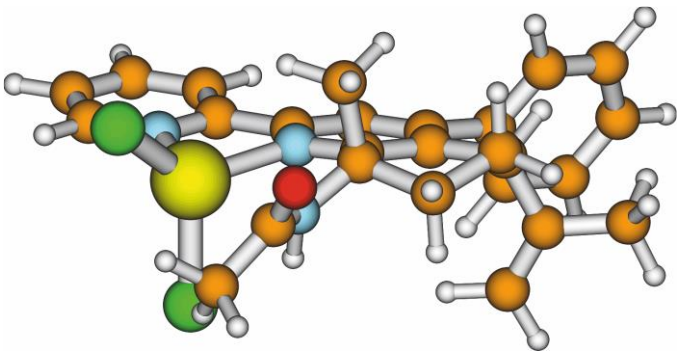
Table S8. Calculated geometry of the conformer **1d** in cartesian (XYZ) coordinates.



E(h) = -3945.0233

C	-4.85070711483183	2.73688636345384	1.57620110909031
C	-5.53141306429858	3.65687792890231	2.56655387092595
C	-6.05487302786922	2.95088110163292	3.83862889414798
C	-6.05656156003399	1.43750668405623	3.79043772587876
C	-5.72682812659401	0.71994956915106	2.63141891289132
C	-5.68580302024093	1.48059242098792	1.31627303859040
C	-6.32385636614941	0.69537935412062	4.94692466601152
C	-6.18885354278014	-0.68373323189687	4.89653990089425
C	-5.71992125529490	-1.28882823570076	3.74736300693942
N	-5.46941715262586	-0.58622410491889	2.63890353182758
C	-6.83282997841765	1.29855115557849	6.20174805756990
C	-5.50605832670664	-2.74686985764860	3.67789958180342
C	-7.35534175413598	3.60552233070889	4.25176658704144
C	-7.18539416768650	4.96951973343354	4.84303326424340
C	-8.54770538624467	3.05049605915362	4.07605066614724
C	-6.07958536681137	2.16580039039409	6.98549140250225
C	-6.63192192157944	2.73731764600204	8.12308428909325
C	-7.93486066788726	2.44376108283669	8.49401221290485
C	-8.68027448357306	1.55255260282820	7.73481736388851
C	-8.12720658756989	0.97616549910078	6.60438884745814
C	-6.11187872105777	-3.64264970592071	4.55268224561514
C	-5.90183276351987	-4.99733814051926	4.37134245924814
C	-5.09708857225322	-5.42946393209975	3.32753932693346
C	-4.52911545466299	-4.47761762756108	2.50189373597576
N	-4.72943596123943	-3.17821276349906	2.68439075526165
N	-7.05681557037510	1.89452639130589	0.99197725759774
C	-5.12211974799207	0.70956685829209	0.13993794963866
C	-8.17101777928566	1.13635782163669	1.14570530674840
C	-9.41469718295556	1.67326905591629	0.48569904532196
O	-8.19393013361425	0.09175779598501	1.77088680340105
H	-4.68407113524249	3.26917660019988	0.63428793005851
H	-3.87144971742652	2.40460174779887	1.93218169483233
H	-4.84533649757854	4.45584443823030	2.85266013565625
H	-6.37623108404004	4.14346552695141	2.07440669997927
H	-5.33848867283975	3.18639899559782	4.63375225345976
H	-6.40192617249377	-1.26698075617367	5.78158932954323
H	-6.70236657605708	5.65218438334451	4.13669431163947
H	-6.54083800032385	4.92234607243236	5.72631033747075
H	-8.14185960272176	5.40035186677401	5.14059082773174
H	-9.45030681414793	3.57716531067962	4.36495326947423
H	-8.66314689987635	2.05045437398268	3.67357701308390
H	-5.05816403661907	2.39892917062370	6.70870942185279
H	-6.03659680742027	3.41287494638213	8.72636535132336
H	-8.36777896344349	2.90510207341642	9.37400016206027
H	-9.69468658645861	1.30334903221080	8.02463701053213
H	-8.71614693241721	0.30190420200558	5.99195635556728
H	-6.76255528261513	-3.28814262070355	5.33964414826445
H	-6.37922009125243	-5.71211131728502	5.03116083347411
H	-4.91686484969607	-6.48016913582064	3.14211776895422
H	-3.91306733006647	-4.74669727381982	1.65207981197125
H	-7.13435841930972	2.70580071636440	0.40188503219587
H	-5.68048721555359	-0.20668382397722	-0.05356735914666
H	-5.19713952708293	1.33431845897857	-0.75259139402259
H	-4.06280478856270	0.48295803864326	0.28364790334674
H	-10.26068838823901	1.48783097175102	1.14582794109621
H	-9.58238036081796	1.10794488385530	-0.43404306608622
H	-9.36251646508042	2.73500210150920	0.24066039548468
Zn	-4.07221580704547	-1.71130313426695	1.35082912172484
Cl	-2.17606384345667	-0.65001619678901	1.84554204557164
Cl	-4.45925837382748	-2.73717989860822	-0.58196910268561

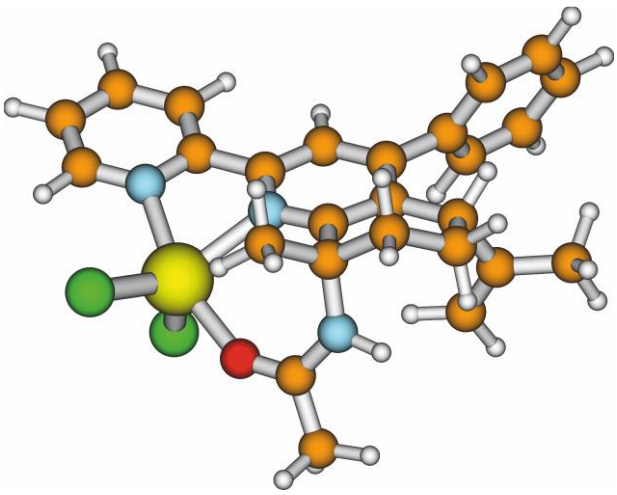
Table S9. Calculated geometry of the conformer **1b** in cartesian (XYZ) coordinates.



E(h) = -3945.0688

Zn	0.47721832196366	7.90519305133145	5.04801577489654
Cl	0.52400281973145	5.69129830475822	5.63623940573563
Cl	-1.41161598378535	9.02742608157961	4.65138521011371
O	-1.21629426498039	9.53460281273413	8.66951025814084
N	2.36534349347323	8.57903706813846	5.72137974318580
N	1.58117484599563	7.90072130642875	3.26446568503047
N	0.41290683957573	8.35154998527438	7.60879266329726
C	1.49865904403963	9.29786285744969	7.86587991044798
C	2.67140816736140	8.91930887756989	6.97555816270239
C	3.99311433759137	9.03083591059419	7.41317729794250
C	4.35143713956152	9.38211173896273	8.83394089555483
C	3.17596091139127	9.98308105422178	9.61182415692450
C	1.89172032488394	9.23833875484920	9.33967837612209
C	4.95188881143693	8.21080205854412	9.58569891789022
C	4.62502699031026	6.94489151528894	9.34604718218556
C	5.93465009242175	8.61025532113634	10.63888893452678
C	1.10880611170198	10.72206287628135	7.43935818848130
C	-0.85355349570287	8.51623382068666	8.10978112761004
C	-1.78226958032117	7.35967807577136	7.88528012825086
C	3.32771128018442	8.37226757117903	4.81895487995296
C	4.66109365284322	8.45367852825385	5.17626605219572
C	5.00663754107713	8.76581608601528	6.48091668938150
C	6.44675938104103	8.79227516580717	6.82893404065554
C	7.17877758512042	7.60824221529785	6.78879406249379
C	8.53388119853660	7.61107765783613	7.08245829562523
C	9.17406375602496	8.80188952639747	7.39712999030536
C	8.45324845429362	9.98749701115249	7.42353517704933
C	7.09421442877375	9.98425128828880	7.14318664107738
C	2.89366509374425	8.08417686662430	3.43626071278924
C	3.76948882678108	8.04558449929940	2.35890697195072
C	3.26074805417510	7.82162835349355	1.09032902766008
C	1.89717728716586	7.64213526400538	0.92644957956811
C	1.08972654721600	7.68816999826426	2.04923039819032
H	0.69335152577895	7.38035864120167	7.51857731952794
H	5.13239532515798	10.14526122274985	8.79002336614205
H	3.40087732379774	9.94944038655397	10.67983452254436
H	3.06435149077167	11.03720557570311	9.34686879558513
H	1.07045933507148	9.65540509466373	9.92407651873268
H	2.00421732529083	8.18803141263137	9.62897873637943
H	5.05740812174908	6.13949685920819	9.93013974220800
H	3.93511724615676	6.66650994389445	8.55653975182142
H	6.78045355467963	9.13086780370204	10.17676040333187
H	6.31371326021388	7.74895065584932	11.19033161853024
H	5.48568592603221	9.30927718088554	11.35142252356951
H	0.67862292843089	10.71098414084790	6.43622471046477
H	1.99744682802679	11.35367035728540	7.42112254372303
H	0.38021693113605	11.14138489243541	8.12754174781272
H	-2.16472316414663	7.02072641754762	8.84984545244683
H	-1.31473320672557	6.53012429850993	7.35735626000911
H	-2.62407929317706	7.72542970851285	7.29536762098844
H	5.44246383811803	8.27229736044440	4.45163579986310
H	6.67648607771520	6.67949978885690	6.54361538455451
H	9.09114607040170	6.68164026480591	7.06328957956501
H	10.23329334743980	8.80491891224129	7.62740049542578
H	8.95011702623984	10.92076007571768	7.66223016940708
H	6.53658543399709	10.91389038720886	7.15307542434765
H	4.82902557994025	8.21132282796770	2.49759334216777
H	3.92693183854062	7.79597731919095	0.23662521181779
H	1.46016852901462	7.47016654118371	-0.04812032471657
H	0.01623724672073	7.55414089668388	1.98124305581565

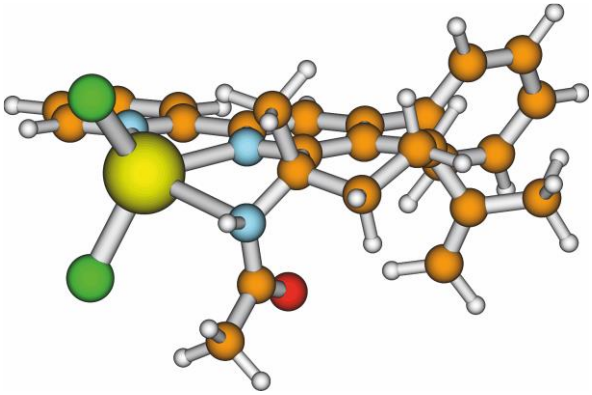
Table S10. Calculated geometry of the conformer **1e** in cartesian (XYZ) coordinates.



E(h) = -3945.0569

C	-8.76666942461584	0.49700358020281	0.56506212322556
C	-8.97595746576501	1.71845374609329	-0.30304002083351
C	-9.28394025907286	2.97914114517547	0.52415149549633
C	-9.67419382815356	2.70912909364373	1.95354534678226
C	-10.07884495345396	1.45544136900113	2.41963759878665
C	-9.93154582221186	0.22730785232934	1.52052453783289
C	-9.67495035400222	3.77645478855054	2.86375740527112
C	-10.06493100472596	3.54208319272235	4.16973174030139
C	-10.48005879112469	2.27646738806021	4.54397395898112
N	-10.51985508304197	1.26911829877197	3.66702396807669
C	-10.82084643206591	1.94159027999110	5.94289901858160
C	-10.66665184949503	2.82804794764441	6.99913342646390
C	-10.92827351828262	2.38425052613977	8.28560802125907
C	-11.32422535230939	1.07237474805782	8.48448192153852
C	-11.48323329749988	0.26136641325833	7.37332617432579
N	-11.24791685503310	0.69457497177651	6.14312011386699
C	-9.24106149566482	5.14448085473146	2.49471266121679
C	-7.90738563028174	5.40775999701017	2.19279729663567
C	-7.49713992854124	6.69678376279796	1.88677830802486
C	-8.41683116658604	7.73681876519650	1.87835542134884
C	-9.74535972013708	7.48177430330621	2.18775399690345
C	-10.15601453414278	6.19356659138646	2.49785698646088
C	-9.60479512041816	-1.04358323874054	2.29851922386657
N	-11.12785100287989	0.05301518696054	0.69676013823786
C	-12.36179767169999	-0.21738178043501	1.12807556694033
C	-13.42994960830711	-0.29198084356587	0.08146868662433
O	-12.65035546513205	-0.39861392637562	2.31327943366893
Zn	-12.12684690933037	-0.12718966983290	4.35469954346575
Cl	-12.04085136612379	-2.32639129566330	4.94388660814188
Cl	-14.05689842982986	1.09509135003355	4.67756866086867
H	-8.61908147591657	-0.38909377163982	-0.05777747507617
H	-7.86967887329963	0.61032239229301	1.17976622723213
H	-9.78935504736102	1.54770208511578	-1.01337756408857
H	-10.03155323402853	4.35036040672281	4.88663272535034
H	-10.32919670445454	3.84183412165501	6.83330728489269
H	-10.81166508646981	3.05828131227799	9.12552022828293
H	-11.52126677323182	0.68167718100642	9.47413047400756
H	-11.82261173347127	-0.76513381086968	7.45695754410727
H	-7.18293861930818	4.60080726798268	2.21481637270900
H	-6.45569750012462	6.88894161656097	1.65550600852354
H	-8.09613815417550	8.74300629203191	1.63422281628919
H	-10.46838319399165	8.28924891154625	2.18701765249318
H	-11.19460251063977	5.99516877823286	2.73716249725388
H	-10.43356734609554	-1.41535244397444	2.89564978620288
H	-8.75603237341204	-0.86668542477261	2.96083017475748
H	-9.32856354503827	-1.82230421950965	1.58497586209125
H	-11.02054602106100	0.19012642769596	-0.29436649003714
H	-13.07367204380398	-0.01501793685441	-0.90983981811526
H	-14.24332075244055	0.37078547022347	0.37886033266677
H	-13.82592063699389	-1.30893532942561	0.05664820271643
H	-8.08753444137400	1.88643075164926	-0.91347079062452
H	-8.36673563107889	3.57143562782683	0.55725127874358
C	-10.31376150338567	3.83277382572592	-0.19206837088887
C	-9.76157436295890	4.63735972024284	-1.32291291592116
C	-11.60437091488528	3.83283387718575	0.12553359817221
H	-11.99478807531769	3.25983652633960	0.95927857969747
H	-12.31357640346878	4.42572397794680	-0.44190375655076
H	-9.02567672332656	5.35509941735196	-0.94440533880534
H	-9.23650607046887	3.99815910658847	-2.04033453614711
H	-10.54390890848842	5.18306144461524	-1.85172995229603

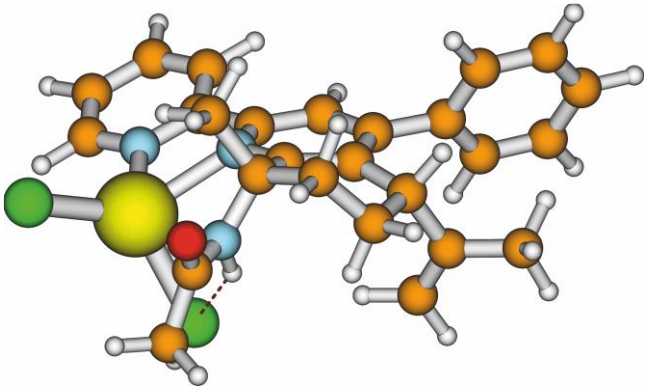
Table S11. Calculated geometry of the conformer **2a** in cartesian (XYZ) coordinates.



E(h) = -2333.6540

Cd	2.18100961354165	5.93169498151623	7.61558496842173
Cl	0.47091004057396	4.35623218216493	8.36883730215935
Cl	2.84615216823664	5.87570054695792	5.26779782824535
O	0.08620913017697	8.07129219159061	9.94947724862390
N	3.04966670347739	7.57594201018647	9.03435861508103
N	3.91673286797422	4.99950136467934	8.86195329031911
N	0.64726791013639	8.17836359654921	7.76002485008099
C	1.66878254958851	9.22423195791169	7.92074765801839
C	2.63589290290868	8.84266805464603	9.03142354534198
C	3.09719832793680	9.78554903054451	9.95552926724558
C	2.65045541952155	11.22742070301545	9.95563447236212
C	1.98677917632012	11.61291189257370	8.63077710514314
C	0.98622354035524	10.56048603757345	8.21654488147071
C	1.75888944262975	11.60022353975630	11.12502337999003
C	0.93446825077004	10.74514468596880	11.72081105094650
C	1.85105506614814	13.03618612160158	11.53389732169966
C	2.43211613043905	9.31605879023004	6.60036950521620
C	-0.23294546086175	7.90662626076455	8.78811800321606
C	-1.58066333663932	7.38833244482818	8.39569873778730
C	3.92403362799344	7.14609806227948	9.94685280375404
C	4.40917625793331	8.01138925855568	10.91295494878938
C	3.99836360067122	9.33578169275548	10.92767663783101
C	4.50402564137156	10.19780608405715	12.02102580413761
C	4.12176109799470	9.89954910539546	13.32663781635986
C	4.61816998149955	10.63457691959927	14.39116179572401
C	5.51193590332594	11.67254334584119	14.16057336159197
C	5.89558139376110	11.97573336589670	12.86189548695598
C	5.39024956466395	11.24643235401915	11.79348891423888
C	4.35258860678821	5.72590454097083	9.89352163919746
C	5.16820417537138	5.16079186887164	10.87028044218453
C	5.53599746767693	3.83115855634316	10.75477557553348
C	5.09290719528071	3.09696115169569	9.66659770988775
C	4.27137402582972	3.72419459137538	8.74744666002703
H	0.22823547765580	8.17844599945353	6.84018779170919
H	3.55231464287092	11.83699174393785	10.05775330958608
H	1.49124965391038	12.58011596137273	8.73499598982361
H	2.75558821910764	11.73894827811536	7.86437893429382
H	0.43719135608426	10.86576833233901	7.32270262089659
H	0.26026747321811	10.42284897724960	9.02074207847306
H	0.29094283990969	11.07370752715609	12.52996415315978
H	0.87036269341097	9.70519517169849	11.42404963848416
H	2.86111468384938	13.26582180023400	11.89019003717073
H	1.14218786521321	13.27075290017179	12.32791174838882
H	1.65087505576284	13.70468430929594	10.69019008968105
H	2.88768559147739	8.36407468918098	6.32502075812613
H	3.22399431035207	10.05985887647188	6.66848204913614
H	1.74705738990268	9.61316126332986	5.80217438392559
H	-1.80164794602600	7.53251982199872	7.33833972733159
H	-2.32414938881050	7.90715430513887	9.00121227359790
H	-1.62463815101833	6.32353376394941	8.63572641340821
H	5.11733200968735	7.67721440610005	11.65750618341023
H	3.42430233203293	9.08827609538612	13.50195407433960
H	4.30634339436523	10.38972154856979	15.40025340061954
H	5.91103759450741	12.24292368839665	14.99121899891279
H	6.59803044028838	12.78006219839431	12.67699620141342
H	5.70734526035737	11.47974353659033	10.78285430747002
H	5.51064812467012	5.74078658837712	11.71500759853001
H	6.16364481442463	3.37473506295805	11.51052020786437
H	5.36692345868243	2.05882824410858	9.53143543643420
H	3.87579182071788	3.18923761930957	7.89163296623123

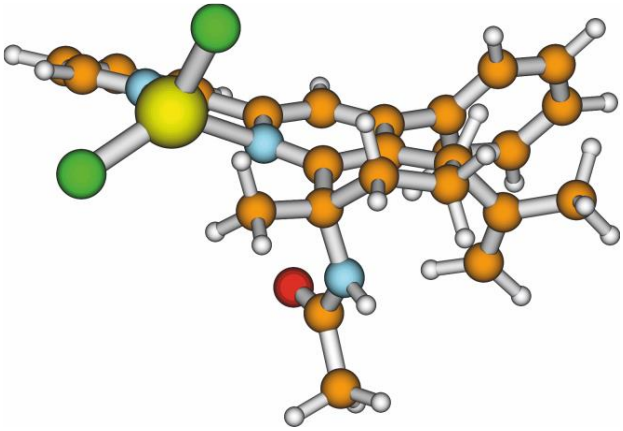
Table S12. Calculated geometry of the conformer **2c** in cartesian (XYZ) coordinates.



