

https://dspace.org/

The solid state structures of metallo-beta-amino alcohol complexes

Reisinger, Sandra Ann

2009-05-25T11:50:06Z
http://hdl.handle.net/10539/6979

Downloaded from a DSpace repository. https://dspace.org/

Appendix A – MM Data

General Methodology to Calculate Charges

Before starting MM calculations, the atoms in the molecule had to be assigned charges. In the Setup menu Semi-empirical was selected. Under the Options tab, the total charge was set to 0, the charge of the free ligand. The spin multiplicity was set to zero. The Restricted Hartree-Fock method (RHF) was selected for spin pairing. The lowest state was selected and the convergence limit was set to 0.0001 kcal mol^{-1} or an iteration limit of 500 was selected in the SCF Controls section. The convergence was accelerated. Once all of these parameters had been set, a single point calculation was performed by selecting Single Point from the Compute menu. The resultant molecule was saved.

To view to charges on each molecule, Labels was selected from the Display menu. In the dialog box, Charges was selected for Atom.

General Methodology to Perform MM Calculations

In order for the MM calculations to be performed, one had to set the MM settings in HyperChem. This was done by selecting the Setup Menu and selecting the AMBER option. In the adjoining Options tab, the dielectric constant, *K*, was set to 76 (the dielectric constant of water), and both the Electrostatic and van der Waals 1-4 scale factors were set to 0.5. These two scaling factors set the scaling of the nonbonded interactions of the atoms that are separated by three atoms. This is the default setting for AMBER. This ensures that the energy is not dominated by van der Waals and electrostatic terms but rather by bond lengths and angles. Under the Cutoffs tab, None was selected. The tabs were then closed. Form the Setup menu, Select Parameter Set was selected. In the window that opened WitsGAFF was selected and the window closed. From the Setup menu, Compile Parameter Set was then selected.

Once all of these parameters had been set, the atom types for each of the atoms in the molecule were selected according to the specifications given by Kollman and his

colleagues.[6] This was done by selecting Atom Type in the Build menu. Once all atom types had been assigned, one could view the types by selecting Labels from the Display menu. In the dialog box, Type was selected for Atom.

Once the desired dielectric constant had been set, the molecule was submitted for a MM geometry optimisation. Under the Compute menu Geometry Optimization was selected. The algorithm used was the Polak-Ribiere (Conjugate gradient). The system was set to be in vacuo, and the termination conditions were set to a root-mean-square, RMS, gradient of less than 0.001 kcal/(Å mol) or at least 5000 cycles. This large number of cycles ensured that the first termination condition was reached first. The window was then closed by selecting OK. This started the calculation.

General Methodology to Perform Simulated Annealing

This method added energy to the system in the form of heat so that the different energy barriers between the different structural isomers could be overcome. This was done by setting the parameters for the simulated annealing in the molecular dynamics menu. This was to be found under Compute. The simulated annealing process was built up in the following manner: the simulation started at a temperature of 0 K and was heated to 800 K over 10 ps. The molecule was then kept at a constant temperature of 800 K for different run times of between 5 and 100 ps, in 5 ps intervals. The molecule was then cooled to 0 K over a period of 20 ps. The step size was set as 1 fs or 0.001 ps. The resulting structures were then saved and MM calculations performed to find the total energy of the molecule.

Cy_2-en Data

Table A.1: Cy_2-en Data After Simulated Annealing

		C-C	C-N	C-O	C-C-C	C-C-N	C-C-O	C-N-C
XRD		Cy2-en_002						
	Average	1.518	1.475	1.427	111.1	110.6	109.8	113.7
	Std Dev	0.006	0.002	0.000	0.7	1.4	0.9	0.0
MM w ZINDO1		Cy2-en_004						

e = 76								
	Average	1.545	1.480	1.432	111.2	110.2	109.3	114.5
	Std Dev	0.005	0.004	0.000	0.4	1.2	0.4	0.0
Annealing	Cy2-en_010							
run time = 10 ps								
	Average	1.546	1.481	1.432	111.2	110.3	109.4	115.5
	Std Dev	0.006	0.003	0.002	0.6	2.1	1.5	1.4
Annealing	Cy2-en_011							
run time = 20 ps								
	Average	1.548	1.484	1.431	111.7	111.2	109.1	117.6
	Std Dev	0.007	0.005	0.000	0.9	2.8	1.7	1.3
Annealing	Cy2-en_012							
run time = 30 ps								
	Average	1.547	1.479	1.432	111.6	110.2	109.1	114.7
	Std Dev	0.006	0.003	0.001	0.8	1.3	0.4	0.2
Annealing	Cy2-en_013							
run time = 40 ps								
	Average	1.546	1.480	1.432	111.4	110.2	109.4	114.8
	Std Dev	0.005	0.004	0.000	0.5	1.4	0.8	0.1
Annealing	Cy2-en_014							
run time = 50 ps								
	Average	1.547	1.480	1.432	111.6	110.5	109.5	114.5
	Std Dev	0.005	0.002	0.000	1.0	0.8	0.5	0.5
Annealing	Cy2-en_015							
run time = 60 ps								
	Average	1.545	1.482	1.432	111.2	110.6	109.3	115.7
	Std Dev	0.004	0.004	0.000	0.4	1.5	0.4	1.7
Annealing	Cy2-en_016							
run time = 70 ps								
	Average	1.546	1.480	1.431	111.2	110.2	109.5	115.7
	Std Dev	0.006	0.003	0.002	0.5	2.0	1.5	1.2
Annealing	Cy2-en_017							
run time = 80 ps								
	Average	1.548	1.482	1.432	111.8	110.7	109.4	115.6
	Std Dev	0.005	0.003	0.000	0.8	1.5	0.4	1.1
Annealing	Cy2-en_018							
run time = 90 ps								
	Average	1.545	1.482	1.432	111.1	111.0	109.4	115.7
	Std Dev	0.004	0.003	0.001	0.3	1.2	0.8	1.1
Annealing	Cy2-en_019							

run time = 100 ps							
Average	1.545	1.482	1.432	111.2	110.7	109.2	115.4
Std Dev	0.004	0.003	0.000	0.3	1.6	0.3	1.6
Annealing	Cy2-en_020						
run time = 5 ps							
Average	1.545	1.480	1.432	111.2	110.0	109.4	115.5
Std Dev	0.006	0.004	0.002	0.6	2.1	1.5	1.4
Annealing	Cy2-en_021						
run time = 15 ps							
Average	1.546	1.484	1.432	111.1	111.3	109.6	116.6
Std Dev	0.004	0.004	0.001	0.4	1.6	0.5	0.3
Annealing	Cy2-en_022						
run time = 25 ps							
Average	1.545	1.482	1.432	111.1	111.0	109.4	115.8
Std Dev	0.005	0.003	0.000	0.3	1.3	0.7	1.2
Annealing	Cy2-en_023						
run time = 35 ps							
Average	1.546	1.482	1.432	111.3	110.9	109.6	115.7
Std Dev	0.005	0.005	0.001	0.5	1.8	0.3	1.3
Annealing	Cy2-en_024						
run time = 45 ps							
Average	1.547	1.482	1.432	111.3	111.1	109.6	115.7
Std Dev	0.005	0.003	0.000	0.5	1.7	0.7	1.3
Annealing	Cy2-en_025						
run time = 55 ps							
Average	1.545	1.482	1.432	111.1	110.8	109.6	115.5
Std Dev	0.005	0.004	0.000	0.4	1.5	0.6	1.4
Annealing	Cy2-en_026						
run time = 65 ps							
Average	1.546	1.480	1.432	111.4	110.4	109.4	114.9
Std Dev	0.005	0.002	0.000	0.5	1.2	0.3	0.1
Annealing	Cy2-en_027						
run time = 75 ps							
Average	1.547	1.480	1.432	111.6	110.4	109.7	115.2
Std Dev	0.005	0.003	0.000	0.5	1.6	0.2	0.0
Annealing	Cy2-en_028						
run time = 85 ps							
Average	1.546	1.481	1.432	111.4	110.4	109.4	114.9
Std Dev	0.005	0.002	0.000	0.5	1.3	0.4	0.2
Annealing	Cy2-en_029						

run time = 95 ps							
Average	1.548	1.483	1.432	111.7	110.8	109.2	116.6
Std Dev	0.007	0.005	0.002	0.9	2.9	1.6	2.5
Comparisons	002 - 004						
Average	0.027	0.005	0.004	0.0	0.4	0.5	0.8
Std Dev	0.001	0.002	0.000	0.3	0.2	0.4	0.0
Comparisons	002 - 010						
Average	0.028	0.006	0.004	0.1	0.3	0.4	1.8
Std Dev	0.000	0.001	0.002	0.2	0.7	0.6	1.4
Comparisons	002 - 011						
Average	0.030	0.009	0.004	0.5	0.6	0.8	3.9
Std Dev	0.001	0.003	0.000	0.2	1.4	0.9	1.3
Comparisons	002 - 012						
Average	0.029	0.005	0.005	0.5	0.4	0.7	1.0
Std Dev	0.001	0.002	0.000	0.1	0.1	0.5	0.1
Comparisons	002 - 013						
Average	0.028	0.005	0.005	0.3	0.3	0.4	1.0
Std Dev	0.000	0.002	0.000	0.2	0.1	0.1	0.1
Comparisons	002 - 014						
Average	0.029	0.005	0.005	0.5	0.1	0.3	0.8
Std Dev	0.000	0.001	0.000	0.2	0.7	0.3	0.5
Comparisons	002 - 015						
Average	0.027	0.007	0.004	0.0	0.0	0.5	2.0
Std Dev	0.001	0.002	0.000	0.3	0.1	0.4	1.7
Comparisons	002 - 016						
Average	0.028	0.006	0.004	0.1	0.3	0.3	2.0
Std Dev	0.000	0.001	0.002	0.2	0.6	0.6	1.1
Comparisons	002 - 017						
Average	0.030	0.007	0.005	0.6	0.1	0.4	1.9
Std Dev	0.000	0.002	0.000	0.1	0.1	0.5	1.1
Comparisons	002 - 018						
Average	0.028	0.007	0.004	0.1	0.4	0.4	2.0
Std Dev	0.001	0.002	0.000	0.4	0.2	0.1	1.1
Comparisons	002 - 019						
Average	0.027	0.007	0.005	0.1	0.2	0.6	1.7
Std Dev	0.002	0.002	0.000	0.4	0.1	0.5	1.6
Comparisons	002 - 020						
Average	0.027	0.005	0.004	0.1	0.6	0.4	1.8

Std Dev	0.000	0.002	0.002	0.2	0.7	0.6	1.4
Comparisons	002 - 021						
Average	0.028	0.009	0.005	0.0	0.7	0.2	2.9
Std Dev	0.002	0.002	0.001	0.3	0.1	0.3	0.3
Comparisons	002 - 022						
Average	0.028	0.007	0.004	0.0	0.4	0.4	2.0
Std Dev	0.001	0.002	0.000	0.4	0.1	0.1	1.2
Comparisons	002 - 023						
Average	0.029	0.007	0.004	0.2	0.3	0.2	2.0
Std Dev	0.001	0.003	0.001	0.2	0.4	0.6	1.2
Comparisons	002 - 024						
Average	0.029	0.007	0.005	0.2	0.5	0.2	2.0
Std Dev	0.001	0.002	0.000	0.2	0.3	0.2	1.2
Comparisons	002 - 025						
Average	0.028	0.007	0.005	0.0	0.2	0.2	1.8
Std Dev	0.001	0.003	0.000	0.4	0.1	0.3	1.3
Comparisons	002 - 026						
Average	0.028	0.005	0.005	0.3	0.2	0.4	1.2
Std Dev	0.001	0.001	0.000	0.2	0.3	0.5	0.0
Comparisons	002 - 027						
Average	0.029	0.005	0.005	0.5	0.2	0.1	1.5
Std Dev	0.001	0.001	0.000	0.2	0.2	0.6	0.0
Comparisons	002 - 028						
Average	0.028	0.006	0.005	0.3	0.2	0.4	1.2
Std Dev	0.001	0.001	0.000	0.2	0.1	0.5	0.2
Comparisons	002 - 029						
Average	0.030	0.008	0.005	0.6	0.2	0.6	2.9
Std Dev	0.001	0.003	0.002	0.2	1.4	0.8	2.5

Cy_2-Otn Data

Table A.2: Charges on Cy_2-Otn Calculated by Semi-empirical Methods Using PM3 and ZINDO/1

Atom	PM3 charge	ZINDO/1 charge
Secondary amine nitrogen, NH	-0.019	-0.324
Secondary amine nitrogen, NH	-0.008	-0.319
Alcohol group on ring, OH	-0.305	-0.398
Alcohol group on ring, OH	-0.309	-0.403
Alcohol group on propylene bridge, OH	-0.313	-0.397
Carbon on propylene bridge bonded to amine, CH_2	-0.122	-0.008

Carbon on propylene bridge bonded to amine, CH_2	-0.096	0.004
Carbon on ring bonded to amine, CH	-0.109	0.076
Carbon on ring bonded to amine, CH	-0.106	0.074
Carbon on ring bonded to alcohol, CH	0.079	0.152
Carbon on ring bonded to alcohol, CH	0.073	0.145
Carbon on propylene bridge boned to alcohol, OH	0.075	0.144

Table A.3: Energies of Cy_2-Otn after Simulated Annealing Runs with Various Run Times Compared to the Energy of the XRD Structure

Run Time	Energy [kcal/mol]
XRD structure	19.563
5 ps	19.257
10 ps	25.740
15 ps	18.620
20 ps	19.735
25 ps	18.951
30 ps	18.763
35 ps	20.588
40 ps	20.141
45 ps	22.103
50 ps	20.107
55 ps	18.592
60 ps	30.107
65 ps	18.001
70 ps	18.816
75 ps	18.319
80 ps	24.677
85 ps	18.463
90 ps	18.213
95 ps	24.722
100 ps	20.332

Table A.4: Cy_2-Otn Data After Simulated Annealing

	C-C	C-N	C-O	C-C-C	C-C-O	C-C-N	C-N-C
XRD	Cy2Otn_001						
Average	1.513	1.463	1.425	111.0	110.6	110.7	113.4
Std Dev	0.007	0.007	0.005	0.8	1.6	1.1	1.7
ZINDO/1 geom	Cy2Otn_004						
Average	1.545	1.481	1.433	111.1	109.5	110.6	114.6
Std Dev	0.005	0.003	0.000	0.6	0.9	1.1	0.2
Annealing Run time = 5 ps	Cy2Otn_005						
Average	1.546	1.480	1.431	111.3	109.1	110.5	115.1
Std Dev	0.004	0.002	0.002	0.6	0.9	1.2	0.1
Annealing Run time = 10 ps	Cy2Otn_006						
Average	1.548	1.481	1.430	111.8	109.1	110.5	115.1
Std Dev	0.007	0.002	0.000	1.0	1.2	2.4	0.3
Annealing Run time = 15 ps	Cy2Otn_007						
Average	1.545	1.481	1.432	111.2	109.5	110.6	114.7
Std Dev	0.004	0.002	0.001	0.4	0.6	1.2	0.3
Annealing Run time = 20 ps	Cy2Otn_008						
Average	1.546	1.482	1.431	111.1	109.3	111.0	115.7
Std Dev	0.004	0.004	0.001	0.3	0.7	1.2	1.0
Annealing Run time = 25 ps	Cy2Otn_009						
Average	1.545	1.480	1.433	111.1	109.6	110.4	114.8
Std Dev	0.004	0.002	0.000	0.5	0.5	1.0	0.0
Annealing Run time = 30 ps	Cy2Otn_010						
Average	1.545	1.480	1.432	111.2	109.3	110.4	114.9
Std Dev	0.004	0.002	0.001	0.4	0.5	1.0	0.0
Annealing Run time = 35 ps	Cy2Otn_011						
Average	1.546	1.482	1.433	111.3	110.0	111.8	115.8
Std Dev	0.004	0.002	0.001	0.6	1.3	1.5	1.4

Annealing	Cy2Otn_012						
Run time = 40 ps							
Average	1.546	1.483	1.432	111.1	109.5	111.3	115.6
Std Dev	0.004	0.003	0.001	0.4	0.8	1.1	1.2
Annealing	Cy2Otn_013						
Run time = 45 ps							
Average	1.546	1.482	1.431	111.1	109.5	111.0	116.5
Std Dev	0.005	0.004	0.001	0.5	1.4	2.2	0.0
Annealing	Cy2Otn_014						
Run time = 50 ps							
Average	1.546	1.482	1.432	111.1	109.7	111.2	115.7
Std Dev	0.004	0.003	0.000	0.3	0.5	1.3	1.3
Annealing	Cy2Otn_015						
Run time = 55 ps							
Average	1.546	1.480	1.432	111.4	109.3	110.4	114.8
Std Dev	0.004	0.003	0.001	0.5	0.4	1.4	0.5
Annealing	Cy2Otn_016						
Run time = 60 ps							
Average	1.549	1.480	1.432	112.2	109.0	110.5	115.0
Std Dev	0.006	0.002	0.001	0.8	0.6	1.7	0.3
Annealing	Cy2Otn_017						
Run time = 65 ps							
Average	1.547	1.482	1.432	111.5	109.9	111.2	114.7
Std Dev	0.004	0.002	0.001	0.7	0.7	1.7	0.1
Annealing	Cy2Otn_018						
Run time = 70 ps							
Average	1.546	1.480	1.431	111.3	109.0	110.5	115.1
Std Dev	0.004	0.002	0.001	0.5	0.8	1.2	0.1
Annealing	Cy2Otn_019						
Run time = 75 ps							
Average	1.545	1.480	1.431	111.2	109.2	110.4	114.9
Std Dev	0.004	0.002	0.000	0.4	0.4	1.0	0.1
Annealing	Cy2Otn_020						
Run time = 80 ps							
Average	1.547	1.480	1.432	111.6	109.3	110.5	114.9
Std Dev	0.005	0.002	0.001	0.9	0.4	1.3	0.0
Annealing	Cy2Otn_021						
Run time = 85 ps							
Average	1.546	1.480	1.432	111.3	109.4	110.5	114.6
Std Dev	0.004	0.001	0.001	0.5	0.4	1.2	0.4

Annealing	Cy2Otn_022						
Run time = 90 ps							
Average	1.545	1.480	1.432	111.1	109.4	110.4	114.7
Std Dev	0.004	0.003	0.001	0.5	0.4	1.1	0.2
Annealing	Cy2Otn_023						
Run time = 95 ps							
Average	1.547	1.482	1.432	111.6	109.2	110.8	115.9
Std Dev	0.005	0.003	0.001	0.8	0.5	1.9	1.1
Annealing	Cy2Otn_024						
Run time = 100 ps							
Average	1.547	1.482	1.432	111.3	109.5	111.1	115.7
Std Dev	0.004	0.004	0.000	0.5	0.7	1.4	1.1
Comparisons	001 - 004						
Average	0.032	0.019	0.008	0.0	1.1	0.1	1.2
Std Dev	0.002	0.004	0.004	0.2	0.8	0.0	1.5
Comparisons	001 - 005						
Average	0.032	0.017	0.007	0.2	1.5	0.2	1.7
Std Dev	0.002	0.005	0.003	0.3	0.7	0.1	1.6
Comparisons	001 - 006						
Average	0.035	0.018	0.006	0.7	1.5	0.2	1.7
Std Dev	0.000	0.005	0.005	0.2	0.5	1.3	1.4
Comparisons	001 - 007						
Average	0.032	0.018	0.008	0.1	1.1	0.1	1.3
Std Dev	0.003	0.005	0.004	0.5	1.0	0.2	1.4
Comparisons	001 - 008						
Average	0.032	0.019	0.007	0.1	1.3	0.3	2.3
Std Dev	0.003	0.003	0.004	0.5	1.0	0.1	0.6
Comparisons	001 - 009						
Average	0.032	0.017	0.008	0.1	1.0	0.3	1.4
Std Dev	0.003	0.004	0.005	0.3	1.1	0.1	1.7
Comparisons	001 - 010						
Average	0.032	0.017	0.007	0.1	1.3	0.3	1.5
Std Dev	0.003	0.004	0.004	0.4	1.1	0.1	1.6
Comparisons	001 - 011						
Average	0.033	0.000	0.000	2.0	1.0	4.3	0.0
Std Dev	0.002	0.000	0.000	0.1	0.0	0.0	0.0
Comparisons	001 - 012						
Average	0.032	0.020	0.007	0.0	1.1	0.6	2.2
Std Dev	0.002	0.004	0.004	0.4	0.9	0.1	0.5

Comparisons	001 - 013						
Average	0.032	0.020	0.007	0.1	1.1	0.3	3.1
Std Dev	0.002	0.003	0.004	0.3	0.3	1.1	1.7
Comparisons	001 - 014						
Average	0.032	0.020	0.008	0.1	0.9	0.5	2.3
Std Dev	0.003	0.003	0.004	0.5	1.1	0.2	0.4
Comparisons	001 - 015						
Average	0.033	0.018	0.007	0.3	1.3	0.3	1.4
Std Dev	0.002	0.004	0.004	0.3	1.2	0.4	1.2
Comparisons	001 - 016						
Average	0.035	0.017	0.007	1.2	1.6	0.2	1.6
Std Dev	0.001	0.005	0.004	0.1	1.0	0.7	1.4
Comparisons	001 - 017						
Average	0.033	0.019	0.007	0.5	0.7	0.5	1.3
Std Dev	0.002	0.005	0.004	0.2	0.9	0.6	1.6
Comparisons	001 - 018						
Average	0.032	0.017	0.006	0.2	1.6	0.2	1.7
Std Dev	0.003	0.005	0.003	0.3	0.8	0.1	1.6
Comparisons	001 - 019						
Average	0.032	0.017	0.007	0.1	1.4	0.3	1.5
Std Dev	0.003	0.004	0.004	0.5	1.3	0.1	1.6
Comparisons	001 - 020						
Average	0.033	0.017	0.007	0.6	1.3	0.3	1.5
Std Dev	0.002	0.005	0.004	0.1	1.2	0.2	1.7
Comparisons	001 - 021						
Average	0.032	0.017	0.007	0.2	1.2	0.2	1.2
Std Dev	0.003	0.005	0.004	0.3	1.2	0.1	1.3
Comparisons	001 - 022						
Average	0.032	0.018	0.008	0.0	1.2	0.3	1.3
Std Dev	0.003	0.004	0.004	0.3	1.3	0.0	1.4
Comparisons	001 - 023						
Average	0.034	0.019	0.007	0.5	1.5	0.1	2.5
Std Dev	0.001	0.003	0.004	0.0	1.1	0.8	0.6
Comparisons	001 - 024						
Average	0.033	0.000	0.001	0.1	0.0	0.1	0.1
Std Dev	0.000	0.000	0.002	0.1	0.8	0.2	1.6

BHEEN Data

Table A.5: Charges on BHEEN Calculated by Semi-empirical Methods Using PM3 and ZINDO/1

Atom	PM3 charge	ZINDO/1 charge
Secondary amine nitrogen, NH	0.844	-0.016
Secondary amine nitrogen, NH	0.788	-0.028
Alcohol group, OH	-0.294	-0.364
Alcohol group, OH	-0.274	-0.352
Carbon on ethylene bridge bonded to both amines, CH_2	-0.247	-0.012
Carbon on ethylene bridge bonded to both amines, CH_2	-0.212	-0.000
Carbon on ethylene bridge between alcohol and amine, bonded to amine, CH_2	-0.244	-0.014
Carbon on ethylene bridge between alcohol and amine, bonded to amine, CH_2	-0.240	-0.012
Carbon bonded to alcohol, CH_2	0.084	0.081
Carbon bonded to alcohol, CH_2	0.087	0.083

Table A.6: Energies of BHEEN after Simulated Annealing Runs with Various Run Times Compared to the Energy of the XRD Structure

Run Time	Energy [kcal/mol]
XRD structure	
5 ps	2.798
10 ps	2.334
15 ps	1.772
20 ps	1.007
25 ps	4.595
30 ps	4.380
35 ps	1.614
40 ps	1.716
45 ps	2.153
50 ps	2.531
55 ps	1.160
60 ps	1.007
65 ps	2.220
70 ps	1.805
75 ps	2.216
80 ps	2.254
85 ps	2.073
90 ps	2.271
95 ps	1.881
100 ps	2.066

Table A.7: BHEEN Data After Simulated Annealing

		C-C	C-N	C-O	C-C-N	C-C-O	C-N-C
XRD		bheen_001					
	Average	1.511	1.486	1.415	109.654	109.639	112.726
	Std Dev	0.005	0.004	0.000	0.252	0.000	0.000
Annealing run time = 5 ps		bheen_006					
	Average	1.542	1.514	1.429	110.978	110.276	112.994
	Std Dev	0.004	0.001	0.001	1.222	0.239	0.001
Annealing run time = 10 ps		bheen_007					
	Average	1.540	1.512	1.428	110.283	109.904	112.234
	Std Dev	0.002	0.003	0.001	1.213	0.371	1.052
Annealing run time = 15 ps		bheen_008					
	Average	1.540	1.512	1.428	110.295	109.697	112.263
	Std Dev	0.003	0.002	0.001	1.227	0.565	1.058
Annealing run time = 20 ps		bheen_009					
	Average	1.538	1.509	1.428	109.427	109.700	111.472
	Std Dev	0.001	0.001	0.001	0.422	0.559	0.015
Annealing run time = 25 ps		bheen_010					
	Average	1.543	1.517	1.428	111.590	109.856	115.015
	Std Dev	0.001	0.001	0.001	0.515	0.515	0.019
Annealing run time = 30 ps		bheen_011					
	Average	1.541	1.514	1.428	110.698	109.566	113.998
	Std Dev	0.003	0.003	0.000	1.087	0.103	1.385
Annealing run time = 35 ps		bheen_012					
	Average	1.540	1.512	1.429	110.401	110.128	112.280
	Std Dev	0.002	0.002	0.000	1.031	0.061	1.027
Annealing run time = 40 ps		bheen_013					
	Average	1.540	1.512	1.428	110.279	109.682	112.282
	Std Dev	0.003	0.002	0.001	1.228	0.543	1.056

