Supplementary data for the article:

Čobeljić, B.; Pevec, A.; Stepanović, S.; Milenković, M. R.; Turel, I.; Gruden, M.; Radanović, D.; Anđelković, K. Structural Diversity of Isothiocyanato Cd(II) and Zn(II) Girard's T Hydrazone Complexes in Solution and Solid State: Effect of H-Bonding on Coordination Number and Supramolecular Assembly of Cd(II) Complex in Solid State. *Structural Chemistry* **2018**, *29* (6), 1797–1806. https://doi.org/10.1007/s11224-018-1155-8

SUPPORTING INFORMATION

Structural diversity of isothiocyanato Cd(II) and Zn(II) Girard's T hydrazone complexes in solution and solid state. Effect of H-bonding on coordination number and supramolecular assembly of Cd(II) complex in solid state

Božidar Čobeljić[a], Andrej Pevec[b], Stepan Stepanović[c], Milica R. Milenković[a], Iztok Turel[b], Maja Gruden[a], Dušanka Radanović[c], Katarina Anđelković[a*]

[a]*Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade, Serbia*

[b]*Faculty of Chemistry and Chemical Technology, University of Ljubljana, Vec˘na pot 113, 1000 Ljubljana, Slovenia*

[c]*Center for Chemistry, IHTM, University of Belgrade, Studentski trg 12-16, Belgrade, Serbia*

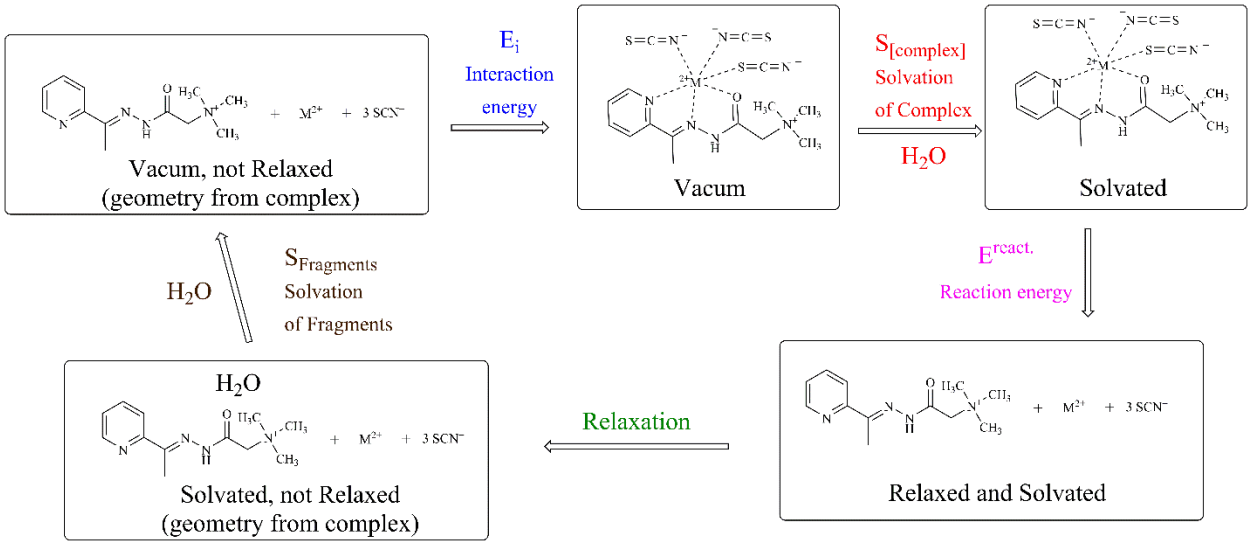

Figure S1. Schematic representation of the thermodinamic cycle used to decompose reaction energetics into four contributions: relaxation of solvated ligands, ligands solvation, complex solvation and vacuum interaction energy obtained from EDA.

*Corresponding author: Katarina Anđelković, e-mail: kka@chem.bg.ac.rs

Table S1. Reaction energies decomposed accordin to Scheme Sx. All values are in kcal/mol.

	Cd^{2+}_penta	Cd^{2+}_hexa	Zn^{2+}_penta	Zn^{2+}_hexa
complex solvation	-34.46	-58.05	-33.97	-57.72
fragment solvation	-481.55	-571.31	-510.59	-600.85
dispersion	3.56	2.42	5.36	4.54
interaction energy	-609.07	-667.98	-687.33	-740.50
ΔE^{react}	-158.42	-152.30	-205.35	-192.83

Table S2. Differencies between the reaction energies for hexa- and penta-coordinated structures, decomposed accordin to Scheme Sx (and obtained from Table Sx1). All values are in kcal/mol.

	Cd^{2+}	Zn^{2+}	Short comment
Complex solvation (penta-hexa)	23.59	23.75	Similar magnitude
Fragment solvation (penta-hexa)	-89.76	-90.26	Similar magnitude
Dispersion (penta-hexa)	-1.14	-0.82	Similar magnitude
Interaction energy (penta-hexa)	**58.91**	**53.17**	Favors pentacoordinated in Zn^{2+} more than in Cd^{2+}
ΔE (penta-hexa)	-6.12	-12.52	

Table S3. EDA of vacum interaction energies for all structures of interest. All values are in kcal/mol.

	Cd^{2+}_penta	Cd^{2+}_hexa	Zn^{2+}_penta	Zn^{2+}_hexa
Pauli	173.56	184.80	197.56	211.56
Electrostatic	-618.71	-680.39	-684.87	-735.36
Orbital	-150.84	-146.51	-186.41	-190.20
Dispersion	-13.08	-25.88	-13.61	-26.49
Interaction energy	-609.07	-667.99	-687.33	-740.50

Table S3. Differencies between the EDA of vacum interaction energies for hexa- and penta-coordinated structures obtained from Table Sx3. All values are in kcal/mol.

	Cd^{2+}	Zn^{2+}	Short comment
Pauli(penta-hexa)	-11.24	-14	Favors pentacoordinated in Zn^{2+} more than in Cd^{2+}
Electrostatic(penta-hexa)	61.68	50.49	Favors pentacoordinated in Zn^{2+} more than in Cd^{2+}
Orbital(penta-hexa)	-4.33	3.79	Favors pentacoordinated in Cd^{2+} more than in Zn^{2+}
Dispersion(penta-hexa)	12.8	12.88	Similar magnitude
Interaction energy(penta-hexa)	58.92	53.17	

Coordinates of all DFT optimized structures.

In order to be completely unambiguous about the methodology we used for EDA, we are providing all coordinates for the thermodynamic cycle necessary to decompose reaction energetics. Some coordinates are shown more than once, so there would be no confusion about the nature of geometry used in any particular situation.

Zn2+ ion 5-coordinated environment entier complex relaxed_structure

N	8.11580000	15.24740000	6.14810000
N	9.15290000	13.20850000	7.44440000
N	9.84480000	12.20050000	8.05660000
N	12.87480000	10.73670000	7.74130000
O	11.70040000	13.62960000	7.81420000
C	7.26570000	14.25940000	6.53000000
C	5.89360000	14.34840000	6.26430000
H	5.21890000	13.55300000	6.57370000
C	5.40150000	15.47300000	5.60070000
H	4.33650000	15.55770000	5.38700000
C	6.28390000	16.48300000	5.21800000
H	5.93940000	17.37650000	4.70040000
C	7.63930000	16.32580000	5.51560000
H	8.37570000	17.08270000	5.24360000
C	7.87010000	13.10720000	7.23440000
C	7.03620000	11.93840000	7.64660000
H	7.66440000	11.17070000	8.10560000
H	6.51770000	11.51200000	6.77630000
H	6.26490000	12.25090000	8.36530000
C	11.14230000	12.53760000	8.16950000
C	11.99460000	11.43900000	8.77720000
H	11.35590000	10.66800000	9.21730000
H	12.67020000	11.84800000	9.53560000
C	13.98520000	11.64240000	7.26820000
H	14.59390000	11.92290000	8.13210000
H	13.54150000	12.52730000	6.80760000
H	14.58570000	11.08800000	6.54200000
C	13.47850000	9.52170000	8.40130000
H	12.67190000	8.84110000	8.68610000
H	14.03510000	9.84570000	9.28490000
H	14.14910000	9.03890000	7.68550000
C	12.04760000	10.30080000	6.55890000
H	11.69780000	11.18870000	6.02530000
H	11.20090000	9.71220000	6.92100000
H	12.68380000	9.70130000	5.90260000
S	12.85340000	12.83300000	3.65620000
N	11.05680000	14.56280000	4.96150000
C	11.81840000	13.82430000	4.41730000

C	10.63630000	17.59310000	8.12420000
S	10.70950000	19.03230000	8.87870000
N	10.59500000	16.54140000	7.57530000
Zn	10.16900000	14.85110000	6.70330000

Zn2+ ion 5-coordinated environment L fragment_solv

N	8.11580000	15.24740000	6.14810000
N	9.15290000	13.20850000	7.44440000
N	9.84480000	12.20050000	8.05660000
N	12.87480000	10.73670000	7.74130000
O	11.70040000	13.62960000	7.81420000
C	7.26570000	14.25940000	6.53000000
C	5.89360000	14.34840000	6.26430000
H	5.21890000	13.55300000	6.57370000
C	5.40150000	15.47300000	5.60070000
H	4.33650000	15.55770000	5.38700000
C	6.28400000	16.48300000	5.21800000
H	5.93940000	17.37650000	4.70040000
C	7.63930000	16.32580000	5.51560000
H	8.37570000	17.08270000	5.24360000
C	7.87010000	13.10720000	7.23440000
C	7.03620000	11.93840000	7.64670000
H	7.66440000	11.17070000	8.10560000
H	6.51770000	11.51200000	6.77630000
H	6.26490000	12.25090000	8.36530000
C	11.14220000	12.53760000	8.16950000
C	11.99460000	11.43900000	8.77720000
H	11.35590000	10.66800000	9.21740000
H	12.67020000	11.84800000	9.53560000
C	13.98520000	11.64240000	7.26820000
H	14.59390000	11.92290000	8.13210000
H	13.54150000	12.52730000	6.80760000
H	14.58570000	11.08800000	6.54200000
C	13.47850000	9.52170000	8.40130000
H	12.67190000	8.84110000	8.68610000
H	14.03510000	9.84570000	9.28490000
H	14.14910000	9.03890000	7.68550000
C	12.04760000	10.30080000	6.55890000
H	11.69780000	11.18870000	6.02530000
H	11.20090000	9.71220000	6.92100000
H	12.68380000	9.70130000	5.90260000

Zn2+ ion 5-coordinated environment L fragment_vacum

N	8.11580000	15.24740000	6.14810000
N	9.15290000	13.20850000	7.44440000
N	9.84480000	12.20050000	8.05660000
N	12.87480000	10.73670000	7.74130000