E(h) = -2333.6481

C	-4.81871681371340	1.22604879544997	3.71756417465633
C	-5.70318839490953	0.00780424601412	3.61677995524679
C	-4.96165755087538	-1.14587009959853	2.94124940958258
C	-4.12711806301691	-0.66396453255179	1.78043962021220
C	-4.09729202267798	0.67326040295064	1.39502214321419
C	-4.53022967797724	1.79563944338607	2.32772122218570
C	-3.39666494554851	-1.57127545257320	0.99577335486819
C	-2.82678879457489	-1.13684651246096	-0.18683704385202
C	-3.00962577784158	0.17985949581326	-0.58788190556542
N	-3.61456604111455	1.05564153630148	0.20985618353514
C	-3.18198677608054	-2.96767544048121	1.43576699381707
C	-2.52545024053607	0.67243084379048	-1.89528236497294
C	-5.95931364890503	-2.21078375973442	2.50553108236269
C	-6.10540086730721	-3.36630871467664	3.43824319939758
C	-6.68944839860126	-2.07396884655444	1.40273983635575
C	-2.38106484718000	-3.19997578329357	2.55119377088229
C	-2.12138110083855	-4.49525358102043	2.97101365407143
C	-2.67599801682317	-5.56994511455214	2.28887053312516
C	-3.48538298689400	-5.34270025762946	1.18301219383146
C	-3.73090142660878	-4.04732227389813	0.75044428449761
C	-1.49996460919399	0.03506016951008	-2.58308057634704
C	-1.08007634088325	0.55302865575739	-3.79475531307817
C	-1.69555284482969	1.68885328906996	-4.29495943533780
C	-2.71149594163870	2.26637556368557	-3.55424265011634
N	-3.11133018153410	1.76908686687406	-2.38768046097441
N	-5.72973256319335	2.39772605749891	1.73791019161523
C	-3.39028745117360	2.81104427937769	2.41977893884389
C	-6.44749552999178	3.40359418031463	2.30808361394325
C	-7.76705308981342	3.68478302611255	1.64376999691745
O	-6.06550549399956	4.02439118825945	3.28759051255726
H	-5.27785304582105	2.01054692615045	4.31844936393352
H	-3.86544532466565	0.96685178276677	4.18882335519447
H	-6.05805703158284	-0.31143741529736	4.59863482611034
H	-6.59141551807949	0.25306108462639	3.02738831412976
H	-4.29168531979923	-1.59658048978554	3.68053337156528
H	-2.27477031647697	-1.83520546794481	-0.80121716345239
H	-6.35091950070615	-3.01679918477151	4.44702547776018
H	-5.16034511622528	-3.91385584285077	3.51150233023323
H	-6.88413786621588	-4.05526865049536	3.11083767378920
H	-7.42997819210789	-2.81651210631060	1.12742229135041
H	-6.57762815510972	-1.22255643655110	0.73786479139269
H	-1.94871216212473	-2.35927892200903	3.08211144412425
H	-1.48694714831995	-4.66419776993619	3.83307807019830
H	-2.47733220213833	-6.58189131160813	2.62342277219140
H	-3.93130020160389	-6.17738373197213	0.65453249577177
H	-4.36918279761294	-3.86764953872893	-0.10667321309163
H	-1.01938763502390	-0.83907971463807	-2.16612062598706
H	-0.27788863147927	0.07272235716126	-4.34171474281002
H	-1.39338228327059	2.12805617220855	-5.23650040632738
H	-3.22345892411301	3.15653334123475	-3.90183700294995
H	-6.23646791546082	1.83554946456608	1.06429956660259
H	-3.19376087951762	3.28762194846458	1.45944339523842
H	-3.64747239197153	3.58134306768490	3.14421021668305
H	-2.48052218212192	2.30338270247808	2.74655001187668
H	-7.93399287572789	3.07979984033683	0.75323826007333
H	-7.81198941699085	4.74173827031482	1.37574046533925
H	-8.55688203532399	3.48627324414977	2.37115156910259
Cd	-4.71161084820907	2.73366057416778	-1.03173835484519
Cl	-4.53484034080554	5.11461382174675	-1.00211529373822
Cl	-6.79124662311793	1.44718543370036	-1.30498076493407

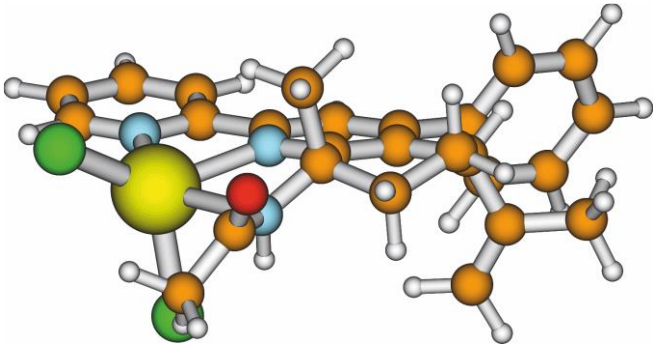
Table S13. Calculated geometry of the conformer **2d** in cartesian (XYZ) coordinates.



E(h) = -2333.6355

C	-4.20315742248137	3.03171276358302	1.96972321428137
C	-4.73186823188214	4.01455669559568	2.98896867031098
C	-4.87392094346309	3.42704146935566	4.40899528454755
C	-4.75991659759265	1.92204505774563	4.50935337370005
C	-4.65349201527741	1.08132281143819	3.39124963691855
C	-4.93773513692548	1.69158361210351	2.01907423595767
C	-4.68482883689085	1.31993994560251	5.77240701564644
C	-4.47378718125704	-0.04650446472959	5.84620235342577
C	-4.29288974416880	-0.79252689393256	4.69536967849243
N	-4.36346345879071	-0.21619621761541	3.49104543555672
C	-4.91106872398782	2.03773443931347	7.04960347722694
C	-4.09113381842854	-2.26176590068243	4.77954369444305
C	-6.09667763123416	4.03789795658823	5.05920112447877
C	-5.89026244644039	5.45053008079836	5.50507019550551
C	-7.25922969222882	3.40876925858003	5.18190401731442
C	-4.09128934846045	3.06655571200368	7.50274697792149
C	-4.36523825941558	3.70220277230640	8.70695537630768
C	-5.46499717356808	3.32292074900883	9.46322184618621
C	-6.27163321133108	2.27861768359113	9.02974898843044
C	-5.99244597422224	1.63746087406872	7.83445596383006
C	-4.20421775885851	-2.95254845798411	5.98305870082592
C	-4.08028068347739	-4.33018705693027	5.99166875901785
C	-3.85383073248707	-5.00098458720056	4.80099144186263
C	-3.73697194852949	-4.24970033435440	3.64685943187209
N	-3.84527941759053	-2.92374357500096	3.64657709573286
N	-6.37731785757324	1.94664780689708	1.93948842725569
C	-4.51641187374504	0.86870330862297	0.81577379659386
C	-7.32596137190358	0.99502816949407	2.08208070336800
C	-8.74244481297127	1.42815974036399	1.81798495024087
O	-7.06177891542503	-0.15475886684393	2.40583022565420
H	-4.29638228575489	3.45436889271379	0.96546014341561
H	-3.14290698560170	2.82280723121102	2.13534380127190
H	-4.07906307031092	4.88801225824015	3.02194459217666
H	-5.70736974200451	4.38560624470308	2.66433028280009
H	-4.01623350713049	3.79775866206300	4.97903202200472
H	-4.43163589843871	-0.50648758925782	6.82205470197530
H	-5.50811227152112	6.07191555650152	4.68835729775798
H	-5.13733830507595	5.48391902129826	6.29916018123699
H	-6.81204232497711	5.89309067567339	5.88453193508193
H	-8.11841624148735	3.91076272186443	5.61304371943913
H	-7.38949884761783	2.37546968170222	4.87912116467258
H	-3.22753932118853	3.36906379483293	6.92274571894422
H	-3.71752965318682	4.50011812498981	9.05116614342119
H	-5.69092217292758	3.83155382125097	10.39328155740984
H	-7.12536218832512	1.96649625742715	9.62035421915561
H	-6.63487244586958	0.83739689050308	7.48397904799226
H	-4.40787407258577	-2.43284945787709	6.90703005206925
H	-4.17317980752829	-4.87521477657050	6.92327648578895
H	-3.76297200431030	-6.07834258423215	4.76203800747197
H	-3.55289356162588	-4.71759977596974	2.68641333484665
H	-6.66917407092587	2.85751530312926	1.62793431731200
H	-5.08132062650514	-0.06155619257458	0.73663070517965
H	-4.74109420223334	1.44179158086147	-0.08516201904162
H	-3.43725247391020	0.68690993888052	0.81237216513747
H	-9.36487903130591	1.11190653818192	2.65555156225323
H	-9.09704984425760	0.90129508985124	0.92957089358954
H	-8.85299170297542	2.50149962602985	1.66203729441678
Cd	-3.48674111151925	-1.65211795029747	1.80312172425397
Cl	-1.15947797016452	-0.90981197786192	1.73858037073445
Cl	-4.53235813812631	-2.77250274905476	-0.07069785567435

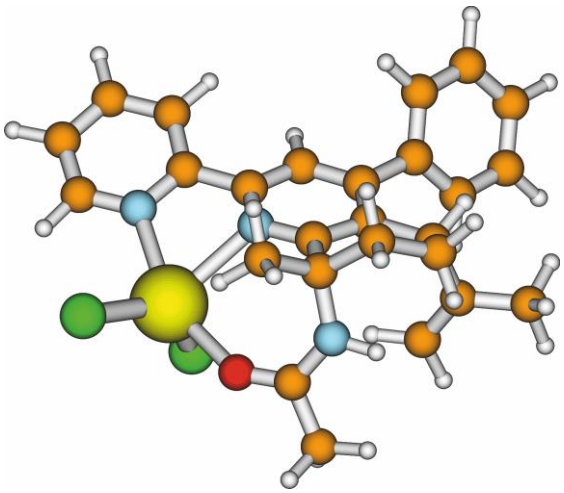
Table S14. Calculated geometry of the conformer **2b** in cartesian (XYZ) coordinates.



E(h) = -2333.6517

Cd	0.38113881996109	7.96124154142905	4.79044311992105
Cl	1.03779507480405	5.66982495627449	5.47261344372928
Cl	-1.84627479360955	8.65045323216164	4.21343850278539
O	-1.27384711779749	9.39948709467985	8.48004475158981
N	2.40142628472479	8.96326497609044	5.44521433642917
N	1.69458948012404	8.24518267166725	2.91482243922839
N	0.50056865329778	8.46462466580562	7.37462942329896
C	1.48237979345572	9.53180835646399	7.62232597314849
C	2.68128996262881	9.30206097470091	6.70480366293446
C	3.98910786204373	9.54048879165803	7.13569770926161
C	4.33109304535359	9.89117144162770	8.55966642166583
C	3.11242668746201	10.35471438962014	9.36265545088349
C	1.90501519983379	9.49126591825438	9.09063161770063
C	5.04992240174925	8.75963347158482	9.26973821142111
C	4.82228680564618	7.47606875059787	9.00976216006088
C	6.02795882650976	9.21438364081650	10.30476599011411
C	0.91644832125681	10.90320911778501	7.23783955586200
C	-0.76607563906171	8.44419037703853	7.92805764497418
C	-1.50489517845316	7.15124597162601	7.72807178317518
C	3.36847649542773	8.85429934133720	4.53453027615396
C	4.69184483442430	9.06279139099815	4.88712103738470
C	5.01504833171041	9.40033191388116	6.18946735843300
C	6.44775631556141	9.58234477999979	6.52400224655597
C	7.30118751134604	8.48244291756962	6.48641892934811
C	8.64969981890627	8.63163834872653	6.76953555830280
C	9.16149712018755	9.88603297363269	7.07233912550544
C	8.31963127440802	10.98950425042479	7.09366201893124
C	6.96716980395015	10.83929377973836	6.82404656163281
C	2.97766642660660	8.54036525455936	3.13846955499419
C	3.88888907461181	8.57647032253984	2.08862162805296
C	3.44741154866342	8.32204067408079	0.80120714129971
C	2.10945630360863	8.04119737451627	0.58380524036753
C	1.26586533157631	8.01080187653320	1.67962432161413
H	0.91410439401365	7.53708362544845	7.33262753220926
H	5.03528004172888	10.72652506392972	8.52819383952066
H	3.35361431453792	10.32013278999340	10.42732500798081
H	2.89165049423355	11.39772451978860	9.12245870498314
H	1.05694595303587	9.81667519721102	9.69538470931606
H	2.12686290060210	8.45413311585822	9.36303147113217
H	5.33571908804561	6.69848888437553	9.56531063741902
H	4.13701340678969	7.15592933585263	8.23223902809755
H	6.82412828574572	9.79769318425426	9.82927977886315
H	6.47914753277714	8.37502720432404	10.83557398145838
H	5.54897784549862	9.87268127117257	11.03656788328503
H	0.54240757616179	10.88931741849060	6.21227464380973
H	1.70782936806755	11.65127014580223	7.29478706466421
H	0.10594765522041	11.18280280810020	7.90559392254527
H	-0.87760221383702	6.34864229674864	7.34189705913838
H	-2.30617484143559	7.34060325130662	7.00984297647068
H	-1.96270473891557	6.85553147419395	8.67225061442751
H	5.48503847132084	8.96662019658482	4.15984516350080
H	6.89927195808170	7.50435641570598	6.24833100744627
H	9.30225847207901	7.76646194142373	6.75159841518132
H	10.21616764168525	10.00349988598920	7.29357492019366
H	8.71798505291262	11.97174813612731	7.32015553319970
H	6.31288224291612	11.70402995500930	6.83153294378450
H	4.92732604592878	8.82128453408529	2.26082598313405
H	4.14636529526626	8.35198200370866	-0.02573556323025
H	1.72036327370815	7.84529183008700	-0.40649278358130
H	0.20990979291270	7.78831793600788	1.57094675828961

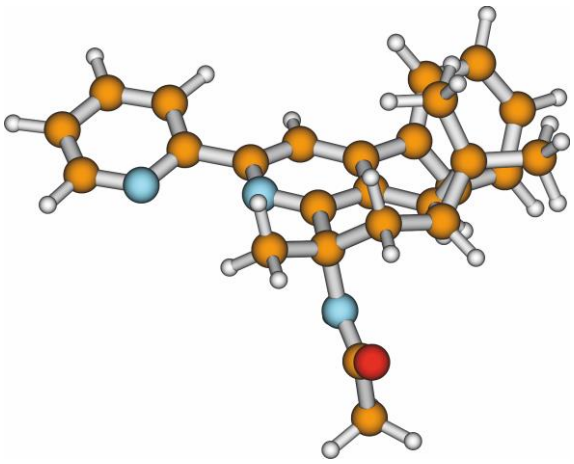
Table S15. Calculated geometry of the conformer **2e** in cartesian (XYZ) coordinates.



E(h) = -2333.6450

C	-8.73308143919801	0.56216084333833	0.59878805259244
C	-8.88542371074084	1.79848402850917	-0.26465069414946
C	-9.44358654586929	3.02626771881494	0.49789287853778
C	-9.74135165540945	2.75945543026946	1.94834495701017
C	-10.08180795095715	1.48345691053302	2.41820558231341
C	-9.94931932117152	0.27742778047940	1.48551086093094
C	-9.64959705517266	3.79539785436450	2.89118555746246
C	-9.91012430437506	3.50424779057369	4.22216514223938
C	-10.30152671633873	2.23081900171729	4.58763604964454
N	-10.40951469002236	1.24861003860331	3.68882299907976
C	-10.57879367871712	1.89414305945478	6.00130521920729
C	-9.99205786966545	2.58983078182782	7.05349701416324
C	-10.27700916162773	2.20169787890809	8.35219477963518
C	-11.13697901565998	1.13676708574823	8.56929647595664
C	-11.67198134066771	0.49144354977935	7.46722558848426
N	-11.39471436361328	0.86518584117463	6.22447359361482
C	-9.21097982624182	5.17474397908175	2.57200123970672
C	-8.08623473060403	5.68377818230357	3.22387146576205
C	-7.65977162935089	6.98164244750093	2.98826335400618
C	-8.35843317911588	7.79402543087101	2.10510209722883
C	-9.48752195800144	7.30115824590205	1.46625668568648
C	-9.91231175505280	6.00147851651991	1.69732915625269
C	-9.67703432603878	-1.02773274296039	2.22630027423683
N	-11.11451308185837	0.16014801737709	0.60778495663931
C	-12.35871037101201	-0.18075164248228	0.95606118207700
C	-13.39324012587521	-0.10454688087864	-0.12344572368917
O	-12.68287896664263	-0.53791006523587	2.09153775204000
Cd	-12.42891718159918	-0.06547688407505	4.35052433215794
Cl	-12.43907459886769	-2.40384255441359	5.05780982288151
Cl	-14.16196305920580	1.68263494017326	4.26028811138868
H	-8.54446320108326	-0.30975235465172	-0.03261906187962
H	-7.87689474404645	0.66261408348528	1.27096139153112
H	-9.53969119048904	1.57983175260601	-1.11337743450850
H	-9.84132823447144	4.29017357820581	4.96227202263970
H	-9.30993099537795	3.40723802565591	6.86217058127624
H	-9.82402095770222	2.72420345499904	9.18621352277924
H	-11.38931550112974	0.80083386735422	9.56680123641015
H	-12.34253686533653	-0.35383249713784	7.57481343047439
H	-7.53517534849075	5.04838244577575	3.90852456345951
H	-6.77911409661427	7.35864382943053	3.49556687156668
H	-8.02095429282017	8.80594163770490	1.91149027681255
H	-10.04875871372719	7.93355436530749	0.78778987715957
H	-10.80423205253664	5.62958872093700	1.21121139882307
H	-10.52227531506307	-1.38059091630569	2.80971286135873
H	-8.82391474385710	-0.90154612653392	2.89393113774875
H	-9.42974301799895	-1.79420314388463	1.48923808401127
H	-10.99267514978972	0.46098138019645	-0.34484173341342
H	-12.97699780087417	0.14814235173439	-1.09782866467541
H	-14.12006462859930	0.65718703214796	0.16711227407153
H	-13.91949695028080	-1.05787766707691	-0.17694918592261
H	-7.91864155613934	2.04513793186128	-0.70582496015371
H	-8.67694710535619	3.80745831718038	0.48152667759288
C	-10.62727061282140	3.59245900271164	-0.26675648887441
C	-10.24964433831732	4.31806627301969	-1.51975655880592
C	-11.89185096766708	3.45489031606184	0.12015297692520
H	-12.16435755758051	2.96214076833680	1.04716737502932
H	-12.70031931018622	3.85939306185750	-0.47892536353225
H	-9.58921242940355	5.15848554371291	-1.28108854705730
H	-9.69221628376583	3.66945364286539	-2.20274608183926
H	-11.12695899980097	4.70366481866276	-2.04018533210532

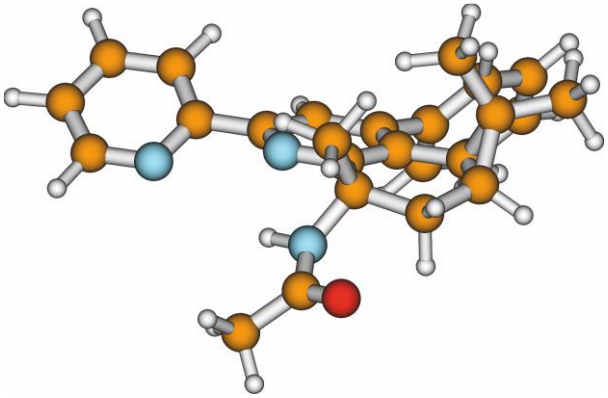
Table S16. Calculated geometry of the conformer **L[1]a** in cartesian (XYZ) coordinates.