Annealing run time = 45 ps		bheen_014					
	Average	1.539	1.511	1.429	109.835	109.865	112.196
	Std Dev	0.002	0.002	0.002	0.940	0.800	1.019
Annealing run time = 50 ps		bheen_015					
	Average	1.540	1.512	1.429	110.336	109.950	112.215
	Std Dev	0.001	0.001	0.002	0.563	1.076	1.067
Annealing run time = 55 ps		bheen_016					
	Average	1.539	1.510	1.428	109.808	109.701	111.509
	Std Dev	0.001	0.001	0.001	0.401	0.560	0.019
Annealing run time = 60 ps		bheen_017					
	Average	1.538	1.509	1.428	109.428	109.698	111.471
	Std Dev	0.001	0.001	0.001	0.422	0.558	0.014
Annealing run time = 65 ps		bheen_018					
	Average	1.540	1.512	1.428	110.293	109.866	112.262
	Std Dev	0.002	0.002	0.001	1.230	0.326	1.058
Annealing run time = 70 ps		bheen_019					
	Average	1.540	1.512	1.428	110.297	109.706	112.255
	Std Dev	0.003	0.003	0.001	1.191	0.569	1.080
Annealing run time = 75 ps		bheen_020					
	Average	1.540	1.512	1.428	110.291	109.866	112.263
	Std Dev	0.002	0.002	0.001	1.228	0.326	1.055
Annealing run time = 80 ps		bheen_021					
	Average	1.540	1.512	1.428	110.295	109.874	112.255
	Std Dev	0.002	0.003	0.001	1.193	0.331	1.081
Annealing run time = 85 ps		bheen_022					
	Average	1.542	1.514	1.429	110.889	110.165	113.082
	Std Dev	0.002	0.001	0.000	1.148	0.077	0.053
Annealing run time = 90 ps		bheen_023					
	Average	1.541	1.514	1.429	110.844	110.168	113.002
	Std Dev	0.003	0.001	0.000	1.276	0.000	0.000

Annealing		bheen_024					
run time = 95 ps							
	Average	1.538	1.510	1.427	109.660	109.246	112.201
	Std Dev	0.002	0.002	0.000	0.967	0.082	1.045
Annealing		bheen_025					
run time = 100 ps							
	Average	1.540	1.511	1.429	110.043	110.268	112.202
	Std Dev	0.000	0.002	0.001	0.810	0.231	1.027
Comparisons		001 - 006					
	Average	0.031	0.028	0.014	1.323	0.636	0.269
	Std Dev	0.001	0.003	0.001	0.970	0.239	0.001
Comparisons		001 - 007					
	Average	0.029	0.026	0.013	0.629	0.265	0.492
	Std Dev	0.002	0.001	0.001	0.961	0.371	1.052
Comparisons		001 - 008					
	Average	0.029	0.026	0.013	0.641	0.058	0.462
	Std Dev	0.002	0.001	0.001	0.975	0.565	1.058
Comparisons		001 - 009					
	Average	0.027	0.023	0.013	0.227	0.061	1.254
	Std Dev	0.004	0.003	0.001	0.170	0.559	0.015
Comparisons		001 - 010					
	Average	0.032	0.031	0.013	1.935	0.216	2.289
	Std Dev	0.004	0.003	0.001	0.262	0.515	0.019
Comparisons		001 - 011					
	Average	0.030	0.029	0.013	1.044	0.073	1.272
	Std Dev	0.002	0.001	0.000	0.834	0.103	1.385
Comparisons		001 - 012					
	Average	0.029	0.026	0.014	0.746	0.489	0.446
	Std Dev	0.003	0.001	0.000	0.779	0.061	1.027
Comparisons		001 - 013					
	Average	0.029	0.026	0.013	0.624	0.043	0.443
	Std Dev	0.002	0.001	0.001	0.976	0.543	1.056
Comparisons		001 - 014					
	Average	0.028	0.025	0.013	0.180	0.226	0.530
	Std Dev	0.003	0.002	0.002	0.688	0.800	1.019
Comparisons		001 - 015					
	Average	0.029	0.026	0.013	0.682	0.311	0.511
	Std Dev	0.004	0.002	0.002	0.311	1.076	1.067

Comparisons		001 - 016					
	Average	0.027	0.024	0.013	0.154	0.061	1.217
	Std Dev	0.004	0.003	0.001	0.149	0.560	0.019
Comparisons		001 - 017					
	Average	0.027	0.023	0.013	0.226	0.059	1.255
	Std Dev	0.004	0.003	0.001	0.169	0.558	0.014
Comparisons		001 - 018					
	Average	0.029	0.026	0.013	0.638	0.227	0.463
	Std Dev	0.003	0.001	0.001	0.977	0.326	1.058
Comparisons		001 - 019					
	Average	0.029	0.026	0.013	0.643	0.066	0.471
	Std Dev	0.002	0.001	0.001	0.938	0.569	1.080
Comparisons		001 - 020					
	Average	0.029	0.026	0.013	0.637	0.227	0.463
	Std Dev	0.003	0.001	0.001	0.976	0.326	1.055
Comparisons		001 - 021					
	Average	0.029	0.026	0.013	0.641	0.235	0.471
	Std Dev	0.003	0.001	0.001	0.941	0.331	1.081
Comparisons		001 - 022					
	Average	0.030	0.028	0.014	1.235	0.526	0.356
	Std Dev	0.003	0.003	0.000	0.895	0.077	0.053
Comparisons		001 - 023					
	Average	0.030	0.028	0.014	1.190	0.529	0.277
	Std Dev	0.002	0.003	0.000	1.023	0.000	0.000
Comparisons		001 - 024					
	Average	0.027	0.025	0.012	0.006	0.393	0.525
	Std Dev	0.003	0.001	0.000	0.715	0.082	1.045
Comparisons		001 - 025					
	Average	0.029	0.026	0.014	0.389	0.629	0.524
	Std Dev	0.004	0.001	0.001	0.557	0.231	1.027

Cy_2-en/Cd Complex Data

Table A.8: Abridged WitsGAFFtyp.txt file

```
ATOM  MASS        REFERENCE
c3    12.01       sp3 C
h3    1.008       H bonded to aliphatic carbon with 3 electrwd. group
hn    1.008       H bonded to nitrogen atoms
ho    1.008       Hydroxyl group
cl    35.45       Chlorine
n3    14.01       sp3 N with three connected atoms
oh    16          Oxygen in hydroxyl group
c0    40.08       calcium added J.R 01.04.05
cu2   63.55       copper(II) added HMM 10.02.06
ni2   58.6        Nickel 2+ HMM 14/08/2007
cd2   112.41      Cadmium 2+ SAR 18/04/2008
```

Table A.9: Abridged WitsGAFFstr.txt file

```
B1    B2    KR          REQ   REFERENCE
c3    c3    303.1       1.535
c3    n3    320.6       1.47
c3    oh    314.1       1.426
cu2   n3a   300.0       1.975
cu2   n3b   300.0       1.975
cu2   oha   150.0       1.970
cu2   ohb   150.0       1.970
ni2   n3a   300.0       2.135 HMM 14/08/2007
ni2   n3b   300.0       2.135 HMM 14/08/2007
ni2   n3c   300.0       2.135 HMM 14/08/2007
ni2   oha   150.0       2.048 HMM 2007
ni2   ohb   150.0       2.048 HMM 2007
ni2   ohc   150.0       2.048 HMM 2007
cd2   n3    300.0       2.390 SAR 18/04/2008
cd2   oh    150.0       2.440 SAR 18/04/2008
cd2   cl    150.0       2.610 SAR 18/04/2008
```

Table A.10: Abridged WitsGAFFben.txt file

```
A1    A2    A3    KTHETA      THETAEQ     REFERENCE
h1    c3    n3a   49.4        109.92      HAR 24/02/2006 from H1-C3-N3
c3    n3a   hn    47.1        109.92      HAR 24/02/2006 from HN-N3-C3
c3    oha   ho    47.1        108.16      HAR 24/02/2006 from ho-oh-C3
h1    c3    oha   51.0        109.88      HAR 24/02/2006 from h1-c3-oh
c3    c3    oha   67.7        109.43      HAR 24/02/2006 from c3-c3-oh
cu2   oh    ho    47.1        108.16      HAR 09/03/2006 from c3-oh-ho
oh    cu2   n3b   72.0        90.000      HAR 09/03/2006 from
                                          cobalamins force field
n3    cd2   n3    0.00        74.00       SAR 18/04/2008
n3    cd2   oh    0.00        70.00       SAR 18/04/2008
n3    cd2   cl    0.00        90.00       SAR 18/04/2008
oh    cd2   cl    0.00        90.00       SAR 18/04/2008
cl    cd2   cl    0.00        90.00       SAR 18/04/2008
cd2   n3    c3    64.0        110.90      SAR 18/04/2008 from c3 n3 c3
cd2   oh    c3    62.1        113.41      SAR 18/04/2008 from c3 os c3
cd2   n3    hn    47.1        109.92      SAR 18/04/2008 from c3 n3 hn
cd2   oh    ho    47.1        108.16      SAR 18/04/2008 from c3 oh ho
```

Table A.11: Abridged WitsGAFFnbd.txt file

ATOM	R_STAR	EPS	REFERENCE
hc	1.487	0.0157	OPLS
hn	0.600	0.0157	!Ferguson base pair geom.
ho	0.000	0.0000	" OPLS Jorgensen, JACS,110,(1988),1657"
oh	1.721	0.2104	OPLS
c3	1.908	0.1094	OPLS
n3	1.824	0.1700	OPLS
cl	1.948	0.2650	"Fox, JPCB,102,8070,(98),flex.mdl CHCl3"
cu2	1.970	0.0440	Cu(II) preliminary values - PCCP, 2002, 4, 5878. HAR 13/02/2006
ni2	1.960	0.0440	Ni(II) preliminary values - PCCP, 2002, 4, 5878. HMM 14/08/2007
cd2	0.970	0.2600	SAR 18/04/2008 R_Star from corr with ionic radius epsilon from corr with third ionisation E

Table A.12: Abridged WitsGAFFtor.txt file

T1	T2	T3	T4	HALF_VN	GAMMA	N	REFERENCE
**	c3	n3	**	6	1.80	0.00	3.00 "Junmei et al, 1999 "
**	c3	n4	**	9	1.40	0.00	3.00 "JCC,7,(1986),230 "
**	c3	oh	**	3	0.50	0.00	3.00 "JCC,7,(1986),230 "
**	oh	oh	**	1	1.60	0.00	2.00
hc	c3	c3	hc	1	0.15	0.00	3.00 "Junmei et al, 1999 "
ni2	n3a	c3	c3	1	0.30	0.00	3.00 HMM 2007 based on c3-c3-n3-c3
ni2	n3a	c3	h1	1	1.80	0.00	3.00 HMM 2007 based on **-c3-n3-**
c3	c3	oha	ni2	1	0.50	0.00	3.00 HMM 2007 based on **-c3-oh-**
h1	c3	oha	ni2	1	0.50	0.00	3.00 HMM 2007 based on **-c3-oh-**
**	cd2	**	**	1	0.00	180.0	1.00 SAR 18/04/2008

Table A.13: Abridged WitsGAFFimp.txt file

T1	T2	T3	T4	HALF_VN	GAMMA	N	REFERENCE
**	o	c	o	1.10	180.00	2.00	" JCC,7,(1986),230"
**	**	c	o	10.50	180.00	2.00	" JCC,7,(1986),230"
**	**	n	hn	1.10	180.00	2.00	" JCC,7,(1986),230"
**	**	n2	Hn	1.10	180.00	2.00	" JCC,7,(1986),230"
**	**	na	hn	1.10	180.00	2.00	" JCC,7,(1986),230"
**	c3	n	c3	1.10	180.00	2.00	" JCC,7,(1986),230"
**	n2	ca	n2	10.50	180.00	2.00	" JCC,7,(1986),230"
c3	o	c	oh	1.10	180.00	2.00	
c2	c3	c2	hc	1.10	180.00	2.00	Junmei et al.1999
c2	c3	ca	hc	1.10	180.00	2.00	Junmei et al.1999
c2	hc	c	o	1.10	180.00	2.00	Junmei et al.1999
c3	ca	ca	n2	1.10	180.00	2.00	
c3	ca	ca	na	1.10	180.00	2.00	
hc	o	c	oh	1.10	180.00	2.00	Junmei et al.1999
hc	o	c	os	1.10	180.00	2.00	
n2	c2	ca	n2	1.10	180.00	2.00	" dac guess, 9/94"
n2	ca	ca	n2	1.10	180.00	2.00	" dac guess, 9/94"
na	n2	ca	n2	1.10	180.00	2.00	" dac, 10/94"
**	**	**	**	1.10	180.00	2.00	" dac, 10/94"
**	**	cd2	**	0.00	180.00	2.00	SAR 18/04/2008

Table A.14: Energies of the Cy_2-en/Cd Complex After the First Simulated Annealing Runs with Various Run Times Compared to the Energy of the XRD Structure

Run Time	Energy [kcal/mol]
XRD structure	22.835
5 ps	18.933
10 ps	19.704
15 ps	19.899
20 ps	18.505
25 ps	18.505
30 ps	25.450
35 ps	19.738
40 ps	25.586
45 ps	19.917
50 ps	19.362
55 ps	20.808
60 ps	19.705
65 ps	18.900
70 ps	18.695
75 ps	19.917
80 ps	18.817
85 ps	19.705
90 ps	19.547
95 ps	18.971
100 ps	18.814

Table A.15: Cy_2-en/Cd Complex Data After the First Simulated Annealing Run

		C-C	C-N	C-O	N-Cd	O-Cd	Cd-Cl	C-C-C	C-C-N	C-C-O	C-N-C	C-N-Cd	C-O-Cd	O-Cd-N	N-Cd-Cl	O-Cd-Cl
XRD		Cy2en_Cd_000														
	Average	1.521	1.480	1.439	2.348	2.382	2.494	110.7	111.0	111.4	113.1	112.5	114.5	108.1	116.5	92.5
	Std Dev	0.009	0.013	0.006	0.020		0.000	0.4	1.9	1.1	2.4	8.2		51.1	25.1	3.3
Drawn file no charges		Cy2en_Cd_001														
	Average	1.545	1.480	1.432	1.619	3.162	2.799	111.2	110.2	109.3	114.5	112.4	91.7	75.3	115.1	114.6
	Std Dev	0.005	0.004	0.000	0.219		0.029	0.4	1.2	0.4	0.0	5.4		15.6	8.8	57.7
MM no charges		Cy2en_Cd_002														
	Average	1.545	1.485	1.431	2.388	2.444	2.610	111.1	111.6	109.1	116.9	108.5	114.7	82.3	104.2	109.2
	Std Dev	0.005	0.005	0.000	0.002		0.000	0.6	3.1	1.6	2.6	0.5		13.7	30.8	72.4
ZINDO1 e = 76		Cy2en_Cd_003														
	Average	1.545	1.480	1.432	1.619	3.162	2.799	111.2	110.2	109.3	114.5	112.4	91.7	75.3	115.1	114.6
	Std Dev	0.005	0.004	0.000	0.219		0.029	0.4	1.2	0.4	0.0	5.4		15.6	8.8	57.7
MM w ZINDO1 e = 76		Cy2en_Cd_004														
	Average	1.545	1.485	1.431	2.388	2.444	2.609	111.1	111.6	109.1	116.9	108.5	114.7	82.3	103.6	108.4
	Std Dev	0.005	0.005	0.000	0.001		0.000	0.6	3.0	1.6	2.6	0.5		13.7	30.8	72.2
Annealing r.t. = 5 ps		Cy2en_Cd_005														
	Average	1.544	1.480	1.431	2.391	2.442	2.610	111.2	109.7	109.0	115.1	109.2	113.9	100.3	114.6	103.8
	Std Dev	0.005	0.005	0.001	0.003		0.000	0.4	2.6	0.7	0.6	1.0		40.2	39.5	7.6

Annealing r.t. = 10 ps	Cy2en_Cd_006														
Average	1.544	1.480	1.431	2.391	2.442	2.610	111.2	109.6	109.0	115.4	109.1	113.9	100.2	146.4	108.5
Std Dev	0.006	0.005	0.002	0.003		0.000	0.4	2.7	1.1	0.4	0.9		40.0	28.1	0.0
Annealing r.t. = 15 ps	Cy2en_Cd_007														
Average	1.546	1.483	1.432	2.390	2.441	2.609	111.4	110.5	109.3	115.6	108.5	113.4	92.4	107.7	122.5
Std Dev	0.005	0.003	0.000	0.003		0.000	0.5	2.0	0.7	0.1	0.7		28.6	35.6	6.4
Annealing r.t. = 20 ps	Cy2en_Cd_008														
Average	1.546	1.483	1.431	2.390	2.442	2.609	111.4	110.6	109.1	115.5	108.5	114.0	91.6	88.6	176.8
Std Dev	0.005	0.003	0.002	0.002		0.000	0.5	2.1	0.7	0.0	0.7		27.9	20.8	0.0
Annealing r.t. = 25 ps	Cy2en_Cd_009														
Average	1.546	1.483	1.431	2.390	2.442	2.609	111.4	110.6	109.1	115.5	108.5	114.0	91.6	88.6	176.8
Std Dev	0.005	0.003	0.002	0.002		0.000	0.5	2.1	0.7	0.0	0.7		27.9	20.8	0.0
Annealing r.t. = 30 ps	Cy2en_Cd_010														
Average	1.546	1.481	1.430	2.391	2.442	2.610	111.7	109.9	108.8	114.8	108.8	113.8	100.8	93.0	91.8
Std Dev	0.007	0.005	0.002	0.000		0.001	0.8	2.3	1.0	1.1	0.8		40.7	13.0	8.2
Annealing r.t. = 35 ps	Cy2en_Cd_011														
Average	1.545	1.480	1.432	2.391	2.441	2.609	111.4	110.0	109.3	114.9	108.7	113.3	101.0	97.8	82.0
Std Dev	0.006	0.005	0.000	0.001		0.000	0.4	2.5	0.7	1.1	0.7		40.7	7.3	12.2
Annealing r.t. = 40 ps	Cy2en_Cd_012														

	Average	1.546	1.480	1.430	2.391	2.442	2.609	111.7	109.9	108.7	114.9	108.7	113.8	100.6	103.5	85.1
	Std Dev	0.007	0.004	0.001	0.000		0.000	0.9	2.7	0.6	1.2	0.7		40.5	11.7	4.0
Annealing r.t. = 45 ps		Cy2en_Cd_013														
	Average	1.545	1.480	1.432	2.390	2.441	2.609	111.5	110.0	109.3	114.8	108.8	113.3	101.1	100.3	73.4
	Std Dev	0.006	0.005	0.000	0.001		0.000	0.4	2.4	0.7	1.2	0.6		40.7	2.1	0.0
Annealing r.t. = 50 ps		Cy2en_Cd_014														
	Average	1.546	1.484	1.432	2.390	2.441	2.609	111.5	110.6	109.3	115.5	108.5	113.4	92.5	88.5	175.3
	Std Dev	0.005	0.003	0.000	0.002		0.000	0.5	2.0	0.7	0.0	0.7		28.7	20.6	0.0
Annealing r.t. = 55 ps		Cy2en_Cd_015														
	Average	1.546	1.481	1.433	2.390	2.441	2.609	111.6	110.0	109.7	114.9	108.7	113.3	101.1	100.3	73.6
	Std Dev	0.006	0.005	0.001	0.000		0.000	0.5	2.4	0.9	1.1	0.6		40.7	2.3	0.0
Annealing r.t. = 60 ps		Cy2en_Cd_016														
	Average	1.545	1.480	1.432	2.391	2.442	2.609	111.5	109.9	109.5	115.1	108.7	113.9	100.6	95.2	90.5
	Std Dev	0.006	0.005	0.003	0.000		0.000	0.5	2.7	1.1	1.0	0.8		40.5	9.0	0.0
Annealing r.t. = 65 ps		Cy2en_Cd_017														
	Average	1.546	1.483	1.431	2.390	2.442	2.609	111.4	110.5	109.1	115.5	108.5	114.0	91.8	84.5	119.1
	Std Dev	0.004	0.003	0.002	0.002		0.000	0.5	2.1	0.7	0.0	0.7		28.1	18.3	0.0
Annealing r.t. = 70 ps		Cy2en_Cd_018														
	Average	1.546	1.483	1.431	2.390	2.442	2.609	111.4	110.6	109.1	115.5	108.5	114.0	91.7	86.5	147.5
	Std Dev	0.005	0.003	0.002	0.002		0.000	0.5	2.1	0.6	0.0	0.7		28.0	19.5	40.2

Annealing r.t. = 75 ps	Cy2en_Cd_019														
	Average	1.545	1.480	1.432	2.390	2.441	2.609	111.5	110.0	109.3	114.8	108.8	113.3	101.1	100.3	73.4
	Std Dev	0.006	0.005	0.000	0.001		0.000	0.4	2.4	0.7	1.2	0.6		40.7	2.2	0.0
Annealing r.t. = 80 ps	Cy2en_Cd_020														
	Average	1.545	1.480	1.431	2.391	2.442	2.609	111.4	109.9	109.1	115.0	108.7	113.9	100.6	94.8	90.8
	Std Dev	0.006	0.005	0.002	0.000		0.000	0.4	2.7	0.7	1.0	0.8		40.5	8.9	0.0
Annealing r.t. = 85 ps	Cy2en_Cd_021														
	Average	1.545	1.480	1.432	2.391	2.442	2.609	111.5	109.9	109.5	115.1	108.7	113.9	100.6	95.2	90.5
	Std Dev	0.006	0.005	0.003	0.000		0.000	0.5	2.7	1.1	1.0	0.8		40.5	9.0	0.0
Annealing r.t. = 90 ps	Cy2en_Cd_022														
	Average	1.546	1.483	1.432	2.390	2.441	2.609	111.5	110.5	109.3	115.5	108.5	113.4	92.6	86.5	146.3
	Std Dev	0.005	0.003	0.000	0.002		0.000	0.5	2.0	0.7	0.0	0.7		28.8	19.5	40.0
Annealing r.t. = 95 ps	Cy2en_Cd_023														
	Average	1.545	1.480	1.431	2.391	2.442	2.609	111.4	110.0	109.1	114.9	108.7	113.8	100.6	98.6	88.6
	Std Dev	0.006	0.005	0.002	0.000		0.000	0.4	2.6	0.7	1.1	0.7		40.5	10.0	3.5
Annealing r.t. = 100 ps	Cy2en_Cd_024														
	Average	1.545	1.480	1.431	2.391	2.442	2.609	111.4	109.9	109.1	115.0	108.7	113.9	100.6	94.9	90.8
	Std Dev	0.006	0.005	0.002	0.000		0.000	0.4	2.7	0.7	1.0	0.8		40.5	8.9	0.0
Comparisons	000 - 001														
	Average	0.024	0.004	0.008	0.040	0.062	0.115	0.4	0.5	2.3	3.8	4.0	0.2	25.8	12.3	16.7
	Std Dev	0.004	0.008	0.006	0.019		0.000	0.2	1.2	0.5	0.2	7.8		37.4	5.7	69.1

Comparisons	000 - 003															
	Average	0.024	0.000	0.007	0.729	0.780	0.304	0.4	0.9	2.1	1.4	0.0	22.9	32.8	1.4	22.1
	Std Dev	0.004	0.009	0.006	0.199		0.028	0.0	0.6	0.7	2.4	2.8		35.5	16.3	54.4
Comparisons	000 - 004															
	Average	0.024	0.004	0.008	0.040	0.062	0.115	0.4	0.5	2.3	3.8	4.0	0.2	25.8	12.9	15.9
	Std Dev	0.004	0.008	0.006	0.019		0.000	0.2	1.2	0.5	0.1	7.7		37.4	5.7	69.0
Comparisons	000 - 005															
	Average	0.023	0.000	0.008	0.043	0.060	0.115	0.5	1.3	2.4	2.0	3.3	0.6	7.8	1.9	11.3
	Std Dev	0.004	0.008	0.004	0.018		0.000	0.0	0.7	0.5	1.8	7.2		10.9	14.4	4.3
Comparisons	000 - 006															
	Average	0.023	0.000	0.008	0.043	0.060	0.115	0.5	1.4	2.4	2.3	3.4	0.6	7.9	29.9	16.0
	Std Dev	0.003	0.008	0.004	0.018		0.000	0.0	0.8	0.1	2.0	7.3		11.1	3.0	3.3
Comparisons	000 - 007															
	Average	0.025	0.003	0.007	0.042	0.059	0.115	0.7	0.5	2.0	2.5	4.0	1.2	15.7	8.8	30.0
	Std Dev	0.005	0.010	0.005	0.018		0.000	0.1	0.2	0.4	2.4	7.5		22.5	10.5	3.2
Comparisons	000 - 008															
	Average	0.024	0.003	0.008	0.042	0.060	0.115	0.7	0.5	2.3	2.4	4.0	0.6	16.5	27.9	84.4
	Std Dev	0.005	0.011	0.004	0.018		0.000	0.1	0.2	0.5	2.4	7.5		23.2	4.3	3.3
Comparisons	000 - 009															
	Average	0.024	0.003	0.008	0.042	0.060	0.115	0.7	0.5	2.3	2.4	4.0	0.6	16.5	27.9	84.3
	Std Dev	0.005	0.011	0.004	0.018		0.000	0.1	0.2	0.5	2.4	7.5		23.2	4.3	3.3
Comparisons	000 - 010															
	Average	0.025	0.001	0.008	0.043	0.060	0.115	1.0	1.1	2.5	1.7	3.6	0.7	7.3	23.4	0.7
	Std Dev	0.002	0.008	0.004	0.020		0.001	0.4	0.4	0.2	1.3	7.5		10.4	12.1	4.9

Comparisons	000 - 011															
	Average	0.024	0.000	0.007	0.042	0.059	0.115	0.7	1.1	2.1	1.8	3.8	1.2	7.1	18.7	10.5
	Std Dev	0.004	0.008	0.006	0.020		0.000	0.0	0.7	0.4	1.3	7.5		10.4	17.8	9.0
Comparisons	000 - 012															
	Average	0.025	0.000	0.009	0.042	0.059	0.114	1.0	1.1	2.6	1.8	3.8	0.7	7.5	13.0	7.4
	Std Dev	0.002	0.009	0.005	0.020		0.000	0.5	0.8	0.5	1.2	7.6		10.6	13.4	0.7
Comparisons	000 - 013															
	Average	0.024	0.000	0.007	0.042	0.059	0.115	0.7	1.0	2.0	1.7	3.7	1.2	7.1	16.2	19.1
	Std Dev	0.004	0.008	0.005	0.020		0.000	0.0	0.5	0.4	1.3	7.7		10.4	23.0	3.3
Comparisons	000 - 014															
	Average	0.025	0.004	0.007	0.042	0.059	0.115	0.7	0.5	2.0	2.4	4.0	1.2	15.6	28.0	82.9
	Std Dev	0.004	0.010	0.005	0.018		0.000	0.1	0.1	0.5	2.4	7.5		22.4	4.5	3.3
Comparisons	000 - 015															
	Average	0.024	0.000	0.006	0.042	0.059	0.114	0.8	1.1	1.6	1.8	3.7	1.2	7.0	16.2	18.9
	Std Dev	0.003	0.009	0.005	0.020		0.000	0.1	0.5	0.2	1.3	7.7		10.4	22.8	3.3
Comparisons	000 - 016															
	Average	0.024	0.000	0.007	0.043	0.060	0.115	0.8	1.2	1.9	2.0	3.8	0.7	7.5	21.3	1.9
	Std Dev	0.003	0.009	0.002	0.020		0.000	0.1	0.8	0.1	1.5	7.4		10.5	16.1	3.3
Comparisons	000 - 017															
	Average	0.024	0.003	0.008	0.042	0.060	0.115	0.7	0.5	2.3	2.4	4.0	0.5	16.3	32.0	26.7
	Std Dev	0.005	0.010	0.004	0.018		0.000	0.1	0.2	0.5	2.4	7.6		23.0	6.8	3.3
Comparisons	000 - 018															
	Average	0.024	0.003	0.008	0.042	0.060	0.115	0.7	0.5	2.3	2.4	4.0	0.6	16.4	30.0	55.1
	Std Dev	0.005	0.010	0.004	0.018		0.000	0.1	0.2	0.5	2.4	7.5		23.1	5.6	36.9