O	11.70040000	13.62960000	7.81420000
C	7.26570000	14.25940000	6.53000000
C	5.89360000	14.34840000	6.26430000
H	5.21890000	13.55300000	6.57370000
C	5.40150000	15.47300000	5.60070000
H	4.33650000	15.55770000	5.38700000
C	6.28400000	16.48300000	5.21800000
H	5.93940000	17.37650000	4.70040000
C	7.63930000	16.32580000	5.51560000
H	8.37570000	17.08270000	5.24360000
C	7.87010000	13.10720000	7.23440000
C	7.03620000	11.93840000	7.64670000
H	7.66440000	11.17070000	8.10560000
H	6.51770000	11.51200000	6.77630000
H	6.26490000	12.25090000	8.36530000
C	11.14220000	12.53760000	8.16950000
C	11.99460000	11.43900000	8.77720000
H	11.35590000	10.66800000	9.21740000
H	12.67020000	11.84800000	9.53560000
C	13.98520000	11.64240000	7.26820000
H	14.59390000	11.92290000	8.13210000
H	13.54150000	12.52730000	6.80760000
H	14.58570000	11.08800000	6.54200000
C	13.47850000	9.52170000	8.40130000
H	12.67190000	8.84110000	8.68610000
H	14.03510000	9.84570000	9.28490000
H	14.14910000	9.03890000	7.68550000
C	12.04760000	10.30080000	6.55890000
H	11.69780000	11.18870000	6.02530000
H	11.20090000	9.71220000	6.92100000
H	12.68380000	9.70130000	5.90260000

Zn2+ ion 5-coordinated environment L relaxed_structure

N	7.63857039	15.68498034	6.81880445
N	9.29903917	13.61961000	7.51928167
N	10.00931092	12.60369393	8.12111231
N	12.87191589	10.71145928	8.08636865
O	12.01137102	13.57598145	7.33468030
C	7.30892207	14.41184444	6.47730574
C	6.20867208	14.14016431	5.63953983
H	5.95719277	13.11552369	5.37121787
C	5.44378077	15.19393242	5.14084690
H	4.59267378	14.99458553	4.48882274
C	5.78696227	16.50053561	5.48906723
H	5.21886509	17.35818112	5.12914150
C	6.89115357	16.68436015	6.32875404
H	7.18652814	17.69355778	6.63001359
C	8.13969225	13.30316889	7.01227007
C	7.61741336	11.89224423	6.91611221

H	8.25941754	11.22542798	7.50048953
H	7.62452021	11.54460123	5.87139303
H	6.58179390	11.82393221	7.27721165
C	11.33577890	12.75593135	8.03838074
C	12.07404783	11.73560564	8.90354162
H	11.36390361	11.15890087	9.50351537
H	12.80046849	12.23502514	9.55562875
C	14.10010824	11.34436427	7.47969286
H	14.74778944	11.68442150	8.29300813
H	13.77907439	12.19361649	6.87268793
H	14.61089128	10.58752756	6.87731876
C	13.30120193	9.60410826	9.01391794
H	12.40910170	9.10122901	9.39756297
H	13.87496766	10.04145209	9.83587943
H	13.92178767	8.90094230	8.45074317
C	12.00752126	10.13727445	6.99479399
H	11.76830139	10.93177535	6.28352103
H	11.09047719	9.74837574	7.44560855
H	12.56521745	9.33738018	6.50018313

Zn2+ ion 5-coordinated environment SCN1 fragment_solv

S	0.18980000	3.68900000	0.00000000
N	-2.36470000	4.87150000	0.00000000
C	-1.28710000	4.36120000	0.00000000

Zn2+ ion 5-coordinated environment SCN1 fragment_vacum

S	0.18980000	3.68900000	0.00000000
N	-2.36470000	4.87150000	0.00000000
C	-1.28710000	4.36120000	0.00000000

Zn2+ ion 5-coordinated environment SCN1 relaxed_structure

S	0.00000000	0.00000000	-14.07557240
N	0.00000000	0.00000000	-11.23194374
C	0.00000000	0.00000000	-12.42114366

Zn2+ ion 5-coordinated environment SCN2 fragment_solv

C	11.17480000	18.86470000	0.00000000
S	11.32440000	20.48440000	0.00000000
N	11.07790000	17.68160000	0.00000000

Zn2+ ion 5-coordinated environment SCN2 fragment_vacum

C	11.17480000	18.86470000	0.00000000
S	11.32440000	20.48440000	0.00000000
N	11.07790000	17.68160000	0.00000000

Zn2+ ion 5-coordinated environment SCN2 relaxed_structure

S	0.00000000	0.00000000	-14.07557240
N	0.00000000	0.00000000	-11.23194374
C	0.00000000	0.00000000	-12.42114366

Zn2+ ion 5-coordinated environment Zn_ fragment_solv

Zn	0.00000000	0.00000000	0.00000000

Zn2+ ion 5-coordinated environment Zn_ fragment_vacum

Zn	0.00000000	0.00000000	0.00000000

Zn2+ ion 6-coordinated environment entier complex relaxed_structure

N	9.90590000	2.18750000	12.00070000
N	8.35650000	0.49630000	10.78380000
N	7.67250000	-0.31550000	9.94280000
H	7.09110000	-1.07390000	10.30210000
N	7.19590000	-0.95260000	6.26880000
O	8.55070000	0.79860000	8.15440000
C	9.08530000	1.43700000	12.77940000
C	9.04800000	1.61470000	14.16450000
H	8.39080000	1.00710000	14.78200000
C	9.85690000	2.59250000	14.74450000
H	9.83690000	2.74710000	15.82240000
C	10.68090000	3.37040000	13.93180000
H	11.32110000	4.14690000	14.34570000
C	10.67650000	3.13170000	12.55790000
H	11.30050000	3.70390000	11.87130000
C	8.22950000	0.45200000	12.07460000
C	7.34060000	-0.46840000	12.84100000
H	6.67840000	-1.05910000	12.20110000
H	6.70850000	0.11360000	13.52190000
H	7.94930000	-1.15990000	13.44010000
C	7.85330000	-0.12200000	8.60000000
C	7.14300000	-1.17280000	7.75950000
H	7.60880000	-2.14540000	7.96290000
H	6.08660000	-1.22650000	8.04680000
C	6.40100000	-2.07310000	5.63170000
H	5.37000000	-2.01920000	5.99050000
H	6.85660000	-3.02730000	5.90920000

H	6.43540000	-1.93410000	4.54860000
C	8.61790000	-1.02090000	5.75320000
H	8.57890000	-0.94360000	4.66400000
H	9.04640000	-1.97980000	6.05700000
H	9.18620000	-0.19590000	6.18270000
C	6.55950000	0.36600000	5.88710000
H	5.53930000	0.37940000	6.27970000
H	6.54770000	0.42540000	4.79620000
H	7.15160000	1.17780000	6.31040000
S	10.66040000	-2.36800000	8.78380000
N	11.19270000	0.26050000	9.64550000
C	10.97590000	-0.85690000	9.27970000
C	10.90300000	4.40090000	9.06330000
N	10.41630000	3.31540000	8.99160000
S	11.56070000	5.88060000	9.12660000
N	5.95220000	2.57340000	12.48320000
S	7.12210000	3.54380000	10.08770000
C	6.42860000	2.99230000	11.47850000
Zn	9.85830000	1.74290000	9.96820000

Zn2+ ion 6-coordinated environment LH fragment_solv

N	9.90590000	2.18750000	12.00070000
N	8.35650000	0.49630000	10.78380000
N	7.67250000	-0.31550000	9.94280000
H	7.09110000	-1.07390000	10.30210000
N	7.19590000	-0.95260000	6.26880000
O	8.55070000	0.79860000	8.15440000
C	9.08530000	1.43700000	12.77940000
C	9.04800000	1.61470000	14.16450000
H	8.39080000	1.00710000	14.78200000
C	9.85690000	2.59250000	14.74450000
H	9.83690000	2.74710000	15.82240000
C	10.68090000	3.37040000	13.93180000
H	11.32110000	4.14690000	14.34570000
C	10.67650000	3.13170000	12.55790000
H	11.30050000	3.70390000	11.87130000
C	8.22950000	0.45200000	12.07460000
C	7.34060000	-0.46840000	12.84100000
H	6.67840000	-1.05910000	12.20110000
H	6.70850000	0.11360000	13.52190000
H	7.94930000	-1.15990000	13.44010000
C	7.85330000	-0.12200000	8.60000000
C	7.14300000	-1.17280000	7.75950000
H	7.60880000	-2.14540000	7.96290000
H	6.08660000	-1.22650000	8.04680000
C	6.40100000	-2.07310000	5.63170000
H	5.37000000	-2.01920000	5.99050000
H	6.85660000	-3.02730000	5.90920000
H	6.43540000	-1.93410000	4.54860000

C	8.61790000	-1.02090000	5.75320000
H	8.57890000	-0.94360000	4.66400000
H	9.04640000	-1.97980000	6.05700000
H	9.18630000	-0.19590000	6.18270000
C	6.55950000	0.36600000	5.88710000
H	5.53930000	0.37940000	6.27970000
H	6.54770000	0.42540000	4.79620000
H	7.15160000	1.17780000	6.31040000

Zn2+ ion 6-coordinated environment LH fragment_vacum

N	9.90590000	2.18750000	12.00070000
N	8.35650000	0.49630000	10.78380000
N	7.67250000	-0.31550000	9.94280000
H	7.09110000	-1.07390000	10.30210000
N	7.19590000	-0.95260000	6.26880000
O	8.55070000	0.79860000	8.15440000
C	9.08530000	1.43700000	12.77940000
C	9.04800000	1.61470000	14.16450000
H	8.39080000	1.00710000	14.78200000
C	9.85690000	2.59250000	14.74450000
H	9.83690000	2.74710000	15.82240000
C	10.68090000	3.37040000	13.93180000
H	11.32110000	4.14690000	14.34570000
C	10.67650000	3.13170000	12.55790000
H	11.30050000	3.70390000	11.87130000
C	8.22950000	0.45200000	12.07460000
C	7.34060000	-0.46840000	12.84100000
H	6.67840000	-1.05910000	12.20110000
H	6.70850000	0.11360000	13.52190000
H	7.94930000	-1.15990000	13.44010000
C	7.85330000	-0.12200000	8.60000000
C	7.14300000	-1.17280000	7.75950000
H	7.60880000	-2.14540000	7.96290000
H	6.08660000	-1.22650000	8.04680000
C	6.40100000	-2.07310000	5.63170000
H	5.37000000	-2.01920000	5.99050000
H	6.85660000	-3.02730000	5.90920000
H	6.43540000	-1.93410000	4.54860000
C	8.61790000	-1.02090000	5.75320000
H	8.57890000	-0.94360000	4.66400000
H	9.04640000	-1.97980000	6.05700000
H	9.18630000	-0.19590000	6.18270000
C	6.55950000	0.36600000	5.88710000
H	5.53930000	0.37940000	6.27970000
H	6.54770000	0.42540000	4.79620000
H	7.15160000	1.17780000	6.31040000