E(h) = -1245.5915

C	-10.83907293844901	0.96618211293163	1.55562201695168
C	-11.25702479812152	-0.32656058020793	0.90602910331132
C	-10.22909206624123	-1.03641914599826	0.07864046878398
C	-8.87159784934371	-0.46117919025482	0.01536155632575
C	-8.64805859875148	0.87395938326482	0.37782775944144
C	-9.85113293954618	1.75827776622460	0.68727329167001
C	-7.76117454222910	-1.21376931974388	-0.37999383625257
C	-6.51149540590850	-0.61041924430274	-0.35909742704233
C	-6.39078599606162	0.72042819942292	0.02742461384337
N	-7.45492205104370	1.44153153199109	0.37986598020325
C	-7.92068169743153	-2.61445622591528	-0.82931899293649
C	-5.07736410167224	1.41315337337609	0.02258700834336
C	-7.27753463010307	-3.65916571397754	-0.17049201694817
C	-7.47850110541445	-4.97332854488603	-0.57285058495076
C	-8.32204730460298	-5.25674642564149	-1.63804442636084
C	-8.94247376019215	-4.21724170610967	-2.31874245480527
C	-8.74121674821372	-2.90763421234465	-1.91700898978874
C	-3.88098043676104	0.69595147005724	0.05287392147392
C	-2.68172409753915	1.38626025754267	0.04091880818916
C	-2.70458945427927	2.77114020534723	0.00371840484418
C	-3.94103887115250	3.39941566478900	-0.02265998044700
N	-5.09673444481339	2.74752228869066	-0.01508897277205
N	-10.41787010149276	2.03811044761526	-0.63826973105566
C	-9.46364033515598	3.05166693460224	1.38286682405816
C	-11.60888091103847	2.59482775737194	-0.91841493518433
C	-11.89143002912414	2.72862893374739	-2.39326262355810
O	-12.40498369299286	2.97882582188762	-0.06836495384167
C	-10.73896888106063	-1.66710091541485	1.35716997247497
C	-11.64190477932367	-2.85837985977352	1.18624245828724
C	-9.83997444573003	-1.77519705624253	2.55550069143614
H	-11.71243726790270	1.58899839559151	1.74294998724382
H	-10.35087866588870	0.79582063881761	2.51812600764291
H	-12.25895534435943	-0.32968388882827	0.48906316254864
H	-10.58559633279767	-1.51589610189104	-0.82320815703071
H	-5.64873947562213	-1.17384302523393	-0.69043742033235
H	-6.63557282150387	-3.44216140585523	0.67599721249359
H	-6.98051555840750	-5.77819412000135	-0.04444531877873
H	-8.49166592206452	-6.28203823435067	-1.94729707814070
H	-9.58681453654065	-4.42652261785589	-3.16477168762442
H	-9.22074565701115	-2.09905268455168	-2.45614376747048
H	-3.88569686438869	-0.38510801885470	0.10164676793403
H	-1.74201857178607	0.84731042880266	0.06807769060939
H	-1.79231959181745	3.35429648331133	-0.00441316675471
H	-4.00406440943744	4.48404368807980	-0.05600319826519
H	-9.84277668114390	1.79542212089790	-1.42702370094048
H	-10.36368831979370	3.64071389483888	1.56335397982775
H	-8.76874212801862	3.62582146983896	0.77199599956612
H	-8.98065096366622	2.83845706042421	2.33853337909603
H	-12.93133502188392	2.46117609225107	-2.58254651763189
H	-11.24180218337272	2.10599478943579	-3.00823947836086
H	-11.74515878016491	3.77211922051908	-2.68363797626309
H	-11.04862393650616	-3.77083767589674	1.06933460666705
H	-12.29051848223771	-2.98481314501234	2.05858427994459
H	-12.27788693334312	-2.75458338963266	0.30424321694652
H	-9.25765518742592	-2.69985189880181	2.50333378808322
H	-9.13359647430135	-0.94884740957988	2.63569535804904
H	-10.43752987482367	-1.80683567451186	3.47200907724693

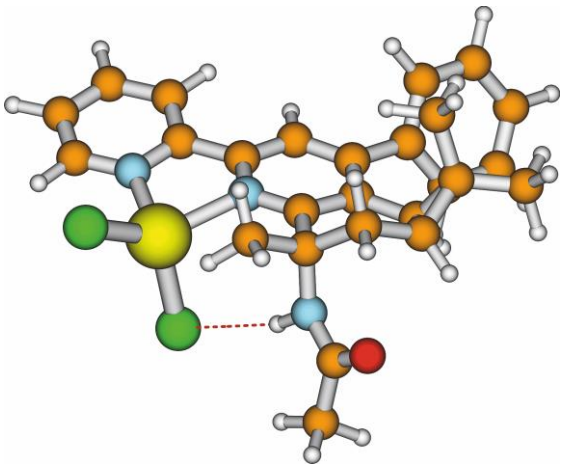
Table S17. Calculated geometry of the conformer **L[1]b** in cartesian (XYZ) coordinates.



E(h) = -1245.5860

C	-10.78675303904264	0.85610146358655	1.94578108764371
C	-11.12838586036746	-0.51980957930185	1.43558504495071
C	-10.19573050093063	-1.21637594546487	0.49796193335692
C	-8.84521187272945	-0.66498202227845	0.34546759523966
C	-8.40322305463007	0.43512694126909	1.08965907479919
C	-9.30176054913898	1.25086152028858	2.03077211464616
C	-7.94764460560670	-1.21077665526394	-0.58671456111656
C	-6.66699823896186	-0.68885364338021	-0.67589848888626
C	-6.30587313195617	0.37412237425421	0.14273837707751
N	-7.17345665243203	0.92460057315569	0.98203818518655
C	-8.35151706071626	-2.28345991328923	-1.52101916329270
C	-4.94589942875495	0.95928413713249	0.08924033797958
C	-8.82875701432686	-3.51352793682209	-1.07365224663815
C	-9.19071597087270	-4.49642794474604	-1.98220014422123
C	-9.09623995363597	-4.25889133619216	-3.34702815486692
C	-8.62357684469075	-3.03657763438186	-3.80167399883446
C	-8.25135842841955	-2.05736828582686	-2.89276507124188
C	-3.82858197245498	0.14293181139630	-0.07671519125635
C	-2.57413817814806	0.72715795351045	-0.11359479378911
C	-2.47505061165072	2.10410163375241	0.00270218026299
C	-3.64486310876418	2.83419311494040	0.16035869815863
N	-4.85281753799786	2.28556155451157	0.21198750557588
N	-9.10332935105594	2.63269420208351	1.56386394393864
C	-8.81412647191215	1.19508888631084	3.48237117954999
C	-9.77343249183624	3.72455151889251	1.97229863634569
C	-9.16339448072136	5.03645526749471	1.54158970740228
O	-10.79884333004848	3.68697989517785	2.64461600170329
C	-10.57874193500689	-1.86171094301082	1.82628928699712
C	-11.54010679957156	-3.01803159773516	1.72085938119761
C	-9.53786509123891	-2.08699685707148	2.88779541245549
H	-11.24839606165371	1.02914998188462	2.91915257027630
H	-11.27145784297273	1.55510349966061	1.26309256807982
H	-12.17031007251293	-0.57371293269263	1.13351129361775
H	-10.60850132053764	-1.68659989408527	-0.38648700413609
H	-5.96652775677001	-1.10048108827538	-1.39236518297684
H	-8.91029950258563	-3.70522874009967	-0.00995938776832
H	-9.55516065312645	-5.45131554560553	-1.62096907185953
H	-9.38975614720729	-5.02675233418341	-4.05325979079287
H	-8.54841330385375	-2.83799718675093	-4.86480895853454
H	-7.89235679902304	-1.09748630585613	-3.24755244892777
H	-3.94285762004417	-0.93132331403998	-0.15615131362963
H	-1.68712470751096	0.11519373359025	-0.22853179334462
H	-1.51645080065877	2.60712227663460	-0.02429557282840
H	-3.60476535725018	3.91610950062823	0.25234322535168
H	-8.18987335655713	2.77684979353322	1.15540261366304
H	-9.36247834189650	1.94785089442083	4.05082436803767
H	-7.74676118241419	1.41692957621640	3.53687268022097
H	-9.00746739132725	0.22715286558513	3.94000467306837
H	-8.74682272264307	5.52414080090673	2.42666478446664
H	-8.36944734965481	4.92236806532774	0.80398991125560
H	-9.94607814037608	5.67821105092255	1.13671960734507
H	-11.00120704504656	-3.94419303466316	1.49776974334122
H	-12.07786097916883	-3.16300143662897	2.66289849184955
H	-12.27749816291434	-2.85817479907955	0.93161140146427
H	-9.13229848821082	-3.09927777319440	2.79098162351249
H	-8.69636923014309	-1.40141159419322	2.82442809452610
H	-9.97996309631973	-2.00102161295481	3.88481900439808

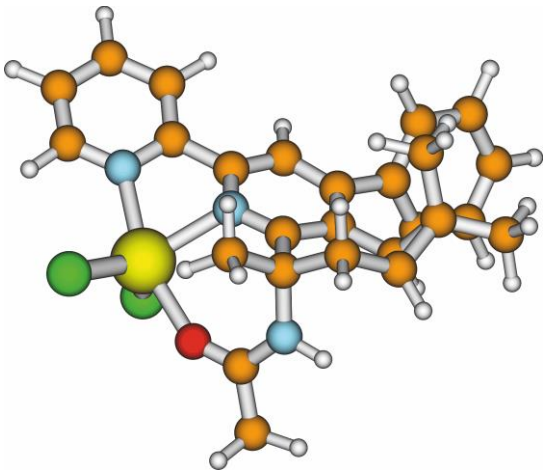
Table S18. Calculated geometry of the conformer **3la** in cartesian (XYZ) coordinates.



E(h) = -3945.0616

C	-10.97327878357143	0.52055910246540	0.72236557692598
C	-11.39353748481930	-0.77686110090639	0.10035972469510
C	-10.31048101615577	-1.54443084681379	-0.58516829085032
C	-8.94910093055553	-0.98039745099598	-0.53590837227303
C	-8.74813049673840	0.39514723672791	-0.34534846219836
C	-9.96794430628255	1.30078460744643	-0.13855723653051
C	-7.82772771154439	-1.80731881718491	-0.65319723113730
C	-6.57008786171278	-1.23155821620548	-0.57615111003569
C	-6.44668137872400	0.13900635430499	-0.45428472738641
N	-7.52616865647714	0.93324132125027	-0.34410281569920
C	-7.94653770899440	-3.26911211495200	-0.83767607654578
C	-5.11948024245275	0.78729788775256	-0.47775351316991
C	-7.37838118279733	-4.13393330081547	0.09495104469534
C	-7.47472260676378	-5.50778212378586	-0.07067804178346
C	-8.13317202327016	-6.03077279623609	-1.17568747394149
C	-8.68962743838063	-5.17357054437427	-2.11541293222870
C	-8.59865132995008	-3.80130567360699	-1.94813347031789
C	-3.92745932392947	0.08226895897087	-0.35583337501775
C	-2.73247876685628	0.77891838964866	-0.37906385454709
C	-2.74694482514710	2.15915321946229	-0.50901204530007
C	-3.96986796707687	2.79190136451403	-0.62799558185888
N	-5.11418591266815	2.11442877877138	-0.62288425157647
N	-10.46250677258643	1.61219416238464	-1.48288709694978
C	-9.63952107764706	2.59065132826256	0.60222510140879
C	-11.72059050103884	1.94217366891764	-1.85654192296195
C	-11.83828703284660	2.41307799054297	-3.28495958748304
O	-12.70790660469645	1.84752355544664	-1.14046361413136
C	-10.96252439622534	-2.10573286272840	0.66173136228746
C	-11.88762305258705	-3.27270685156586	0.45423224377213
C	-10.19347434515479	-2.18691214997741	1.95197305007978
H	-11.84166476510576	1.14913215391419	0.89802025897454
H	-10.48350248782736	0.36418193013188	1.68643412425840
H	-12.35184609824002	-0.75189165036073	-0.40540659995406
H	-10.56949470937100	-2.04809563676220	-1.50775986844256
H	-5.69523563238372	-1.85899832794837	-0.67133277866209
H	-6.86982087283849	-3.72569299072938	0.96122581520035
H	-7.03305569804102	-6.17019037623447	0.66468028590863
H	-8.20886855876885	-7.10348306027633	-1.31204042211719
H	-9.19714492794302	-5.57630331927438	-2.98413665708103
H	-9.01972713689949	-3.13670771400854	-2.69292881225852
H	-3.92713762488319	-0.99048172204543	-0.22530348129593
H	-1.79502319777967	0.24484527304650	-0.28338489170333
H	-1.83323279095383	2.73784001903750	-0.52036995993399
H	-4.05141889695860	3.86783012807321	-0.72951853733854
H	-9.73248085657677	1.88223043708552	-2.13267203437884
H	-10.57485249662517	3.06379930054608	0.90694047872648
H	-9.12571467709745	3.32112201357340	-0.02467795409892
H	-9.03947162423438	2.40089010637200	1.49322074778206
H	-12.25413742092521	1.60085718896951	-3.88584443161129
H	-10.88598233963020	2.72388658857430	-3.71601227852837
H	-12.54212608045216	3.24366080271862	-3.32180986670099
H	-11.32640535689323	-4.21182871747190	0.47976918914625
H	-12.64487417638114	-3.30995462145243	1.24332587266767
H	-12.40377819021712	-3.21003015995796	-0.50606429030949
H	-9.69330252469437	-3.15624542184574	2.02827643188461
H	-9.42723306334531	-1.41674421166802	2.04545410153666
H	-10.87428644076481	-2.09397384956455	2.80366129183687
Zn	-6.98172432320578	2.94795455150371	-0.83752924714901
Cl	-7.70563633569577	2.98007995207140	-2.97384397362809
Cl	-6.79260127761619	4.85431043726230	0.30298898732960

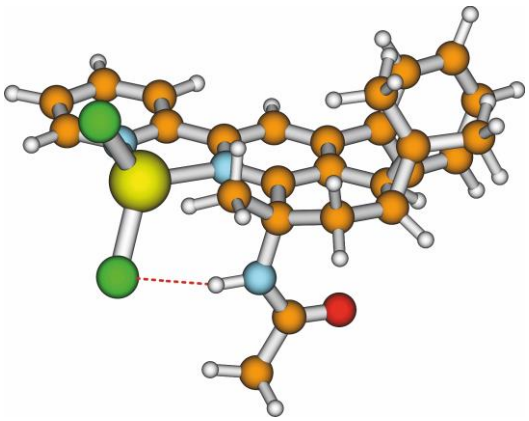
Table S19. Calculated geometry of the conformer **3II** in cartesian (XYZ) coordinates.



E(h) = -3945.0602

C	-7.57321410922588	2.43526421254578	1.53900231007194
C	-8.90416155270188	3.13398478705101	1.57640205264423
C	-10.05864087591036	2.40332219376215	0.95050017443370
C	-9.78106476006174	1.04520502875258	0.43547844938892
C	-8.48499737018804	0.68243008745355	0.05297415277787
C	-7.33789187072289	1.68000859928172	0.22563667454325
C	-10.78573600271335	0.07175093226332	0.36989356760903
C	-10.43849977893041	-1.22015413190052	0.00427331649168
C	-9.13964710448106	-1.48547818366044	-0.38859994261242
N	-8.20353066966894	-0.53037877648310	-0.41623908619859
C	-8.68957555917742	-2.82531575244887	-0.81151612666893
C	-9.33982557933199	-3.99470248561842	-0.44397942470807
C	-8.79814231745326	-5.20543613425362	-0.84313405168759
C	-7.63213990177799	-5.21594047278248	-1.59171079319926
C	-7.05339613923876	-4.00296246035838	-1.92765010032588
N	-7.57556772660682	-2.84626338179116	-1.54623996729548
C	-12.19363512618293	0.38112971513564	0.69585880998238
C	-12.82773888854583	-0.25816198931622	1.75812961466112
C	-14.15622860431965	0.01437616478811	2.04892406890742
C	-14.87059941107086	0.91028706226405	1.26520876355218
C	-14.24791831148852	1.53711118405334	0.19313752176601
C	-12.91554944829692	1.27964048695265	-0.08726134019657
C	-10.04099226417450	2.65983377533301	2.44113534998773
C	-10.96498039084488	3.73225271254206	2.95004880416437
C	-9.84129100498343	1.51706849116923	3.39635931689219
C	-5.96890084632931	1.02174350598651	0.31908535321995
N	-7.39226129425305	2.66352308672740	-0.85674332180294
C	-7.27837568051818	2.36517010808980	-2.15373082377322
C	-7.48341448029096	3.47935363751842	-3.13054288181515
O	-7.01577440432085	1.23157703369655	-2.55981450438065
Zn	-7.06688068163608	-0.89543222052085	-2.30423907739321
Cl	-4.82468500878144	-1.14419398195925	-2.53370513099827
Cl	-8.66613605353592	-1.00476047219177	-3.95616885562726
H	-6.76262083746838	3.15712217089968	1.66395480351648
H	-7.46613672141668	1.70930172965937	2.34731431320479
H	-8.87602391667541	4.20562085022986	1.40976820712778
H	-10.77032713301660	2.98737810690508	0.37884053579914
H	-11.19392887755361	-1.99449827494485	-0.02400514393557
H	-10.23714192991170	-3.96299803794312	0.15929383233184
H	-9.28014818492354	-6.13372518932548	-0.56042181795969
H	-7.17663752599854	-6.14215195465974	-1.91692207867577
H	-6.14736605388732	-3.94620739825950	-2.52019204892067
H	-12.26922857780029	-0.95923212625229	2.36832155396921
H	-14.63634047297649	-0.48089256537640	2.88490674939592
H	-15.90811626769314	1.12608908444766	1.49369028675406
H	-14.80439219689505	2.22589154181293	-0.43183239742300
H	-12.43455970674227	1.76435247158481	-0.92947398296047
H	-11.94288055929491	3.31617552174531	3.20900482991772
H	-10.54554703348621	4.20044013989574	3.84608604578225
H	-11.11375628226561	4.51282769963711	2.20059454358587
H	-10.80725034089302	1.08781891341880	3.67536436348837
H	-9.35193896424407	1.86646655629995	4.31020268235651
H	-9.23815236934849	0.71200170869472	2.97609848406132
H	-5.62913179920050	0.58988346930620	-0.61856712045310
H	-5.98801903306755	0.23297592284681	1.07273065157264
H	-5.24528477190307	1.77769935504088	0.63168121553849
H	-7.66190589419712	3.60350216502186	-0.61634492704929
H	-7.81073073100061	4.40485420735042	-2.65797038611383
H	-8.22909307028881	3.15487283072500	-3.85744820545092
H	-6.55046997008689	3.65194125915739	-3.67000373187056

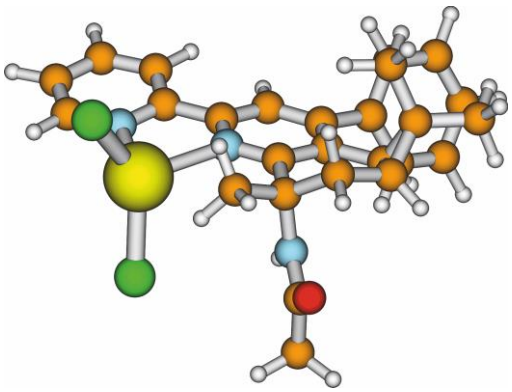
Table S20. Calculated geometry of the conformer **3Ib** in cartesian (XYZ) coordinates.