Comparisons		000 - 019														
	Average	0.024	0.000	0.007	0.042	0.059	0.115	0.7	1.0	2.0	1.7	3.7	1.2	7.0	16.2	19.1
	Std Dev	0.004	0.008	0.005	0.020		0.000	0.0	0.5	0.4	1.3	7.7		10.4	22.9	3.2
Comparisons		000 - 020														
	Average	0.024	0.000	0.008	0.043	0.060	0.115	0.6	1.1	2.3	1.9	3.8	0.7	7.5	21.6	1.6
	Std Dev	0.004	0.008	0.004	0.020		0.000	0.0	0.8	0.4	1.4	7.4		10.6	16.2	3.3
Comparisons		000 - 021														
	Average	0.024	0.000	0.007	0.043	0.060	0.115	0.8	1.2	1.9	2.0	3.8	0.7	7.5	21.3	2.0
	Std Dev	0.003	0.009	0.002	0.020		0.000	0.1	0.8	0.1	1.5	7.4		10.5	16.1	3.3
Comparisons		000 - 022														
	Average	0.025	0.003	0.007	0.042	0.059	0.115	0.7	0.5	2.0	2.4	4.0	1.2	15.5	30.0	53.8
	Std Dev	0.005	0.010	0.005	0.018		0.000	0.1	0.1	0.5	2.4	7.6		22.3	5.6	36.7
Comparisons		000 - 023														
	Average	0.024	0.000	0.008	0.043	0.060	0.115	0.7	1.1	2.3	1.8	3.7	0.7	7.5	17.9	3.9
	Std Dev	0.004	0.009	0.004	0.020		0.000	0.0	0.7	0.4	1.3	7.5		10.6	15.1	0.2
Comparisons		000 - 024														
	Average	0.024	0.000	0.008	0.043	0.060	0.115	0.7	1.1	2.3	1.9	3.8	0.7	7.5	21.6	1.6
	Std Dev	0.004	0.008	0.004	0.020		0.000	0.1	0.8	0.4	1.4	7.4		10.6	16.2	3.3

Table A.16: Energies of the Cy_2-en/Cd Complex After the Second Simulated Annealing Runs with Various Run Times Compared to the Energy of the XRD Structure

Run Time	Energy [kcal/mol]
XRD structure	22.835
Sample 1: 5 ps	20.034
Sample 1: 10 ps	19.372
Sample 1: 100 ps	18.597
Sample 2: 5 ps	25.083
Sample 2: 10 ps	23.919
Sample 2: 100 ps	18.951
Sample 3: 5 ps	21.589
Sample 3: 10 ps	18.951
Sample 3: 100 ps	25.822
Sample 4: 5 ps	19.559
Sample 4: 10 ps	26.551
Sample 4: 100 ps	21.329
Sample 5: 5 ps	20.034
Sample 5: 10 ps	19.753
Sample 5: 100 ps	18.497

Table A.17: Cy_2-en/Cd Complex Data After the Second Simulated Annealing Process

		C-C	C-N	C-O	N-Cd	O-Cd	Cd-Cl	C-C-C	C-C-N	C-C-O	C-N-C	C-N-Cd	C-O-Cd	O-Cd-N	N-Cd-Cl	O-Cd-Cl
XRD		Cy2en_Cd_000														
	Average	1.521	1.480	1.439	2.348	2.382	2.494	110.7	111.0	111.4	113.1	112.5	114.5	108.1	116.5	92.5
	Std Dev	0.009	0.013	0.006	0.020		0.000	0.4	1.9	1.1	2.4	8.2		51.1	25.1	3.3
Annealing Sample 1		Cy2en_Cd_035														
r.t. = 5 ps	Average	1.545	1.481	1.432	2.392	2.442	2.610	111.5	110.0	109.3	115.2	109.4	113.2	100.8	150.1	70.9
	Std Dev	0.006	0.006	0.000	0.002		0.000	0.5	3.0	0.8	0.7	1.7		40.5	9.7	0.0
Annealing Sample 1		Cy2en_Cd_025														
r.t. = 10 ps	Average	1.546	1.484	1.432	2.390	2.441	2.609	111.5	110.6	109.3	115.5	108.5	113.4	92.5	88.5	175.4
	Std Dev	0.005	0.003	0.000	0.002		0.000	0.5	2.0	0.7	0.0	0.7		28.7	20.6	0.0
Annealing Sample 1		Cy2en_Cd_026														
r.t. = 100 ps	Average	1.544	1.481	1.431	2.391	2.442	2.610	111.2	109.9	109.0	114.9	109.3	114.0	100.4	82.1	100.1
	Std Dev	0.005	0.005	0.001	0.003		0.000	0.4	2.4	0.7	0.7	1.1		40.3	5.9	0.0
Annealing Sample 2		Cy2en_Cd_036														
r.t. = 5 ps	Average	1.547	1.481	1.431	2.391	2.442	2.611	112.0	110.4	109.0	114.4	109.0	113.9	100.8	78.9	101.1
	Std Dev	0.006	0.006	0.002	0.001		0.000	1.2	2.1	0.7	1.3	0.9		40.8	6.1	0.0
Annealing Sample 2		Cy2en_Cd_027														
r.t. = 10 ps	Average	1.546	1.483	1.431	2.390	2.443	2.610	111.6	110.5	108.8	115.5	108.4	114.2	89.8	113.8	111.2
	Std Dev	0.005	0.002	0.002	0.004		0.000	0.8	2.1	0.4	0.4	1.1		25.3	39.3	76.1

Annealing		Cy2en_Cd_028														
Sample 2																
r.t. = 100 ps	Average	1.545	1.480	1.431	2.391	2.442	2.609	111.4	110.0	109.1	114.9	108.7	113.8	100.6	98.6	88.8
	Std Dev	0.006	0.005	0.002	0.000		0.000	0.4	2.6	0.7	1.1	0.7		40.5	10.1	3.3
Annealing		Cy2en_Cd_037														
Sample 3																
r.t. = 5 ps	Average	1.546	1.483	1.432	2.388	2.445	2.610	111.3	111.6	109.3	116.2	108.8	114.9	82.1	126.1	57.7
	Std Dev	0.004	0.006	0.000	0.001		0.000	0.5	2.2	0.3	3.4	0.7		13.7	22.3	0.0
Annealing		Cy2en_Cd_029														
Sample 3																
r.t. = 10 ps	Average	1.545	1.480	1.431	2.391	2.442	2.609	111.4	110.0	109.1	114.9	108.7	113.8	100.6	98.6	88.8
	Std Dev	0.006	0.005	0.002	0.000		0.000	0.4	2.6	0.7	1.1	0.7		40.5	10.1	3.3
Annealing		Cy2en_Cd_030														
Sample 3																
r.t. = 100 ps	Average	1.546	1.479	1.430	2.392	2.444	2.610	111.8	109.7	109.2	115.4	109.1	111.7	101.2	145.4	107.7
	Std Dev	0.006	0.004	0.003	0.003		0.000	1.0	3.1	2.0	0.6	0.9		40.6	26.9	0.0
Annealing		Cy2en_Cd_038														
Sample 4																
r.t. = 5 ps	Average	1.546	1.483	1.432	2.390	2.441	2.609	111.5	110.5	109.3	115.5	108.5	113.4	92.6	86.5	146.3
	Std Dev	0.005	0.003	0.000	0.002		0.000	0.5	2.0	0.7	0.0	0.7		28.9	19.5	39.9
Annealing		Cy2en_Cd_031														
Sample 4																
r.t. = 10 ps	Average	1.546	1.480	1.432	2.390	2.441	2.609	111.7	109.9	109.4	114.8	108.8	113.3	101.1	100.1	74.1
	Std Dev	0.007	0.005	0.000	0.001		0.000	0.7	2.2	0.8	1.2	0.6		40.7	2.7	0.1
Annealing		Cy2en_Cd_032														
Sample 4																
r.t. = 100 ps	Average	1.545	1.483	1.432	2.389	2.441	2.609	111.3	110.9	109.4	115.8	109.3	113.3	97.0	80.1	140.5

	Std Dev		0.004	0.004	0.000	0.003		0.000	0.5	2.2	0.9	0.1	1.3		34.8	13.0	25.4
Annealing Sample 5		Cy2en_Cd_039															
r.t. = 5 ps	Average		1.545	1.481	1.432	2.392	2.442	2.610	111.5	110.0	109.3	115.2	109.4	113.2	100.8	150.1	70.9
	Std Dev		0.006	0.006	0.000	0.002		0.000	0.5	3.0	0.8	0.7	1.7		40.5	9.7	0.0
Annealing Sample 5		Cy2en_Cd_033															
r.t. = 10 ps	Average		1.544	1.480	1.432	2.391	2.442	2.610	111.2	109.6	109.2	115.3	109.1	113.4	100.6	122.9	88.4
	Std Dev		0.006	0.005	0.001	0.003		0.000	0.4	2.6	0.7	0.6	1.0		40.2	30.7	28.7
Annealing Sample 5		Cy2en_Cd_034															
r.t. = 100 ps	Average		1.546	1.483	1.431	2.390	2.442	2.609	111.4	110.6	109.1	115.5	108.5	114.0	91.6	88.6	176.8
	Std Dev		0.005	0.003	0.002	0.002		0.000	0.5	2.0	0.6	0.0	0.7		27.8	20.8	0.0
Comparisons		000 - 035															
	Average		0.024	0.001	0.007	0.043	0.060	0.116	0.8	1.1	2.1	2.1	3.0	1.3	7.3	33.6	21.6
	Std Dev		0.003	0.007	0.005	0.018		0.000	0.2	1.1	0.3	1.8	6.5		10.6	15.4	3.2
Comparisons		000 - 025															
	Average		0.025	0.004	0.007	0.042	0.059	0.115	0.7	0.5	2.0	2.4	4.0	1.2	15.6	28.0	82.9
	Std Dev		0.005	0.010	0.005	0.018		0.000	0.1	0.1	0.4	2.4	7.5		22.4	4.5	3.3
Comparisons		000 - 026															
	Average		0.023	0.001	0.008	0.043	0.060	0.115	0.4	1.2	2.4	1.8	3.2	0.6	7.7	34.4	7.6
	Std Dev		0.004	0.008	0.004	0.018		0.000	0.0	0.6	0.5	1.7	7.1		10.8	19.2	3.3
Comparisons		000 - 036															
	Average		0.025	0.001	0.008	0.043	0.060	0.116	1.2	0.7	2.3	1.3	3.5	0.6	7.3	37.6	8.7
	Std Dev		0.003	0.008	0.003	0.020		0.000	0.8	0.3	0.5	1.1	7.3		10.2	19.0	3.3

Comparisons	000 - 027															
	Average	0.025	0.003	0.008	0.041	0.061	0.115	0.9	0.6	2.5	2.4	4.0	0.4	18.3	2.7	18.8
	Std Dev	0.004	0.011	0.004	0.016		0.000	0.4	0.2	0.7	2.1	7.1		25.8	14.2	72.8
Comparisons	000 - 028															
	Average	0.024	0.000	0.008	0.043	0.059	0.115	0.7	1.1	2.3	1.8	3.7	0.7	7.5	17.9	3.7
	Std Dev	0.004	0.009	0.004	0.020		0.000	0.0	0.7	0.4	1.3	7.5		10.6	15.0	0.0
Comparisons	000 - 037															
	Average	0.024	0.003	0.007	0.040	0.063	0.115	0.6	0.6	2.1	3.1	3.7	0.4	26.0	9.6	34.8
	Std Dev	0.005	0.007	0.005	0.020		0.000	0.2	0.4	0.8	1.0	7.5		37.4	2.8	3.3
Comparisons	000 - 029															
	Average	0.024	0.000	0.008	0.043	0.059	0.115	0.7	1.1	2.3	1.8	3.7	0.7	7.5	17.9	3.7
	Std Dev	0.004	0.009	0.004	0.020		0.000	0.0	0.7	0.4	1.3	7.5		10.6	15.0	0.0
Comparisons	000 - 030															
	Average	0.024	0.001	0.009	0.044	0.061	0.115	1.1	1.3	2.2	2.2	3.4	2.9	6.9	28.9	15.3
	Std Dev	0.003	0.009	0.003	0.017		0.000	0.6	1.3	0.9	1.8	7.4		10.5	1.8	3.3
Comparisons	000 - 038															
	Average	0.025	0.003	0.007	0.042	0.059	0.115	0.7	0.5	2.0	2.4	4.0	1.2	15.5	30.0	53.8
	Std Dev	0.005	0.010	0.005	0.018		0.000	0.1	0.1	0.4	2.4	7.6		22.2	5.6	36.6
Comparisons	000 - 031															
	Average	0.025	0.000	0.007	0.042	0.059	0.115	1.0	1.2	1.9	1.7	3.7	1.2	7.0	16.4	18.4
	Std Dev	0.002	0.009	0.005	0.020		0.000	0.3	0.3	0.3	1.2	7.7		10.4	22.4	3.2
Comparisons	000 - 032															
	Average	0.024	0.003	0.006	0.041	0.058	0.115	0.6	0.1	2.0	2.7	3.1	1.2	11.1	36.4	48.0
	Std Dev	0.005	0.010	0.005	0.018		0.000	0.1	0.3	0.3	2.3	6.9		16.3	12.1	22.1
Comparisons	000 - 039															

	Average		0.024	0.001	0.007	0.043	0.060	0.116	0.8	1.1	2.1	2.1	3.0	1.3	7.3	33.6	21.6
	Std Dev		0.003	0.007	0.005	0.018		0.000	0.2	1.1	0.3	1.8	6.5		10.6	15.4	3.2
Comparisons		000 - 033															
	Average		0.022	0.000	0.007	0.043	0.060	0.115	0.5	1.4	2.1	2.2	3.3	1.1	7.5	6.5	4.1
	Std Dev		0.004	0.008	0.005	0.018		0.000	0.0	0.8	0.4	1.8	7.2		10.9	5.6	25.5
Comparisons		000 - 034															
	Average		0.024	0.003	0.008	0.042	0.060	0.115	0.7	0.5	2.3	2.4	4.0	0.6	16.5	27.9	84.4
	Std Dev		0.005	0.011	0.004	0.018		0.000	0.1	0.2	0.5	2.4	7.5		23.2	4.3	3.3

Table A.18: Abridged WitsGAFFtyp.txt file for the first geometry optimisation run

ATOM	MASS	REFERENCE
cd2	112.41	Cadmium 2+ SAR 18/04/2008
clx	35.45	Chlorine coordinated to cd2 in an axial manner SAR 06/05/2008
cly	35.45	Chlorine coordinated to cd2 in an axial manner SAR 06/05/2008
n3x	14.01	nitrogen coordinated to cd2 and trans to cly SAR 06/05/2008
n3y	14.01	nitrogen coordinated to cd2 and at right angle to cly SAR 06/05/2008

Table A.19: Abridged WitsGAFFstr.txt file for the first geometry optimisation run

B1	B2	KR	REQ	REFERENCE
cd2	n3	320.0	2.390	SAR 01/05/2008
cd2	oh	175.0	2.440	SAR 01/05/2008
cd2	cl	200.0	2.610	SAR 01/05/2008
cd2	n3x	350.0	2.390	SAR 06/05/2008
cd2	n3y	350.0	2.390	SAR 06/05/2008
cd2	oh	150.0	2.440	SAR 06/05/2008
cd2	clx	200.0	2.610	SAR 06/05/2008
cd2	cly	200.0	2.610	SAR 06/05/2008
hn	n3x	394.1	1.018	SAR 06/05/2008
hn	n3y	394.1	1.018	SAR 06/05/2008

Table A.20: Abridged WitsGAFFben.txt file for the first geometry optimisation run

A1	A2	A3	KTHETA	THETAEQ	REFERENCE
n3x	cd2	n3y	20.00	90.00	SAR 06/05/2008 co-planar nitrogens
n3x	cd2	oh	70.00	90.00	SAR 06/05/2008 co-planar cis atoms
n3y	cd2	oh	70.00	180.00	SAR 06/05/2008 co-planar trans atoms
n3x	cd2	cly	50.00	180.00	SAR 06/05/2008 co-planar trans atoms
n3y	cd2	cly	50.00	90.00	SAR 06/05/2008 co-planar cis atoms
oh	cd2	cly	50.00	90.00	SAR 06/05/2008 co-planar trans atoms
clx	cd2	cly	50.00	90.00	SAR 06/05/2008 axial and equatorial atoms
oh	cd2	clx	50.00	90.00	SAR 06/05/2008 axial cl to equatorial o
n3x	cd2	clx	50.00	90.00	SAR 06/05/2008 axial cl to equatorial n3x
n3y	cd2	clx	50.00	90.00	SAR 06/05/2008 axial cl to equatorial n3y
cd2	n3x	c3	64.0	110.90	SAR 06/05/2008 from c3 n3 c3
cd2	n3y	c3	64.0	110.90	SAR 06/05/2008 from c3 n3 c3
cd2	oh	c3	62.1	113.41	SAR 06/05/2008 from c3 os c3
cd2	n3x	hn	47.1	109.92	SAR 06/05/2008 from c3 n3 hn
cd2	n3y	hn	47.1	109.92	SAR 06/05/2008 from c3 n3 hn
c3	n3x	hn	47.1	109.92	SAR 06/05/2008 from c3 n3 hn
c3	n3y	hn	47.1	109.92	SAR 06/05/2008 from c3 n3 hn

Table A.21: Abridged WitsGAFFnbd.txt file for the first geometry optimisation run

```
ATOM  R_STAR      EPS         REFERENCE
cd2   0.970       0.2600      SAR 18/04/2008 R_Star from corr with
                              ionic radius epsilon from corr with third
                              ionisation E
n3x   1.824       0.1700      SAR 06/05/2008
n3y   1.824       0.1700      SAR 06/05/2008
clx   1.948       0.2650      SAR 06/05/2008
cly   1.948       0.2650      SAR 06/05/2008
```

Table A.22: Abridged WitsGAFFtor.txt file for the first geometry optimisation run

```
T1    T2    T3    T4    HALF_VN     GAMMA N     REFERENCE
**    cd2   **    **    1     0.00  180.0 1.00  SAR 18/04/2008
clx   cd2   oh    ho    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
clx   cd2   oh    c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
clx   cd2   n3x   hn    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
clx   cd2   n3x   c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
clx   cd2   n3y   hn    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
clx   cd2   n3y   c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
cly   cd2   oh    ho    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
cly   cd2   oh    c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
cly   cd2   n3x   hn    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
cly   cd2   n3x   c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
cly   cd2   n3y   hn    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
cly   cd2   n3y   c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
n3x   c3    c3    n3y   1     1.40  0.00  3.00  SAR 06/05/2008 based on
**-c3-c3-**
n3x   cd2   oh    ho    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
n3y   cd2   oh    ho    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
n3x   cd2   oh    c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
n3y   cd2   oh    c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
n3x   cd2   n3y   hn    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
n3y   cd2   n3x   hn    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
n3x   cd2   n3y   c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
n3y   cd2   n3x   c3    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
n3x   c3    c3    hc    1     1.40  0.00  3.00  SAR 06/05/2008 based on
**-c3-c3-**
n3y   c3    c3    hc    1     1.40  0.00  3.00  SAR 06/05/2008 based on
**-c3-c3-**
```

```
n3x   c3    c3    h1    1     1.40  0.00  3.00  SAR 06/05/2008 based on
**-c3-c3-**
n3y   c3    c3    h1    1     1.40  0.00  3.00  SAR 06/05/2008 based on
**-c3-c3-**
hn    n3x   cd2   oh    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
hn    n3y   cd2   oh    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
c3    c3    n3x   hn    6     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
c3    c3    n3y   hn    6     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
h1    c3    n3x   hn    6     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
h1    c3    n3y   hn    6     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
c3    n3x   cd2   oh    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
c3    n3y   cd2   oh    1     0.00  180.0 2.00  SAR    06/05/2008    all
torsions **-**-cd2-** set to zero
c3    c3    n3x   c3    6     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
c3    c3    n3y   c3    6     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
h1    c3    n3x   c3    6     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
h1    c3    n3y   c3    6     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
cd2   n3x   c3    c3    1     0.30  0.00  3.00  SAR 06/05/2008 based on
c3-c3-n3-c3
cd2   n3y   c3    c3    1     0.30  0.00  3.00  SAR 06/05/2008 based on
c3-c3-n3-c3
cd2   n3x   c3    h1    1     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
cd2   n3y   c3    h1    1     1.80  0.00  3.00  SAR 06/05/2008 based on
**-c3-n3-**
```

Table A.23: Abridged WitsGAFFben.txt file for the second geometry optimisation run

```
A1    A2    A3    KTHETA      THETAEQ     REFERENCE
n3x   cd2   cly   50.00       96.00       SAR 06/05/2008 co-planar
                                           trans atoms
n3y   cd2   cly   50.00       106.00      SAR 06/05/2008 co-planar cis
                                           atoms
oh    cd2   cly   50.00       95.00       SAR 06/05/2008 co-planar
                                           trans atoms
clx   cd2   cly   50.00       106.00      SAR 06/05/2008 axial and
                                           equatorial atoms
oh    cd2   clx   50.00       90.00       SAR 06/05/2008 axial cl to
                                           equatorial o
n3x   cd2   clx   50.00       153.00      SAR 06/05/2008 axial cl to
                                           equatorial n3x
n3y   cd2   clx   50.00       111.00      SAR 06/05/2008 axial cl to
                                           equatorial n3y
cd2   n3x   c3    64.0        110.00      SAR 06/05/2008 from c3 n3 c3
cd2   n3y   c3    64.0        115.00      SAR 06/05/2008 from c3 n3 c3
cd2   oh    c3    62.1        115.00      SAR 06/05/2008 from c3 os c3
cd2   n3x   hn    47.1        107.00      SAR 06/05/2008 from c3 n3 hn
cd2   n3y   hn    47.1        105.00      SAR 06/05/2008 from c3 n3 hn
c3    n3x   hn    47.1        107.00      SAR 06/05/2008 from c3 n3 hn
c3    n3y   hn    47.1        105.00      SAR 06/05/2008 from c3 n3 hn
```

Table A.24: Abridged WitsGAFFstr.txt file for the third geometry optimisation run

```
B1    B2    KR          REQ         REFERENCE
cd2   n3x   350.0       2.390       SAR 06/05/2008
cd2   n3y   350.0       2.390       SAR 06/05/2008
cd2   oh    150.0       2.440       SAR 06/05/2008
cd2   clx   225.0       2.605       SAR 07/05/2008
cd2   cly   225.0       2.605       SAR 07/05/2008
hn    n3x   394.1       1.018       SAR 06/05/2008
hn    n3y   394.1       1.018       SAR 06/05/2008
```

Table A.25: Abridged WitsGAFFben.txt file for the third geometry optimisation run

```
A1    A2    A3    KTHETA      THETAEQ     REFERENCE
cd2   n3x   c3    64.0        110.00      SAR 06/05/2008 from c3 n3 c3
cd2   n3y   c3    64.0        115.00      SAR 06/05/2008 from c3 n3 c3
cd2   oh    c3    62.1        115.00      SAR 06/05/2008 from c3 os c3
cd2   n3x   hn    47.1        107.00      SAR 06/05/2008 from c3 n3 hn
cd2   n3y   hn    47.1        105.00      SAR 06/05/2008 from c3 n3 hn
c3    n3x   hn    47.1        109.92      SAR 07/05/2008 from c3 n3 hn
c3    n3y   hn    47.1        109.92      SAR 07/05/2008 from c3 n3 hn
```

Table A.26: Abridged WitsGAFFstr.txt file for the fourth geometry optimisation run

```
B1    B2    KR          REQ         REFERENCE
cd2   n3x   350.0       2.390       SAR 06/05/2008
cd2   n3y   350.0       2.390       SAR 06/05/2008
cd2   oh    150.0       2.440       SAR 06/05/2008
cd2   clx   250.0       2.590       SAR 07/05/2008
cd2   cly   250.0       2.590       SAR 07/05/2008
hn    n3x   394.1       1.018       SAR 06/05/2008
hn    n3y   394.1       1.018       SAR 06/05/2008
```

Table A.27: Abridged WitsGAFFben.txt file for the fourth geometry optimisation run

```
A1    A2    A3    KTHETA      THETAEQ     REFERENCE
oh    cd2   cly   50.00       90.00       SAR    07/05/2008    co-planar
trans atoms
oh    cd2   clx   50.00       90.00       SAR  06/05/2008  axial  cl  to
equatorial o
n3x   cd2   clx   50.00       153.00      SAR  06/05/2008  axial  cl  to
equatorial n3x
n3y   cd2   clx   50.00       111.00      SAR  06/05/2008  axial  cl  to
equatorial n3y
cd2   n3x   c3    64.0        110.00      SAR 06/05/2008 from c3 n3 c3
cd2   n3y   c3    64.0        115.00      SAR 06/05/2008 from c3 n3 c3
cd2   oh    c3    62.1        115.00      SAR 06/05/2008 from c3 os c3
cd2   n3x   hn    47.1        107.00      SAR 06/05/2008 from c3 n3 hn
cd2   n3y   hn    47.1        105.00      SAR 06/05/2008 from c3 n3 hn
c3    n3x   hn    47.1        109.92      SAR 07/05/2008 from c3 n3 hn
c3    n3y   hn    47.1        109.92      SAR 07/05/2008 from c3 n3 hn
```

Table A.28: Abridged WitsGAFFstr.txt file for the fifth geometry optimisation run

B1	B2	KR	REQ	REFERENCE
cd2	oh	150.0	2.440	SAR 01/05/2008
cd2	n3x	300.0	2.390	SAR 07/05/2008
cd2	n3y	300.0	2.390	SAR 07/05/2008
cd2	clx	250.0	2.500	SAR 07/05/2008
cd2	cly	250.0	2.500	SAR 07/05/2008

Table A.29: Abridged WitsGAFFstr.txt file for the sixth geometry optimisation run

B1	B2	KR	REQ	REFERENCE
cd2	oh	125.0	2.440	SAR 01/05/2008
cd2	n3x	275.0	2.390	SAR 07/05/2008
cd2	n3y	275.0	2.390	SAR 07/05/2008
cd2	clx	250.0	2.500	SAR 07/05/2008
cd2	cly	250.0	2.500	SAR 07/05/2008