Zn2+ ion 6-coordinated environment LH relaxed_structure

N	9.54231994	2.61404776	12.08460757
N	8.57457593	0.48087871	10.69132832
N	7.91656943	-0.43994473	9.92503733
H	7.21159262	-1.05835767	10.33352512
N	6.76596769	-1.33224235	6.69024825
O	9.11430921	0.07021230	8.02718599
C	8.95062887	1.58783814	12.74139538
C	9.06232019	1.42484414	14.13206207
H	8.58981359	0.58198279	14.63398299
C	9.81603052	2.34153418	14.86590868
H	9.92453144	2.22562002	15.94430047
C	10.42426421	3.40096291	14.19475899
H	11.01618970	4.14735048	14.72397805
C	10.25411467	3.49019860	12.80817913
H	10.70994266	4.31264164	12.25092162
C	8.19063932	0.60069767	11.92736731
C	7.07625659	-0.19660099	12.54912623
H	6.18868559	-0.18710226	11.89938336
H	6.77282477	0.21567730	13.51470485
H	7.37528407	-1.24528477	12.69987931
C	8.26969311	-0.61256341	8.61532364
C	7.52214399	-1.76197555	7.93900019
H	8.24767669	-2.52440567	7.63536464
H	6.78621137	-2.22037535	8.60690919
C	5.87672131	-2.48359446	6.28090213
H	5.15131403	-2.66748779	7.07795578
H	6.50278827	-3.36510903	6.11898448
H	5.36511433	-2.20457358	5.35605323
C	7.70998180	-1.02243871	5.54985911
H	7.10457604	-0.73450067	4.68636990
H	8.28665800	-1.92480763	5.32878685
H	8.37173542	-0.21103007	5.85559867
C	5.91000762	-0.12598546	6.98857774
H	5.26820346	-0.35722851	7.84342602
H	5.30327045	0.08821385	6.10535287
H	6.56198045	0.72262646	7.21059829

Zn2+ ion 6-coordinated environment SCN1 fragment_solv

S	11.11230000	0.30910000	0.00000000
N	11.66710000	3.07080000	0.00000000
C	11.44070000	1.89690000	0.00000000

Zn2+ ion 6-coordinated environment SCN1 fragment_vacum

S	11.11230000	0.30910000	0.00000000
N	11.66710000	3.07080000	0.00000000
C	11.44070000	1.89690000	0.00000000

Zn2+ ion 6-coordinated environment SCN1 relaxed_structure

S	0.00000000	0.00000000	-14.07557240
N	0.00000000	0.00000000	-11.23194374
C	0.00000000	0.00000000	-12.42114366

Zn2+ ion 6-coordinated environment SCN2 fragment_solv

C	12.73200000	3.60130000	0.00000000
N	12.18900000	2.54040000	0.00000000
S	13.43940000	5.05930000	0.00000000

Zn2+ ion 6-coordinated environment SCN2 fragment_vacum

C	12.73200000	3.60130000	0.00000000
N	12.18900000	2.54040000	0.00000000
S	13.43940000	5.05930000	0.00000000

Zn2+ ion 6-coordinated environment SCN2 relaxed_structure

S	0.00000000	0.00000000	-14.07557240
N	0.00000000	0.00000000	-11.23194374
C	0.00000000	0.00000000	-12.42114366

Zn2+ ion 6-coordinated environment SCN3 fragment_solv

N	-2.60010000	-7.63380000	0.00000000
S	-0.57690000	-5.64500000	0.00000000
C	-1.76580000	-6.78780000	0.00000000

Zn2+ ion 6-coordinated environment SCN3 fragment_vacum

N	-2.60010000	-7.63380000	0.00000000
S	-0.57690000	-5.64500000	0.00000000
C	-1.76580000	-6.78780000	0.00000000

Zn2+ ion 6-coordinated environment SCN3 relaxed_structure

S	0.00000000	0.00000000	-14.07557240
N	0.00000000	0.00000000	-11.23194374
C	0.00000000	0.00000000	-12.42114366

Zn2+ ion 6-coordinated environment Zn_ fragment_solv

Zn	0.00000000	0.00000000	0.00000000

Zn2+ ion 6-coordinated environment Zn_ fragment_vacum

Zn	0.00000000	0.00000000	0.00000000

Cd2+ ion 5-coordinated environment Cd_ fragment_solv

Cd	0.00000000	0.00000000	0.00000000

Cd2+ ion 5-coordinated environment Cd_ fragment_vacum

Cd	0.00000000	0.00000000	0.00000000

Cd2+ ion 5-coordinated environment entier complex relaxed_structure

Cd	10.34310000	15.00990000	6.64190000
N	8.02710000	15.23280000	6.14800000
N	9.20890000	13.15180000	7.39010000
N	9.90590000	12.14150000	7.99030000
N	12.82980000	10.53540000	7.74680000
O	11.81870000	13.52770000	7.80030000
C	7.26620000	14.15960000	6.48760000
C	5.88750000	14.15300000	6.23040000
H	5.28040000	13.29260000	6.50310000
C	5.29600000	15.26220000	5.62610000
H	4.22530000	15.26700000	5.42350000
C	6.08750000	16.35950000	5.29040000
H	5.66680000	17.24640000	4.81980000
C	7.45370000	16.29700000	5.57170000
H	8.11960000	17.12600000	5.32930000
C	7.93780000	13.00910000	7.14140000
C	7.15680000	11.77630000	7.47590000
H	7.82280000	11.01370000	7.88740000
H	6.66090000	11.37990000	6.57880000
H	6.37120000	12.00230000	8.21160000
C	11.20520000	12.45450000	8.13050000
C	12.01230000	11.33350000	8.76310000
H	11.34440000	10.61810000	9.25140000
H	12.72660000	11.73970000	9.48680000
C	13.92280000	11.38190000	7.14270000
H	14.56570000	11.74460000	7.94910000
H	13.46640000	12.21870000	6.61020000
H	14.49190000	10.75330000	6.45250000
C	13.45520000	9.37320000	8.47810000

H	12.65760000	8.73820000	8.87260000
H	14.07080000	9.76420000	9.29250000
H	14.07230000	8.81340000	7.77030000
C	11.93870000	10.00870000	6.65080000
H	11.56350000	10.85040000	6.06280000
H	11.10980000	9.46100000	7.10630000
H	12.53630000	9.34910000	6.01600000
S	12.54550000	12.38560000	3.64490000
N	11.28620000	14.69770000	4.65340000
C	11.81700000	13.71100000	4.23640000
S	10.44270000	19.06790000	9.31110000
N	10.83480000	16.95550000	7.49010000
C	10.65420000	17.83750000	8.26900000

Cd2+ ion 5-coordinated environment L fragment_solv

N	8.02710000	15.23280000	6.14800000
N	9.20890000	13.15180000	7.39010000
N	9.90590000	12.14150000	7.99030000
N	12.82980000	10.53540000	7.74680000
O	11.81870000	13.52770000	7.80030000
C	7.26620000	14.15960000	6.48760000
C	5.88750000	14.15300000	6.23040000
H	5.28040000	13.29260000	6.50310000
C	5.29600000	15.26220000	5.62610000
H	4.22530000	15.26700000	5.42350000
C	6.08750000	16.35950000	5.29040000
H	5.66680000	17.24640000	4.81980000
C	7.45370000	16.29700000	5.57170000
H	8.11960000	17.12600000	5.32930000
C	7.93780000	13.00910000	7.14140000
C	7.15680000	11.77630000	7.47590000
H	7.82280000	11.01370000	7.88740000
H	6.66090000	11.37990000	6.57880000
H	6.37120000	12.00230000	8.21160000
C	11.20520000	12.45450000	8.13050000
C	12.01230000	11.33350000	8.76310000
H	11.34440000	10.61810000	9.25140000
H	12.72660000	11.73970000	9.48680000
C	13.92280000	11.38190000	7.14270000
H	14.56570000	11.74460000	7.94910000
H	13.46640000	12.21870000	6.61020000
H	14.49190000	10.75330000	6.45250000
C	13.45520000	9.37320000	8.47810000
H	12.65760000	8.73820000	8.87260000
H	14.07080000	9.76420000	9.29250000
H	14.07230000	8.81340000	7.77030000
C	11.93870000	10.00870000	6.65080000
H	11.56350000	10.85040000	6.06280000
H	11.10980000	9.46100000	7.10630000

H	12.53630000	9.34910000	6.01600000

Cd2+ ion 5-coordinated environment L fragment_vacum

N	8.02710000	15.23280000	6.14800000
N	9.20890000	13.15180000	7.39010000
N	9.90590000	12.14150000	7.99030000
N	12.82980000	10.53540000	7.74680000
O	11.81870000	13.52770000	7.80030000
C	7.26620000	14.15960000	6.48760000
C	5.88750000	14.15300000	6.23040000
H	5.28040000	13.29260000	6.50310000
C	5.29600000	15.26220000	5.62610000
H	4.22530000	15.26700000	5.42350000
C	6.08750000	16.35950000	5.29040000
H	5.66680000	17.24640000	4.81980000
C	7.45370000	16.29700000	5.57170000
H	8.11960000	17.12600000	5.32930000
C	7.93780000	13.00910000	7.14140000
C	7.15680000	11.77630000	7.47590000
H	7.82280000	11.01370000	7.88740000
H	6.66090000	11.37990000	6.57880000
H	6.37120000	12.00230000	8.21160000
C	11.20520000	12.45450000	8.13050000
C	12.01230000	11.33350000	8.76310000
H	11.34440000	10.61810000	9.25140000
H	12.72660000	11.73970000	9.48680000
C	13.92280000	11.38190000	7.14270000
H	14.56570000	11.74460000	7.94910000
H	13.46640000	12.21870000	6.61020000
H	14.49190000	10.75330000	6.45250000
C	13.45520000	9.37320000	8.47810000
H	12.65760000	8.73820000	8.87260000
H	14.07080000	9.76420000	9.29250000
H	14.07230000	8.81340000	7.77030000
C	11.93870000	10.00870000	6.65080000
H	11.56350000	10.85040000	6.06280000
H	11.10980000	9.46100000	7.10630000
H	12.53630000	9.34910000	6.01600000

Cd2+ ion 5-coordinated environment L relaxed_structure

N	7.63857039	15.68498034	6.81880445
N	9.29903917	13.61961000	7.51928167
N	10.00931092	12.60369393	8.12111231
N	12.87191589	10.71145928	8.08636865
O	12.01137102	13.57598145	7.33468030
C	7.30892207	14.41184444	6.47730574
C	6.20867208	14.14016431	5.63953983

H	5.95719277	13.11552369	5.37121787
C	5.44378077	15.19393242	5.14084690
H	4.59267378	14.99458553	4.48882274
C	5.78696227	16.50053561	5.48906723
H	5.21886509	17.35818112	5.12914150
C	6.89115357	16.68436015	6.32875404
H	7.18652814	17.69355778	6.63001359
C	8.13969225	13.30316889	7.01227007
C	7.61741336	11.89224423	6.91611221
H	8.25941754	11.22542798	7.50048953
H	7.62452021	11.54460123	5.87139303
H	6.58179390	11.82393221	7.27721165
C	11.33577890	12.75593135	8.03838074
C	12.07404783	11.73560564	8.90354162
H	11.36390361	11.15890087	9.50351537
H	12.80046849	12.23502514	9.55562875
C	14.10010824	11.34436427	7.47969286
H	14.74778944	11.68442150	8.29300813
H	13.77907439	12.19361649	6.87268793
H	14.61089128	10.58752756	6.87731876
C	13.30120193	9.60410826	9.01391794
H	12.40910170	9.10122901	9.39756297
H	13.87496766	10.04145209	9.83587943
H	13.92178767	8.90094230	8.45074317
C	12.00752126	10.13727445	6.99479399
H	11.76830139	10.93177535	6.28352103
H	11.09047719	9.74837574	7.44560855
H	12.56521745	9.33738018	6.50018313