E(h) = -3945.0591

C	-9.08662480513822	1.58744738237122	0.45259566909330
C	-9.56514927749073	0.17417548974472	0.26820997037893
C	-8.55532237597263	-0.89474781213550	0.06703320540324
C	-7.13051920563500	-0.56193020234967	0.10502281353387
C	-6.65460880219488	0.75365991590289	0.18462420354087
C	-7.62304822138977	1.94192148537392	0.08934214739221
C	-6.20457142684021	-1.60964464462260	0.08285842289440
C	-4.86059415246452	-1.30970437244002	0.14603914571636
C	-4.45205600888159	0.00988484081191	0.22657037804428
N	-5.33949127193628	1.01881673836494	0.24768379986286
C	-3.01057551212204	0.33530848737483	0.26816416548353
C	-2.01645899510196	-0.63789761770210	0.28963360129057
C	-0.69140647279894	-0.24441529704243	0.32595907228840
C	-0.37826896401301	1.10585688692122	0.34882215787186
C	-1.41717363371045	2.01576439986166	0.33205197827573
N	-2.68963806191298	1.63174257249869	0.28467209076187
C	-6.62782238562722	-3.02815609159807	-0.00943560985241
C	-6.67851318499874	-3.81606432301193	1.13625059479480
C	-7.04381493338495	-5.15233043225619	1.04988026426739
C	-7.35033220351060	-5.71035707078218	-0.18295607801251
C	-7.30531279170671	-4.92670151589792	-1.32819139247877
C	-6.94816125647439	-3.58906393827163	-1.24330147387133
C	-9.37492645840195	-0.85983511168705	1.34664976519606
C	-10.41427937367449	-1.93912608994295	1.46898770524552
C	-8.71572245858105	-0.49925777081421	2.65150021302288
C	-7.25232598516610	3.08004160707901	1.03175084272393
N	-7.49659596426117	2.49314474159579	-1.26276389517065
C	-7.87862552671468	1.89833531916136	-2.41340130616229
C	-7.48457564754488	2.63568970492311	-3.66886599684630
O	-8.51754352553901	0.85577001282411	-2.45401099127116
Zn	-4.29716310235556	2.88860449061969	0.34919163634043
Cl	-4.02989911374034	4.00721348121310	2.27718919650707
Cl	-4.55746997884117	4.06501427921192	-1.55270736532035
H	-9.71090044707612	2.26420661764012	-0.13180257706194
H	-9.23164967483765	1.87643693492292	1.49702427010781
H	-10.46778946982121	0.07063695910399	-0.32137708885985
H	-8.80352036720699	-1.69867185078546	-0.61355050283029
H	-4.13980362652108	-2.11343799305076	0.12046858190467
H	-2.26140352924452	-1.68999936539133	0.28209167802020
H	0.09236035112485	-0.99204221961879	0.34095548357014
H	0.64588643664417	1.45190500675668	0.38342028450421
H	-1.23658307454422	3.08368518602629	0.36186242783800
H	-6.43326612528090	-3.37968973530487	2.09796477106880
H	-7.08820752335414	-5.75859172893232	1.94731506474286
H	-7.63456178275757	-6.75428060870686	-0.25130278340662
H	-7.55191136955049	-5.35798855337480	-2.29166577043560
H	-6.91556492468102	-2.97476492923141	-2.13635271607697
H	-9.96816840253564	-2.85865459617707	1.86194229893797
H	-11.21347880877403	-1.63600488129746	2.15274059631089
H	-10.86519195342500	-2.16680689590611	0.50087070180936
H	-8.25602557298385	-1.38464154604616	3.10197175823391
H	-9.45564384784829	-0.10893764246936	3.35653622884424
H	-7.93264792751950	0.25317323967070	2.54881645820364
H	-6.38130209607676	3.65376220311952	0.71398691899931
H	-7.07586333950075	2.71141450839696	2.04187842931874
H	-8.08095797003345	3.79020766229399	1.05410727074762
H	-6.82088664394620	3.24188724973843	-1.35735279104079
H	-6.77633882159790	3.44350487980223	-3.49018358680422
H	-8.38600040562186	3.05055493989978	-4.12572600634995
H	-7.04784100490364	1.92069061362151	-4.36680833124073

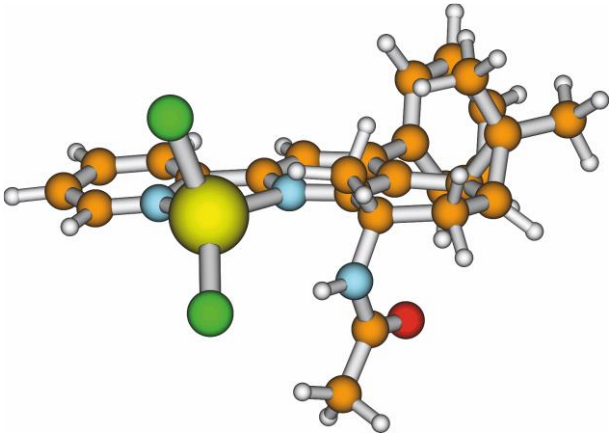
Table S21. Calculated geometry of the conformer **4Ia** in cartesian (XYZ) coordinates.



E(h) = -2333.6404

C	-11.12632606207170	0.55157721482033	0.66314962720376
C	-11.43541090275884	-0.85466816424909	0.22604696334417
C	-10.30272489228561	-1.63822686028833	-0.35451579648035
C	-8.96924276300146	-1.01884485411544	-0.40467197014235
C	-8.78780842381272	0.36183257354799	-0.24021742028909
C	-10.04088337076987	1.24105537215203	-0.18037544479225
C	-7.84029242854931	-1.80841071703010	-0.63523449476333
C	-6.59605344127923	-1.20706161162430	-0.60747231255841
C	-6.48718474247950	0.16161727528216	-0.41997976947395
N	-7.58031828469489	0.92787814822800	-0.26836341286057
C	-7.96662640691929	-3.24611195889522	-0.95929691931778
C	-5.14915592617848	0.80357039339586	-0.44498349587816
C	-7.49041341705699	-4.22941810913817	-0.09880511601588
C	-7.62115050099215	-5.57129835217229	-0.43139540344729
C	-8.22431904284980	-5.93860360641058	-1.62587006242078
C	-8.69127512152569	-4.95906088174826	-2.49247520870433
C	-8.56545118716915	-3.62091866483576	-2.16026840770936
C	-3.97200562149776	0.05854243687649	-0.40796524935089
C	-2.75441768428636	0.71319647509871	-0.45082271514236
C	-2.72474887058408	2.09701467541410	-0.51680327082309
C	-3.93072063762640	2.77050326938416	-0.53831016809744
N	-5.09856643557598	2.13488098521511	-0.51036463477101
N	-10.43888227728241	1.32723022784951	-1.58839253063105
C	-9.81899197723125	2.62865432401482	0.41309309653120
C	-11.52504631291159	1.95958456074020	-2.07831046336393
C	-11.57256315169225	2.01685235880987	-3.58117441192047
O	-12.39888470731556	2.45193296851828	-1.37734290941830
C	-10.91128726582880	-2.05226196374187	0.97343411232935
C	-11.73640979064454	-3.31077117795255	0.95436854700477
C	-10.13987797848122	-1.87864667181749	2.25169721915073
H	-12.02200465571664	1.16632522205808	0.59579129824193
H	-10.79368209973345	0.59043241355940	1.70311238311198
H	-12.39209776180783	-0.98992153965670	-0.26662648168384
H	-10.53007225362454	-2.30429595213087	-1.17621756832545
H	-5.72048486429791	-1.81214011927288	-0.79242714376888
H	-7.02584931301791	-3.94255359356965	0.83800507052720
H	-7.24979520529076	-6.33080177966249	0.24657071179505
H	-8.32884551435243	-6.98534703954065	-1.88769242029165
H	-9.15823432130459	-5.23838376195290	-3.42976722541748
H	-8.92674061032725	-2.85638102972513	-2.83915179027276
H	-3.99609260142740	-1.01860419037983	-0.33142528659224
H	-1.83440000069931	0.14235064405802	-0.42374196274125
H	-1.79369805958852	2.64691198826894	-0.54764908841277
H	-3.97102580949536	3.85303927912274	-0.57963683396550
H	-9.73748668659412	1.07623365013524	-2.26526130885110
H	-10.77800625902690	3.04733126809589	0.71845097440861
H	-9.43037897638603	3.32604732889893	-0.33428583452043
H	-9.17238749306764	2.59712041836682	1.29102312691961
H	-12.57944212120603	1.76706130393863	-3.91649740131095
H	-10.85664584937614	1.34618641235855	-4.05522516422782
H	-11.34681638713497	3.03915068520390	-3.89426451649404
H	-11.10319654030250	-4.18153659929457	1.14979619781750
H	-12.50931895506263	-3.27875169673341	1.72861810618427
H	-12.22990668436490	-3.45325833178698	-0.00944361917589
H	-9.50992387722308	-2.75399206611091	2.43141982730318
H	-9.49128571969633	-1.00260979452391	2.25061268922371
H	-10.83138110619152	-1.78804371356253	3.09489095437235
Cd	-7.07326715649020	3.25672264897670	-0.44411349311749
Cl	-7.75210425167497	3.86447377367638	-2.68884167286666
Cl	-6.79725156016509	4.55354668585707	1.57909801493924

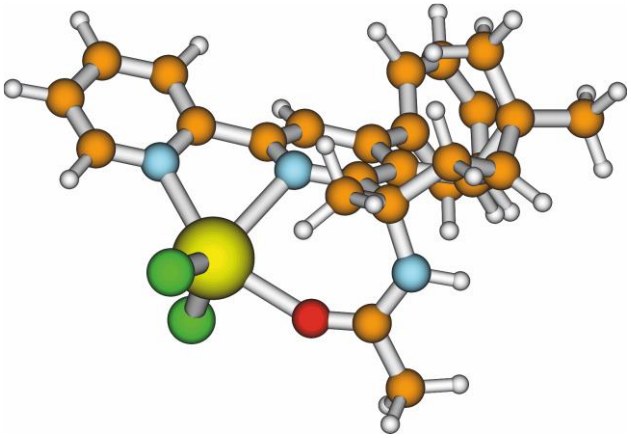
Table S22. Calculated geometry of the conformer **4Ib** in cartesian (XYZ) coordinates.



E(h) = -2333.6395

C	-9.14807139714685	1.53826155684113	0.21372417250811
C	-9.58143064491461	0.10814365899725	0.07788203931128
C	-8.55463845935039	-0.96643856207698	0.03255809691351
C	-7.13650375396467	-0.62601845893958	0.14373348198711
C	-6.67510883609113	0.69226905032432	0.19431310574829
C	-7.63361211491092	1.89065415820249	0.13864754291983
C	-6.19160720923993	-1.65785036332982	0.15984417705527
C	-4.84999593602779	-1.33495405335539	0.18681694714008
C	-4.45726921385776	-0.00595023182041	0.18289127512846
N	-5.36676668997109	0.97778484786622	0.20278647009011
C	-3.01421276608938	0.33475144885043	0.10719592451113
C	-2.02060506367585	-0.64071940828506	0.15550651081210
C	-0.69442949844088	-0.26562753707996	0.04575113772272
C	-0.37147453637531	1.07331807680513	-0.10354976235423
C	-1.40572789394501	1.98724349130887	-0.12996220818487
N	-2.68122420843961	1.62018089966229	-0.03417608008931
C	-6.59439602853746	-3.08310533852044	0.14447440689199
C	-6.43415000950744	-3.85521435414798	1.29061324679514
C	-6.81433710619328	-5.19022122299063	1.29547404547070
C	-7.34942163185537	-5.76523276013822	0.15239048854031
C	-7.49968917973876	-5.00241825929979	-0.99823039294310
C	-7.12645328147290	-3.66738927917263	-1.00273217436828
C	-9.49403531066725	-0.86415062028240	1.21998963762658
C	-10.54624492002045	-1.93576339125225	1.28958148077355
C	-8.96435647192998	-0.42935320083142	2.55822348272251
C	-7.39522226981595	2.85538760995720	1.29710496478518
N	-7.34259544357567	2.59763388221811	-1.10785794578236
C	-7.44878435835480	2.01600194157790	-2.32001141408151
C	-7.11043474033804	2.88006233429898	-3.50170707728701
O	-7.81829390109948	0.85497793184946	-2.45111905332604
Cd	-4.34034918566516	3.10169390681169	0.26635157053717
Cl	-3.80573493136478	3.78234023669547	2.55565273576047
Cl	-4.93739846217694	4.82502089410583	-1.31341295661271
H	-9.63007511988935	2.12289842519021	-0.56858641568716
H	-9.53181778600597	1.93311106604099	1.15777645375361
H	-10.42533271738074	-0.03682741444710	-0.58673919520732
H	-8.75161084711396	-1.80351648062315	-0.62210554775876
H	-4.12156353558161	-2.13148946243780	0.17159789666062
H	-2.26685215668852	-1.68407590701061	0.28472639025296
H	0.08301975502712	-1.01899221775358	0.08170830699430
H	0.65310475344378	1.40905475913483	-0.19112477007882
H	-1.21356877440665	3.04929102513390	-0.22948745269816
H	-6.02168158676765	-3.40259126454283	2.18541586430254
H	-6.69371507804875	-5.78082478382022	2.19625406455452
H	-7.65203173176922	-6.80609223375479	0.15706946228208
H	-7.91228453753232	-5.44819232511203	-1.89617377844537
H	-7.24819464143714	-3.07251393861523	-1.90131795465866
H	-10.14620704748212	-2.83946588840252	1.75993588252045
H	-11.40487948154735	-1.59927318213971	1.87910642141669
H	-10.90402658609618	-2.20318946273326	0.29279350383529
H	-8.58230552108767	-1.29143850413829	3.11291290266129
H	-9.75680516134950	0.03515029371824	3.15256712446252
H	-8.14747883694490	0.28827369075773	2.48244106621281
H	-6.37368714755536	3.21870814975574	1.40985445223407
H	-7.65532031070291	2.37063181462275	2.23740659850492
H	-8.04094220826374	3.72619489115624	1.16869698732780
H	-6.97117691745364	3.53694507192877	-1.06177941718221
H	-6.54001811777453	3.76630378170153	-3.22849961497131
H	-8.04136078450209	3.18989471671084	-3.98340991270845
H	-6.54446542033414	2.28341949482953	-4.21690719530240

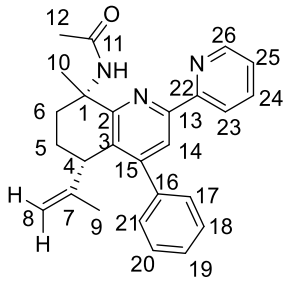
Table S23. Calculated geometry of the conformer **4II** in cartesian (XYZ) coordinates.



E(h) = -2333.6475

C	-7.50704233062124	2.37068553137972	1.57811735231822
C	-8.82702049335349	3.09185626341260	1.63275605806423
C	-9.98365937432264	2.41889378470827	0.94615458167005
C	-9.73388370621343	1.06214000470709	0.40730230391545
C	-8.43453200242470	0.67516324864169	0.05505749101149
C	-7.29346354400594	1.68001403394046	0.22282186422177
C	-10.75186645270389	0.10332676966369	0.31737789062198
C	-10.40569344975915	-1.19608061676816	-0.02937801207629
C	-9.09478611604859	-1.49150156535533	-0.35607016292253
N	-8.14391973527449	-0.55227686204123	-0.36238721998324
C	-8.66791661467304	-2.86117921594531	-0.71425575825183
C	-9.32955307462398	-3.98498660022204	-0.23501624067624
C	-8.84546460032507	-5.23813210703242	-0.56957779113399
C	-7.71647336501535	-5.33738658602362	-1.36668032436239
C	-7.71868952587084	-4.16910439225336	-1.80867960161009
N	-7.58564389333279	-2.96839929486035	-1.48855912091270
C	-12.16620184257724	0.41587393797455	0.60122457889339
C	-12.89052011453275	-0.37677671811288	1.49056372068372
C	-14.22894479842040	-0.11378786888028	1.73711331973459
C	-14.86555127462449	0.93390957114690	1.08515842334302
C	-14.15538611166946	1.71719061244564	0.18449676903268
C	-12.81565579620196	1.46051689749731	-0.05519318675043
C	-10.00243478301201	2.62206149331662	2.44606848039790
C	-10.90536715074191	3.70952310948414	2.96299130169824
C	-9.86989871485403	1.43892909503436	3.36286199991361
C	-5.91010203475393	1.05237122915911	0.22308319228512
N	-7.41288031833708	2.71361175363058	-0.80749793175242
C	-7.41124481397961	2.48669675619353	-2.12445976249216
C	-7.73449981304849	3.65098539396177	-3.00804608031805
O	-7.17238784491481	1.38313803513725	-2.61867555857806
Cd	-6.94400316611461	-0.94984216898876	-2.51303188061999
Cl	-4.52203556221241	-1.11587638258040	-2.64952842685436
Cl	-8.68178529367400	-1.08957556873164	-4.24411893209691
H	-6.68629070856333	3.07340978367699	1.74088696380302
H	-7.41690711703577	1.60352229461886	2.34993737312418
H	-8.77215026015173	4.16864247758711	1.51057099204949
H	-10.65278875929774	3.04907364658602	0.37370269288896
H	-11.17191040113401	-1.95781139158723	-0.09104729257011
H	-10.19537853107528	-3.88105888922710	0.40496947515867
H	-9.34030815815193	-6.12811500266694	-0.19943054086748
H	-7.30224114320372	-6.29685092571773	-1.64810632300624
H	-6.23913465726184	-4.19139301251673	-2.44249736011840
H	-12.39376256555486	-1.19152428897817	2.00574099323219
H	-14.77785678719732	-0.73176887367284	2.43802194579689
H	-15.91039908390214	1.14438090033831	1.28303340094313
H	-14.65011055978425	2.52434756592520	-0.34302475929232
H	-12.27408404982937	2.05937737593999	-0.77743170097427
H	-11.90296430785434	3.31939617708054	3.18409108638004
H	-10.49630652450200	4.13964972431131	3.88250165951369
H	-11.00835513851475	4.51442941727289	2.23184611353835
H	-10.85339052663809	1.00701771642135	3.56689012541979
H	-9.43248235553050	1.74716447295360	4.31689605417433
H	-9.24691418216796	0.64758320747084	2.94567640365979
H	-5.60220132091416	0.68489808981142	-0.75271815863057
H	-5.87278384031898	0.22172951998478	0.92876711597595
H	-5.18933377690961	1.80901871382007	0.54031618949737
H	-7.67200129066324	3.63729893787053	-0.50227274330905
H	-8.04648732671600	4.53480654647049	-2.45244066335671
H	-8.53279311606174	3.34351289565295	-3.68482868876293
H	-6.86067823882741	3.89064386693402	-3.61659956068149

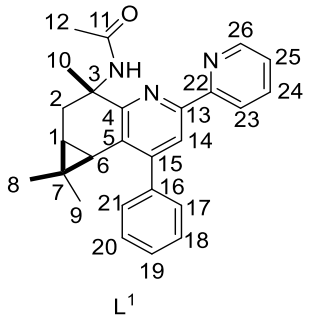
Table S24. Parameters of ^{1}H and ^{13}C NMR spectra of **L** and the complexes **1** and **2**.