Table A.30: Abridged WitsGAFFstr.txt file for the seventh geometry optimisation run

B1	B2	KR	REQ	REFERENCE
cd2	oh	125.0	2.400	SAR 01/05/2008
cd2	n3x	275.0	2.380	SAR 07/05/2008
cd2	n3y	275.0	2.380	SAR 07/05/2008
cd2	clx	250.0	2.500	SAR 07/05/2008
cd2	cly	250.0	2.500	SAR 07/05/2008
hn	n3x	394.1	1.018	SAR 06/05/2008
hn	n3y	394.1	1.018	SAR 06/05/2008

Table A.31: Cy_2-en/Cd Data After the Various Geometry Optimisations

		C-C	C-N	C-O	N-Cd	O-Cd	Cd-Cl	C-C-C	C-C-N	C-C-O	C-N-C	C-N-Cd	C-O-Cd	O-Cd-N	N-Cd-Cl	O-Cd-Cl
XRD		Cy2en_Cd_040														
	Average	1.521	1.480	1.439	2.348	2.382	2.494	110.7	111.0	111.4	113.1	112.5	114.5	108.1	116.5	92.5
	Std Dev	0.009	0.013	0.006	0.020		0.000	0.4	1.9	1.1	2.4	8.2		51.1	25.1	3.3
Geom op		Cy2en_Cd_041														
initial guess	Average	1.550	1.492	1.448	2.356	2.390	2.611	111.2	110.6	110.8	115.9	106.0	104.4	120.7	114.9	92.9
run 1	Std Dev	0.014	0.007	0.022	0.030		0.000	0.2	1.6	2.6	5.7	6.0		56.0	42.7	6.3
Geom op		Cy2en_Cd_042														
run 2	Average	1.550	1.490	1.446	2.360	2.395	2.610	111.195	110.444	110.571	116.932	109.226	105.061	118.100	115.823	48.040
	Std Dev	0.013	0.003	0.018	0.023		0.001	0.313	1.773	2.305	3.196	8.123		53.517	25.616	55.378
Geom op		Cy2en_Cd_043														
run 3	Average	1.550	1.491	1.446	2.360	2.394	2.605	111.199	110.476	110.565	116.153	108.436	105.089	118.462	116.148	85.857
	Std Dev	0.013	0.002	0.018	0.023		0.001	0.345	2.083	2.336	3.379	7.828		53.976	25.449	2.426
Geom op		Cy2en_Cd_044														
run 4	Average	1.545	1.485	1.432	2.386	2.431	2.590	111.109	109.415	109.618	112.411	111.499	112.639	106.824	117.439	90.592
	Std Dev	0.004	0.003	0.001	0.002		0.001	0.445	2.584	0.777	0.239	3.815		49.391	24.721	1.191
Geom op		Cy2en_Cd_045														
run 5	Average	1.545	1.485	1.432	2.386	2.430	2.500	111.108	109.446	109.616	112.371	111.548	112.658	106.829	117.452	90.527
	Std Dev	0.004	0.003	0.001	0.003		0.001	0.445	2.615	0.784	0.277	3.916		49.389	24.701	1.165
Geom op		Cy2en_Cd_046														
run 6	Average	1.545	1.485	1.432	2.385	2.428	2.500	111.108	109.441	109.616	112.369	111.549	112.681	106.842	117.452	90.523
	Std Dev	0.004	0.003	0.001	0.003		0.001	0.443	2.622	0.787	0.280	3.916		49.386	24.704	1.154

Geom op		Cy2en_Cd_047														
run 7	Average	1.545	1.484	1.432	2.376	2.391	2.500	111.100	109.350	109.609	112.309	111.585	113.075	107.156	117.444	90.409
	Std Dev	0.003	0.003	0.001	0.002		0.001	0.425	2.764	0.872	0.296	3.911		49.347	24.765	0.932
Comparisons		040 - 041														
	Average	0.029	0.012	0.009	0.007	0.008	0.117	0.476	0.469	0.604	2.768	6.428	10.172	12.563	1.543	0.423
	Std Dev	0.005	0.006	0.016	0.010		0.000	0.184	0.253	1.502	3.289	2.209		4.893	17.634	3.074
Comparisons		040 - 042														
	Average	0.028	0.010	0.007	0.012	0.013	0.116	0.457	0.605	0.799	3.824	3.240	9.479	9.997	0.657	44.438
	Std Dev	0.003	0.011	0.013	0.003		0.001	0.079	0.102	1.164	0.769	0.109		2.422	0.515	52.102
Comparisons		040 - 043														
	Average	0.028	0.011	0.007	0.012	0.012	0.111	0.462	0.573	0.805	3.045	4.030	9.450	10.359	0.332	6.621
	Std Dev	0.004	0.011	0.013	0.003		0.001	0.046	0.207	1.195	0.952	0.405		2.880	0.349	0.850
Comparisons		040 - 044														
	Average	0.024	0.004	0.007	0.038	0.049	0.096	0.372	1.635	1.752	0.696	0.967	1.901	1.279	0.958	1.886
	Std Dev	0.006	0.010	0.004	0.018		0.000	0.053	0.709	0.365	2.188	4.417		1.704	0.380	2.085
Comparisons		040 - 045														
	Average	0.024	0.005	0.007	0.037	0.047	0.006	0.370	1.604	1.754	0.737	0.918	1.881	1.274	0.972	1.951
	Std Dev	0.006	0.010	0.004	0.018		0.000	0.053	0.740	0.358	2.150	4.317		1.707	0.399	2.111
Comparisons		040 - 046														
	Average	0.024	0.005	0.007	0.037	0.045	0.006	0.370	1.608	1.754	0.739	0.917	1.858	1.260	0.972	1.955
	Std Dev	0.006	0.010	0.004	0.018		0.000	0.052	0.746	0.355	2.147	4.317		1.710	0.397	2.122
Comparisons		040 - 047														
	Average	0.024	0.004	0.007	0.028	0.009	0.006	0.363	1.699	1.761	0.798	0.881	1.465	0.947	0.964	2.069
	Std Dev	0.006	0.010	0.004	0.018		0.000	0.033	0.888	0.270	2.132	4.322		1.749	0.336	2.344

Table A.32: The Calculated Energies for Selected M-N and M-O Bond Lengths

M-O	M-N	E
2.000	2.000	25.368
2.000	2.100	22.964
2.000	2.200	21.464
2.000	2.300	20.837
2.000	2.400	21.038
2.000	2.500	22.017
2.000	2.600	23.722
2.100	2.000	24.676
2.100	2.100	22.302
2.100	2.200	20.827
2.100	2.300	20.219
2.100	2.400	20.434
2.100	2.500	21.419
2.100	2.600	23.121
2.200	2.000	24.237
2.200	2.100	21.885
2.200	2.200	20.429
2.200	2.300	19.835
2.200	2.400	20.058
2.200	2.500	21.043
2.200	2.600	22.736
2.300	2.000	24.054
2.300	2.100	21.718
2.300	2.200	20.274
2.300	2.300	19.688
2.300	2.400	19.913
2.300	2.500	20.893
2.300	2.600	22.573
2.400	2.000	24.132
2.400	2.100	21.807
2.400	2.200	20.368
2.400	2.300	19.784
2.400	2.400	20.004
2.400	2.500	20.972
2.400	2.600	22.633
2.500	2.000	24.477
2.500	2.100	22.155

2.500	2.200	20.716
2.500	2.300	20.126
2.500	2.400	20.336
2.500	2.500	21.287
2.500	2.600	22.922
2.600	2.000	25.093
2.600	2.100	22.767
2.600	2.200	21.322
2.600	2.300	20.721
2.600	2.400	20.913
2.600	2.500	21.840
2.600	2.600	23.443