Cd2+ ion 5-coordinated environment SCN1 fragment_solv

S	0.74630000	8.48540000	0.00000000
N	-1.12320000	10.59580000	0.00000000
C	-0.34010000	9.69260000	0.00000000

Cd2+ ion 5-coordinated environment SCN1 fragment_vacum

S	0.74630000	8.48540000	0.00000000
N	-1.12320000	10.59580000	0.00000000
C	-0.34010000	9.69260000	0.00000000

Cd2+ ion 5-coordinated environment SCN1 relaxed_structure

S	0.00000000	0.00000000	-14.07557240
N	0.00000000	0.00000000	-11.23194374
C	0.00000000	0.00000000	-12.42114366

Cd2+ ion 5-coordinated environment SCN2 fragment_solv

S	4.40100000	22.67260000	0.00000000
N	5.55710000	20.10450000	0.00000000
C	5.04970000	21.18140000	0.00000000

Cd2+ ion 5-coordinated environment SCN2 fragment_vacum

S	4.40100000	22.67260000	0.00000000
N	5.55710000	20.10450000	0.00000000
C	5.04970000	21.18140000	0.00000000

Cd2+ ion 5-coordinated environment SCN2 relaxed_structure

S	0.00000000	0.00000000	-14.07557240
N	0.00000000	0.00000000	-11.23194374
C	0.00000000	0.00000000	-12.42114366

Cd2+ ion 6-coordinated environment Cd_ fragment_solv

Cd	0.00000000	0.00000000	0.00000000

Cd2+ ion 6-coordinated environment Cd_ fragment_vacum

Cd	0.00000000	0.00000000	0.00000000

Cd2+ ion 6-coordinated environment entier complex relaxed_structure

Cd	9.59930000	2.11120000	9.69530000
S	10.61960000	-2.27220000	8.88220000
S	11.96020000	6.02520000	10.05080000
N	6.12790000	2.69230000	12.05810000
N	9.83650000	2.19010000	12.03610000
N	8.33360000	0.37130000	10.78690000
N	7.64360000	-0.49550000	10.00530000
H	7.18470000	-1.31180000	10.41440000
N	7.00490000	-1.41520000	6.41850000
N	11.16920000	0.47670000	9.21940000
N	10.82040000	3.76390000	8.80690000
S	7.40580000	3.69590000	9.72240000
O	8.23130000	0.61590000	8.08260000
C	9.12270000	1.31550000	12.78850000
C	9.19020000	1.34980000	14.18630000
H	8.62360000	0.64270000	14.78700000
C	9.99610000	2.30300000	14.81000000
H	10.05710000	2.33790000	15.89700000

C	10.71340000	3.20480000	14.02750000
H	11.35000000	3.96760000	14.47180000
C	10.60210000	3.10980000	12.63950000
H	11.14060000	3.79290000	11.98040000
C	8.27170000	0.32100000	12.08030000
C	7.43180000	-0.62690000	12.87630000
H	6.73900000	-1.20890000	12.26150000
H	6.82930000	-0.06460000	13.60070000
H	8.06750000	-1.32690000	13.43530000
C	7.69430000	-0.34650000	8.64580000
C	7.02670000	-1.51190000	7.92290000
H	7.56580000	-2.43140000	8.18110000
H	5.98840000	-1.60910000	8.26070000
C	6.31140000	-2.66180000	5.91110000
H	5.29750000	-2.68990000	6.31890000
H	6.88160000	-3.53600000	6.23600000
H	6.28200000	-2.60960000	4.82020000
C	8.40670000	-1.38170000	5.84710000
H	8.32080000	-1.42090000	4.75860000
H	8.95200000	-2.25120000	6.22430000
H	8.89360000	-0.46070000	6.16720000
C	6.22060000	-0.20650000	5.95740000
H	5.21470000	-0.26960000	6.38080000
H	6.17600000	-0.23610000	4.86600000
H	6.73150000	0.69430000	6.29810000
C	10.94260000	-0.68650000	9.07630000
C	11.29910000	4.71880000	9.34330000
C	6.66040000	3.10600000	11.08720000

Cd2+ ion 6-coordinated environment LH fragment_solv

N	9.83650000	2.19010000	12.03610000
N	8.33360000	0.37130000	10.78690000
N	7.64360000	-0.49550000	10.00530000
H	7.18470000	-1.31180000	10.41440000
N	7.00490000	-1.41520000	6.41850000
O	8.23130000	0.61590000	8.08260000
C	9.12270000	1.31550000	12.78850000
C	9.19020000	1.34980000	14.18630000
H	8.62360000	0.64270000	14.78700000
C	9.99610000	2.30300000	14.81000000
H	10.05710000	2.33790000	15.89700000
C	10.71340000	3.20480000	14.02750000
H	11.35000000	3.96760000	14.47180000
C	10.60210000	3.10980000	12.63950000
H	11.14060000	3.79290000	11.98040000
C	8.27170000	0.32100000	12.08030000
C	7.43180000	-0.62690000	12.87630000
H	6.73900000	-1.20890000	12.26150000
H	6.82930000	-0.06460000	13.60070000

H	8.06750000	-1.32690000	13.43530000
C	7.69430000	-0.34650000	8.64580000
C	7.02670000	-1.51190000	7.92290000
H	7.56580000	-2.43140000	8.18110000
H	5.98840000	-1.60910000	8.26070000
C	6.31140000	-2.66180000	5.91110000
H	5.29750000	-2.68990000	6.31890000
H	6.88160000	-3.53600000	6.23600000
H	6.28200000	-2.60960000	4.82020000
C	8.40670000	-1.38170000	5.84710000
H	8.32080000	-1.42090000	4.75860000
H	8.95200000	-2.25120000	6.22430000
H	8.89360000	-0.46070000	6.16720000
C	6.22060000	-0.20650000	5.95740000
H	5.21470000	-0.26960000	6.38080000
H	6.17600000	-0.23610000	4.86600000
H	6.73150000	0.69430000	6.29810000

Cd2+ ion 6-coordinated environment LH fragment_vacum

N	9.83650000	2.19010000	12.03610000
N	8.33360000	0.37130000	10.78690000
N	7.64360000	-0.49550000	10.00530000
H	7.18470000	-1.31180000	10.41440000
N	7.00490000	-1.41520000	6.41850000
O	8.23130000	0.61590000	8.08260000
C	9.12270000	1.31550000	12.78850000
C	9.19020000	1.34980000	14.18630000
H	8.62360000	0.64270000	14.78700000
C	9.99610000	2.30300000	14.81000000
H	10.05710000	2.33790000	15.89700000
C	10.71340000	3.20480000	14.02750000
H	11.35000000	3.96760000	14.47180000
C	10.60210000	3.10980000	12.63950000
H	11.14060000	3.79290000	11.98040000
C	8.27170000	0.32100000	12.08030000
C	7.43180000	-0.62690000	12.87630000
H	6.73900000	-1.20890000	12.26150000
H	6.82930000	-0.06460000	13.60070000
H	8.06750000	-1.32690000	13.43530000
C	7.69430000	-0.34650000	8.64580000
C	7.02670000	-1.51190000	7.92290000
H	7.56580000	-2.43140000	8.18110000
H	5.98840000	-1.60910000	8.26070000
C	6.31140000	-2.66180000	5.91110000
H	5.29750000	-2.68990000	6.31890000
H	6.88160000	-3.53600000	6.23600000
H	6.28200000	-2.60960000	4.82020000
C	8.40670000	-1.38170000	5.84710000
H	8.32080000	-1.42090000	4.75860000

H	8.95200000	-2.25120000	6.22430000
H	8.89360000	-0.46070000	6.16720000
C	6.22060000	-0.20650000	5.95740000
H	5.21470000	-0.26960000	6.38080000
H	6.17600000	-0.23610000	4.86600000
H	6.73150000	0.69430000	6.29810000

Cd2+ ion 6-coordinated environment LH relaxed_structure

N	9.54231994	2.61404776	12.08460757
N	8.57457593	0.48087871	10.69132832
N	7.91656943	-0.43994473	9.92503733
H	7.21159262	-1.05835767	10.33352512
N	6.76596769	-1.33224235	6.69024825
O	9.11430921	0.07021230	8.02718599
C	8.95062887	1.58783814	12.74139538
C	9.06232019	1.42484414	14.13206207
H	8.58981359	0.58198279	14.63398299
C	9.81603052	2.34153418	14.86590868
H	9.92453144	2.22562002	15.94430047
C	10.42426421	3.40096291	14.19475899
H	11.01618970	4.14735048	14.72397805
C	10.25411467	3.49019860	12.80817913
H	10.70994266	4.31264164	12.25092162
C	8.19063932	0.60069767	11.92736731
C	7.07625659	-0.19660099	12.54912623
H	6.18868559	-0.18710226	11.89938336
H	6.77282477	0.21567730	13.51470485
H	7.37528407	-1.24528477	12.69987931
C	8.26969311	-0.61256341	8.61532364
C	7.52214399	-1.76197555	7.93900019
H	8.24767669	-2.52440567	7.63536464
H	6.78621137	-2.22037535	8.60690919
C	5.87672131	-2.48359446	6.28090213
H	5.15131403	-2.66748779	7.07795578
H	6.50278827	-3.36510903	6.11898448
H	5.36511433	-2.20457358	5.35605323
C	7.70998180	-1.02243871	5.54985911
H	7.10457604	-0.73450067	4.68636990
H	8.28665800	-1.92480763	5.32878685
H	8.37173542	-0.21103007	5.85559867
C	5.91000762	-0.12598546	6.98857774
H	5.26820346	-0.35722851	7.84342602
H	5.30327045	0.08821385	6.10535287
H	6.56198045	0.72262646	7.21059829