L

		L ($CDCl_3$)		**1** ($CDCl_3$)		**2** ($CDCl_3$)	
		δ_{Ci}	δ_{Hi}, (J_{H-H}/Hz)	δ_{Hi}, (J_{H-H}/Hz)	$\delta\delta_{Hi}$,	δ_{Hi}, (J_{H-H}/Hz)	$\delta\delta_{Hi}$,
1		57.19					
2		159.15					
3		131.52					
4		41.49	3.43 d (5.4)	3.91 d (6)	0.48	3.47 d (5.4)	0.04
5	*pro-S*	23.06	1.94 dddd (13.9, 13.9, 5.8, 2.6)	2.05 dddd (14.1, 14.1, 6.2, 2.7)	0.09	2.08 dddd (13.9, 13.9, 5.8, 2.6)	0.14
	pro-R		1.75 dm. (13.9)	1.76 dm. (13.9)	0.01	1.62 dm. (13.9)	-0.13
6	*pro-S*	29.39	2.28 ddd (13.9, 13.9, 2.8)	2.33 ddd (13.9, 13.9, 2.8)	0.05	2.91 ddd (13.9, 13.9, 2.8)	*0.63*
	pro-R		2.75 dd (13.9, 2.8, 2.8)	2.68 dd (13.9, 3.0, 3.0)	-0.07	1.78 dd (13.9, 2.8, 2.8)	-0.97
7		148.26					
8		115.07	4.07 s	4.09 s	0.02	4.77 s	0.70
			4.81 s	4.72 s	-0.09	4.99 s	0.18
9		24.63	1.40 s	1.38 s	-0.02	1.89 s.	0.49
10		22.56	1.67 s	1.68 s	0.01	1.34 s	-0.33
11		168.98					
12		27.88	2.02 s	2.02 s	0.00	2.05 s and 2.04 s	0.02
13		152.42					
14		120.55	8.15 s	8.03 s	-0.12	7.88 s	-0.27
15		153.30					
16		139.61					
17, 21		127.82	7.23-7.27 m	7.32 ddd (7.3, 1.1, 1.1)	0.05	7.42-7.46 m.	0.20
18, 20		127.69	7.30-7.36 m	7.46 m	0.10	7.42-7.46 m.	0.10
19		127.46	7.30-7.36 m	7.40 m	0.06	7.42-7.46 m.	0.10
22		155.94					
23		121.41	8.40 ddd (7.9, 1.0, 1.0)	8.02m	-0.38	8.12 d (7.9)	-0.28
24		136.45	7.80 ddd (7.8, 7.8, 1.7.)	7.74 ddd (7.8, 7.8, 1.7.)	-0.06	8.00 ddd (7.8, 7.8, 1.7.)	0.20
25		123.44	7.23-7.27 m	7.28 ddd (7.6, 4.9, 1.0)	0.01	7.61 ddd (7.1, 5.1, 1.8)	0.34
26		149.08	8.59 ddd (4.8, 1.8, 0.8.)	8.65 ddd (4.8, 1.8, 0.8.)	0.06	8.84 br.d (4.8)	0.25

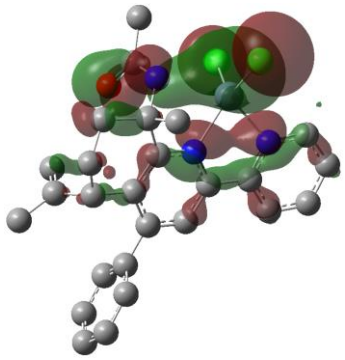
Table S25. Parameters of ^{1}H and ^{13}C NMR spectra of **L[1]** and the complexes **3** and **4**.



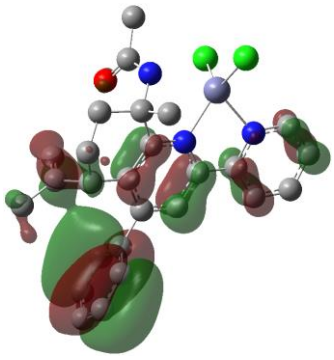
L[1]

		L[1] ($CDCl_3$)		**3** ($CDCl_3$)		**4** ($CDCl_3$)	
		δ_{Ci}	δ_{Hi}, (J_{H-H}/Hz)	δ_{Hi}, (J_{H-H}/Hz)	$\delta\delta_{Hi}$,	δ_{Hi}, м.д. (J_{H-H}/Hz)	$\delta\delta_{Hi}$,
1		20.18	1.21 ddd (8.5, 8.5, 6.9)	1.44 ddd (8.9, 8.9, 4.5)	0.23	1.45br.d (7.4)	0.24
2	*pro-S*	30.85	1.40 dd (15.0, 6.9)	1.78 dd (15.5, 4.9)	0.38	1.48 br.s $W_{1/2}$=43Hz	0.08
	pro-R		3.52 dd (15.0, 9.3)	3.13 dd (15.5, 9.2)	-0.39	2.76 br.s $W_{1/2}$=110 Hz	-0.76
3		57.27					
4		159.85					
5		129.55					
6		24.54	1.64 d (8.5)	1.75 d (8.2)	0.11	1.54 br.s $W_{1/2}$=30 Hz	-0.1
7		25.05					
8		16.16	0.69 s	0.76 s	0.07	0.58 br.s	-0.11
9		27.25	0.94 s	0.95 s	0.01	0.88 br.s	-0.06
10		23.31	1.93 s	2.11 s	0.17	2.10 br.s	0.17
11		168.95					
12		24.55	1.90 s	2.06 s	0.16	2.07 br.s	0.17
13		152,21					
14		120.80	8.31 s	7.99 s	-0.32	7.95 br.s $W_{1/2}$= 32 Hz	-0.36
15		152.45					
16		139.49					
17, 21		128.00	7.35-7.44 m	7.35-7.44 m.	0.00	7.40-7.45 m	0.05
18, 20		128.75	7.35-7.44 m	7.49-7.57 m.	0.13	7.44-7.55 m	0.1
19		127.90	7.35-7.44 m	7.49-7.57 m.	0.13	7.44-7.55 m	0.1
22		156.20					
23		121.04	8.48 ddd (8.1, 1.1., 0.8)	8.12 m	-0.36	8.02 br.m $W_{1/2}$=57 Hz	-0.46
24		136.57	7.77 ddd (8.1, 7.5, 1,8)	7.68 ddd (8.8, 5.2, 1.6)	-0.09	7.95 br.m $W_{1/2}$=32 Hz	0.18
25		123.35	7.23 ddd (7.4, 4.8, 1.1.)	8.10 m	0.84	7.44-7.55 br.m $W_{1/2}$=53 Hz	0.20
26		148.91	8.58 ddd (4.9, 1.8, 0,8)	8.85 d (4.8)	0.27	8.89 br.m $W_{1/2}$=33 Hz	0.31
N-H			4.81 s	6.77 br.s			

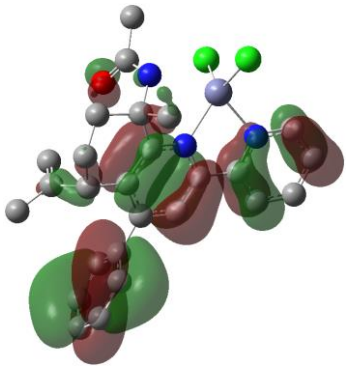
Table S26. Iso-surface contour plots (iso-value = 0.02) of the molecular orbitals of the complex **1** as calculated at the B3LYP/LANL2DZ theory level in the ground state (S_0) geometry.



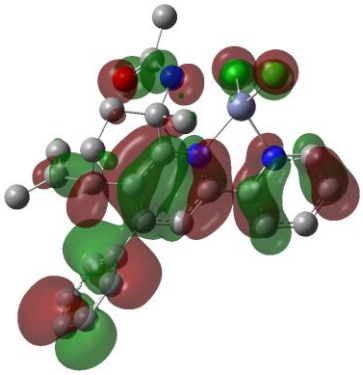
HOMO-11



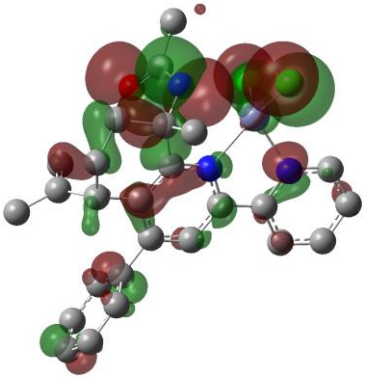
HOMO-10



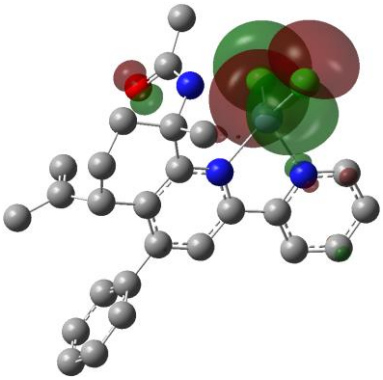
HOMO-9



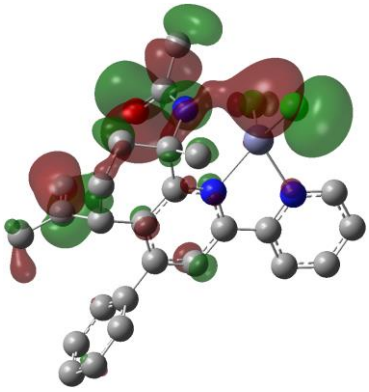
HOMO-8



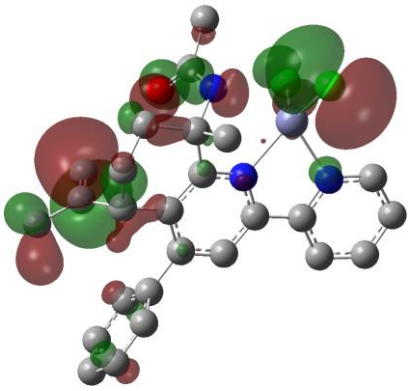
HOMO-7



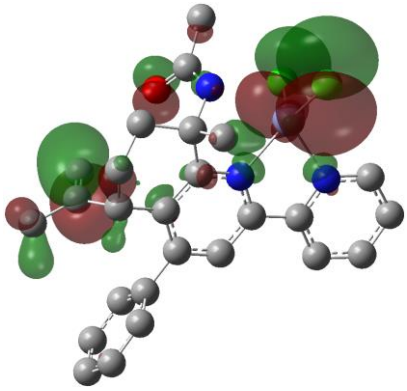
HOMO-6



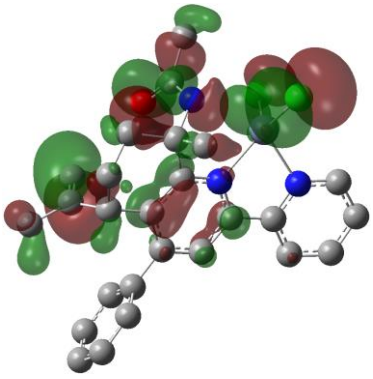
HOMO-5



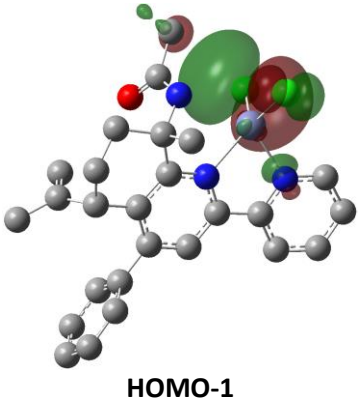
HOMO-4



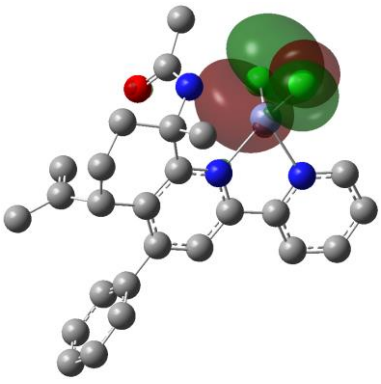
HOMO-3



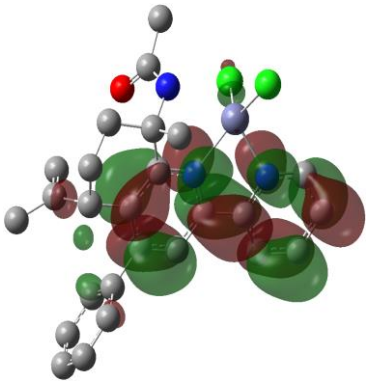
HOMO-2



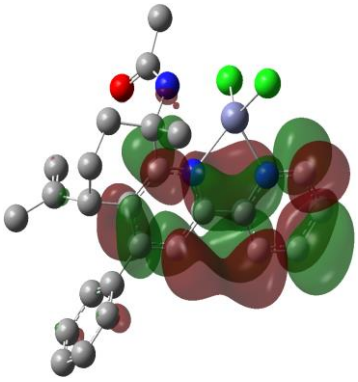
HOMO-1



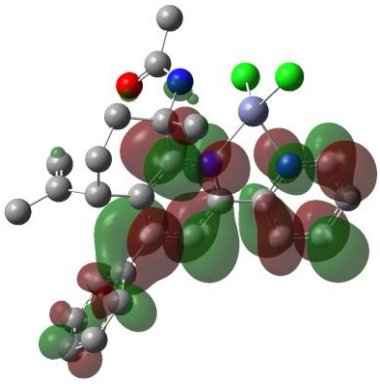
HOMO



LUMO

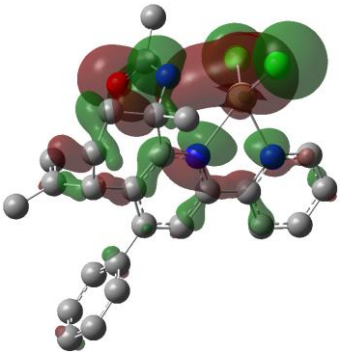


LUMO+1

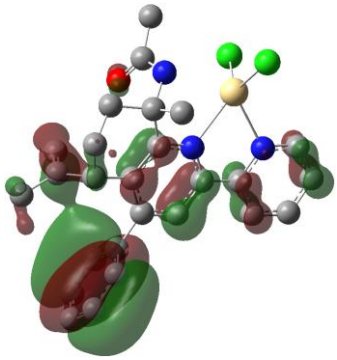


LUMO+2

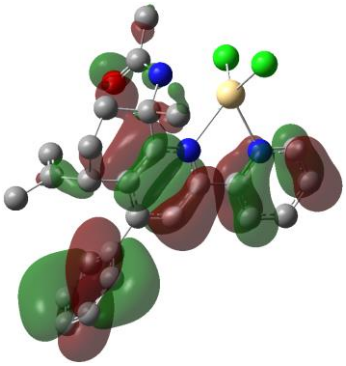
Table S27. Iso-surface contour plots (iso-value = 0.02) of the molecular orbitals of the complex **2** as calculated at the B3LYP/LANL2DZ theory level in the ground state (S_0) geometry.



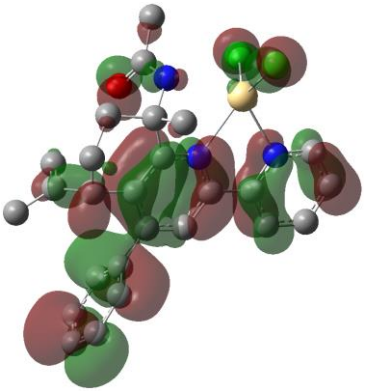
HOMO-11



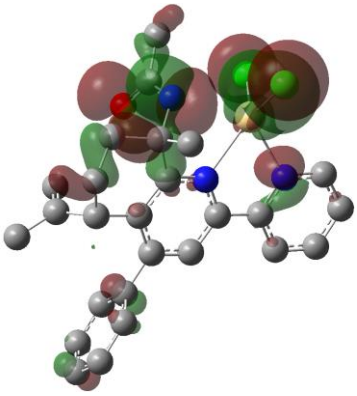
HOMO-10



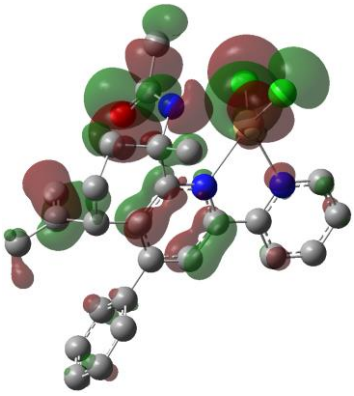
HOMO-9



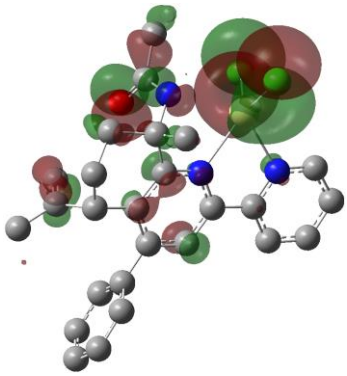
HOMO-8



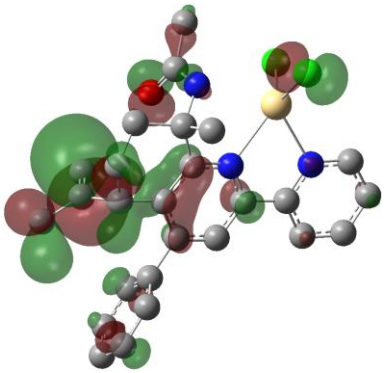
HOMO-7



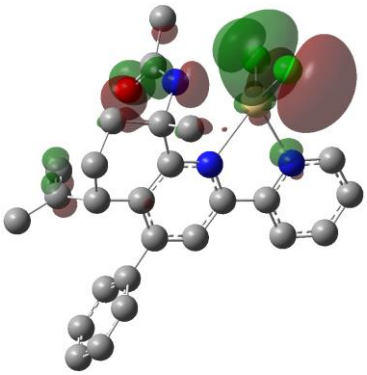
HOMO-6



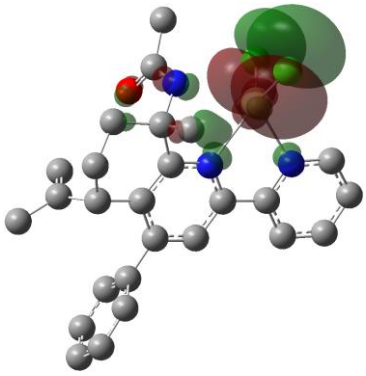
HOMO-5



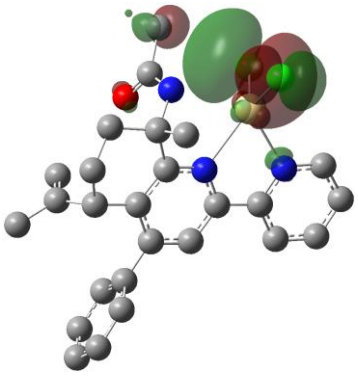
HOMO-4



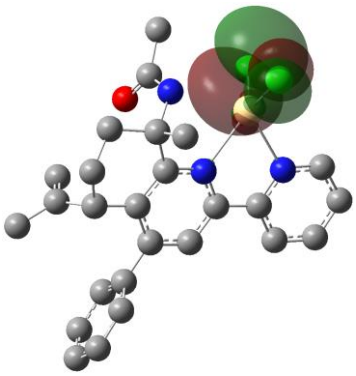
HOMO-3



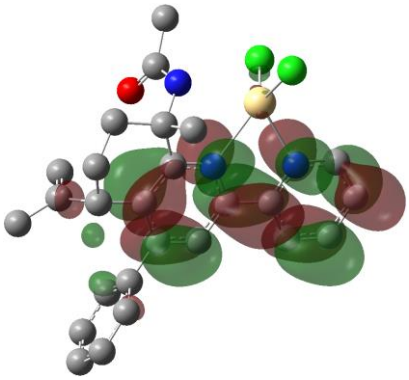
HOMO-2



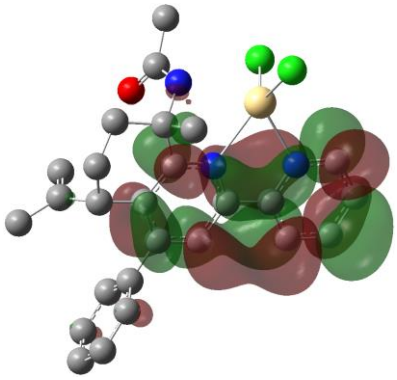
HOMO-1



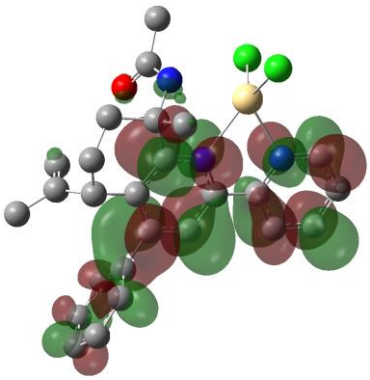
HOMO



LUMO



LUMO+1



LUMO+2

Table S28. Excited state properties of the complex **1** obtained from TD-DFT calculations for the gas phase relaxed geometry of the ground state (S_0). Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	2.93	424	HOMO → LUMO (99.6 %)	0.0015	XLCT
S2	2.99	414	HOMO-1 → LUMO (99.4 %)	0.0028	XLCT
S3	3.29	377	HOMO-2 → LUMO (84.5 %), HOMO-3 → LUMO (14.3 %)	0.0102	XLCT + LC
S4	3.34	372	HOMO-3 → LUMO (82.1 %),	0.0129	XLCT + LC