Figure A.1: The VISTA histogram of the Cd(II)—O(H)(C) bond length

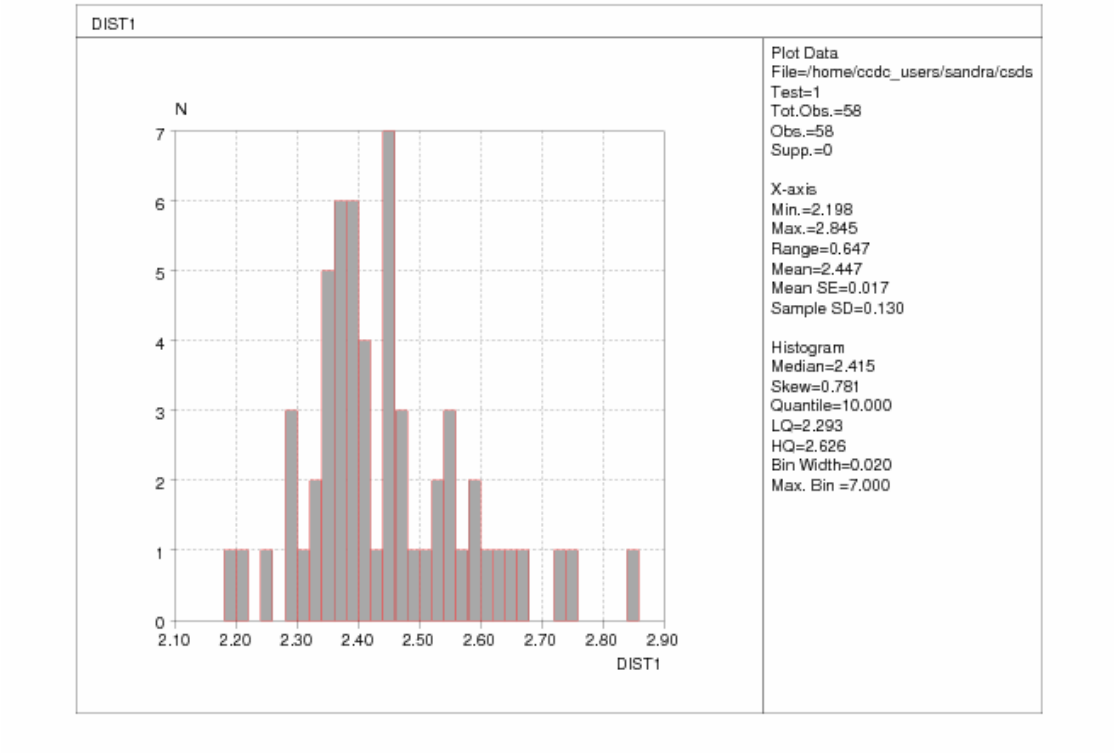


Figure A.2: The VISTA histogram of the Cd(II) —O(C) bond length

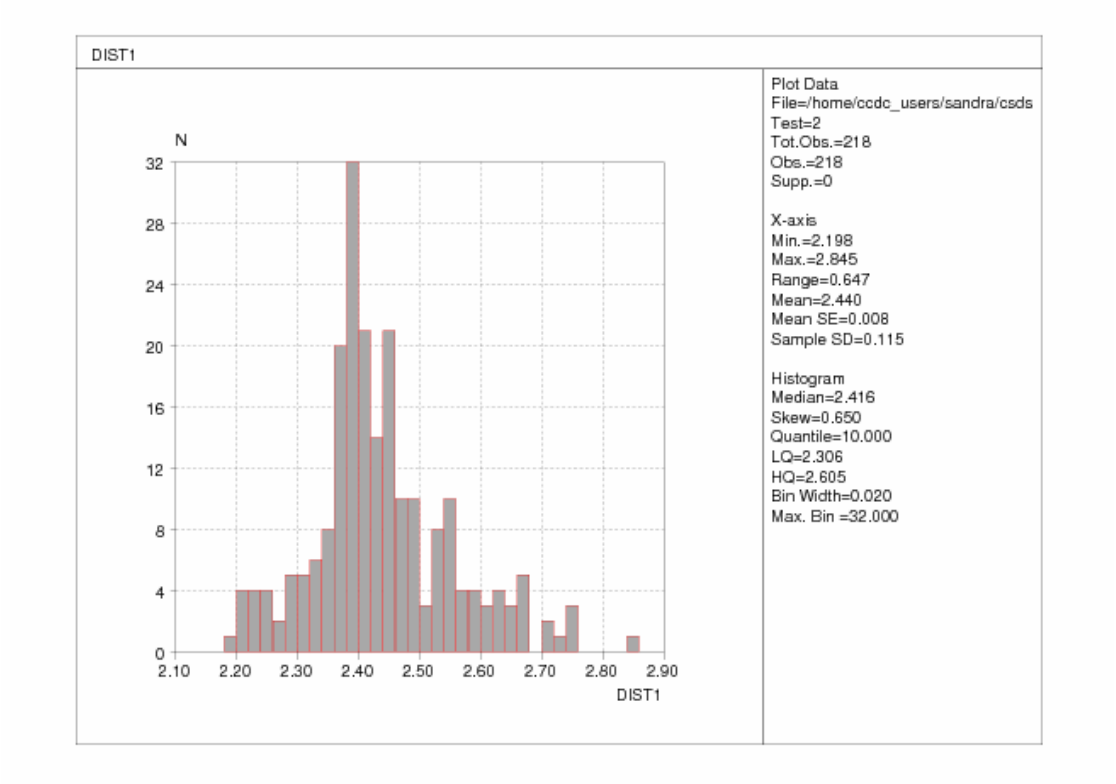


Figure A.3: The VISTA histogram of the Cd(II) —N(H)(C)(C) bond length

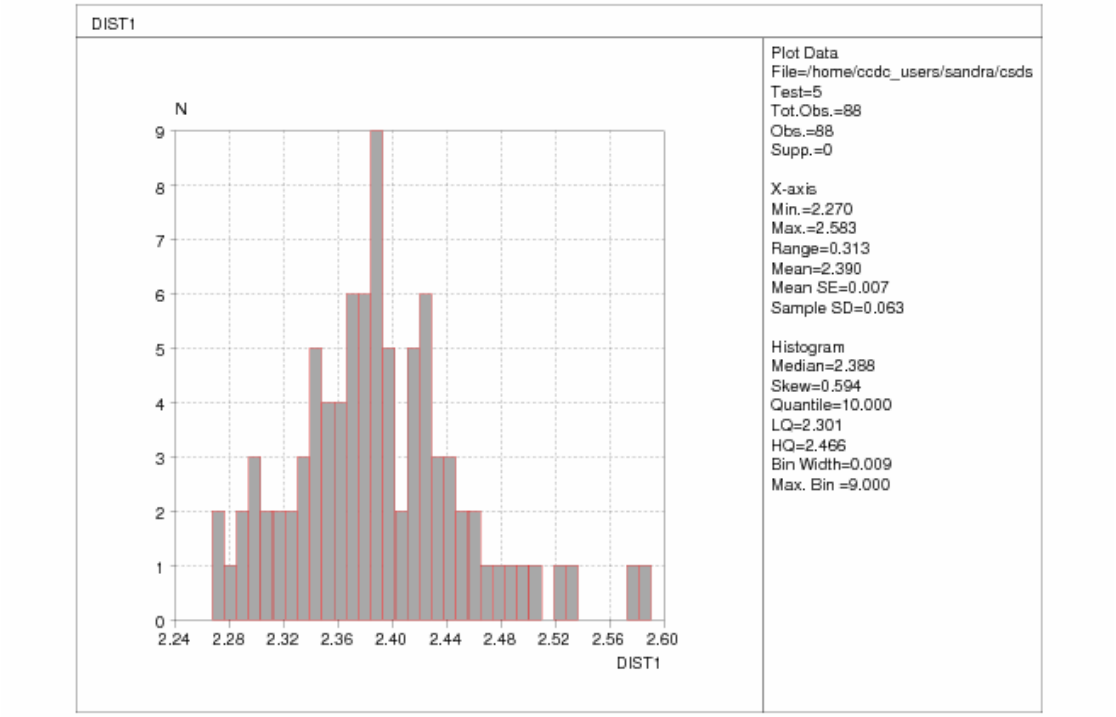


Figure A.4: The VISTA histogram of the Cd(II) —Cl bond length

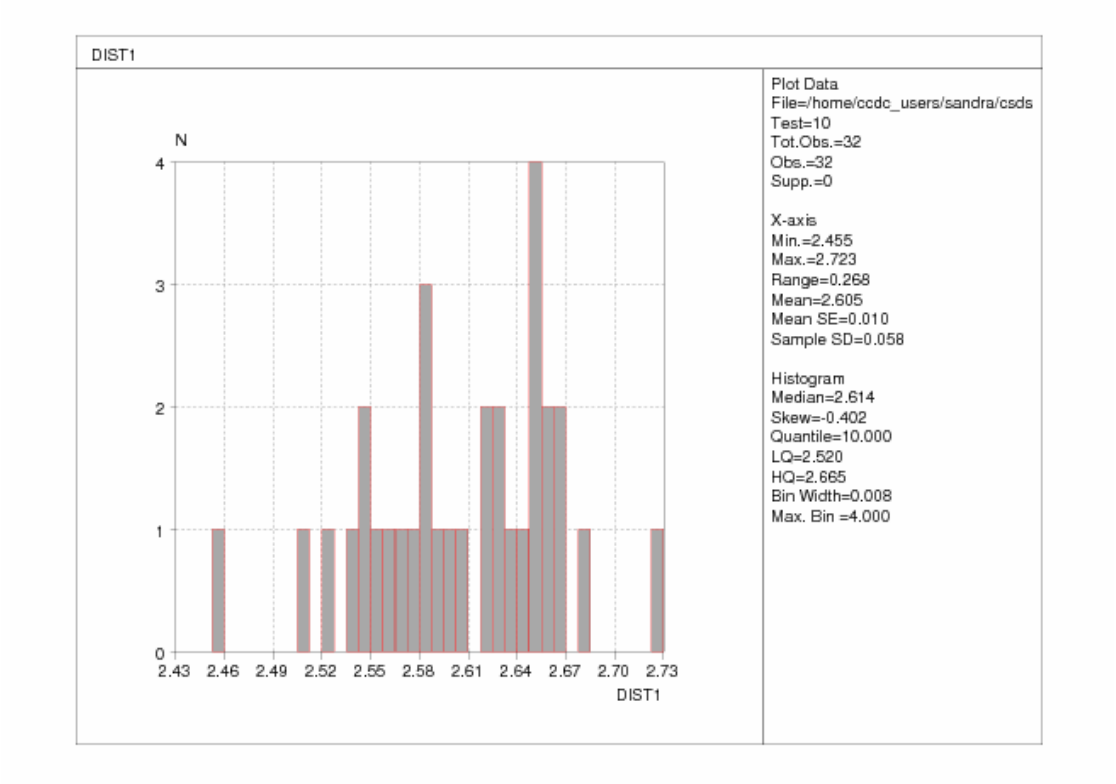


Figure A.5: The VISTA histogram of the N—Cd(II) —N bond angle

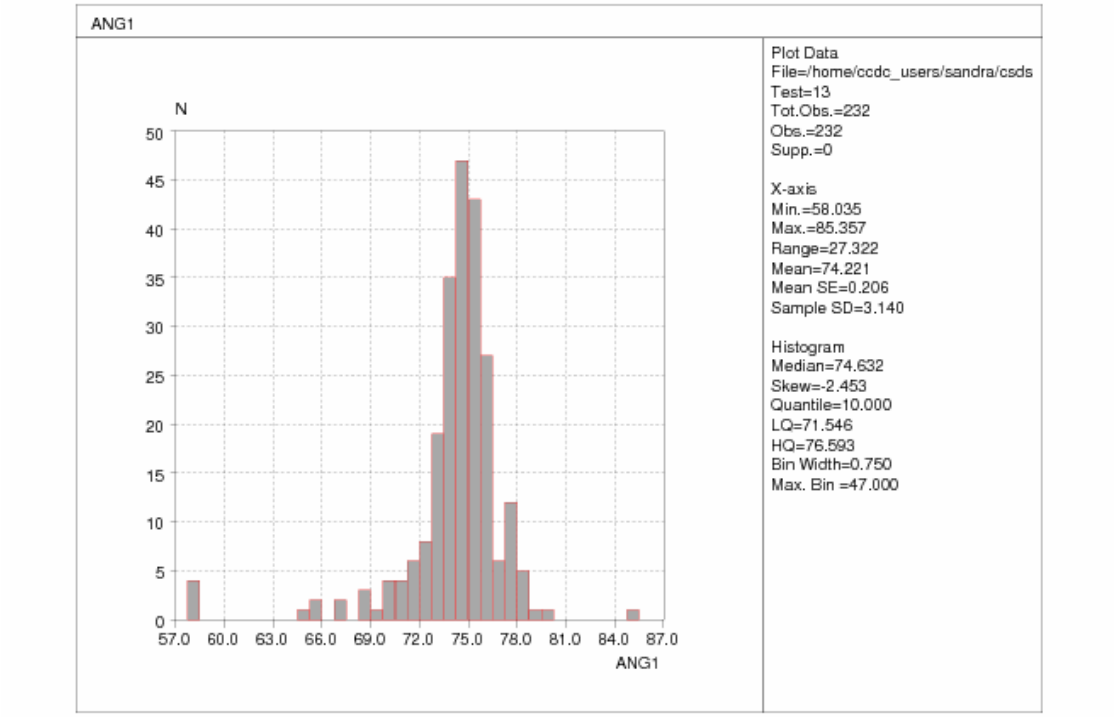


Figure A.6: The VISTA histogram of the N—Cd(II) —O bond angle

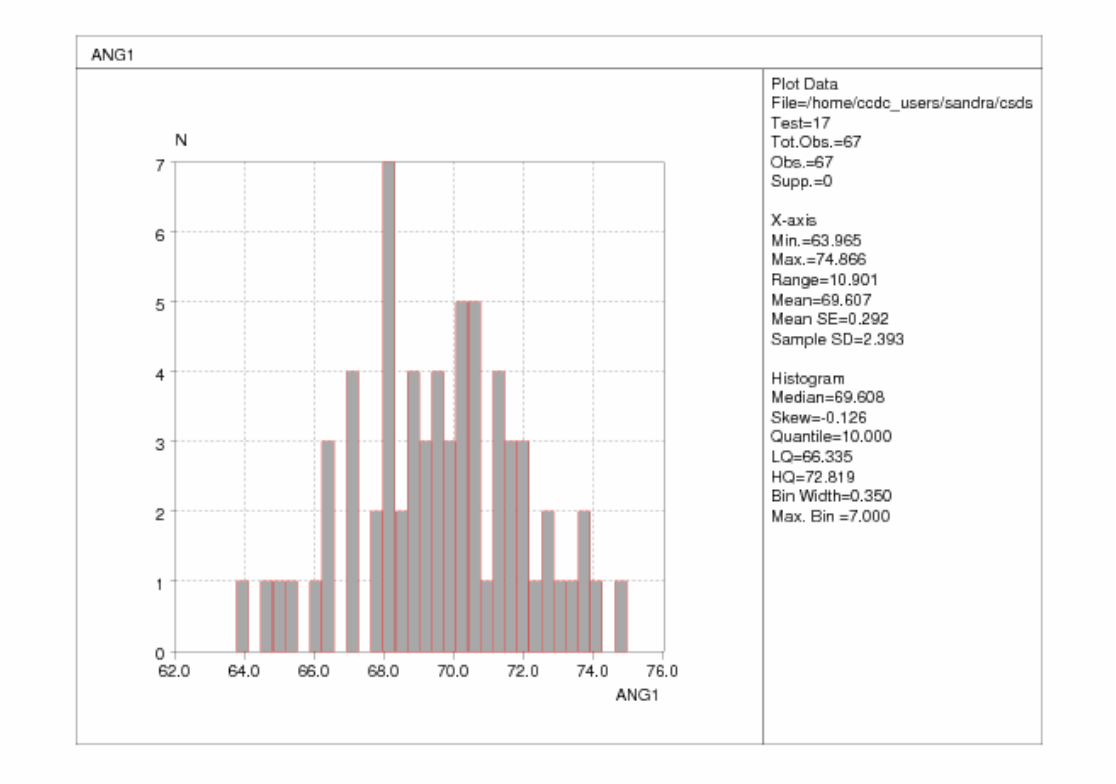


Figure A.7: The VISTA histogram of the Cl—Cd(II) —Cl bond angle

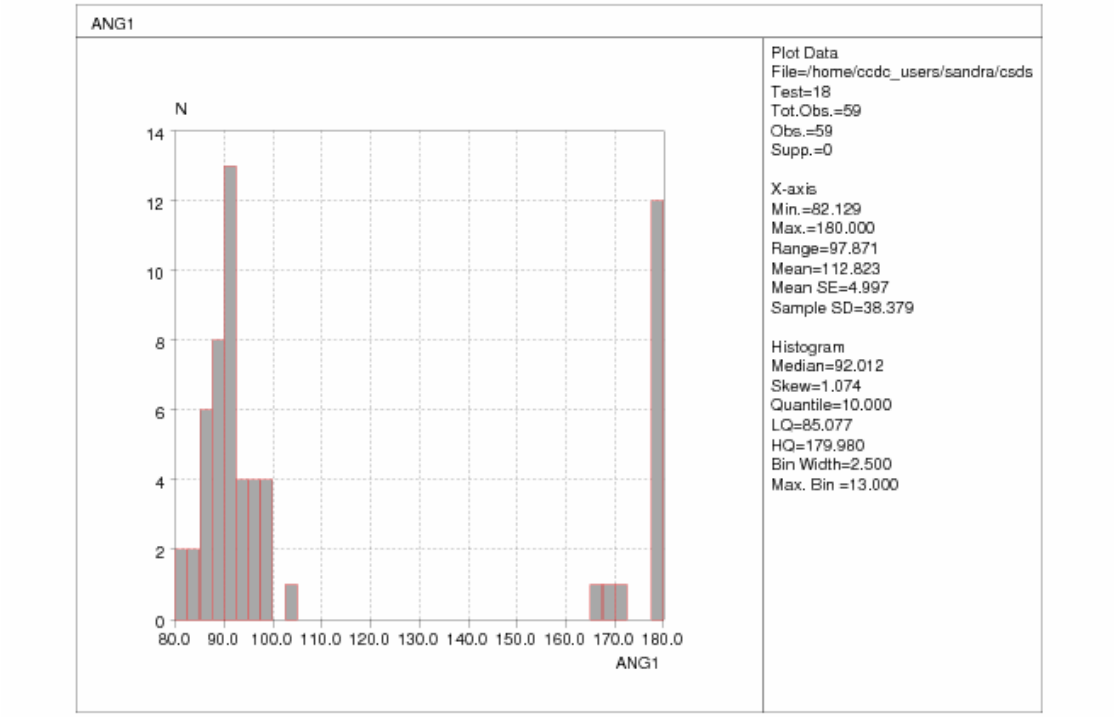


Figure A.8: The VISTA histogram of the Cl—Cd(II) —O(H)(R) bond angle

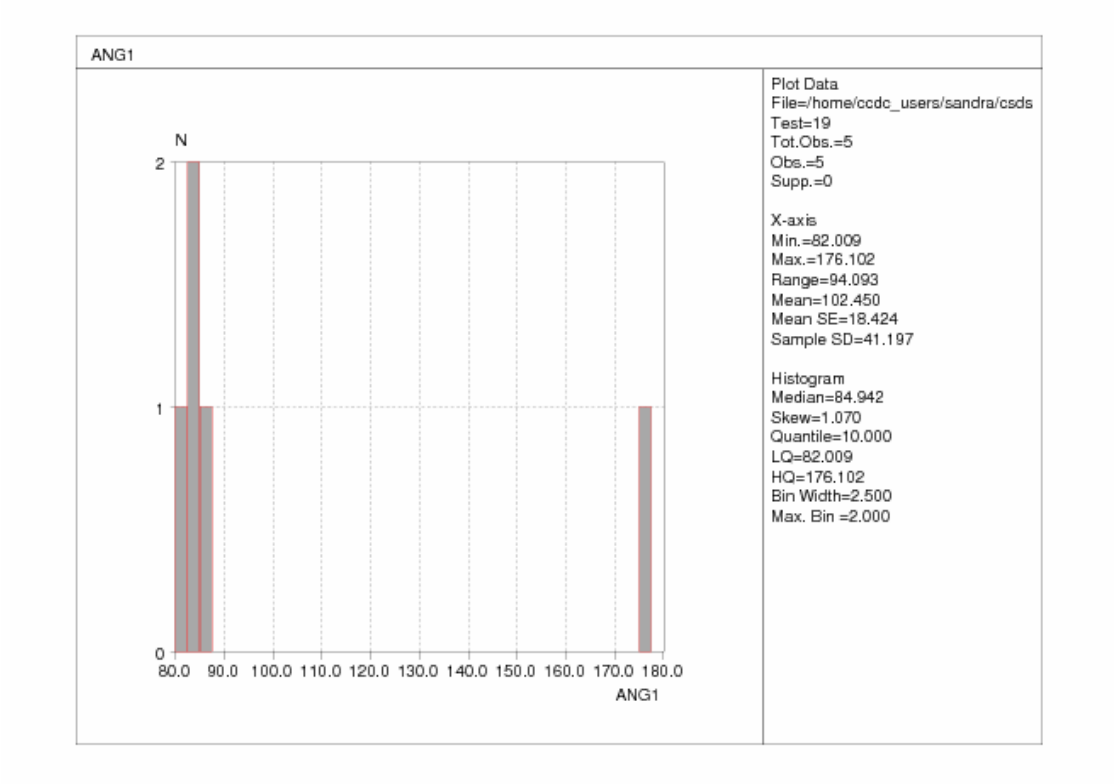
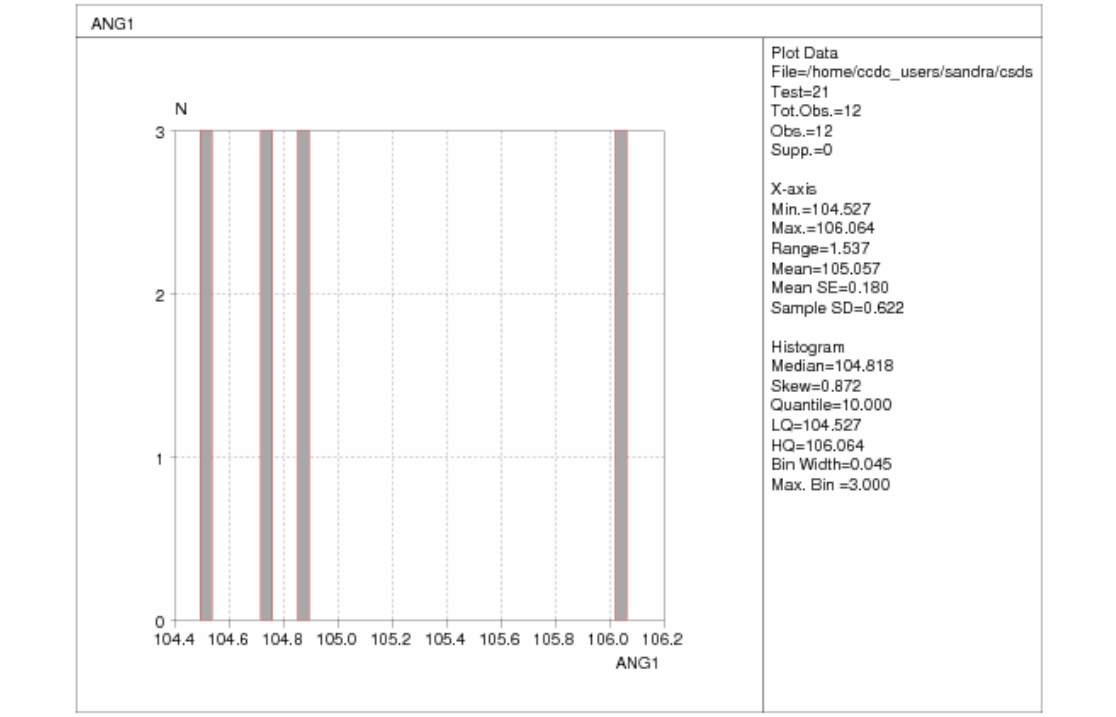


Figure A.9: The VISTA histogram of the Cl—Cd(II) —N(H)(R) bond angle



Appendix B – NMR Data

All NMR data was generated in the manner described in Chapter 2.

Figure B.1: The ^{1}H NMR of Cy_2-en (Sample 1)

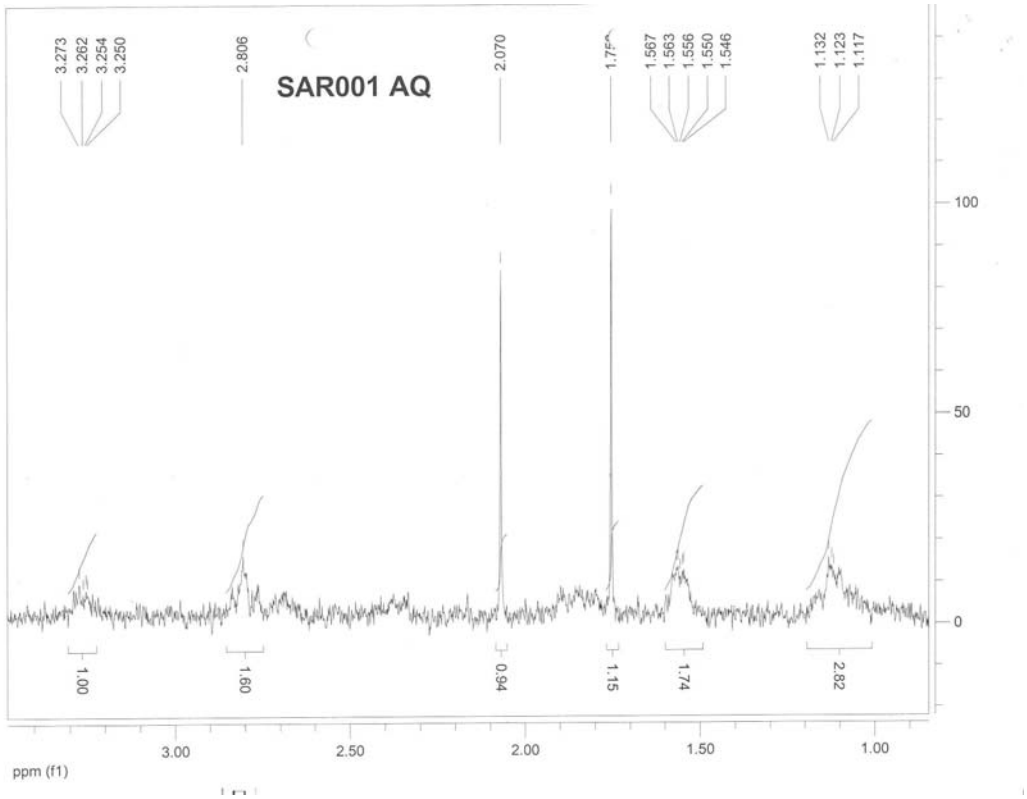


Figure B.2: The ^{13}C NMR of Cy_2-en (Sample 1)

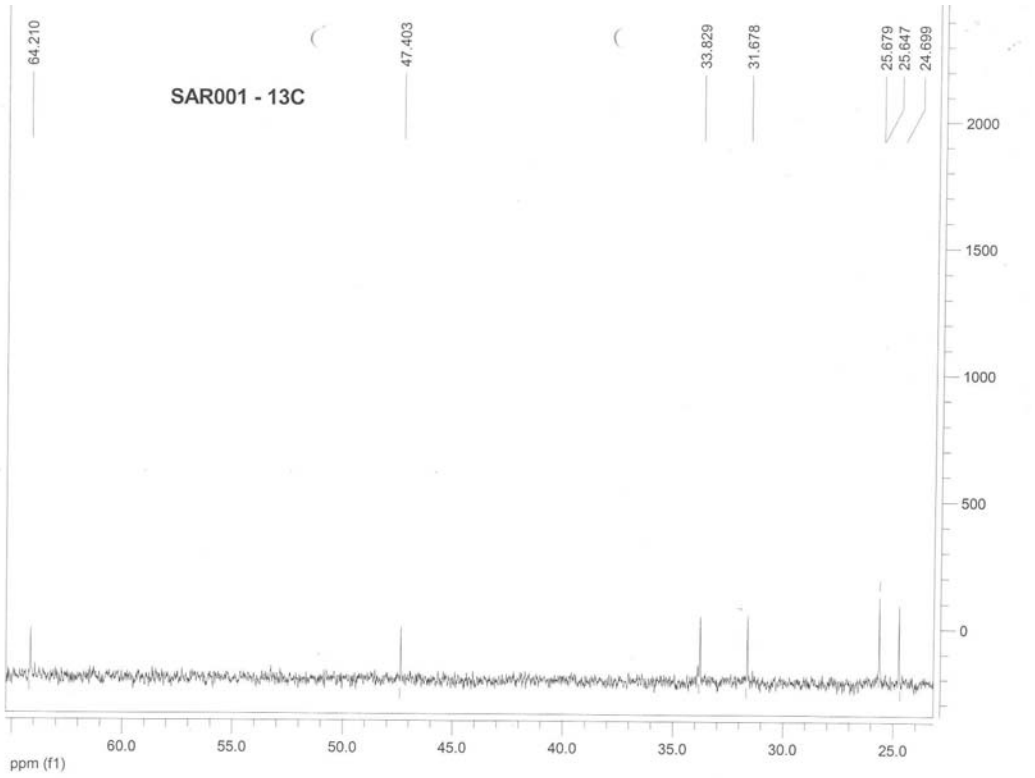


Figure B.3: The ^{1}H NMR of Cy_2-en (Sample 2)

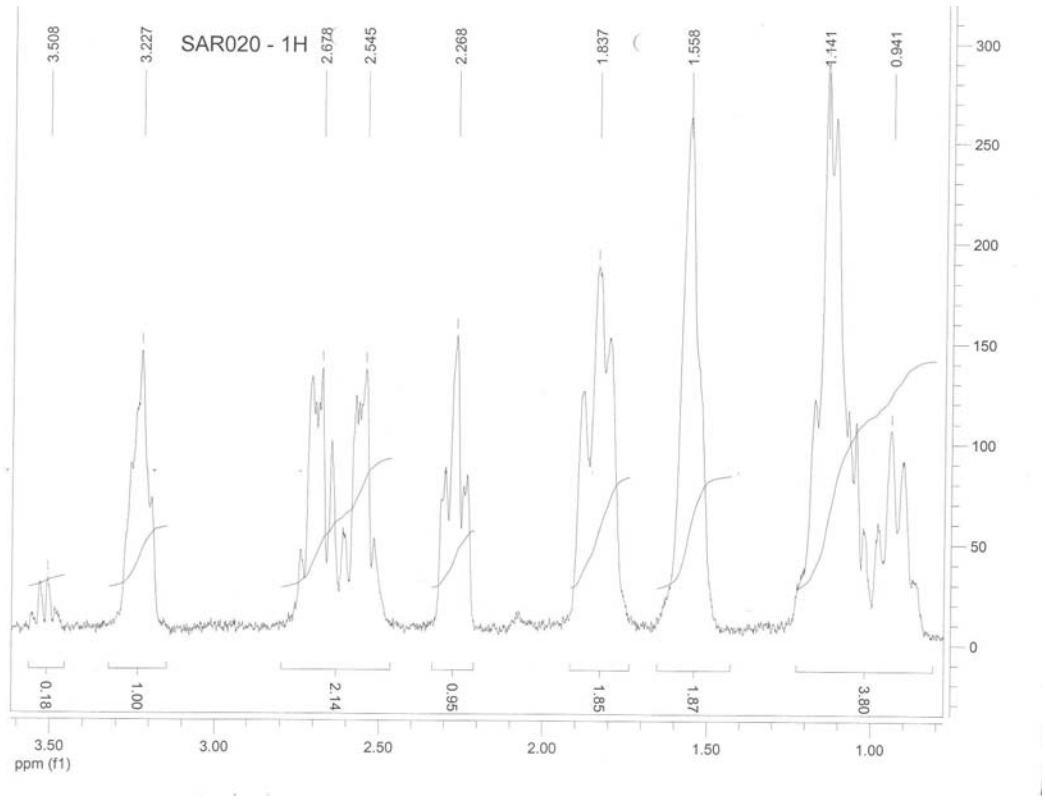


Figure B.4: The ^{13}C NMR of Cy_2-en (Sample 2)

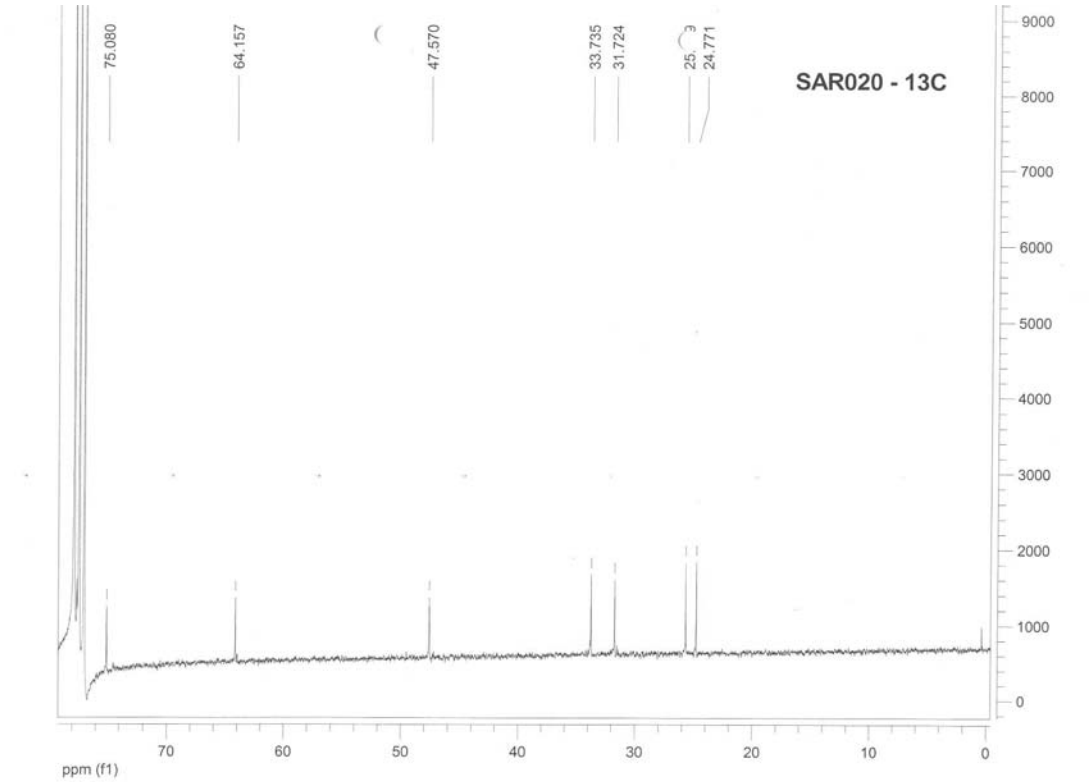


Figure B.5: The ^{1}H NMR of Cy_2-en (Sample 3)

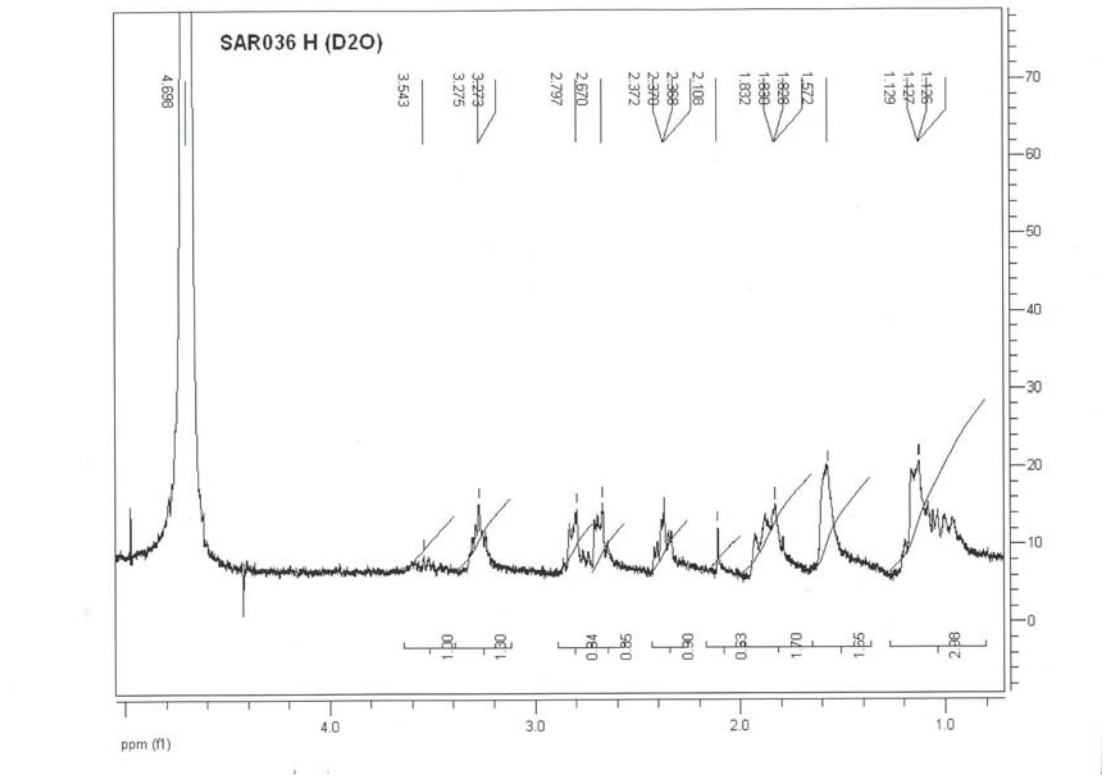


Figure B.6: The ^{13}C NMR of Cy_2-en (Sample 3)

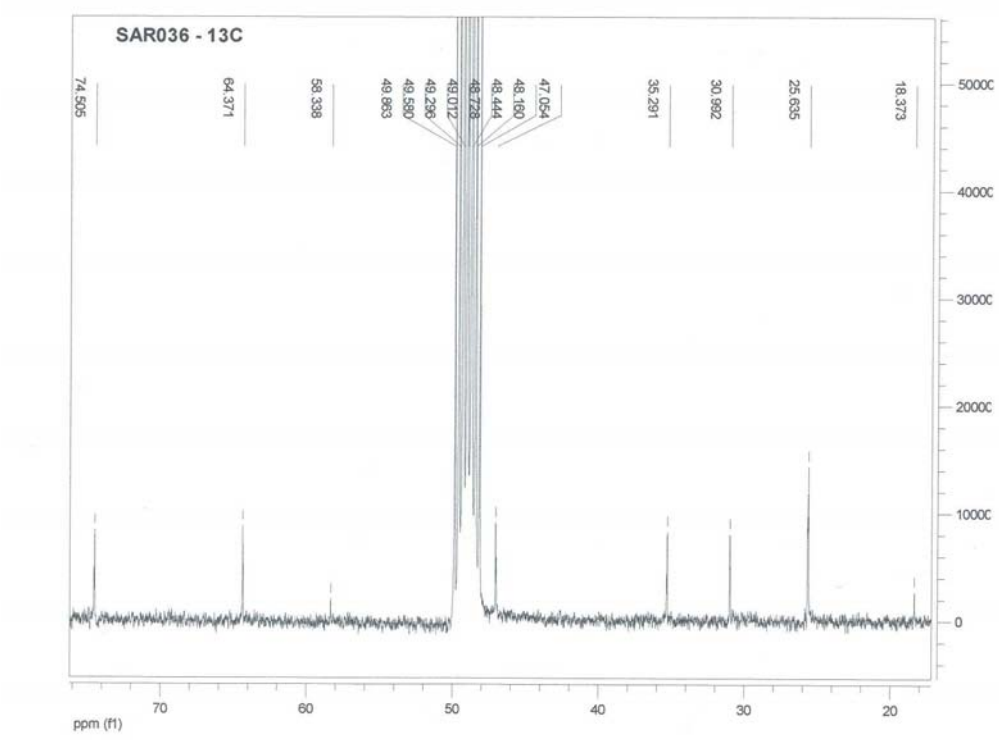


Figure B.7: The ^{1}H NMR of Cy_2-tn (Sample 1)

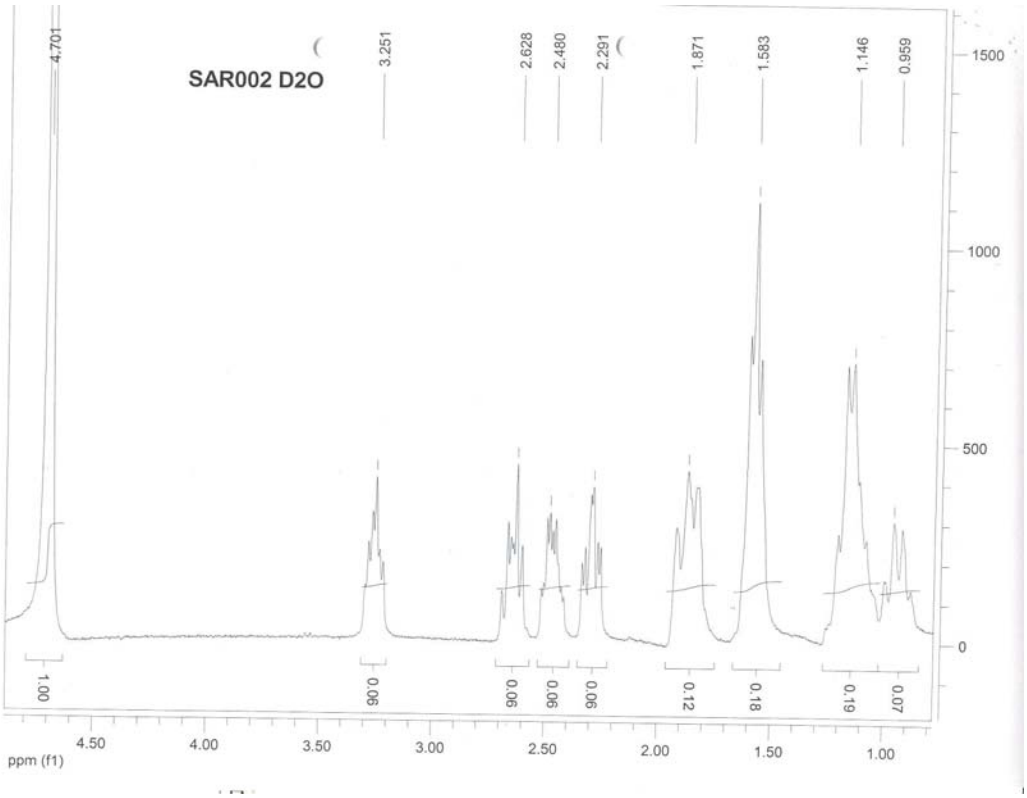


Figure B.8: The ^{13}C NMR of Cy_2-tn (Sample 1)

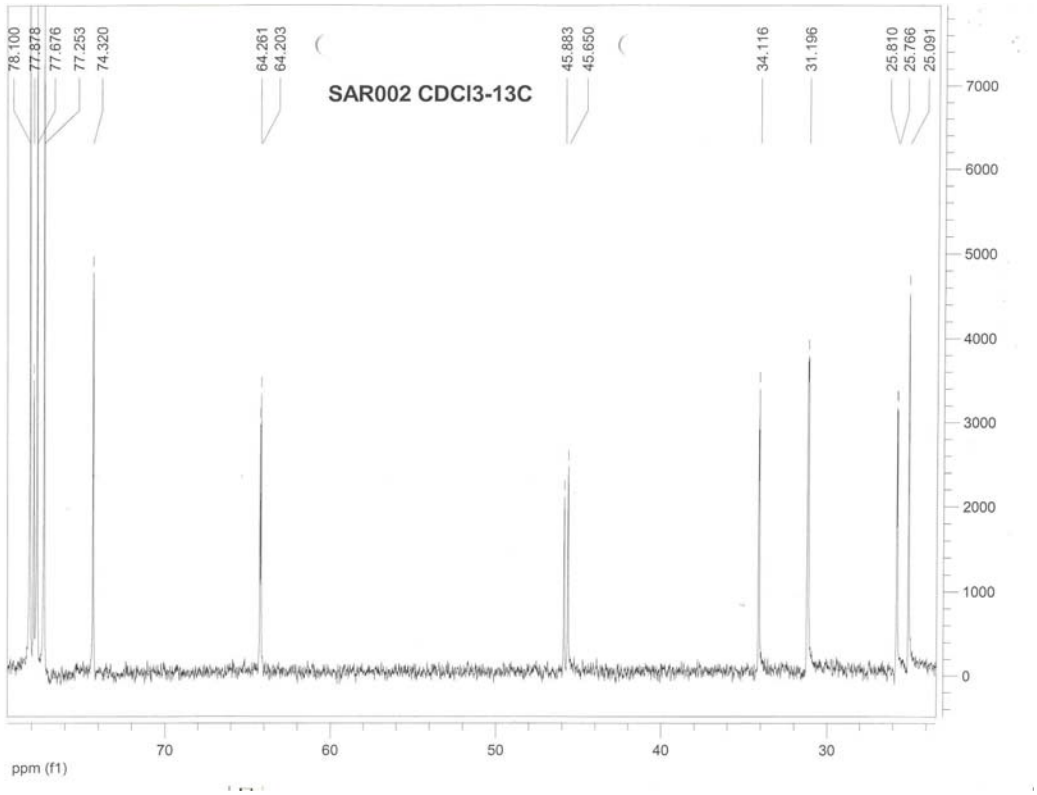


Figure B.9: The ^{1}H NMR of Cy_2-tn (Sample 2)