Cd2+ ion 6-coordinated environment SCN1 fragment_solv

S	9.95250000	-0.99730000	0.00000000

N 10.49010000 1.77460000 0.00000000
C 10.26860000 0.60170000 0.00000000

Cd2+ ion 6-coordinated environment SCN1 fragment_vacum

S 9.95250000 -0.99730000 0.00000000
N 10.49010000 1.77460000 0.00000000
C 10.26860000 0.60170000 0.00000000

Cd2+ ion 6-coordinated environment SCN1 relaxed_structure

S 0.00000000 0.00000000 -14.07557240
N 0.00000000 0.00000000 -11.23194374
C 0.00000000 0.00000000 -12.42114366

Cd2+ ion 6-coordinated environment SCN2 fragment_solv

C -1.26360000 12.64850000 0.00000000
N -1.36880000 11.45790000 0.00000000
S -1.09510000 14.26600000 0.00000000

Cd2+ ion 6-coordinated environment SCN2 fragment_vacum

C -1.26360000 12.64850000 0.00000000
N -1.36880000 11.45790000 0.00000000
S -1.09510000 14.26600000 0.00000000

Cd2+ ion 6-coordinated environment SCN2 relaxed_structure

S 0.00000000 0.00000000 -14.07557240
N 0.00000000 0.00000000 -11.23194374
C 0.00000000 0.00000000 -12.42114366

Cd2+ ion 6-coordinated environment SCN3 fragment_solv

C -5.03280000 -1.34130000 0.00000000
S -3.60330000 -0.49120000 0.00000000
N -6.05200000 -1.94000000 0.00000000

Cd2+ ion 6-coordinated environment SCN3 fragment_vacum

C -5.03280000 -1.34130000 0.00000000
S -3.60330000 -0.49120000 0.00000000
N -6.05200000 -1.94000000 0.00000000

Cd2+ ion 6-coordinated environment SCN3 relaxed_structure

S	0.00000000	0.00000000	-14.07557240
N	0.00000000	0.00000000	-11.23194374
C	0.00000000	0.00000000	-12.42114366

Cd2+ ion 6-coordinated environment dimer relaxed_structure

Cd	8.86875245	3.33877029	10.26527713
S	12.29658803	0.82111164	9.74161391
S	12.45719068	5.44722359	12.04246389
N	7.04161877	6.75748869	11.55986323
N	9.28193457	2.41994449	12.39696978
N	8.53373245	0.89665698	10.33376325
N	8.35347721	0.24331411	9.15595387
H	8.55476618	-0.75566934	9.08061914
N	9.12240509	0.27700206	5.93839798
N	10.49548035	2.76504108	8.77856053
N	9.97085932	5.25703359	10.73516483
S	6.44205724	4.24064020	10.38450765
O	7.57145167	2.12455934	8.09055814
C	9.24672312	1.07346145	12.56380826
C	9.39813925	0.50003704	13.83110045
H	9.35078741	-0.57832935	13.96129869
C	9.58506847	1.32976051	14.93769951
H	9.69574853	0.89648764	15.93083767
C	9.62459271	2.70972354	14.75459571
H	9.77443613	3.39206268	15.58920296
C	9.46710957	3.21175241	13.46141987
H	9.49380391	4.28211711	13.25516298
C	9.02048503	0.24890064	11.35087262
C	9.34597666	-1.21190268	11.31150289
H	8.43764920	-1.81035029	11.15027793
H	9.82968012	-1.55661827	12.22679855
H	10.04512564	-1.40790782	10.48412156
C	7.89938334	0.93315698	8.06400509
C	7.85670890	0.12324379	6.77578764
H	7.72147183	-0.94810148	6.95527450
H	7.02540425	0.50071386	6.17490369
C	8.87420562	-0.42066522	4.61985285
H	8.04157961	0.07544798	4.11505215
H	8.63567421	-1.46836209	4.82028508
H	9.78509799	-0.34462457	4.02102582
C	10.29781519	-0.37791564	6.62190924
H	11.16285330	-0.29664830	5.95970847
H	10.05715913	-1.42966600	6.79902487
H	10.50517805	0.13858623	7.56223022
C	9.43564627	1.73259087	5.68127128

H	8.55362739	2.20034387	5.23656078
H	10.27985861	1.77050325	4.98848354
H	9.69754086	2.21318224	6.63001518
C	11.27782182	1.96084777	9.19506907
C	11.03923061	5.32206788	11.26805585
C	6.79077341	5.69857220	11.10017384
Cd	11.83649329	10.01480696	9.22150147
S	13.29866929	5.40786392	8.11655821
S	14.46921201	13.73616394	9.22465166
N	9.57563165	11.47765237	12.50822507
N	12.71174028	9.95093474	11.41170948
N	10.50199188	8.64865387	10.67142914
N	9.41572328	8.04367780	10.12902193
H	8.83723094	7.38976289	10.68152372
N	8.60734418	6.41981010	7.05482386
N	12.90944937	8.18799555	8.38884742
N	13.16759103	11.47722321	8.14575927
S	10.03709590	12.00302801	9.75129362
O	9.84662279	8.92361225	8.04400642
C	12.03276566	9.24347767	12.34757003
C	12.52521218	9.12111337	13.65236607
H	11.98378289	8.54258241	14.39661736
C	13.72721661	9.74324960	13.99158986
H	14.12332589	9.65026575	15.00205223
C	14.40719720	10.48235940	13.02617317
H	15.34389173	10.99018435	13.24892981
C	13.85879653	10.55802540	11.74463870
H	14.34722872	11.12613422	10.95145651
C	10.75549953	8.59510801	11.94155614
C	9.90070311	7.95847391	12.98929534
H	9.70080482	8.68797915	13.78468579
H	10.43437414	7.10595825	13.43232888
H	8.94237000	7.60060245	12.60323567
C	9.20694963	8.15886117	8.78940761
C	8.12684965	7.22834213	8.25333201
H	7.82092963	6.50611309	9.01525252
H	7.25285362	7.80502786	7.93362269
C	7.65342810	5.26594176	6.87110251
H	6.63705006	5.65776470	6.77979933
H	7.72560629	4.59905618	7.73458272
H	7.93659244	4.73562678	5.95832309
C	9.99787911	5.87674354	7.29990489
H	10.22651490	5.15815999	6.50966122
H	10.03321968	5.38935436	8.27938975
H	10.70304060	6.70815455	7.26614232
C	8.60128986	7.25948527	5.79740505
H	7.57309423	7.57399807	5.59928003
H	8.97518640	6.63783959	4.97979498
H	9.24696495	8.12386985	5.95736316
C	13.07456008	7.01288286	8.29187675
C	13.71331512	12.43486893	8.60865918