			HOMO-2 → LUMO (12.8 %)		
S5	3.40	364	HOMO-4 → LUMO (94.5 %)	0.0053	XLCT + LC
S6	3.55	349	HOMO-5 → LUMO (98.9 %)	0.0044	LC + XLCT
S7	3.76	330	HOMO → LUMO+1 (81.6 %), HOMO-6 → LUMO (14.6 %)	0.0007	XLCT
S8	3.80	327	HOMO-6 → LUMO (75.0 %), HOMO → LUMO+1 (11.9 %)	0.0209	XLCT
S9	3.82	324	HOMO-1 → LUMO+1 (85.5 %)	0.0038	XLCT
S10	3.82	324	HOMO-7 → LUMO (91.7 %)	0.0028	LC + XLCT
S11	4.06	306	HOMO → LUMO+2 (96.0 %)	0.0001	XLCT
S12 (S_1*)	**4.12**	**301**	**HOMO-8 → LUMO (67.7 %), HOMO-9 → LUMO (21.9 %)**	**0.0202**	**LC**
S13	4.13	300	HOMO-2 → LUMO+1 (84.1 %)	0.0138	LC + XLCT
S14	4.13	300	HOMO-1 → LUMO+2 (93.9 %)	0.0037	XLCT
S15	4.16	298	HOMO-3 → LUMO+1 (85.9 %)	0.0070	XLCT + LC
S16	4.23	293	HOMO-4 → LUMO+1 (81.9 %)	0.0059	LC + XLCT
S17 (S_2*)	**4.27**	**290**	**HOMO-9 → LUMO (62.2 %), HOMO-10 → LUMO (10.7 %), HOMO-8 → LUMO (10.3 %)**	**0.2149**	**LC**
S18 (S_3*)	**4.32**	**287**	**HOMO-10 → LUMO (82.0 %)**	**0.1694**	**LC**
S19	4.37	284	HOMO-5 → LUMO+1 (47.9 %), HOMO-2 → LUMO+2 (31.4 %), HOMO-4 → LUMO+2 (11.3 %)	0.0271	LC + XLCT
S20	4.40	282	HOMO-2 → LUMO+2 (43.7 %), HOMO-5 → LUMO+1 (29.6 %), HOMO-3 → LUMO+2 (16.2 %)	0.0034	LC + XLCT
T1	2.87	432	HOMO → LUMO (20.6 %), HOMO-8 → LUMO (18.6 %), HOMO-1 → LUMO (14.5 %), HOMO-2 → LUMO (12.9 %), HOMO-9 → LUMO+1 (10.0 %)	0.0000	XLCT + LC
T2	2.91	426	HOMO → LUMO (77.4 %)	0.0000	XLCT
T3	2.97	418	HOMO-1 → LUMO (82.2 %)	0.0000	XLCT
T4	3.27	379	HOMO-3 → LUMO (58.1 %), HOMO-2 → LUMO (36.3 %)	0.0000	XLCT + LC
T5	3.34	371	HOMO-4 → LUMO (51.2 %), HOMO-2 → LUMO (22.6 %), HOMO-3 → LUMO (15.0 %)	0.0000	LC + XLCT
T6	3.40	365	HOMO-4 → LUMO (42.7 %), HOMO-3 → LUMO (18.2 %), HOMO-2 → LUMO (13.6 %)	0.0000	LC + XLCT
T7	3.52	352	HOMO-5 → LUMO (88.4 %)	0.0000	LC + XLCT
T8	3.62	342	HOMO-9 → LUMO+4 (13.8 %), HOMO-8 → LUMO+3 (13.4 %), HOMO-6 → LUMO (12.5 %), HOMO-10 → LUMO+3 (10.4 %)	0.0000	LC + XLCT
T9	3.69	336	HOMO-6 → LUMO (50.3 %)	0.0000	XLCT
T10	3.75	331	HOMO → LUMO+1 (75.9 %), HOMO-6 → LUMO (12.7 %)	0.0000	XLCT

Table S29. Excited state properties of the complex **2** obtained from TD-DFT calculations for the gas phase relaxed geometry of the ground state (S_0). Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	2.98	416	HOMO → LUMO (99.4 %)	0.0011	XLCT
S2	3.06	405	HOMO-1 → LUMO (99.1 %)	0.0019	XLCT
S3	3.24	382	HOMO-2 → LUMO (99.2 %)	0.0019	XLCT
S4	3.35	370	HOMO-3 → LUMO (99.1 %)	0.0032	XLCT + LC
S5	3.47	357	HOMO-4 → LUMO (98.3 %)	0.0234	LC
S6	3.66	339	HOMO-5 → LUMO (98.5 %)	0.0178	XLCT + LC
S7	3.70	335	HOMO-6 → LUMO (96.8 %)	0.0167	LC + XLCT
S8	3.77	329	HOMO → LUMO+1 (95.9 %)	0.0006	XLCT
S9	3.85	322	HOMO-1 → LUMO+1 (95.4 %)	0.0012	XLCT
S10	3.95	314	HOMO-7 → LUMO (97.2 %)	0.0005	LC + XLCT
S11	4.05	306	HOMO-2 → LUMO+1 (96.8 %)	0.0016	XLCT
S12	4.11	301	HOMO → LUMO+2 (95.9 %)	0.0001	XLCT
S13 (S_1*)	**4.15**	**299**	**HOMO-8 → LUMO (77.9 %), HOMO-9 → LUMO (16.2 %)**	**0.0264**	**LC**
S14	4.15	299	HOMO-3 → LUMO+1 (91.8 %)	0.0032	XLCT + LC
S15	4.20	295	HOMO-1 → LUMO+2 (92.9 %)	0.0005	XLCT
S16	4.25	292	HOMO-4 → LUMO+1 (60.7 %), HOMO-9 → LUMO (17.4 %), HOMO-4 → LUMO+2 (10.4 %)	0.0332	LC
S17 (S_2*)	**4.32**	**287**	**HOMO-9 → LUMO (50.2 %), HOMO-4 → LUMO+1 (16.5 %)**	**0.1945**	**LC**
S18	4.35	285	HOMO-2 → LUMO+2 (76.4 %), HOMO-10 → LUMO (13.8 %)	0.0089	XLCT + LC
S19 (S_3*)	**4.37**	**284**	**HOMO-10 → LUMO (73.8 %), HOMO-2 → LUMO+2 (10.0 %)**	**0.1134**	**LC + XLCT**
S20	4.43	280	HOMO-11 → LUMO (68.5 %), HOMO-3 → LUMO+2 (13.9 %)	0.0382	XLCT + LC
T1	2.91	426	HOMO-8 → LUMO (24.3 %), HOMO-4 → LUMO (17.5 %), HOMO-9 → LUMO (15.8 %)	0.0000	LC
T2	2.96	418	HOMO → LUMO (89.5 %)	0.0000	XLCT
T3	3.04	407	HOMO-1 → LUMO (96.8 %)	0.0000	XLCT
T4	3.22	385	HOMO-2 → LUMO (96.8 %)	0.0000	XLCT
T5	3.35	371	HOMO-3 → LUMO (89.5 %)	0.0000	XLCT + LC
T6	3.48	357	HOMO-4 → LUMO (67.8 %)	0.0000	LC
T7	3.59	345	HOMO-5 → LUMO (65.1 %)	0.0000	XLCT + LC
T8	3.63	341	HOMO-6 → LUMO (65.5 %)	0.0000	LC + XLCT
T9	3.65	340	HOMO-9 → LUMO+4 (15.0 %), HOMO-8 → LUMO+3 (13.9 %), HOMO-10 → LUMO+3 (13.1 %), HOMO-10 → LUMO+4 (10.1 %), HOMO-5 → LUMO (10.0 %)	0.0000	LC + XLCT
T10	3.76	330	HOMO → LUMO+1 (86.7 %)	0.0000	XLCT

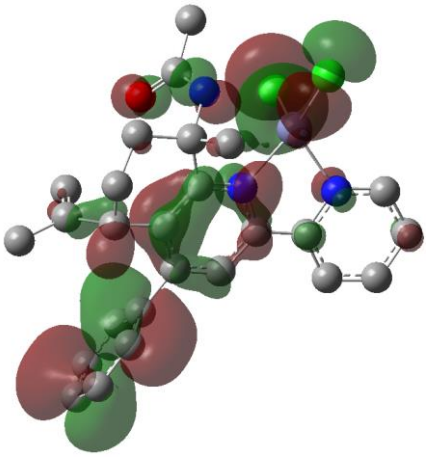
Table S30. Orbital energies and characters resulting from Mulliken population analysis calculated for the complex **1** at the ground state (S_0) optimized geometry.

Orbital	Energy (eV)	Contributions (%)		
		Zn	Cl^-	L
HOMO-11	-7.92	12	56	32
HOMO-10	-7.60	0	0	100
HOMO-9	-7.52	0	0	100
HOMO-8	-7.41	1	4	95
HOMO-7	-7.23	3	22	75
HOMO-6	-7.16	10	85	4
HOMO-5	-6.89	1	28	70
HOMO-4	-6.74	2	45	53
HOMO-3	-6.68	4	68	29
HOMO-2	-6.63	1	36	63
HOMO-1	-6.40	2	95	3
HOMO	-6.32	2	97	1
LUMO	-2.76	1	1	99
LUMO+1	-1.95	0	0	99
LUMO+2	-1.68	0	0	100
LUMO+3	-0.92	0	0	100
LUMO+4	-0.89	0	0	100

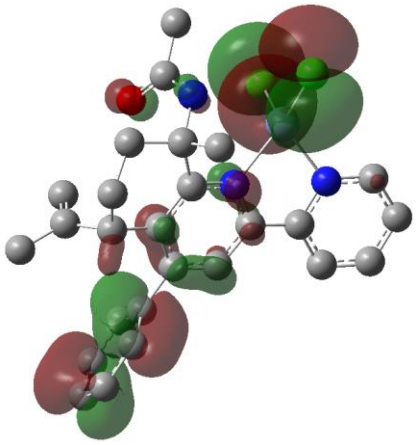
Table S31. Orbital energies and characters resulting from Mulliken population analysis calculated for the complex **2** at the ground state (S_0) optimized geometry.

Orbital	Energy (eV)	Contributions (%)		
		Cd	Cl^-	L
HOMO-11	-7.82	9	34	57
HOMO-10	-7.61	0	0	100
HOMO-9	-7.53	0	0	100
HOMO-8	-7.41	1	5	94
HOMO-7	-7.30	6	34	60
HOMO-6	-7.00	3	29	67
HOMO-5	-6.95	7	65	28
HOMO-4	-6.74	0	4	96
HOMO-3	-6.63	4	84	12
HOMO-2	-6.52	4	92	4
HOMO-1	-6.39	2	95	4
HOMO	-6.30	2	97	1
LUMO	-2.72	1	0	99
LUMO+1	-1.94	0	0	100
LUMO+2	-1.64	0	0	100
LUMO+3	-0.93	0	0	100
LUMO+4	-0.90	0	0	100

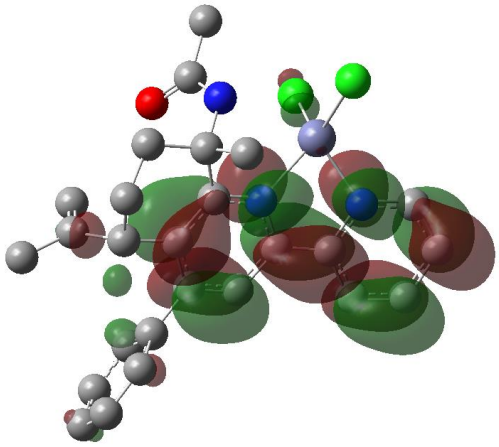
Table S32. Iso-surface contour plots (iso-value = 0.02) of the molecular orbitals of the complex **1** as calculated at the B3LYP/LANL2DZ theory level in the singlet excited state (S_{12} = $\mathbf{S_1}$*) optimized geometry.



HOMO-8



HOMO-7

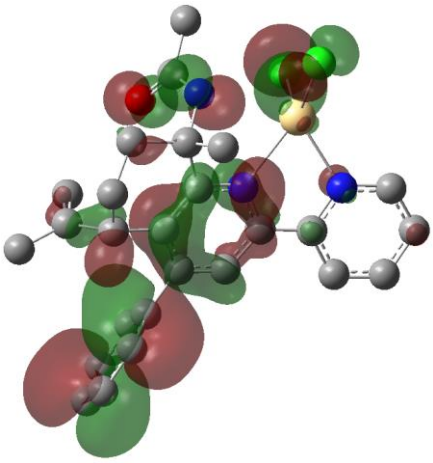


LUMO

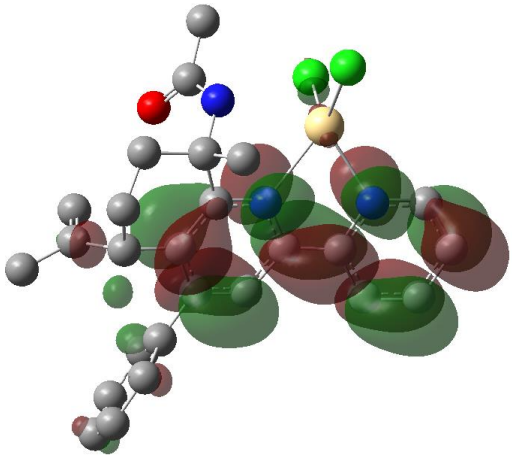
Table S33. Orbital energies and characters resulting from Mulliken population analysis calculated for the complex **1** at the singlet excited state (S_{12} = $\mathbf{S_1}$*) optimized geometry.

Orbital	Energy (eV)	Contributions (%)		
		Zn	Cl^-	L
HOMO-8	-7.20	3	26	70
HOMO-7	-7.13	7	64	29
LUMO	-3.27	1	1	99

Table S34. Iso-surface contour plots (iso-value = 0.02) of the molecular orbitals of the complex **2** as calculated at the B3LYP/LANL2DZ theory level in the singlet excited state (S_{13} = **S_1***) optimized geometry.



HOMO-8

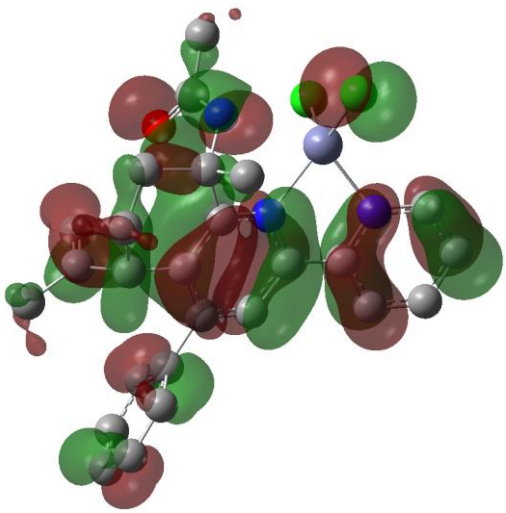


LUMO

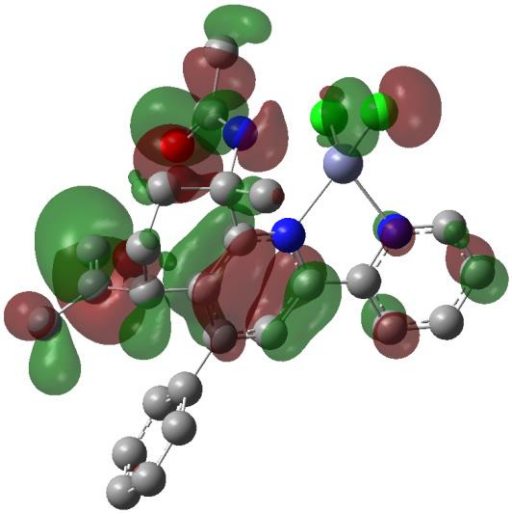
Table S35. Orbital energies and characters resulting from Mulliken population analysis calculated for the complex 2 at the singlet excited state (S_{13}=**S_1***) optimized geometry.

Orbital	Energy (eV)	Contributions (%)		
		Cd	Cl^-	L
HOMO-8	-7.15	1	10	89
LUMO	-3.25	1	0	99

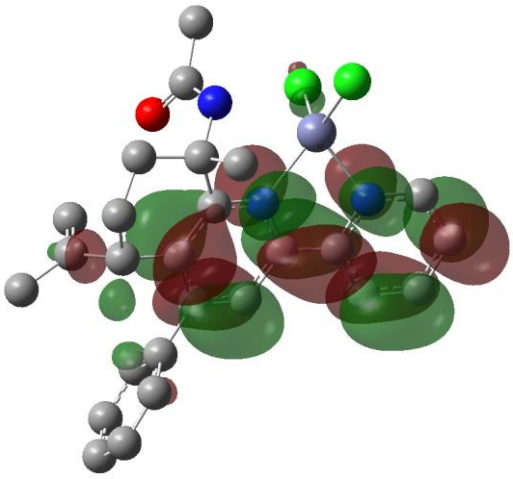
Table S36. Iso-surface contour plots (iso-value = 0.02) of the molecular orbitals of the complex 1 as calculated at the B3LYP/LANL2DZ theory level in the triplet excited state (T_1) optimized geometry.