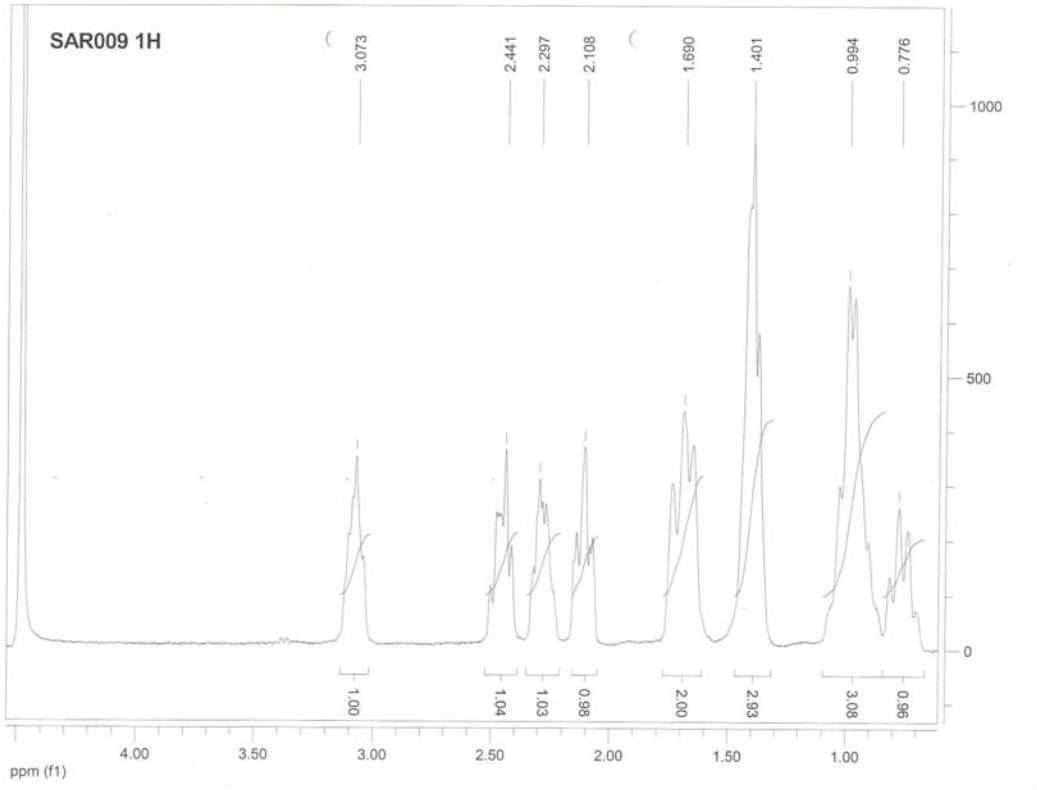


Figure B.10: The ^{13}C NMR of Cy_2-tn (Sample 2)

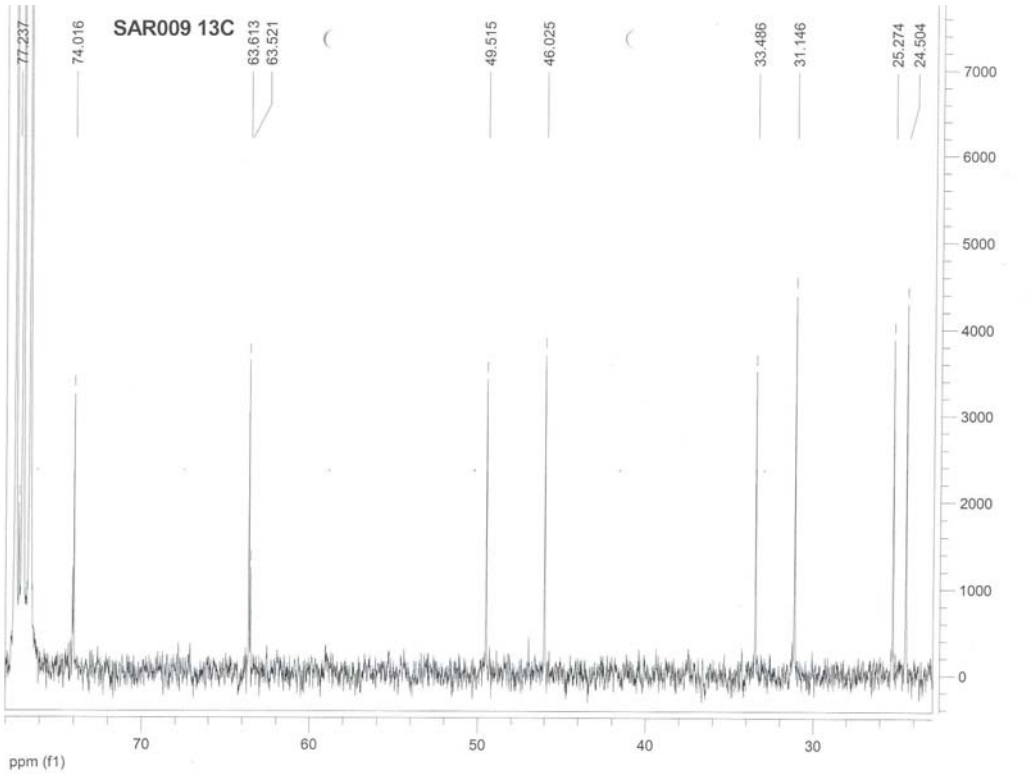


Figure B.11: The ^{1}H NMR of Cy_2-dien (Sample 1)

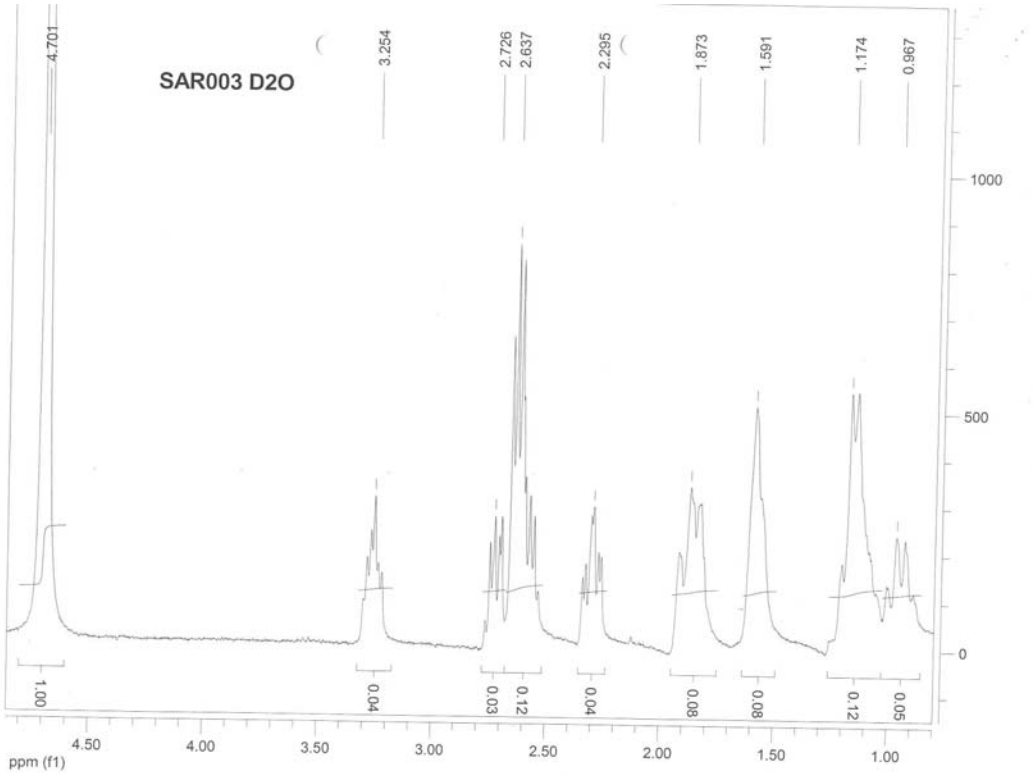


Figure B.12: The ^{13}C NMR of Cy_2-dien (Sample 1)

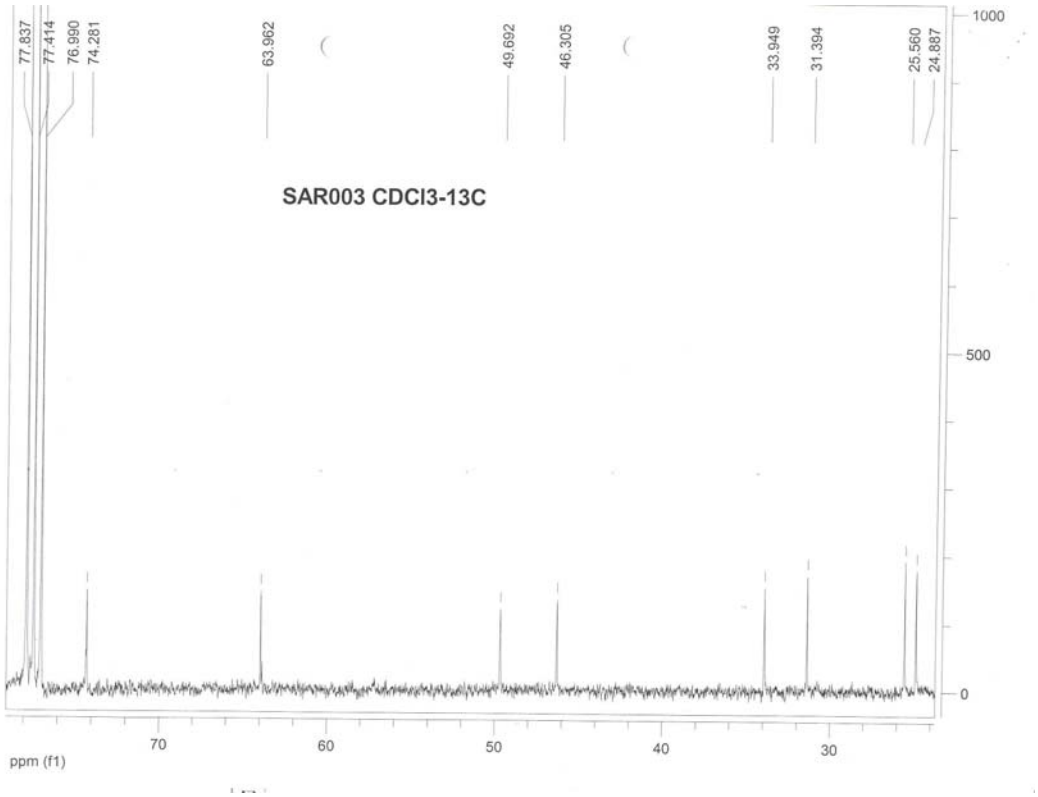


Figure B.13: The ^{1}H NMR of Cy_2-dien (Sample 2)

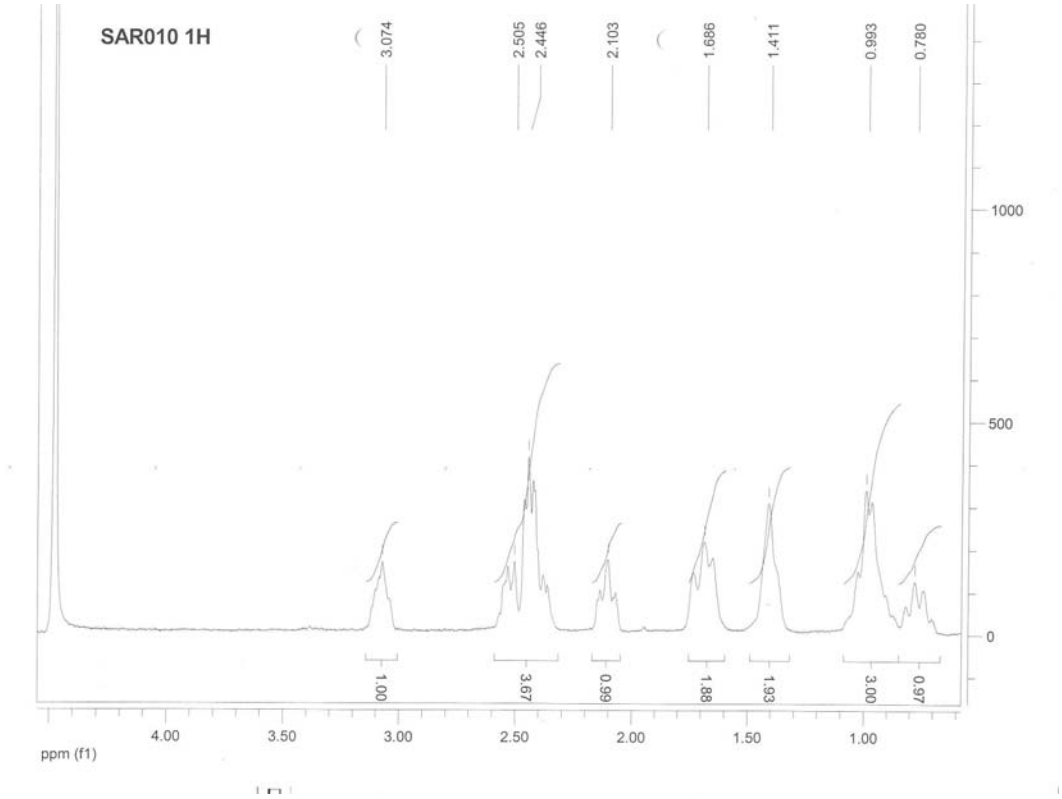


Figure B.14: The ^{13}C NMR of Cy_2-dien (Sample 2)

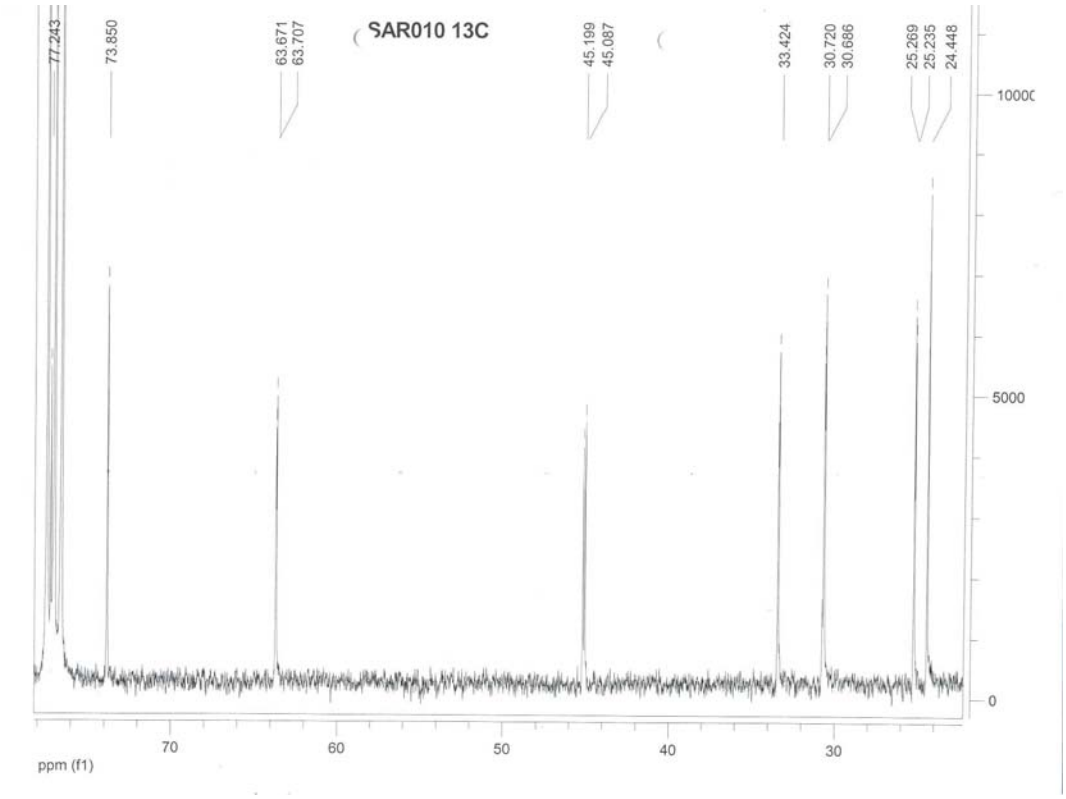


Figure B.15: The ^{1}H NMR of Cy_2-Otn (Sample 1)

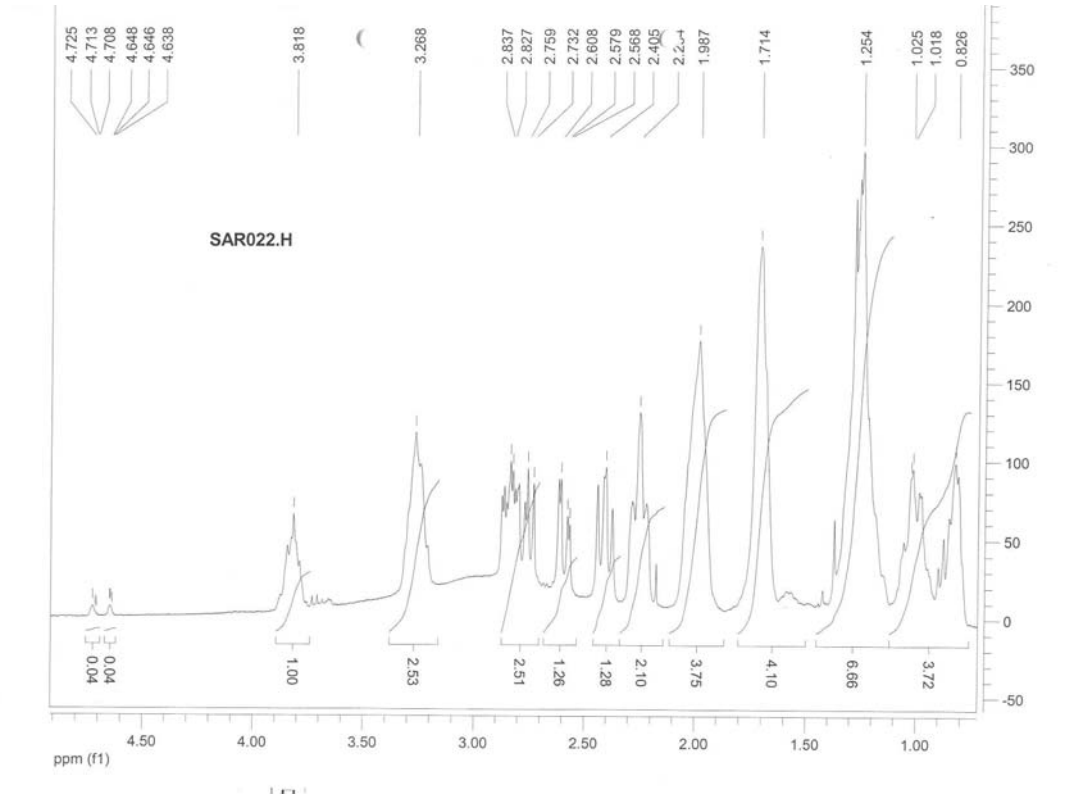


Figure B.16: The ^{13}C NMR of Cy_2-Otn (Sample 1)

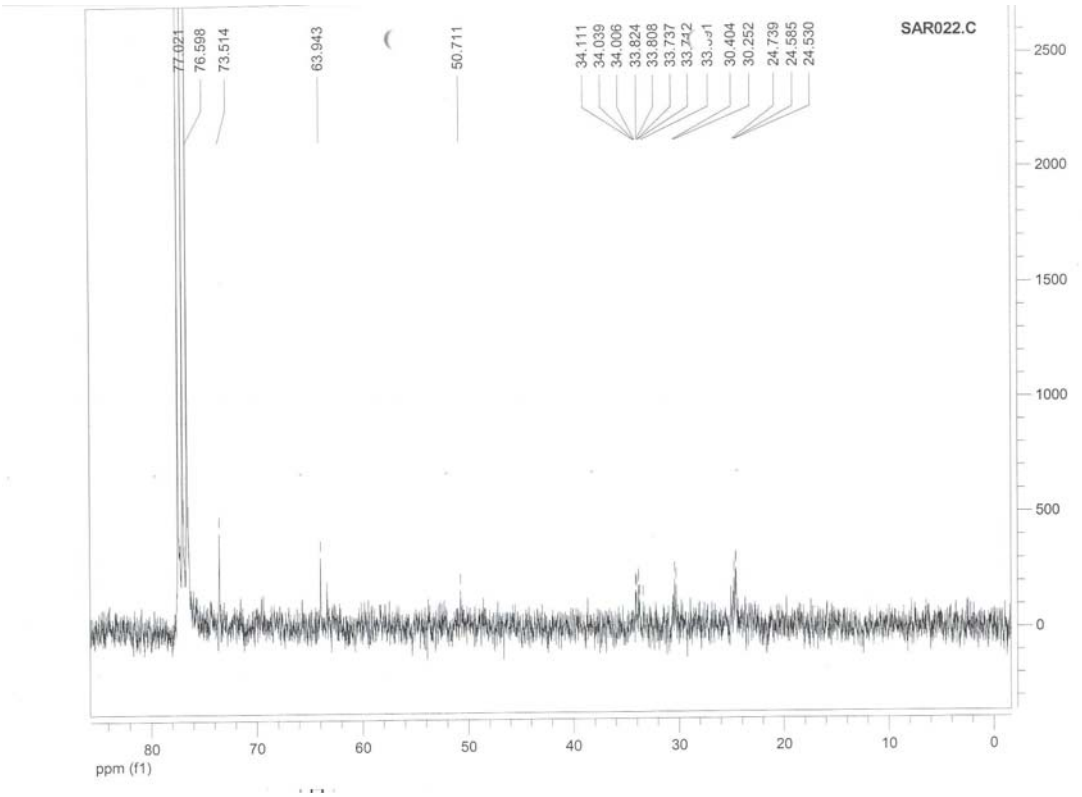


Figure B.17: The ^{1}H NMR of Cy_2-Otn (Sample 2)

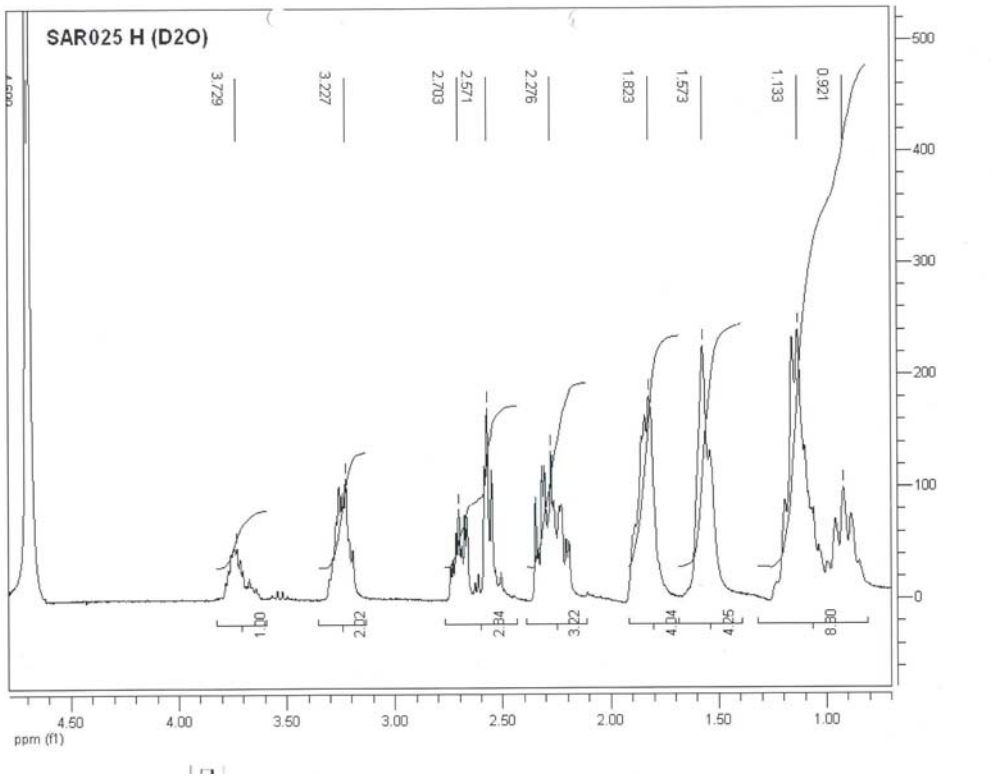


Figure B.18: The ^{13}C NMR of Cy_2-Otn (Sample 2)

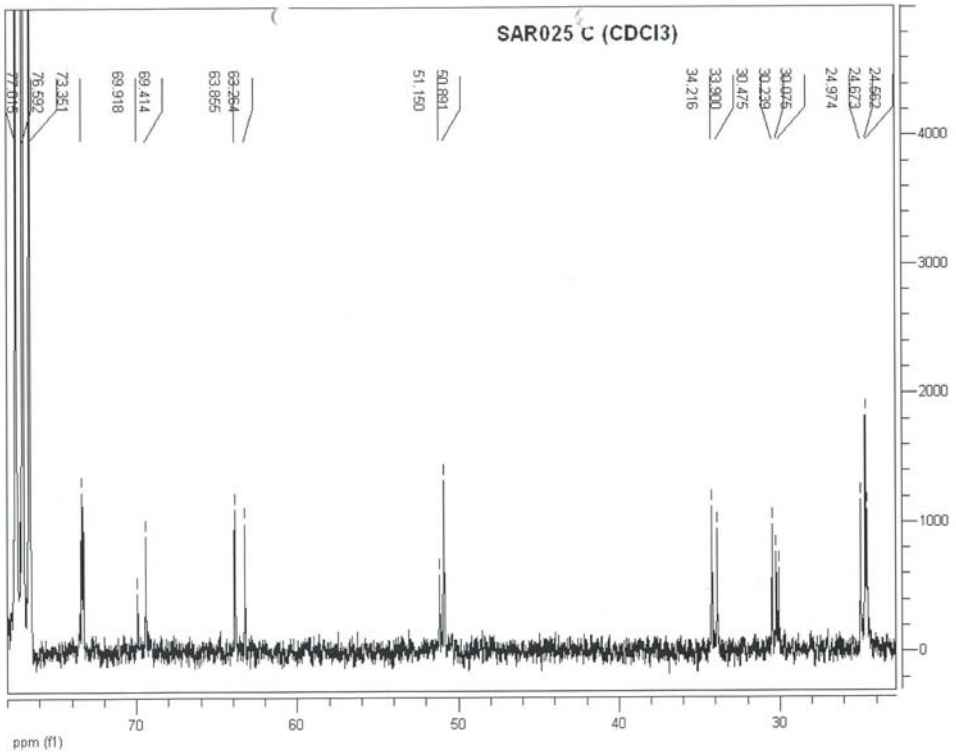


Figure B.19: The ^{1}H NMR of Cy_2-Otn (Sample 3)