C 9.76965872 11.69434675 11.36194830

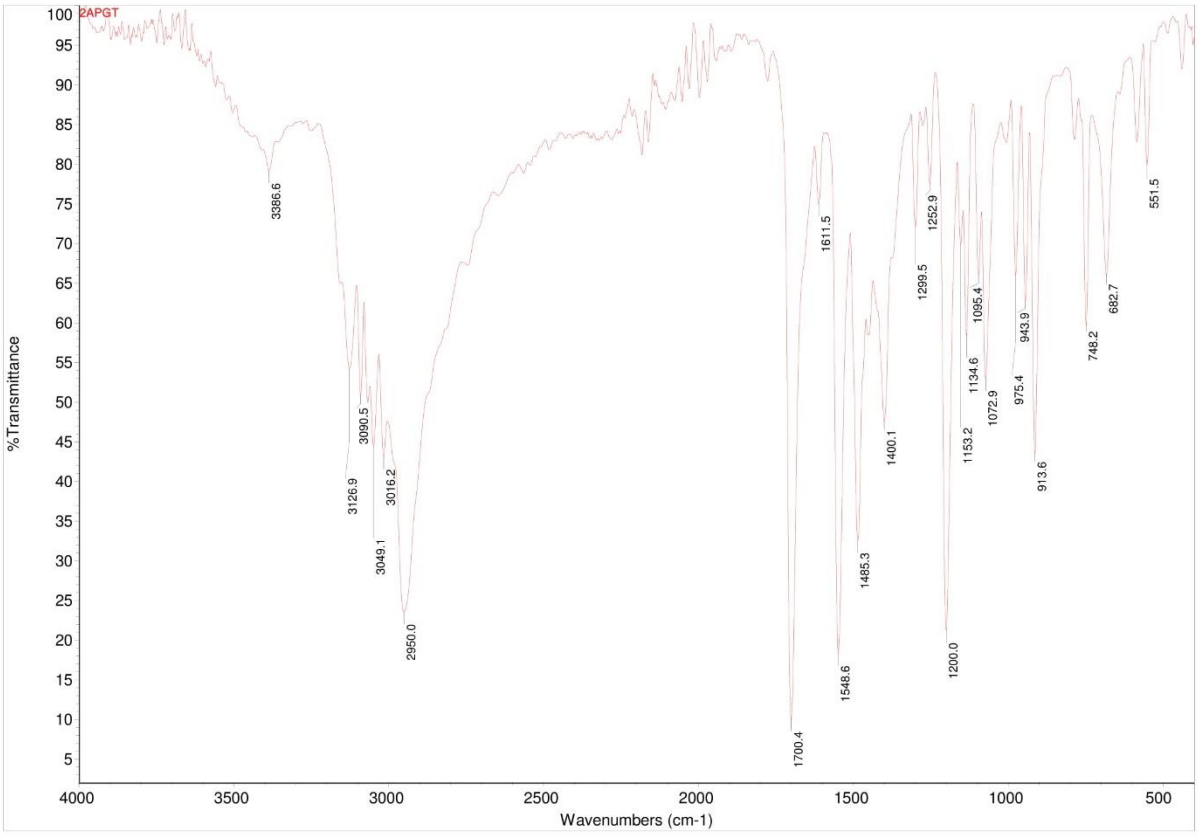

Figure S2. IR spectrum of **HL**Cl

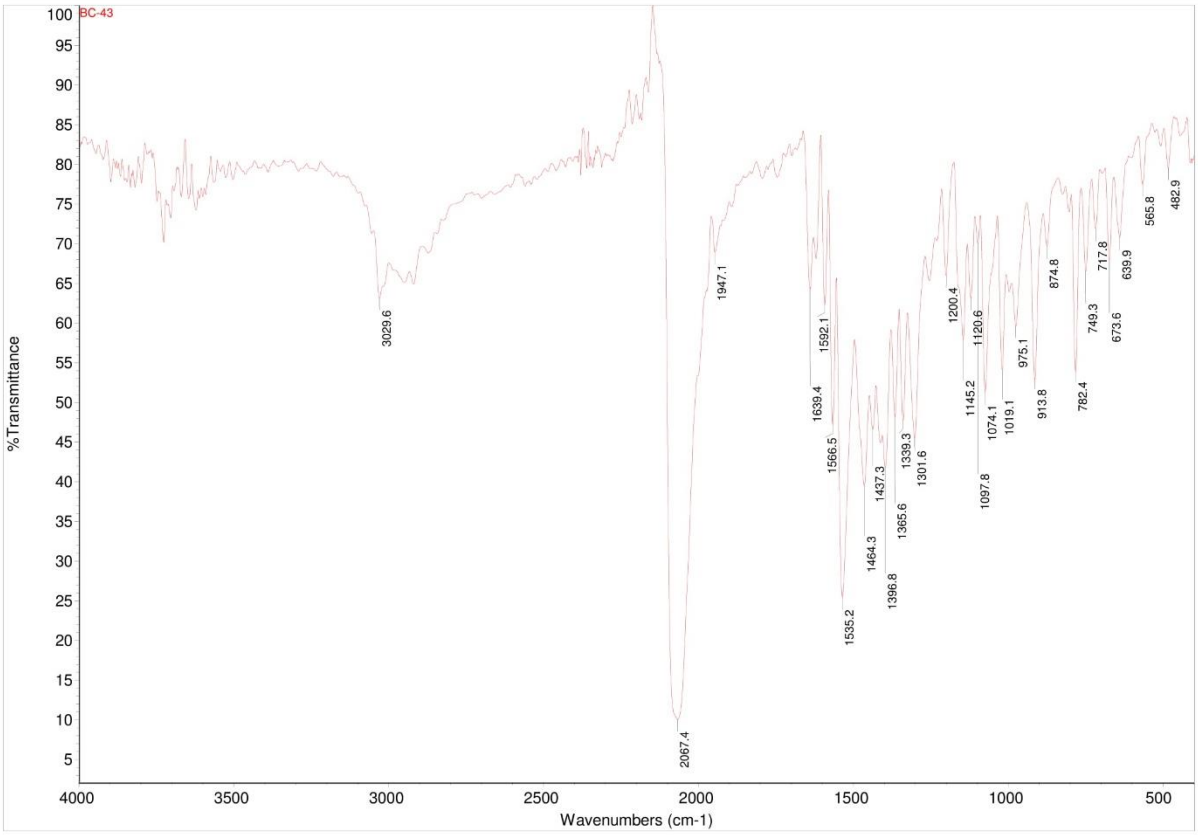

Figure S3. IR spectrum of **1**

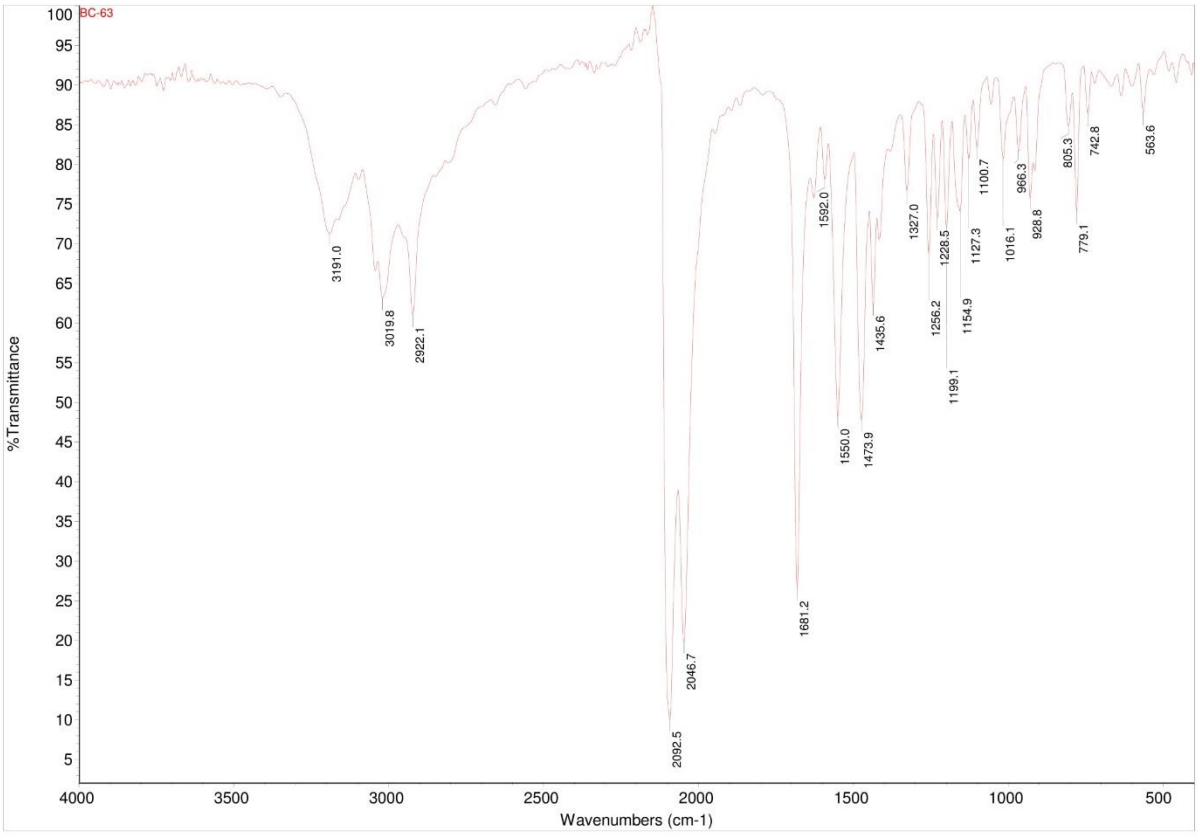

Figure S4. IR spectrum of **2**

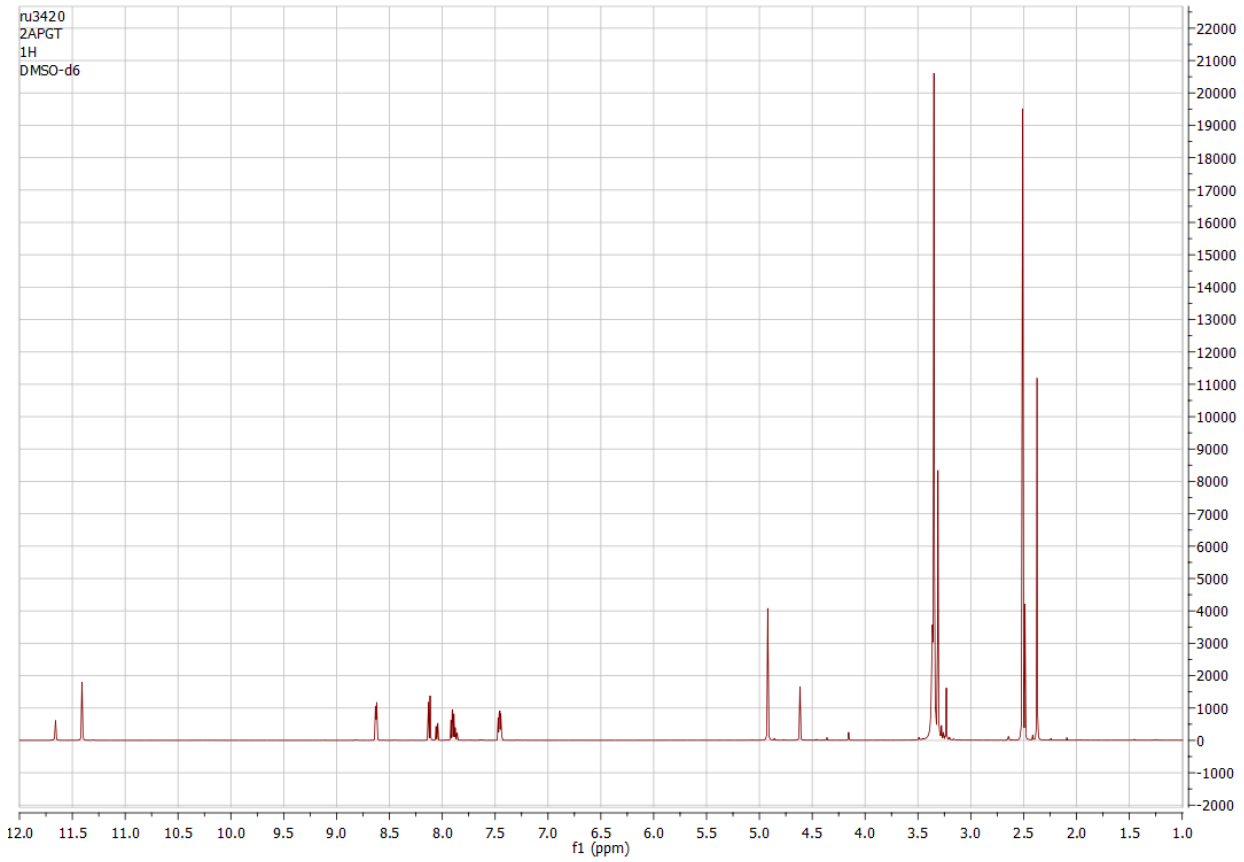

Figure S5. ^{1}H NMR spectrum of **HL**Cl