HOMO-6



HOMO-2

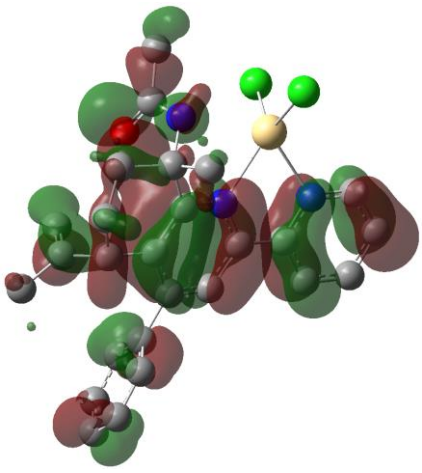


LUMO

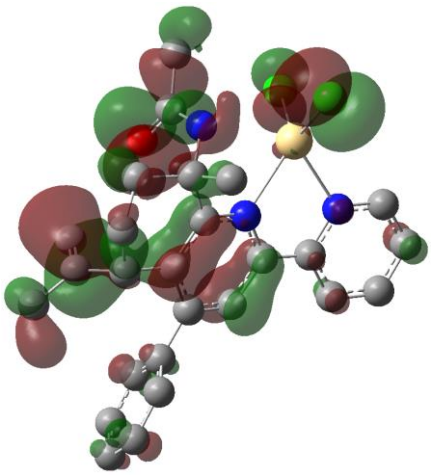
Table S37. Orbital energies and characters resulting from Mulliken population analysis calculated for the complex 1 at the triplet excited state (T_1) optimized geometry.

Orbital	Energy (eV)	Contributions (%)		
		Zn	Cl^-	L
HOMO-6	-7.16	1	8	91
HOMO-2	-6.63	0	7	93
LUMO	-2.76	0	1	99

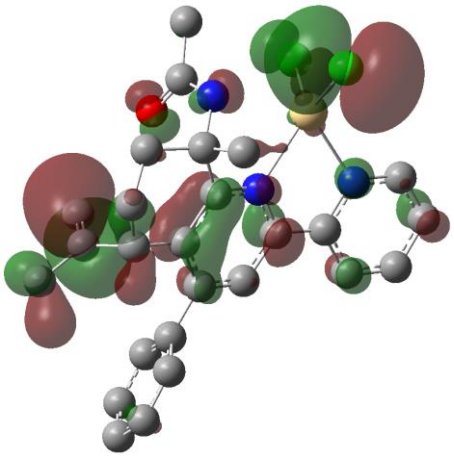
Table S38. Iso-surface contour plots (iso-value = 0.02) of the molecular orbitals of the complex 2 as calculated at the B3LYP/LANL2DZ theory level in the triplet excited state (T_1) optimized geometry.



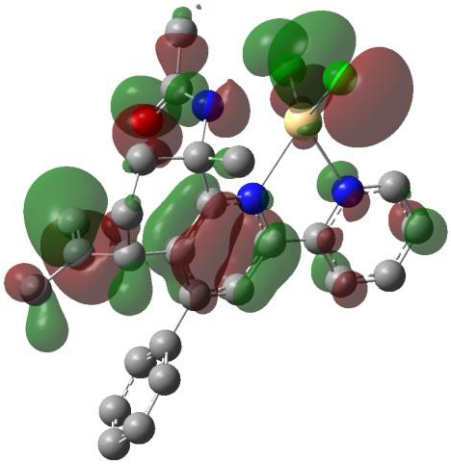
HOMO-7



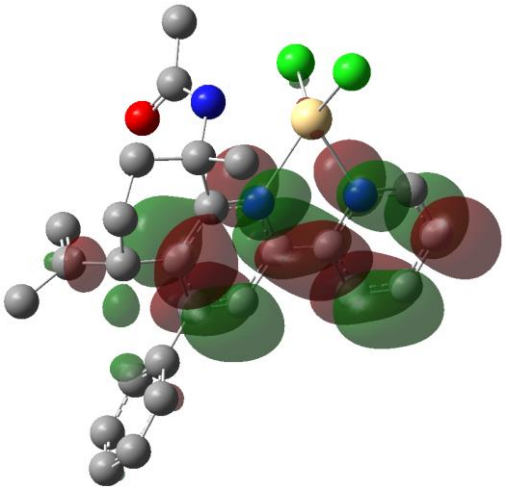
HOMO-5



HOMO-4



HOMO-3



LUMO

Table S39. Orbital energies and characters resulting from Mulliken population analysis calculated for the complex 2 at the triplet excited state (T_1) optimized geometry.

Orbital	Energy (eV)	Contributions (%)		
		Cd	Cl^-	L
HOMO-7	-7.1230	0	0	100
HOMO-5	-6.8957	1	14	85
HOMO-4	-6.7008	2	49	49
HOMO-3	-6.6065	2	41	57
LUMO	-3.2260	0	0	100

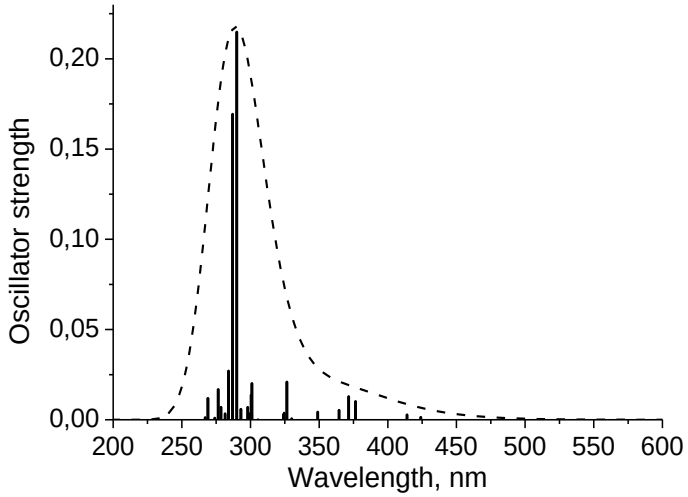


Figure S12. Simulated absorption spectrum of the complex 1. Vertical bars display the positions and oscillator strengths of the computed electronic transitions.

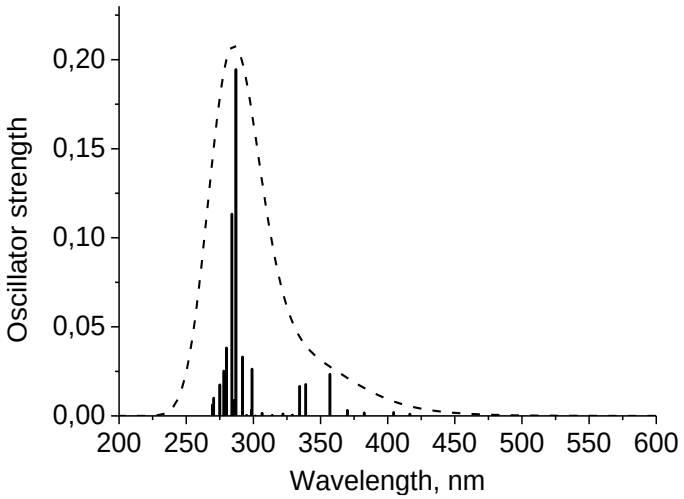


Figure S13. Simulated absorption spectrum of the complex 2. Vertical bars display the positions and oscillator strengths of the computed electronic transitions.

Table S40. Calculated (B3LYP/LANL2DZ) gas phase geometries of the complex **1** in cartesian (XYZ) coordinates

Ground state (S_0)				Singlet excited state ($S_{12} = S_1$*)			
Zn	-2.725143	-0.036142	0.083500	Zn	-2.756857	0.038306	-0.008339
Cl	-3.496614	-0.119798	-2.113506	Cl	-3.275382	-0.189051	-2.300406
Cl	-4.008546	-0.927778	1.822668	Cl	-4.089985	-1.238539	1.474979
O	-0.375694	-2.517693	-1.850496	O	-0.125674	-2.683942	-1.782188
N	-0.601527	0.270364	0.350918	N	-0.644612	0.260104	0.369276
N	-2.598983	2.088856	0.196404	N	-2.691112	2.072908	0.281588
N	-1.411472	-2.450638	0.211510	N	-1.305847	-2.540350	0.199267
H	-2.231930	-2.712070	0.755391	H	-2.209283	-2.659069	0.658984
C	-0.191068	-2.077883	0.980762	C	-0.174582	-2.071839	1.039104

C	0.338059	-0.696664	0.537123	C	0.324090	-0.674577	0.594779
C	1.728017	-0.409464	0.460713	C	1.700435	-0.363764	0.546530
C	2.800299	-1.482962	0.639681	C	2.807279	-1.385659	0.783480
H	3.593005	-1.050104	1.263664	H	3.579956	-0.903174	1.414235
C	2.254358	-2.726157	1.397211	C	2.278781	-2.596802	1.603769
H	2.977205	-3.546688	1.308358	H	3.029567	-3.396966	1.608275
H	2.172210	-2.496618	2.468791	H	2.132267	-2.293179	2.649803
C	0.898457	-3.176831	0.832228	C	0.967897	-3.126094	1.003313
H	0.544892	-4.072865	1.358207	H	0.625922	-4.008291	1.559398
H	1.018537	-3.432828	-0.223156	H	1.146065	-3.428759	-0.031240
C	3.480393	-1.890977	-0.685045	C	3.552188	-1.852416	-0.484214
C	2.824617	-1.983437	-1.861839	C	2.964392	-1.939674	-1.697242
H	3.346149	-2.315965	-2.757976	H	3.516540	-2.322603	-2.554707
H	1.764980	-1.773087	-1.971909	H	1.915959	-1.707835	-1.858481
C	4.952939	-2.233811	-0.547329	C	4.994786	-2.271887	-0.253420
H	5.536290	-1.347543	-0.257080	H	5.606646	-1.432430	0.114202
H	5.363512	-2.620869	-1.486305	H	5.453640	-2.650682	-1.173159
H	5.116647	-2.993917	0.231558	H	5.064220	-3.064701	0.505823
C	-0.612712	-1.957274	2.475337	C	-0.711798	-1.933690	2.493545
H	-1.420114	-1.232474	2.612380	H	-1.540276	-1.222576	2.551991
H	0.239157	-1.655641	3.092054	H	0.083997	-1.596732	3.166027
H	-0.968317	-2.929937	2.838200	H	-1.075978	-2.905719	2.848353
C	-1.381154	-2.780575	-1.142496	C	-1.190360	-2.887217	-1.133564
C	-2.611261	-3.472552	-1.695602	C	-2.403490	-3.545896	-1.762792
H	-2.970720	-2.908655	-2.560366	H	-2.719707	-2.946729	-2.621297
H	-3.425703	-3.544825	-0.967671	H	-3.248556	-3.629450	-1.072337
H	-2.328226	-4.480175	-2.025713	H	-2.117664	-4.544768	-2.115424
C	-0.237932	1.564442	0.124301	C	-0.322710	1.602733	0.155465
C	1.116628	1.912949	0.031396	C	1.049816	1.944191	-0.036933
H	1.417599	2.938114	-0.145756	H	1.314884	2.958998	-0.312162
C	2.110680	0.931994	0.190764	C	2.034226	0.987814	0.164211
C	3.543149	1.364996	0.089291	C	3.444364	1.429607	-0.013176
C	4.100392	1.681509	-1.168920	C	3.906055	1.875245	-1.288986
H	3.502439	1.552970	-2.067613	H	3.228160	1.824200	-2.133185
C	5.429224	2.134459	-1.265897	C	5.212365	2.323688	-1.446006
H	5.848950	2.366550	-2.241508	H	5.571864	2.641537	-2.419805
C	6.213289	2.285028	-0.105830	C	6.108872	2.358260	-0.319402
H	7.239106	2.637291	-0.181176	H	7.124409	2.719742	-0.455279
C	5.660802	1.978821	1.153057	C	5.667880	1.936061	0.958220
H	6.256799	2.100420	2.054245	H	6.340462	1.982831	1.808093
C	4.334291	1.519827	1.249882	C	4.359598	1.484567	1.115890
H	3.909528	1.299651	2.227111	H	3.985225	1.209928	2.096069
C	-1.334966	2.571117	0.039182	C	-1.389663	2.573720	0.151606
C	-1.118804	3.948865	-0.168762	C	-1.195704	3.986707	0.053209
H	-0.118481	4.341707	-0.306656	H	-0.195630	4.395376	-0.050994
C	-2.221541	4.818490	-0.198682	C	-2.284382	4.849419	0.109870
H	-2.070000	5.882007	-0.360257	H	-2.134675	5.923567	0.040063
C	-3.518819	4.302265	-0.022410	C	-3.602078	4.315687	0.264200
H	-4.392941	4.944046	-0.041424	H	-4.474336	4.957595	0.311781
C	-3.665574	2.918795	0.166914	C	-3.742760	2.927424	0.335850
H	-4.639701	2.456209	0.285822	H	-4.723324	2.468992	0.430159
Triplet excited state (T_1)							
Zn	-2.777967	0.025908	0.024233				

Cl	-3.473542	-0.042694	-2.196428
Cl	-4.065804	-1.050007	1.662114
O	-0.325060	-2.486690	-1.810090
N	-0.653115	0.217452	0.304517
N	-2.594227	2.110819	0.275362
N	-1.429693	-2.505447	0.207964
H	-2.298167	-2.684472	0.711005
C	-0.243003	-2.100410	0.998870
C	0.270306	-0.716197	0.540092
C	1.703623	-0.434964	0.500370
C	2.754927	-1.503482	0.723465
H	3.536947	-1.063988	1.358942
C	2.199183	-2.740009	1.479522
H	2.925994	-3.559287	1.412410
H	2.095988	-2.499644	2.546814
C	0.855657	-3.198309	0.895133
H	0.488376	-4.082873	1.430215
H	0.994670	-3.476388	-0.152339
C	3.480810	-1.907263	-0.583412
C	2.848745	-2.034567	-1.772899
H	3.399563	-2.364790	-2.652188
H	1.785331	-1.863362	-1.905818
C	4.961959	-2.187598	-0.415339
H	5.507174	-1.270762	-0.148633
H	5.399552	-2.589053	-1.335787
H	5.141302	-2.913535	0.392055
C	-0.693252	-1.951573	2.483520
H	-1.518589	-1.241823	2.584177
H	0.139591	-1.615956	3.108866
H	-1.033617	-2.923733	2.860634
C	-1.361331	-2.770669	-1.148729
C	-2.574695	-3.423236	-1.778765
H	-2.891687	-2.822888	-2.635434
H	-3.416766	-3.509794	-1.085046
H	-2.291535	-4.422442	-2.133848
C	-0.261162	1.571482	0.067359
C	1.154203	1.879882	-0.088368
H	1.455212	2.888763	-0.342081
C	2.119465	0.928010	0.141465
C	3.558748	1.328344	0.035386
C	4.092212	1.726638	-1.211096
H	3.470087	1.666612	-2.100728
C	5.424103	2.167940	-1.311894
H	5.822507	2.461492	-2.279905
C	6.239807	2.227146	-0.165372
H	7.268308	2.570914	-0.242771
C	5.713546	1.842154	1.083255
H	6.331603	1.898241	1.976008
C	4.383896	1.394258	1.182572
H	3.978647	1.129839	2.157080
C	-1.273762	2.558262	0.079470
C	-1.030699	3.977321	-0.079264
H	-0.025748	4.342833	-0.253141

C	-2.089945	4.873198	-0.001227	
H	-1.912360	5.938526	-0.117734	
C	-3.408174	4.389621	0.228922	
H	-4.258435	5.059679	0.293476	
C	-3.600435	2.988381	0.348200	
H	-4.594715	2.574169	0.488543	

Table S41. Calculated (B3LYP/LANL2DZ) gas phase geometries of the complex **2** in cartesian (XYZ) coordinates

Ground state (S_0)				Singlet excited state (S_{13}=S_1*)			
Cd	-2.726546	-0.057646	0.137179	Cd	-2.749830	0.034547	-0.031841
Cl	-3.816750	-0.022063	-2.109513	Cl	-3.425871	-0.084979	-2.450858
Cl	-3.881881	-1.061327	2.113187	Cl	-4.006721	-1.455369	1.582872
O	-0.226845	-2.313713	-1.959189	O	0.033613	-2.596268	-1.794965
N	-0.366317	0.296169	0.346193	N	-0.407937	0.289596	0.402079
N	-2.317925	2.251451	0.175080	N	-2.415292	2.242813	0.349311
N	-1.242012	-2.416397	0.113265	N	-1.147281	-2.494301	0.188585
H	-2.014908	-2.804857	0.651517	H	-2.037783	-2.665078	0.660926
C	-0.008404	-2.087225	0.891940	C	-0.006381	-2.062723	1.038535
C	0.548755	-0.700819	0.496725	C	0.533841	-0.674117	0.609851
C	1.947081	-0.452991	0.428202	C	1.920348	-0.406321	0.554454
C	2.993986	-1.557798	0.562526	C	2.996322	-1.461843	0.782878
H	3.797019	-1.169131	1.202121	H	3.782488	-1.007201	1.416169
C	2.420820	-2.817454	1.268625	C	2.431650	-2.659827	1.598544
H	3.122153	-3.651718	1.143407	H	3.159069	-3.481062	1.601477
H	2.345155	-2.632084	2.348886	H	2.292179	-2.355563	2.645337
C	1.052881	-3.206083	0.688190	C	1.107059	-3.147884	0.994071
H	0.677641	-4.116869	1.172491	H	0.740900	-4.024858	1.542820
H	1.164633	-3.415859	-0.378785	H	1.277476	-3.446132	-0.043230
C	3.663573	-1.927794	-0.778473	C	3.728227	-1.944500	-0.486206
C	3.006773	-1.951898	-1.958137	C	3.142755	-2.001433	-1.702288
H	3.519759	-2.260089	-2.867745	H	3.686162	-2.394277	-2.560732
H	1.954354	-1.703880	-2.058232	H	2.103045	-1.734518	-1.865084
C	5.126825	-2.313671	-0.656550	C	5.155473	-2.412936	-0.254565
H	5.732153	-1.452931	-0.336109	H	5.793110	-1.597107	0.122317
H	5.526490	-2.676722	-1.609714	H	5.604676	-2.798132	-1.176310
H	5.272483	-3.104876	0.094263	H	5.196931	-3.214128	0.497766
C	-0.415961	-2.020624	2.392750	C	-0.544732	-1.925213	2.491874
H	-1.206699	-1.287329	2.572244	H	-1.349818	-1.188694	2.556089
H	0.448443	-1.762475	3.011790	H	0.259529	-1.621321	3.170308
H	-0.789224	-2.998799	2.722015	H	-0.942573	-2.887634	2.835359
C	-1.213319	-2.663383	-1.263379	C	-1.030821	-2.817801	-1.152018
C	-2.441471	-3.323446	-1.856713	C	-2.254323	-3.432990	-1.803506
H	-3.072124	-3.809827	-1.104242	H	-3.002638	-3.764883	-1.076252
H	-2.120506	-4.059518	-2.600523	H	-1.935852	-4.278980	-2.421829
H	-3.040336	-2.556937	-2.365303	H	-2.718814	-2.682292	-2.454825
C	0.030956	1.582418	0.141821	C	-0.058546	1.622211	0.194292
C	1.398399	1.894268	0.067033	C	1.321756	1.913832	-0.045351
H	1.732327	2.913246	-0.080531	H	1.612132	2.912845	-0.350660
C	2.365843	0.886212	0.207103	C	2.284350	0.932540	0.154469