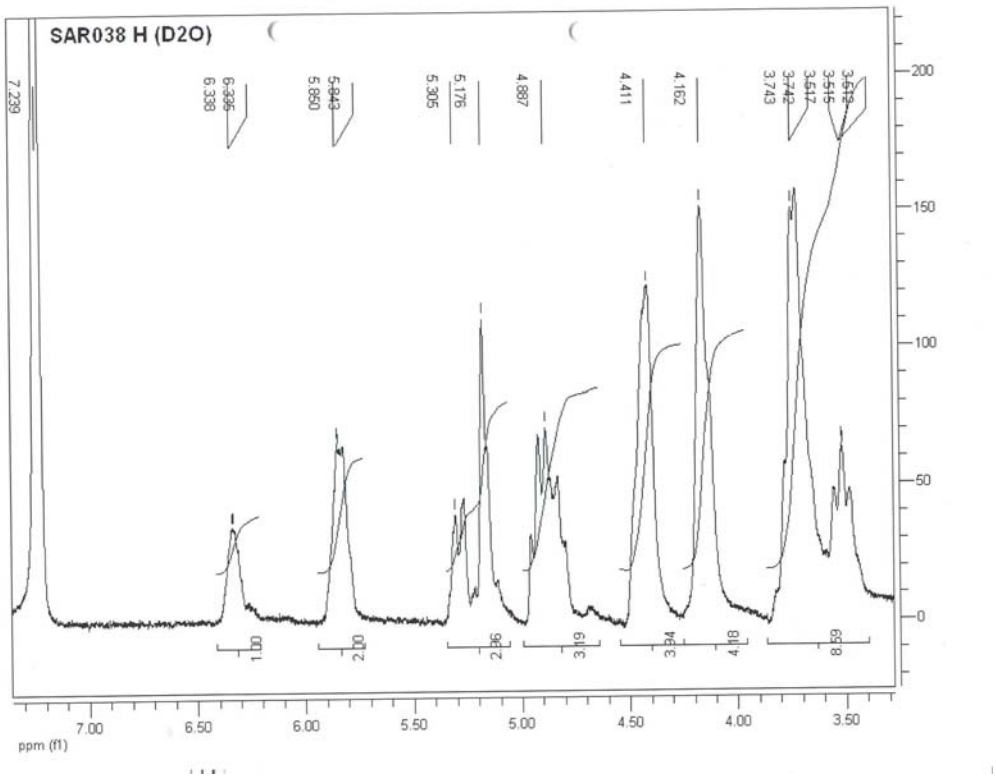


Figure B.20: The ^{13}C NMR of Cy_2-Otn (Sample 3)

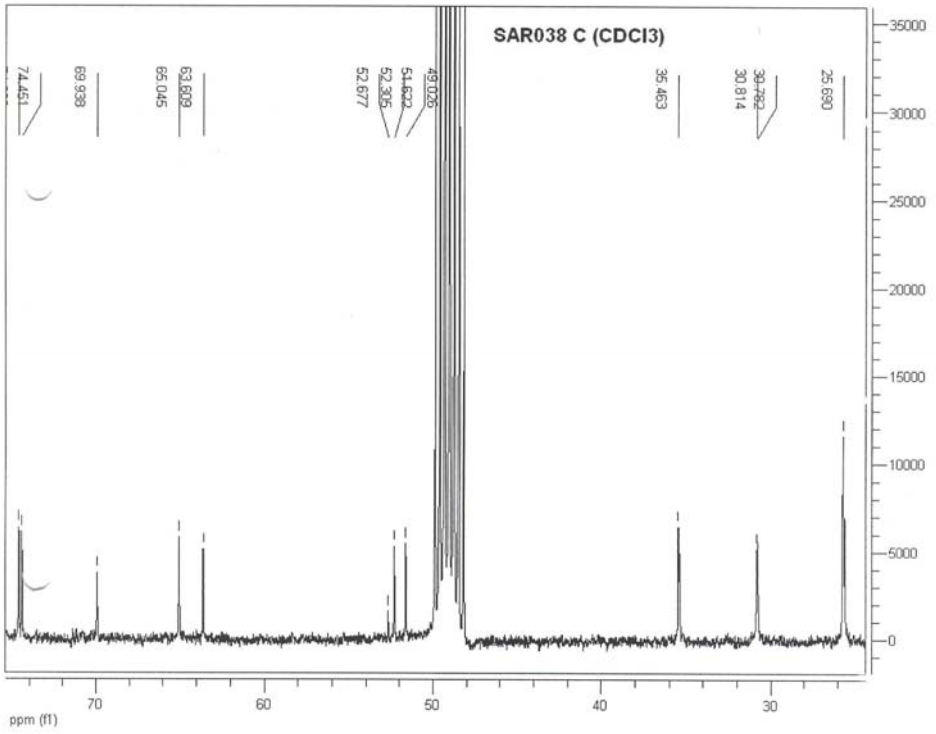


Figure B.21: The ^{1}H NMR of the Imidazolinium Salt

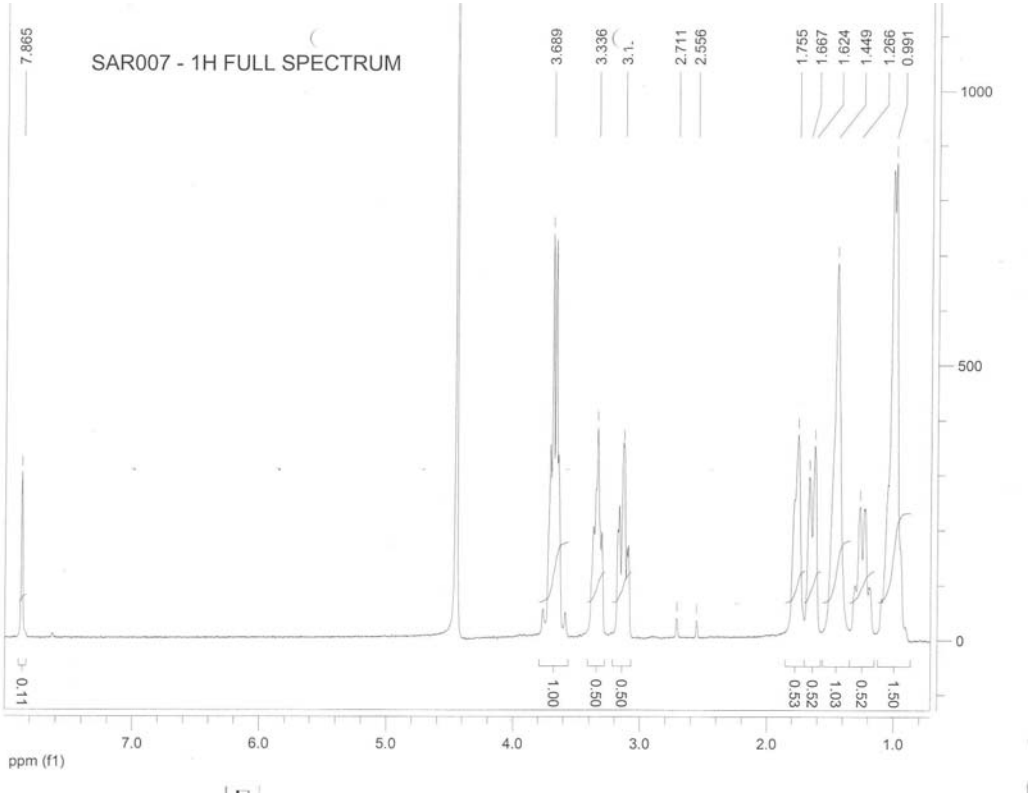


Figure B.22: The ^{13}C NMR of the Imidazolinium Salt

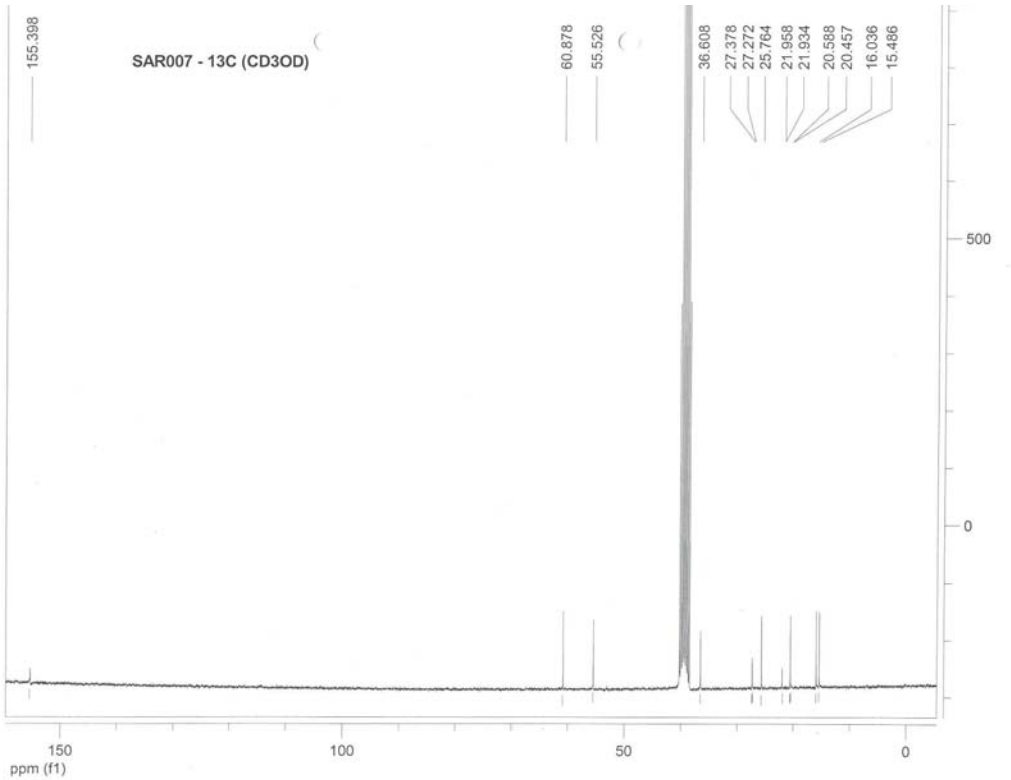
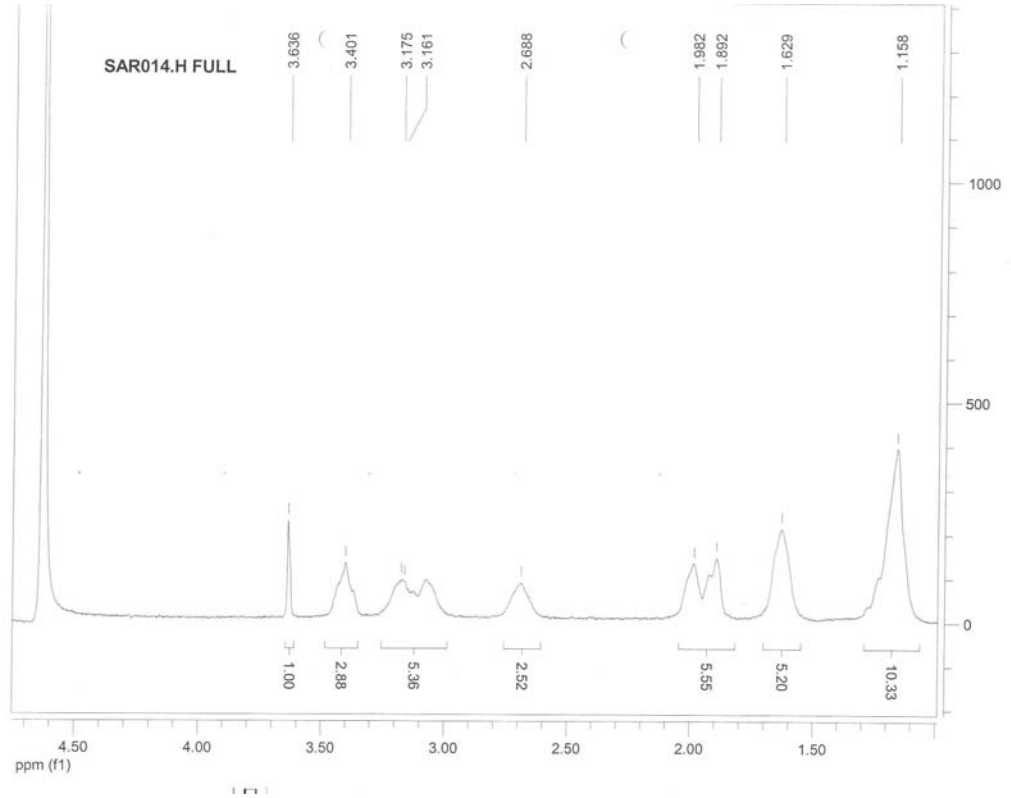


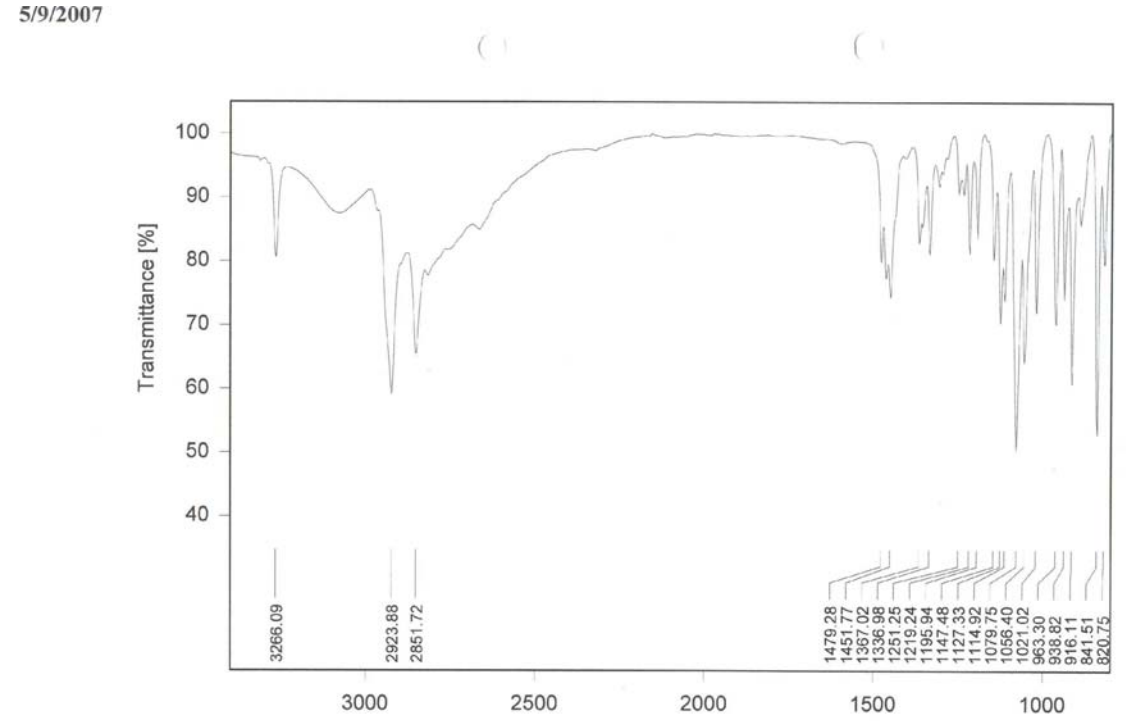
Figure B.23: The ^{1}H NMR of the Protonated Cy_2-en Chloride Salt



Appendix C – IR Data

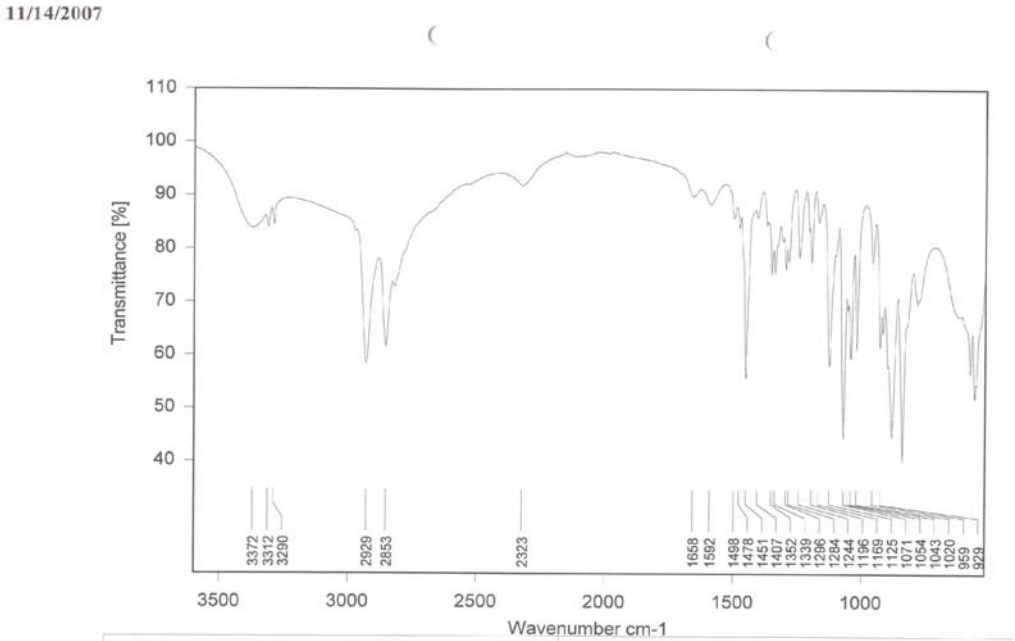
All IR data was generated in the manner described in Chapter 2.

Figure C.1: The IR of Cy_2-en (Sample 1)



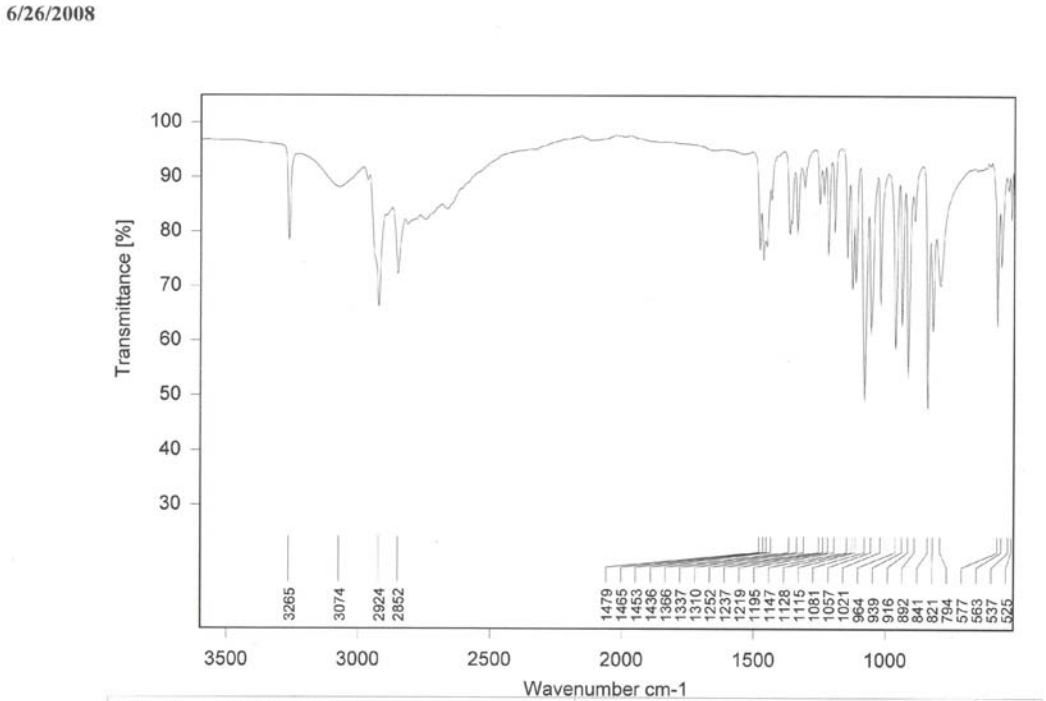
Path of File C:\WITS\SANDRA	Filename SANDRA.0
Sample Name BACKGROUND	Sample Form SOLID ATR
Date of Measurement	Time of Measurement
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.737

Figure C.2: The IR of Cy_2-en (Sample 2)



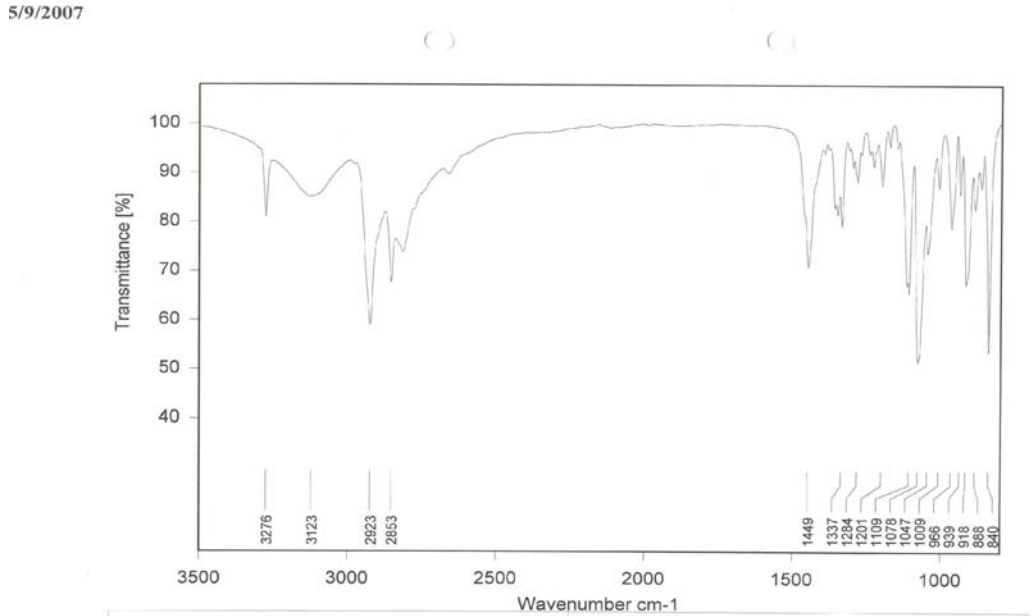
Path of File C:\WITS\SANDRA	Filename SAR020.0
Sample Name SAR020	Sample Form SOLID
Date of Measurement 14/11/2007	Time of Measurement 09:38:03.580 (GMT+1)
Resolution 4	Signal Gain, Sample Automatic

Figure C.3: The IR of Cy_2-en (Sample 3)



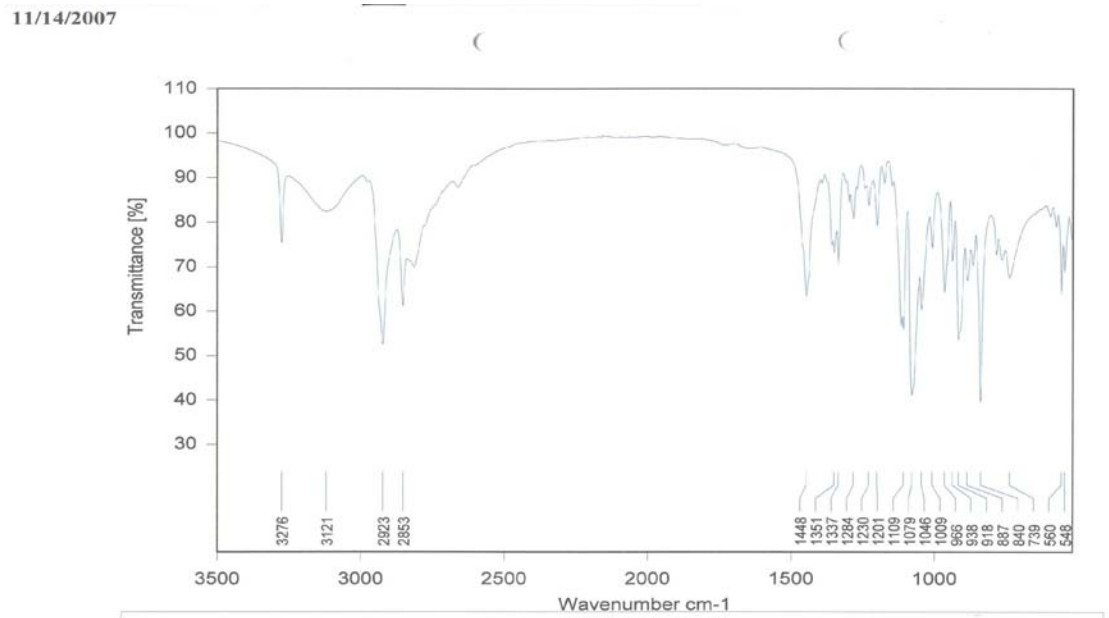
Path of File C:\WITS\SANDRA	Filename SAR036.0
Sample Name SAR036	Sample Form SOLID
Date of Measurement 26/06/2008	Time of Measurement 14:41:19.689 (GMT+2)

Figure C.4: The IR of Cy_2-tn (Sample 1)



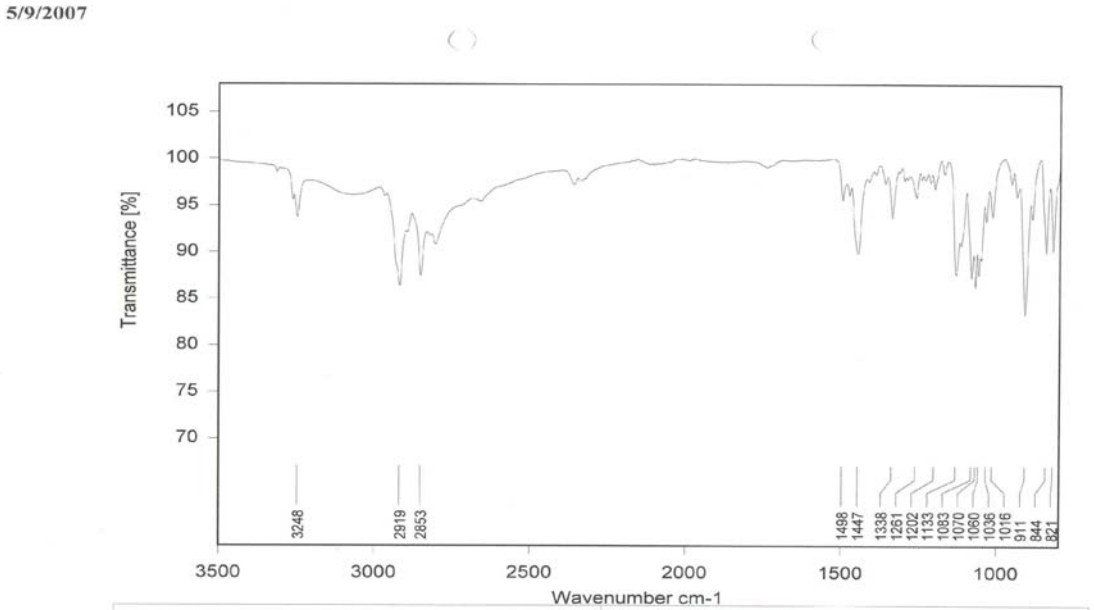
Path of File C:\WITS\SANDRA	Filename SANDRA.5
Sample Name SAR002	Sample Form SOLID ATR
Date of Measurement 09/05/2007	Time of Measurement 15:24:18.467 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.737