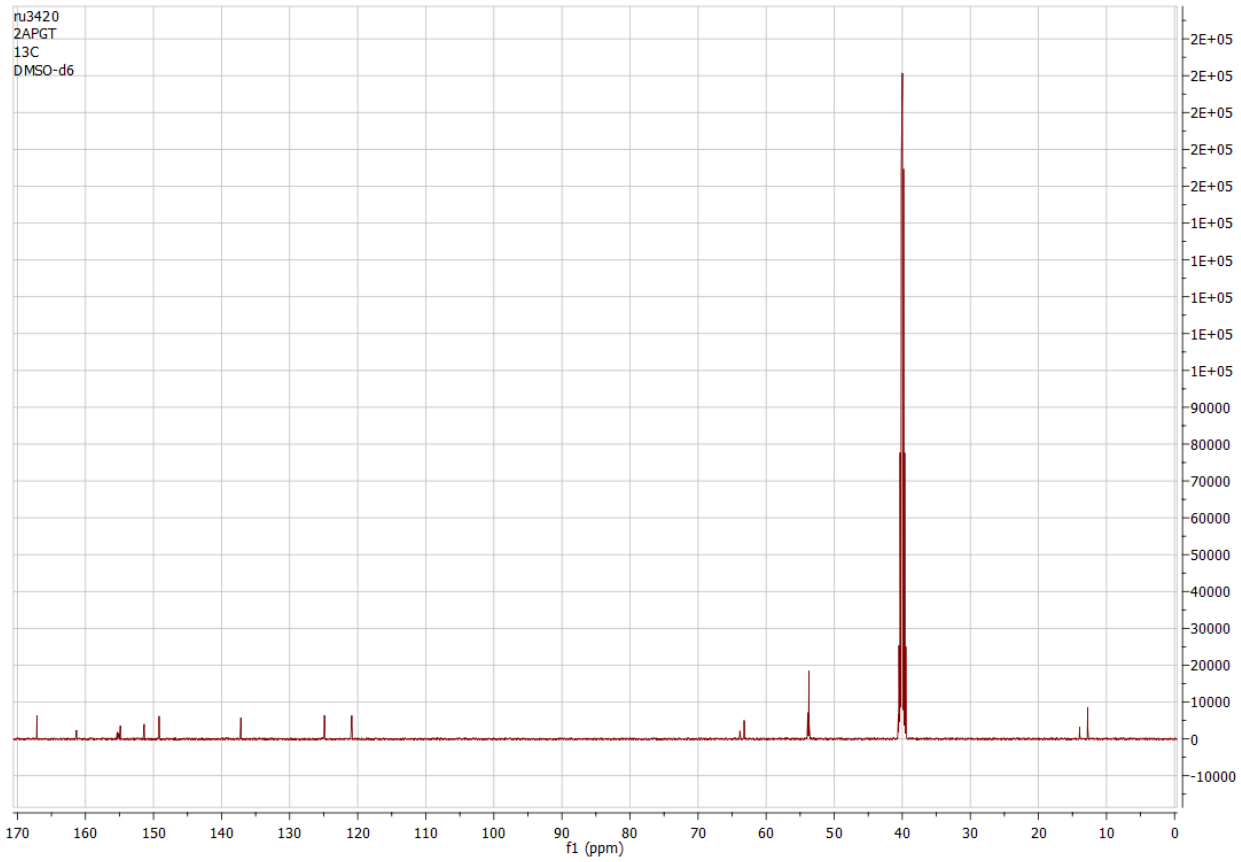

Figure S6. ^{13}C NMR spectrum of **HL**Cl

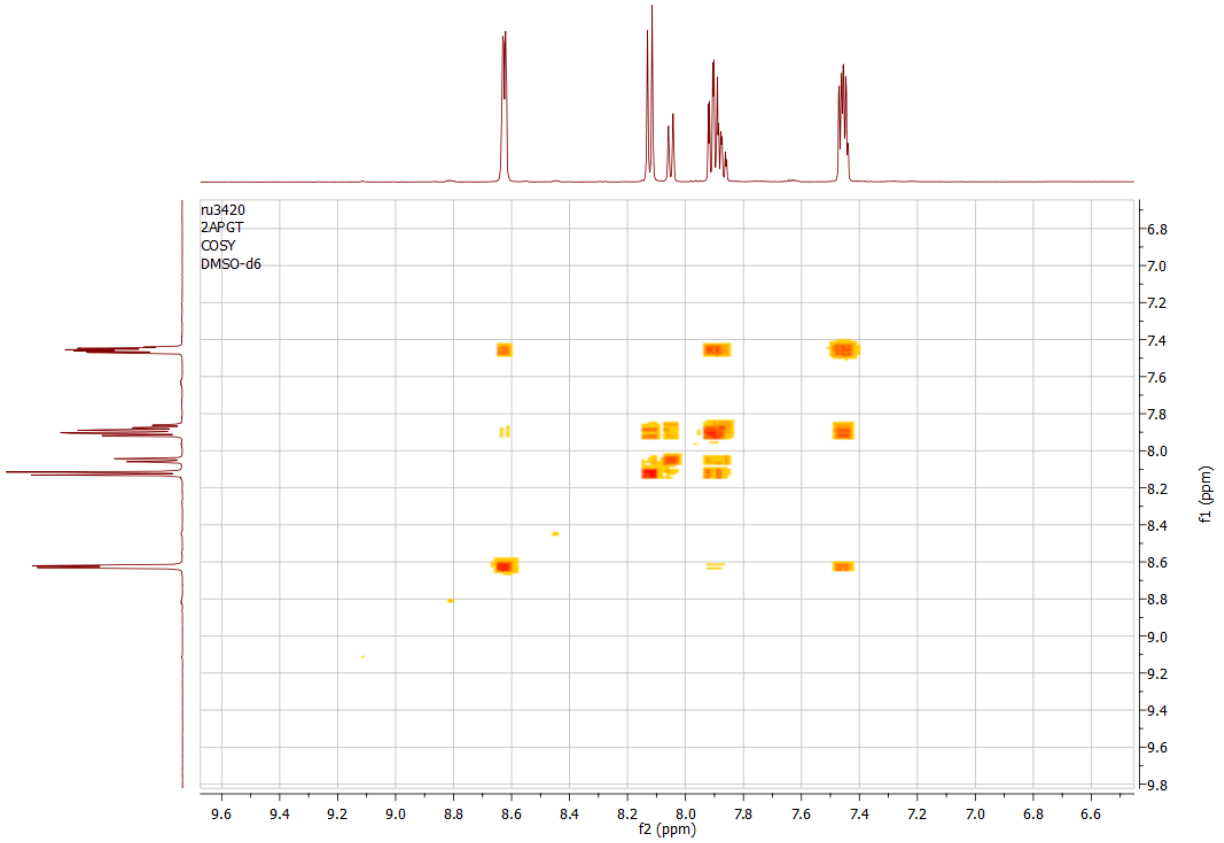

Figure S7. COSY spectrum of **HL**Cl

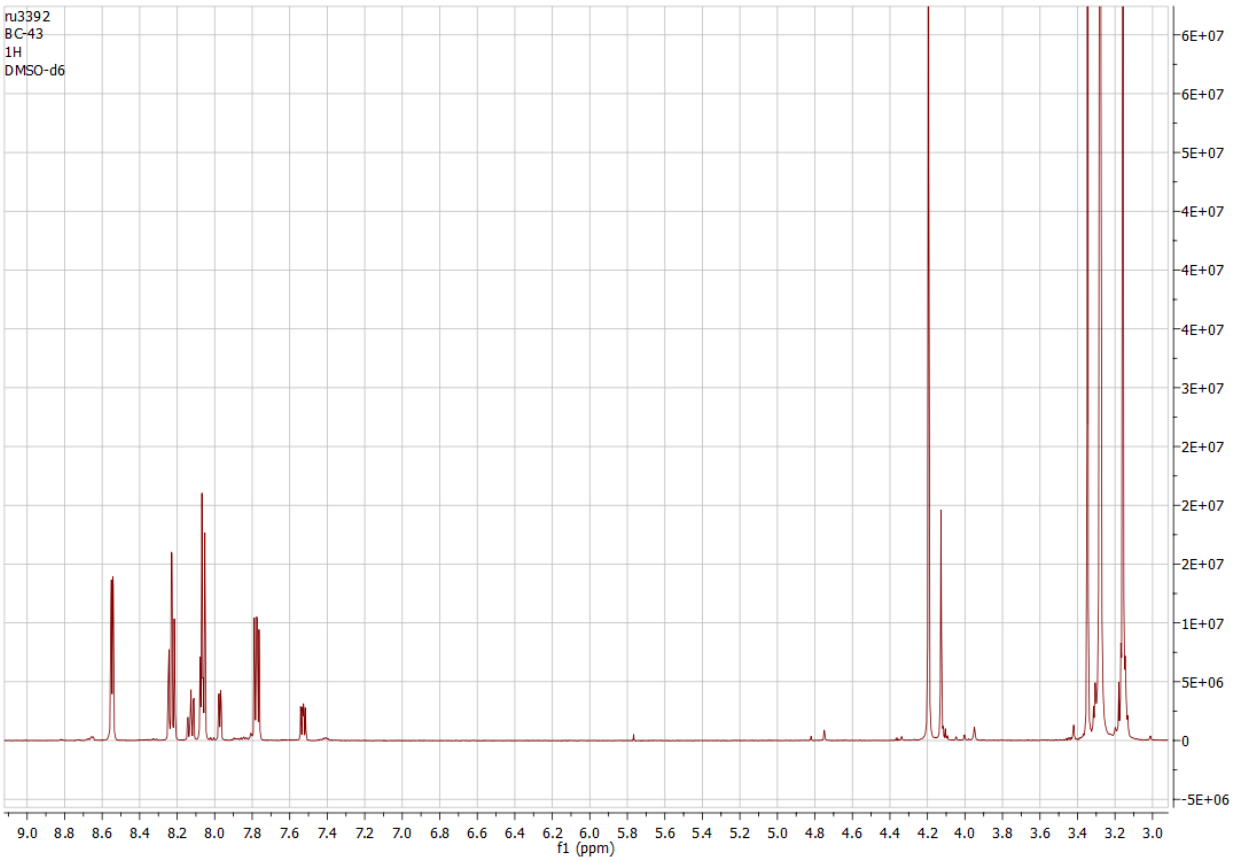

Figure S8. ^{1}H NMR spectrum of **1**

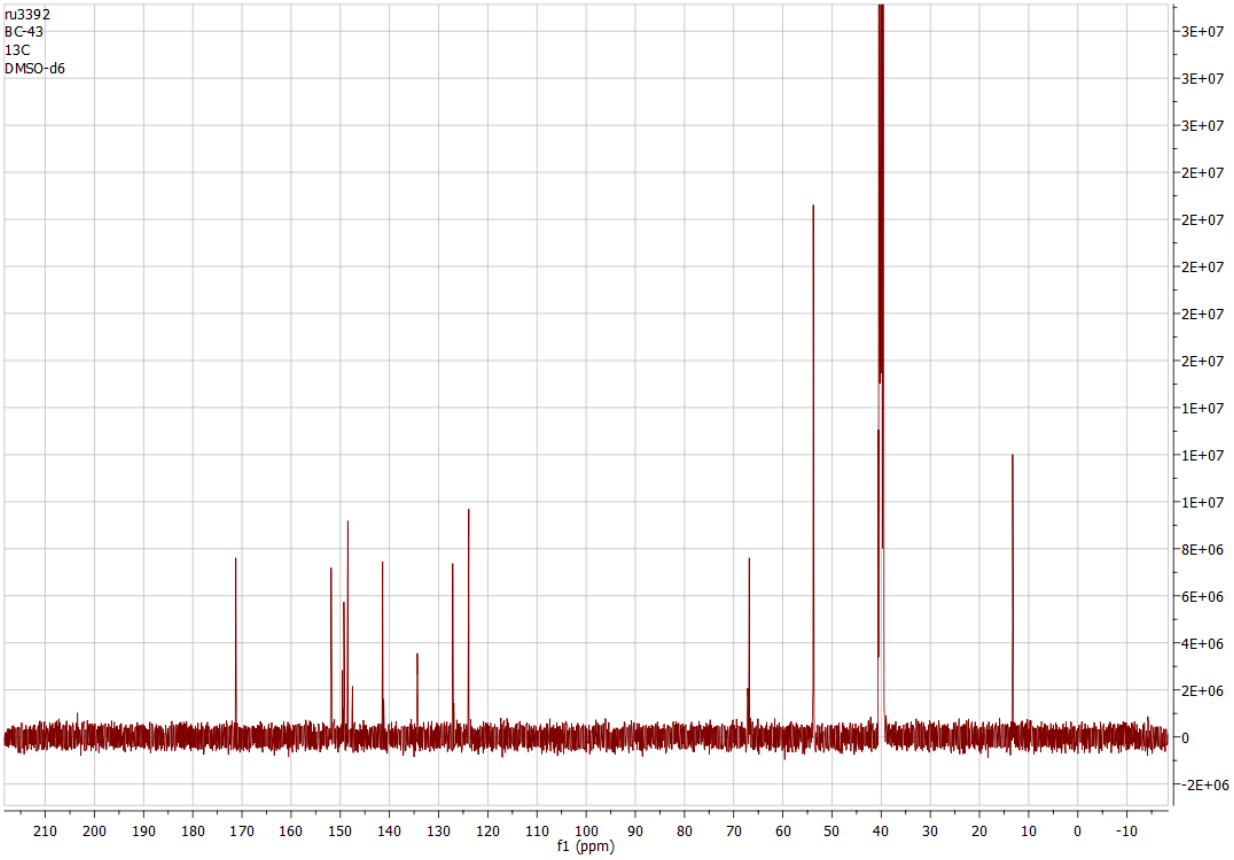

Figure S9. ^{13}C NMR spectrum of **1**