C	3.809349	1.287722	0.134508	C	3.696476	1.353840	-0.035814
C	4.387427	1.639865	-1.104617	C	4.128024	1.866758	-1.301646
H	3.796363	1.560584	-2.013548	H	3.422628	1.874500	-2.124715
C	5.727201	2.065377	-1.170706	C	5.438050	2.292158	-1.478762
H	6.162605	2.325809	-2.132221	H	5.774042	2.651340	-2.446477
C	6.502130	2.152376	0.001941	C	6.367349	2.247112	-0.383086
H	7.536372	2.483682	-0.049483	H	7.386298	2.594333	-0.529957
C	5.929410	1.809749	1.242337	C	5.954889	1.768847	0.886766
H	6.518270	1.881862	2.153480	H	6.654000	1.762887	1.716387
C	4.591752	1.378534	1.307845	C	4.644747	1.334682	1.064351
H	4.151239	1.130358	2.271306	H	4.295553	1.025118	2.043053
C	-1.019985	2.641865	0.037619	C	-1.078022	2.647795	0.225485
C	-0.709898	4.001515	-0.189473	C	-0.781388	4.047667	0.166663
H	0.315761	4.326650	-0.311459	H	0.246904	4.383628	0.081800
C	-1.746358	4.945144	-0.265252	C	-1.797609	4.991762	0.246222
H	-1.515818	5.992047	-0.441153	H	-1.564117	6.052400	0.208776
C	-3.080047	4.521998	-0.120281	C	-3.152288	4.556448	0.385633
H	-3.909043	5.218770	-0.180468	H	-3.974478	5.259960	0.449840
C	-3.321766	3.155935	0.091956	C	-3.394044	3.180862	0.424819
H	-4.330802	2.767912	0.185436	H	-4.409436	2.802313	0.511656
Triplet excited state (T_1)							
Cd	-2.766048	0.015813	0.065415				
Cl	-3.779370	0.000827	-2.212772				
Cl	-3.925658	-1.153691	1.957607				
O	-0.219188	-2.360206	-1.880744				
N	-0.410426	0.250110	0.304880				
N	-2.303663	2.279988	0.244215				
N	-1.273578	-2.456152	0.163599				
H	-2.093273	-2.747753	0.694474				
C	-0.057326	-2.097042	0.939437				
C	0.485351	-0.712720	0.512787				
C	1.931814	-0.476500	0.476590				
C	2.952082	-1.584788	0.640175				
H	3.759727	-1.195291	1.276133				
C	2.371003	-2.830688	1.357857				
H	3.070849	-3.668698	1.248532				
H	2.289598	-2.628692	2.434736				
C	1.006712	-3.223131	0.775106				
H	0.619180	-4.117463	1.279175				
H	1.123746	-3.462497	-0.284819				
C	3.638171	-1.958613	-0.697439				
C	2.978094	-2.013972	-1.876961				
H	3.498891	-2.323442	-2.781689				
H	1.919375	-1.797497	-1.979638				
C	5.111393	-2.297801	-0.573014				
H	5.693328	-1.413782	-0.274657				
H	5.517642	-2.670204	-1.519645				
H	5.279457	-3.066945	0.195851				
C	-0.465400	-1.982373	2.439042				
H	-1.276535	-1.264304	2.583303				
H	0.389993	-1.677319	3.049485				
H	-0.811838	-2.958120	2.801506				
C	-1.231735	-2.689583	-1.205601				

C	-2.459809	-3.318302	-1.829963
H	-3.116584	-3.791392	-1.091998
H	-2.139358	-4.059177	-2.569263
H	-3.028704	-2.535988	-2.349448
C	0.017824	1.597406	0.086054
C	1.449046	1.865988	-0.054601
H	1.785404	2.868346	-0.285773
C	2.387679	0.885240	0.159399
C	3.836457	1.249564	0.072945
C	4.380359	1.697344	-1.152788
H	3.755308	1.702180	-2.042423
C	5.724657	2.102924	-1.235541
H	6.129331	2.435712	-2.188172
C	6.545267	2.074266	-0.091318
H	7.583880	2.389231	-0.154514
C	6.010349	1.637626	1.136503
H	6.632417	1.624388	2.028108
C	4.667767	1.226721	1.217552
H	4.258393	0.922501	2.178605
C	-0.947480	2.631469	0.086810
C	-0.605295	4.036547	-0.065112
H	0.426706	4.337378	-0.194951
C	-1.600095	5.005089	-0.037058
H	-1.342639	6.054427	-0.147865
C	-2.957982	4.614919	0.133083
H	-3.764268	5.339993	0.150419
C	-3.246159	3.229921	0.259265
H	-4.273510	2.891045	0.360246

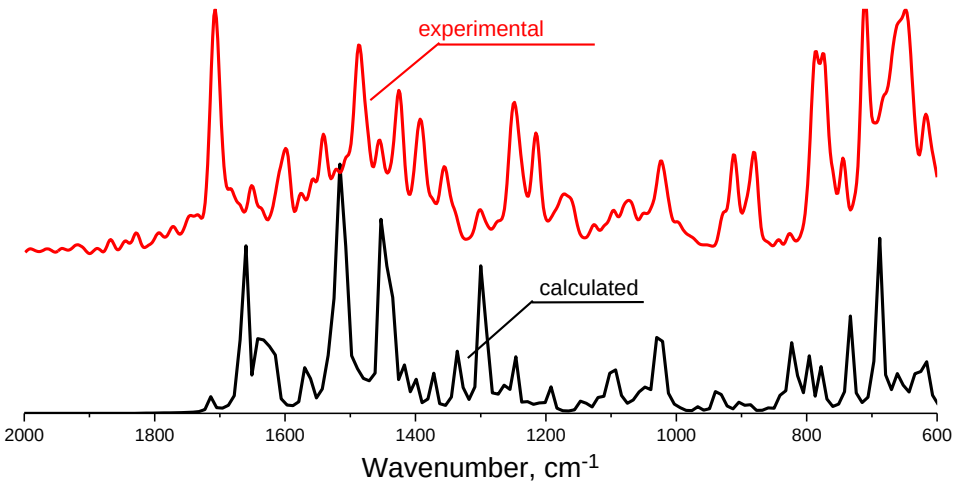


Figure S14. IR spectra for the complex **1** at 2000–600 cm^{-1}. Red curve is an experimental IR spectrum, black one is a calculated IR spectrum.

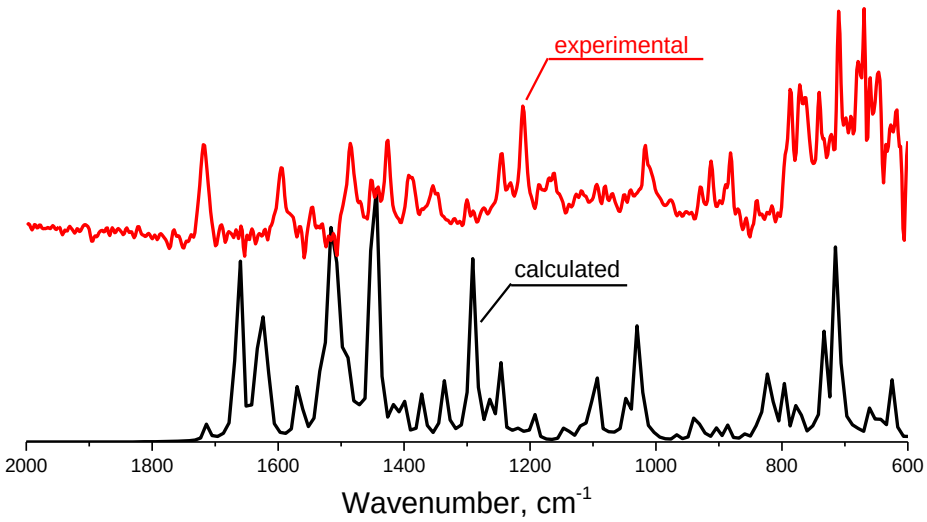


Figure S15. IR spectra for the complex **2** at 2000–600 cm^{-1}. Red curve is an experimental IR spectrum, black one is a calculated IR spectrum.

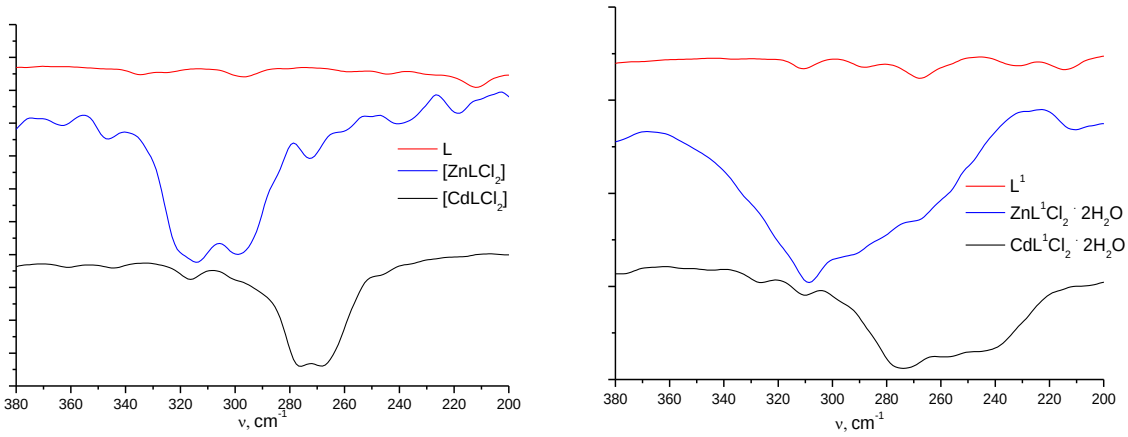


Figure S16. The far-IR spectra of **L**, **1**, and **2** (left) and **L**^{1}, **3**, and **4** (right).

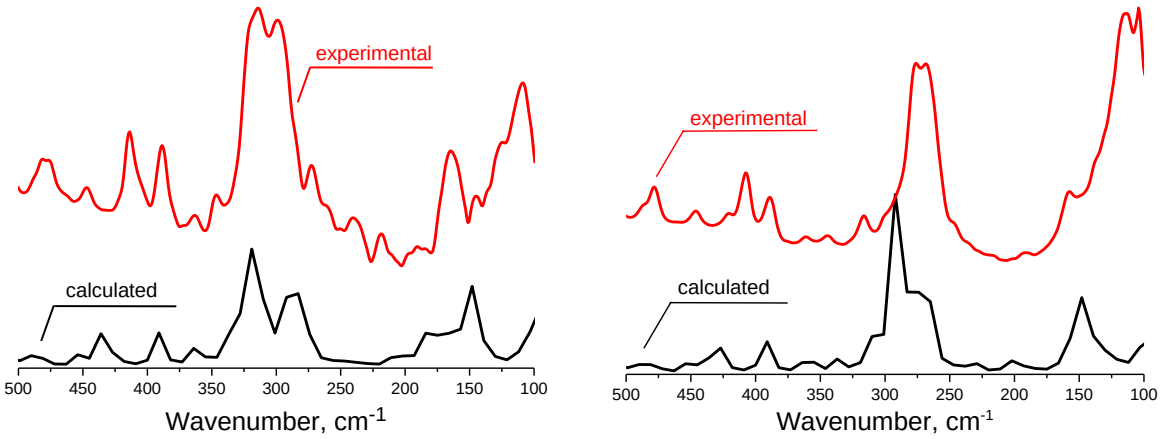
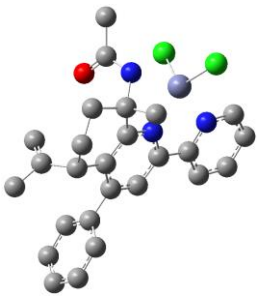


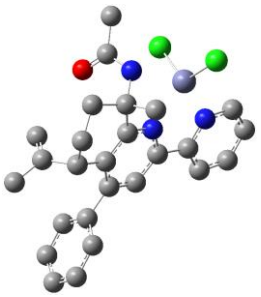
Figure S17. IR spectra for the complexes **1** (left) and **2** (right) at 500–100 cm^{-1}. Red curves are experimental IR spectra, black ones are calculated IR spectra.

Table S42. The most intensive bands in the IR spectrum of the complex **1** at 500–100 cm^{-1} and their assignment.



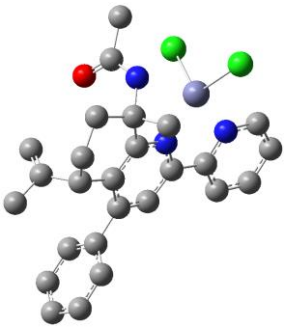
δ(C–C), δ(Zn–Cl)

146 cm^{-1}



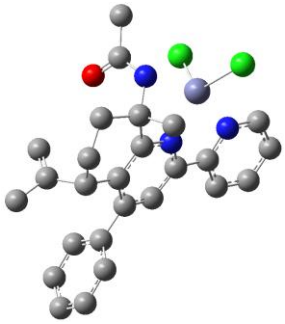
δ(C–C), δ(Zn–Cl)

170 cm^{-1}



ν(Zn–Cl)

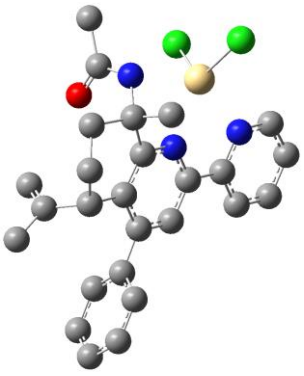
288 cm^{-1}



ν(Zn–Cl)

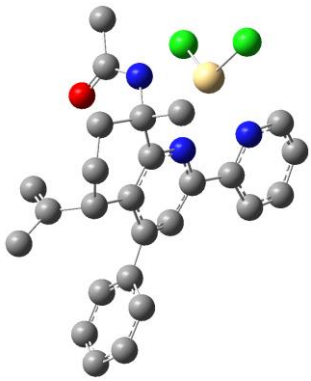
322 cm^{-1}

Table S43. The most intensive bands in the IR spectrum of the complex **2** at 500–100 cm^{-1} and their assignment.



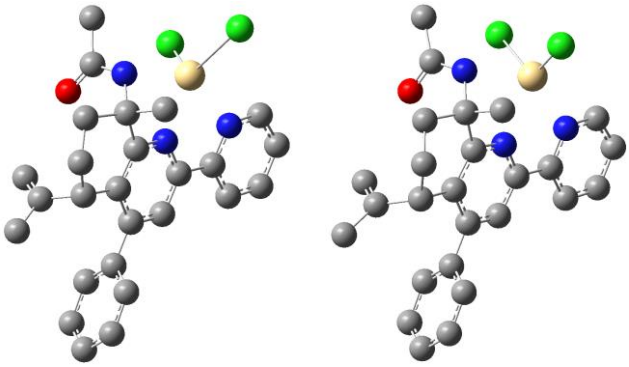
δ(C–C), δ(Cd–Cl)

144 cm^{-1}



ν(Cd–Cl)

270 cm^{-1}



ν(Cd–Cl)

292 cm^{-1}

Table S44. Main vibrational frequencies (cm^{-1}) in the IR spectra of the ligands **L** and **L^1** and the complexes **1** – **4**.

L	**1** $ZnLCl_2$	**2** $CdLCl_2$	**L^1**	**3** $ZnL^1Cl_2 \cdot 2H_2O$	**4** CdL^1Cl_2 $2H_2O$	vibration
3404	3364	3303	3289, 3196	3447, 3277	3389 broad	ν(NH), ν(H_2O)*
1673,	1707,	1719,	1634	1641	1638	ν(C=O), δ(NH)
1647, 1604, 1583, 1566, 1541	1652, 1596, 1578, 1542	1654, 1594, 1578, 1545	1579, 1564, 1538, 1500	1612, 1558, 1542	1596, 1574, 1543	ν(C=C), ν(C=N)
	399	316		382	328, 312	ν(M–N)
	332, 301	276, 268		308, 297 sh., 270 sh.	274, 258 sh., 247 sh.	ν(M–Cl), ν(M–N)

*for the complexes **3** and **4**.

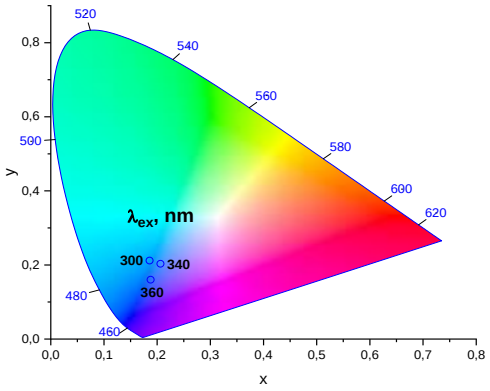


Figure S18. CIE 1931 chromaticity diagram showing chromaticity of emission of the complex **1** recorded at different excitations.

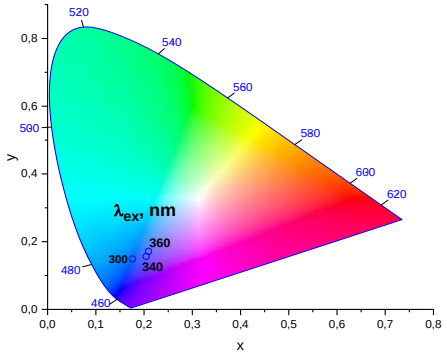


Figure S19. CIE 1931 chromaticity diagram showing chromaticity of emission of the complex **2** recorded at different excitations.

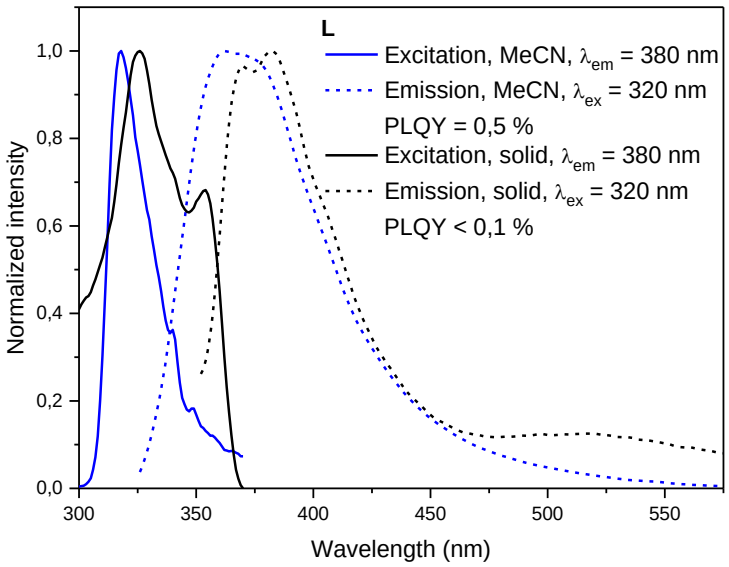


Figure S20. Comparison of the excitation and emission spectra of **L** in solid state and in MeCN.

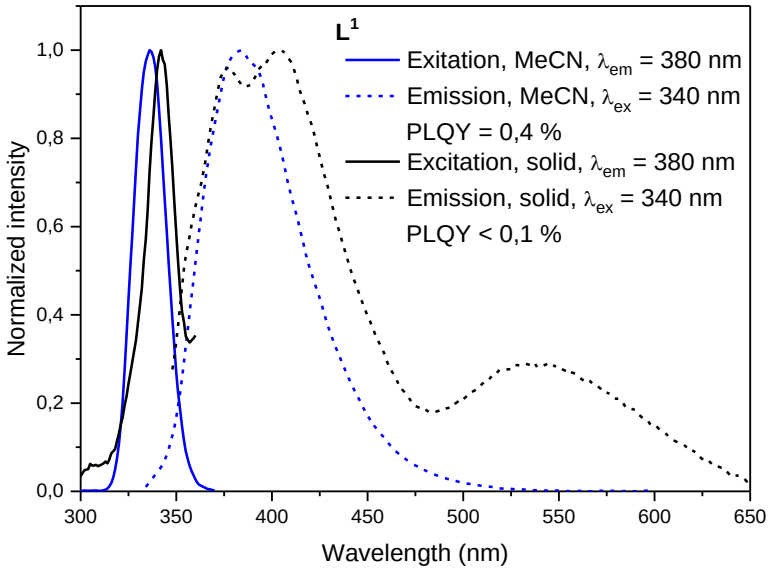


Figure S21. Comparison of the excitation and emission spectra of **L**^{1} in solid state and in MeCN.