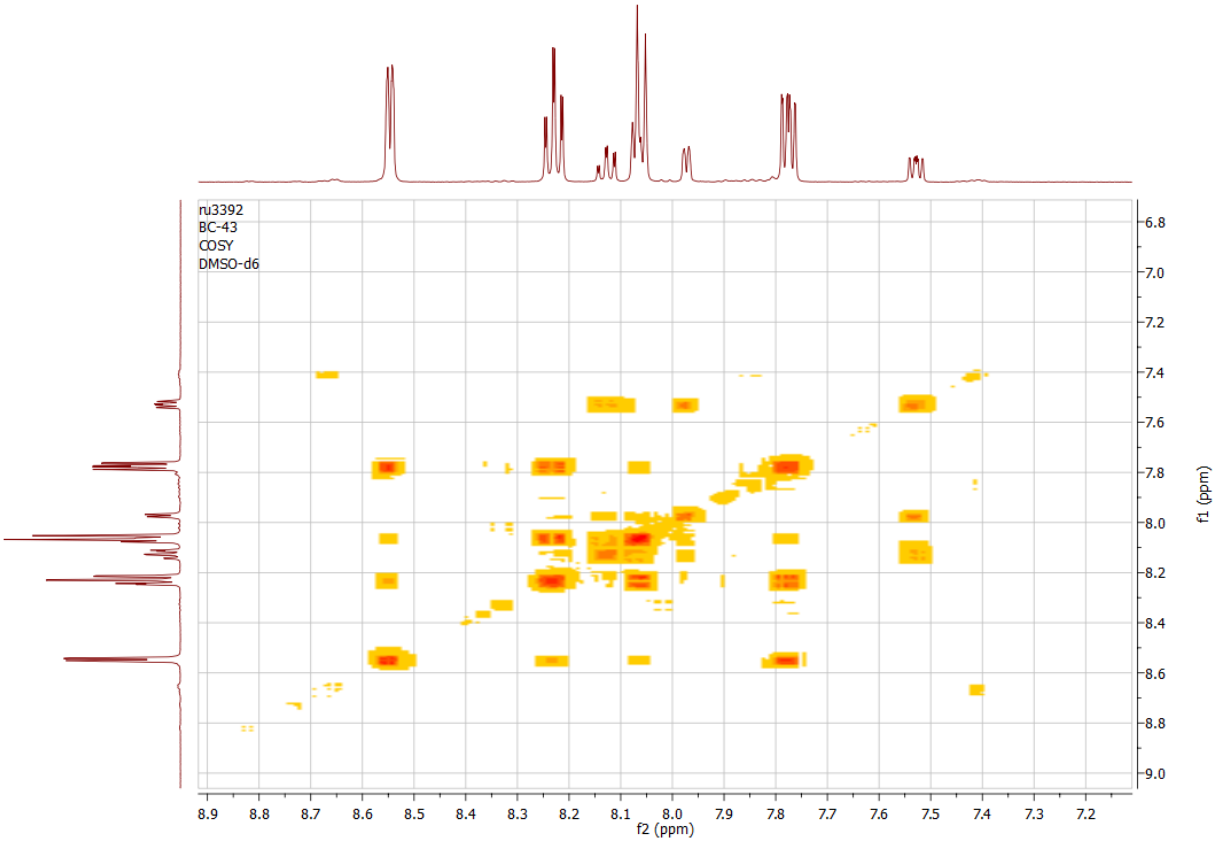

Figure S10. COSY spectrum of **1**

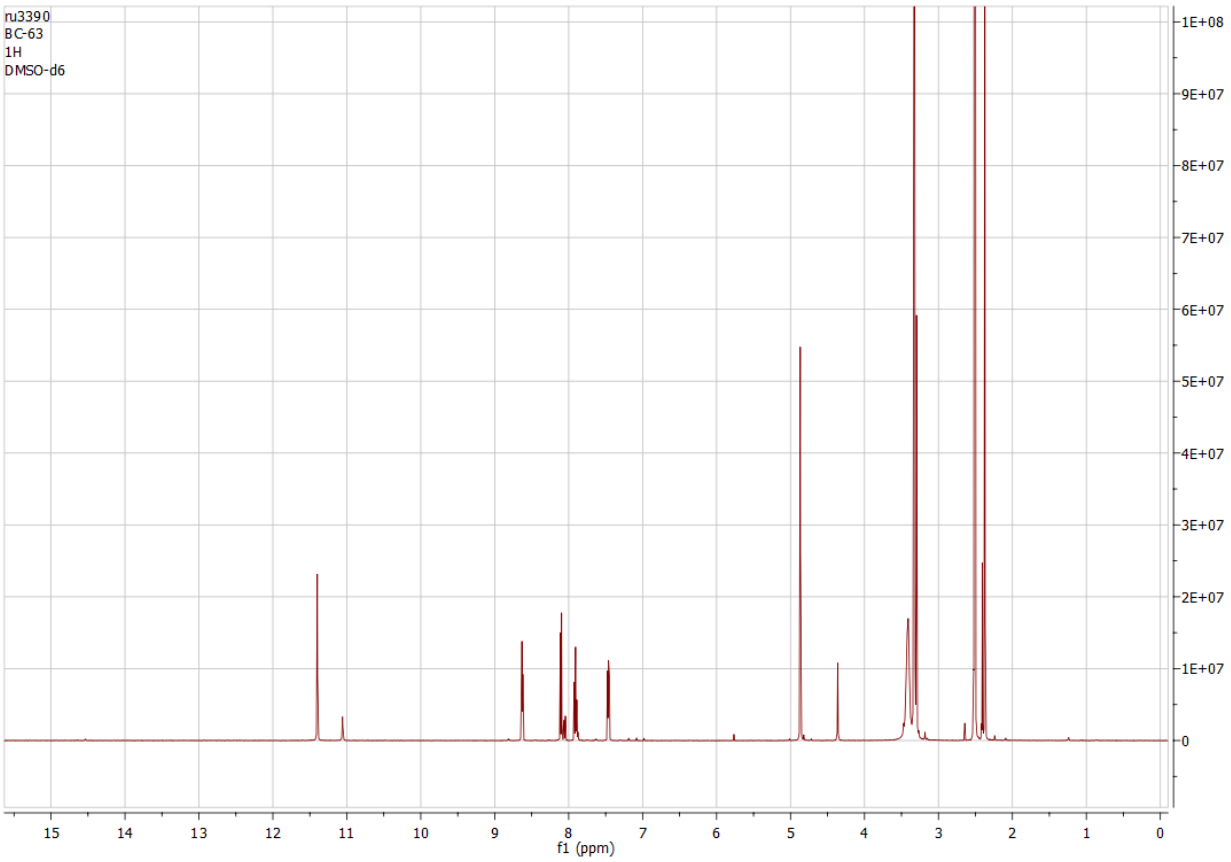

Figure S11. ^{1}H NMR spectrum of **2**

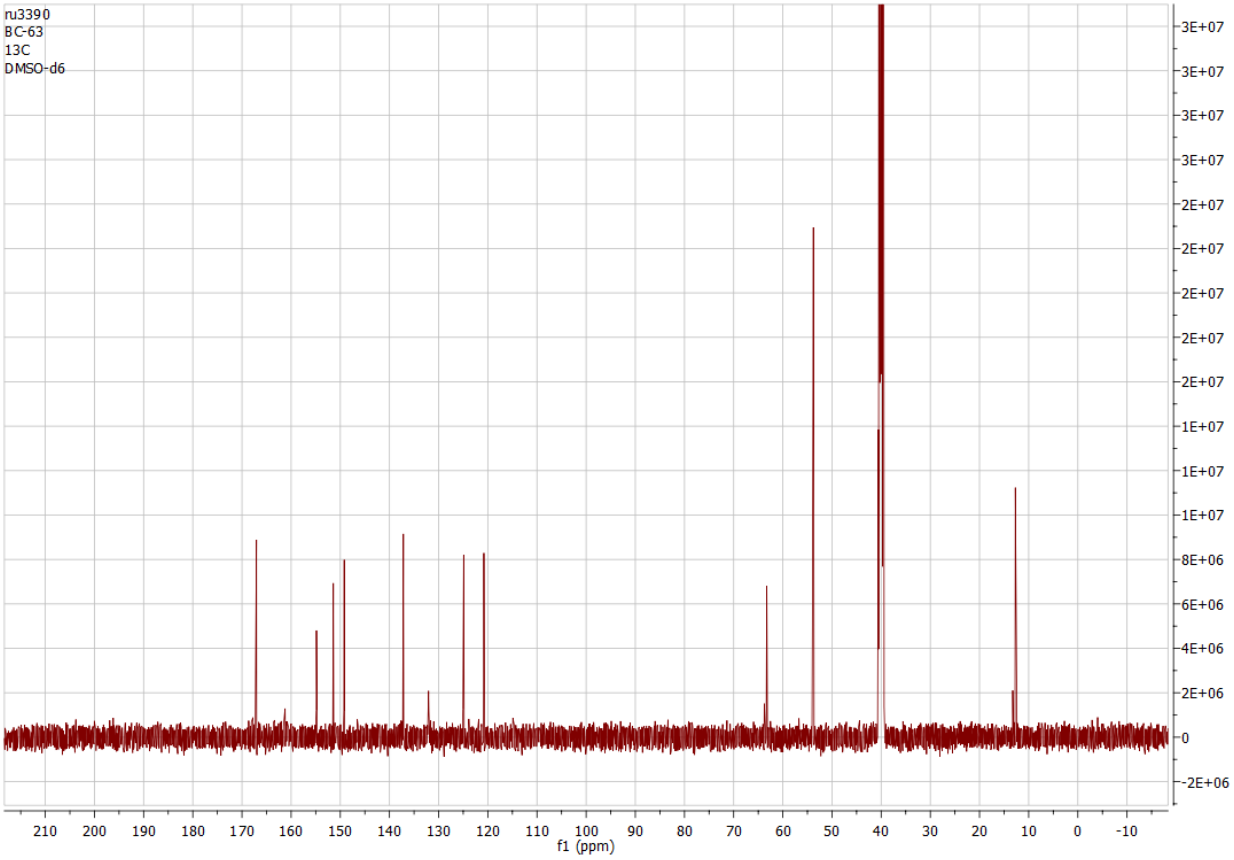

Figure S12. ^{13}C NMR spectrum of **2**

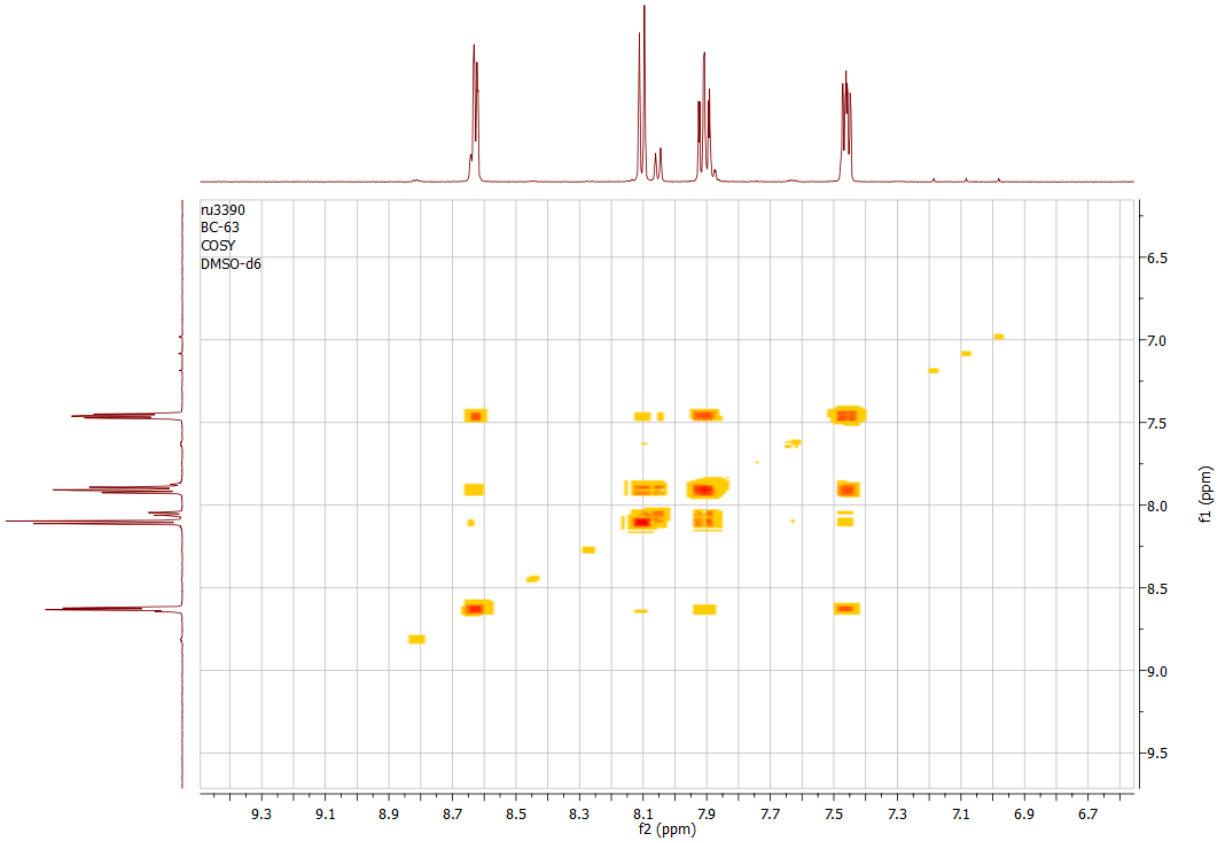

Figure S13. COSY spectrum of **2**