Figure C.5: The IR of Cy_2-tn (Sample 2)



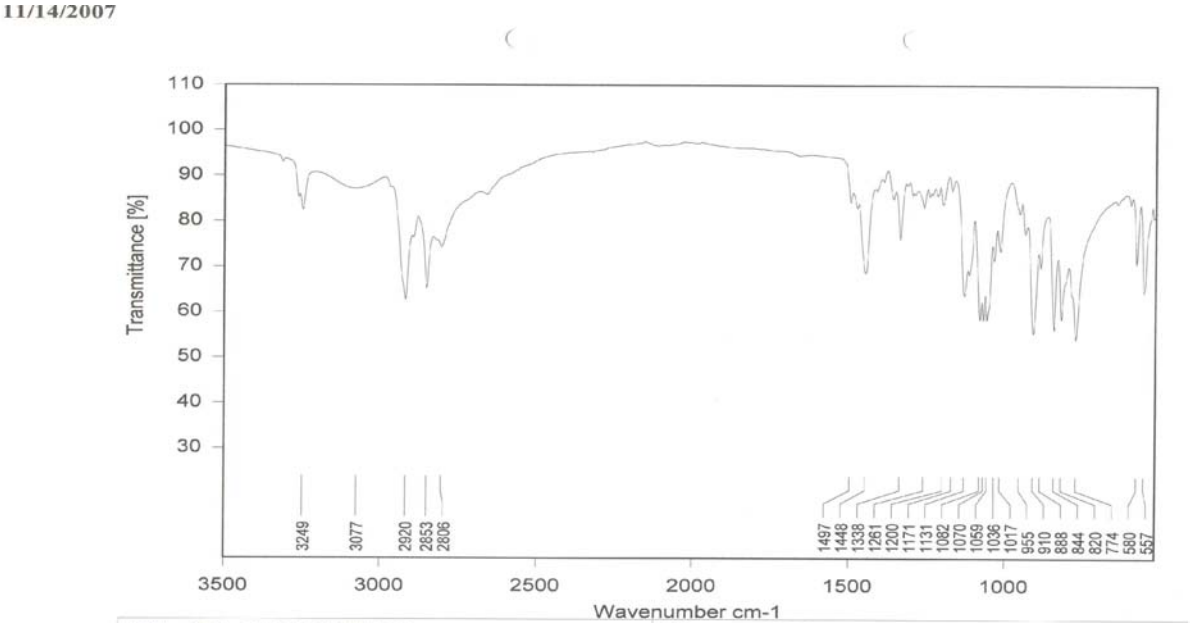
Path of File C:\WITS\SANDRA	Filename SAR009.2
Sample Name SAR009	Sample Form SOLID
Date of Measurement 14/11/2007	Time of Measurement 09:19:44.621 (GMT+1)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.747

Figure C.6: The IR of Cy_2-dien (Sample 1)



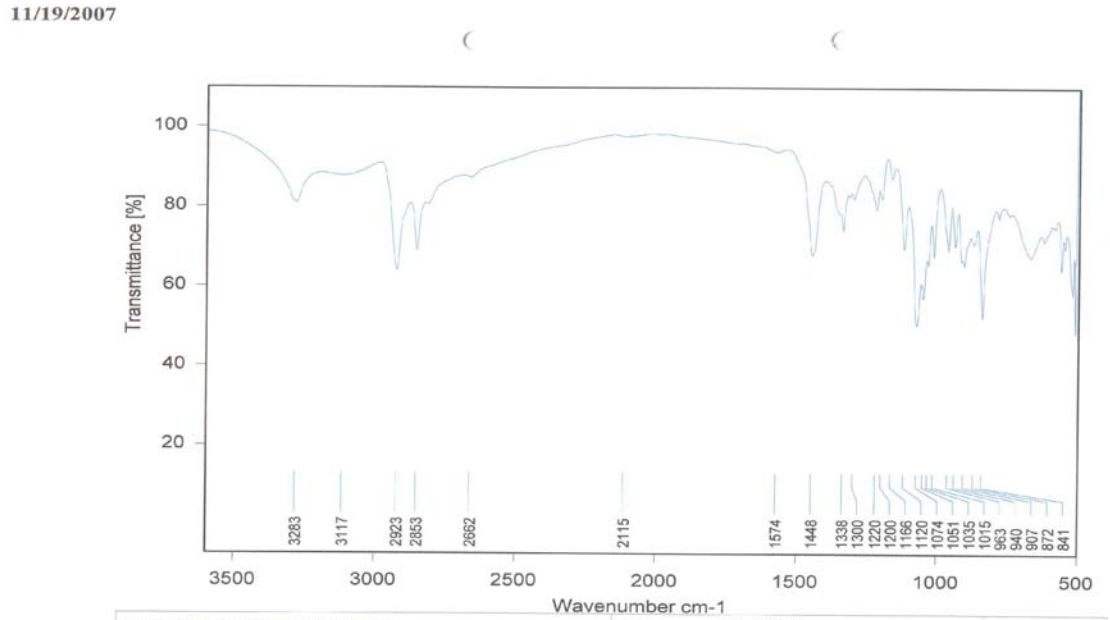
Path of File C:\WITS\SANDRA	Filename SANDRA.6
Sample Name SAR003	Sample Form SOLID ATR
Date of Measurement 09/05/2007	Time of Measurement 15:28:39.464 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.737

Figure C.7: The IR of Cy_2-dien (Sample 2)



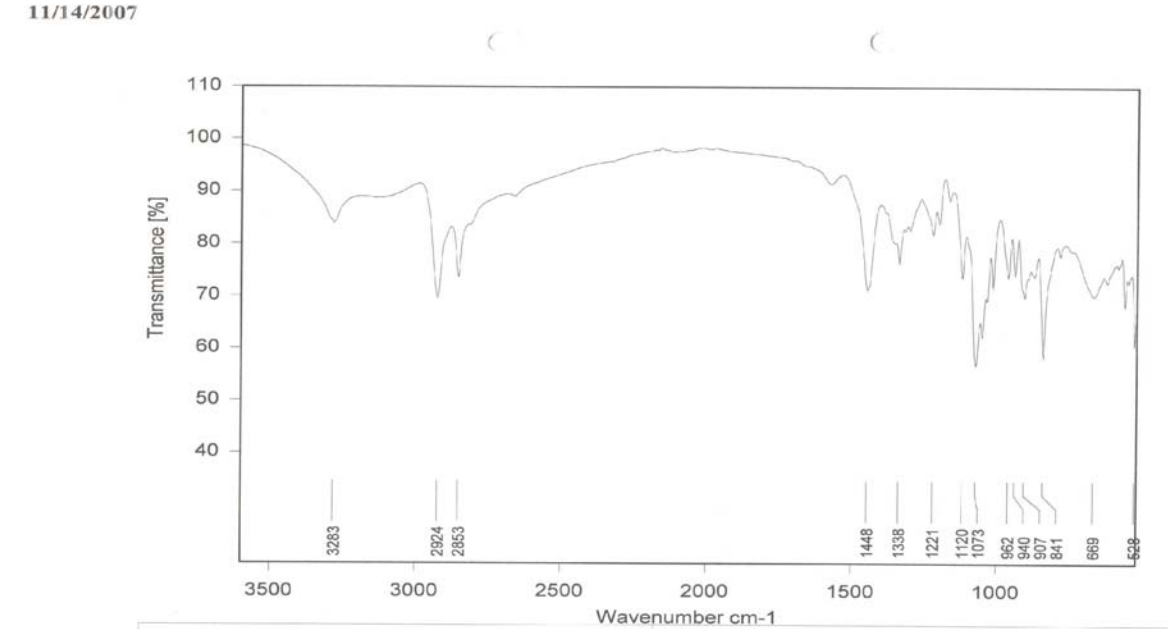
Path of File C:\WITS\SANDRA	Filename SAR010.0
Sample Name SAR010	Sample Form SOLID
Date of Measurement 14/11/2007	Time of Measurement 09:23:55.640 (GMT+1)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.744

Figure C.8: The IR of Cy_2-Otn (Sample 1)



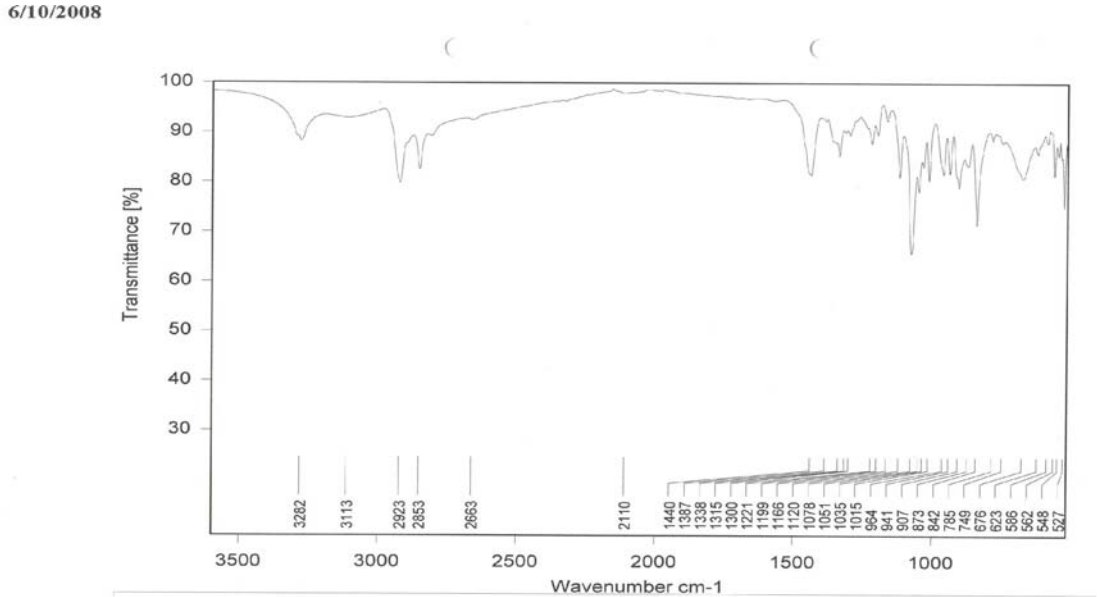
Path of File C:\WITS\SANDRA	Filename SAR022.0
Sample Name SAR022	Sample Form SOLID
Date of Measurement 14/11/2007	Time of Measurement 09:46:47.252 (GMT+1)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.743

Figure C.9: The IR of Cy_2-Otn (Sample 2)



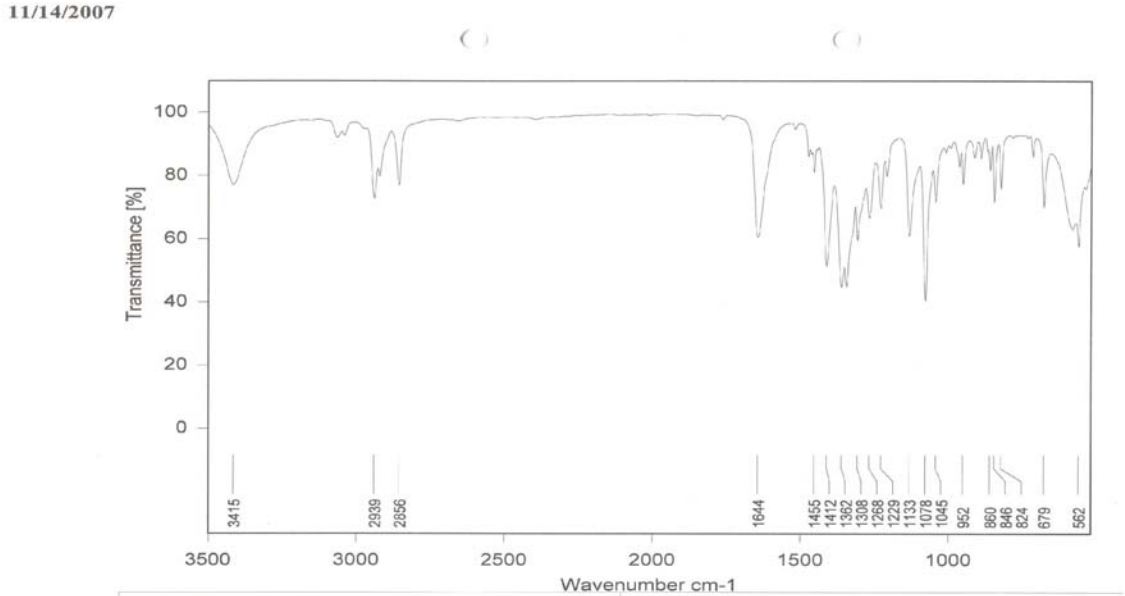
Path of File C:\WITS\SANDRA	Filename SAR025.0
Sample Name SAR025	Sample Form SOLID
Date of Measurement 14/11/2007	Time of Measurement 09:52:58.320 (GMT+1)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.747

Figure C.10: The IR of Cy_2-Otn (Sample 3)



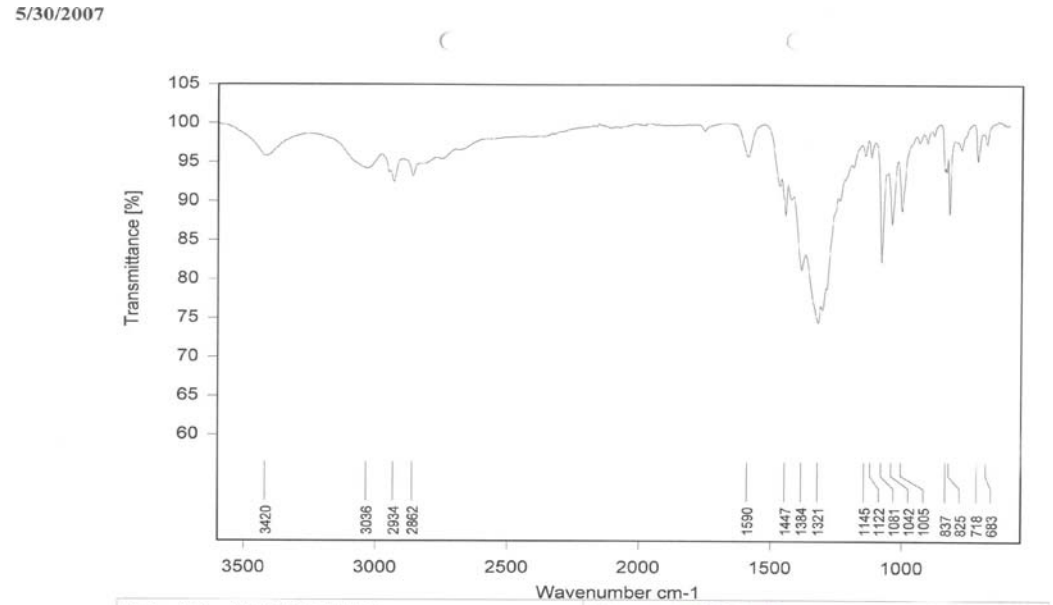
Path of File C:\WITS\SANDRA	Filename SAR038.0
Sample Name SAR038	Sample Form SOLID
Date of Measurement 29/05/2008	Time of Measurement 09:12:34.612 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.736

Figure C.11: The IR of the Imidazolinium Salt from the Attempted Cy_2-en/Pb(II) Reaction (Method 1)



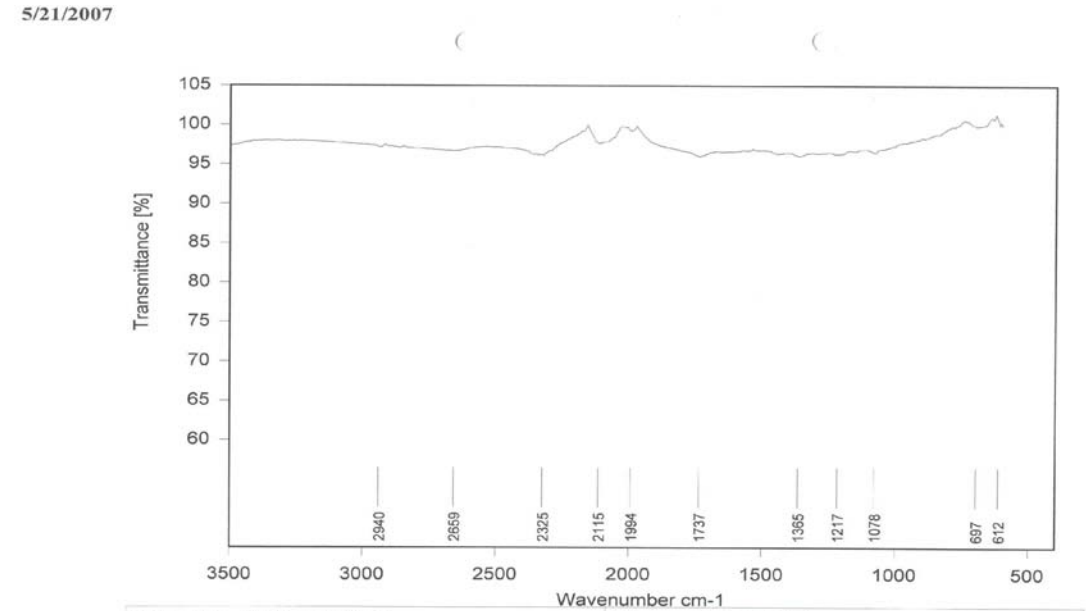
Path of File C:\WITS\SANDRA	Filename SAR007.0
Sample Name SAR007 PRODUCT	Sample Form SOLID
Date of Measurement 14/11/2007	Time of Measurement 09:07:13.462 (GMT+1)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.744

Figure C.12: The IR of the Attempted Cy_2-en/Pb(II) Reaction (Method 2)



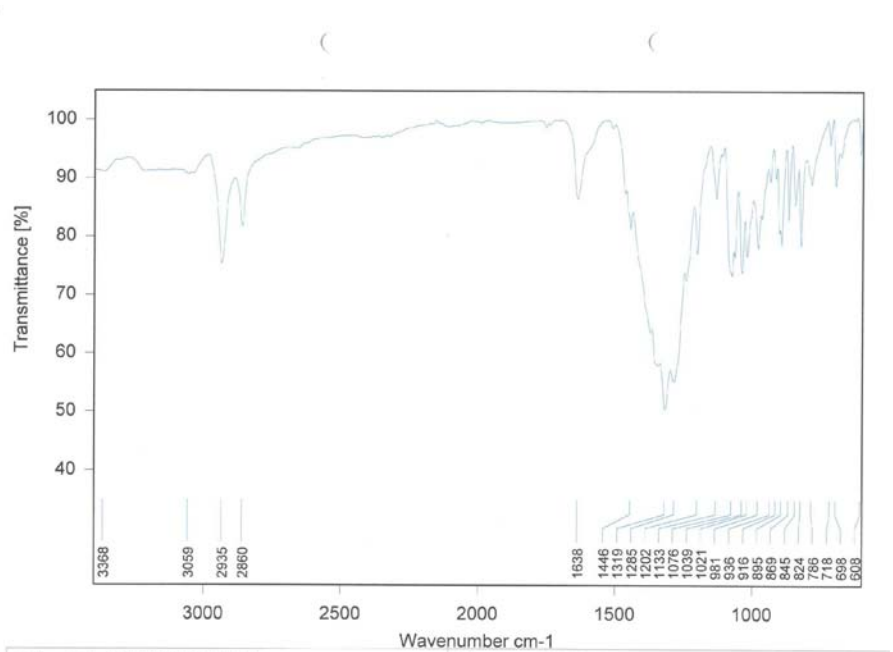
Path of File C:\WITS\SANDRA	Filename SANDRA.16
Sample Name SAR013	Sample Form SOLID ATR
Date of Measurement 30/05/2007	Time of Measurement 13:15:19.948 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.731

Figure C.13: The IR of the Attempted Cy_2-en/Pb(II) Reaction (Method 3)



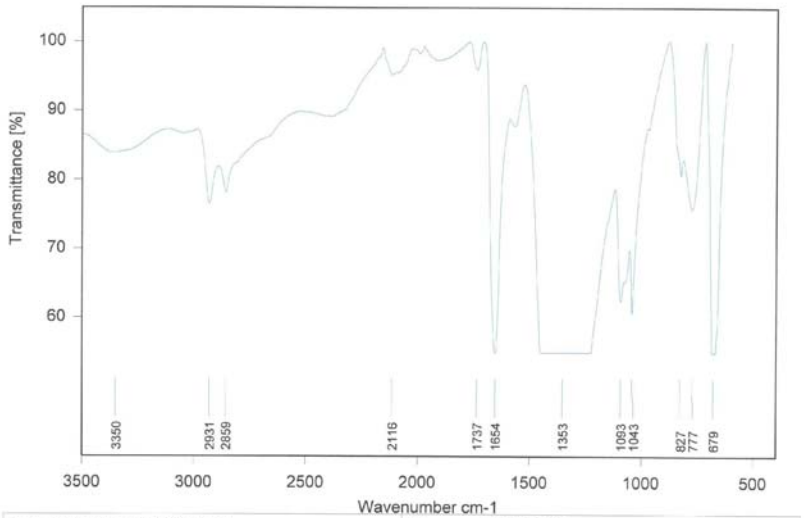
Path of File C:\WITS\SANDRA	Filename SANDRA.15
Sample Name SAR014	Sample Form SOLID ATR
Date of Measurement 21/05/2007	Time of Measurement 11:24:25.814 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.732

Figure C.14: The IR of the Successful Cy_2-en/Pb(II) Complex (Method 5)



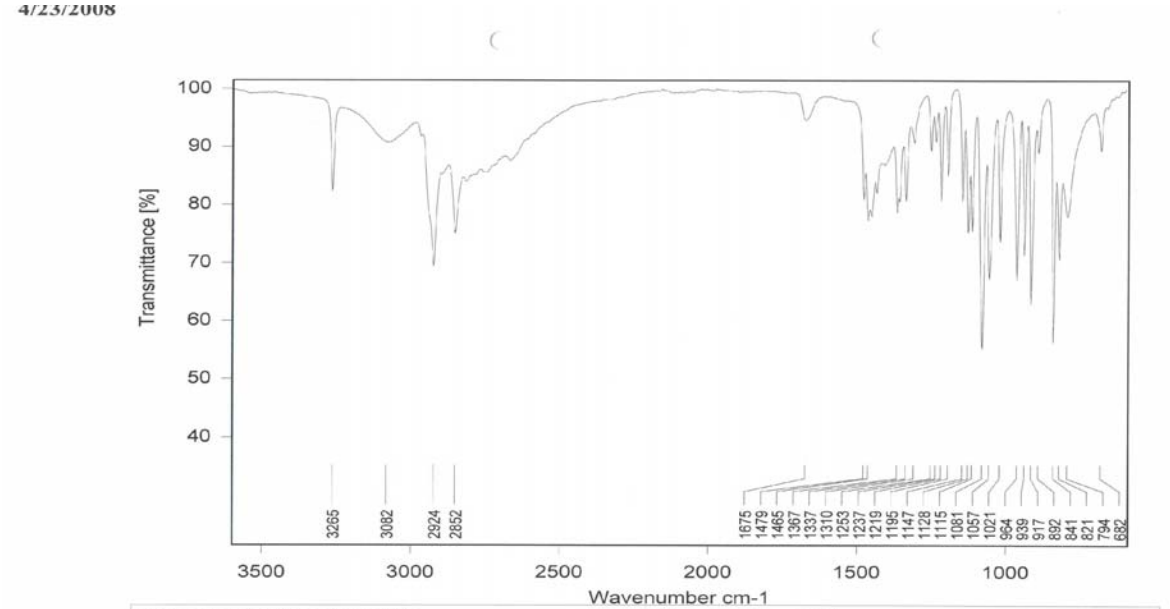
Path of File C:\WITS\SANDRA	Filename SANDRA.27
Sample Name SAR008	Sample Form SOLID ATR
Date of Measurement 16/07/2007	Time of Measurement 11:14:53.918 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 27.572

Figure C.15: The IR of the Attempted Cy_2-tn/Pb(II) Complex



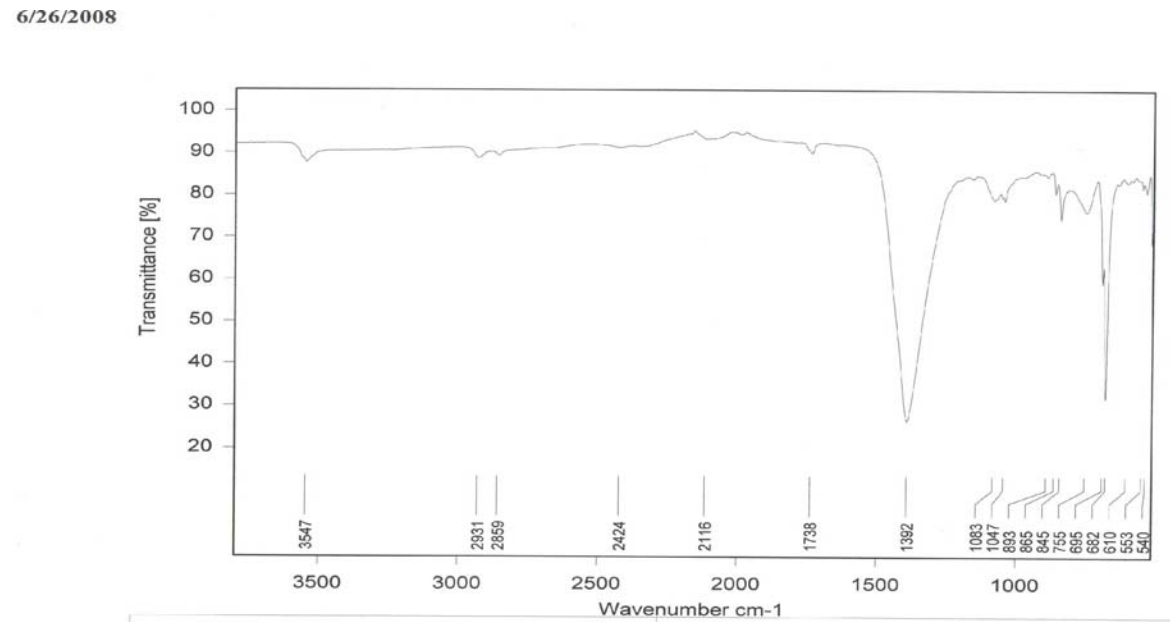
Path of File C:\WITS\SANDRA	Filename SANDRA.12
Sample Name SAR011	Sample Form SOLID ATR
Date of Measurement 21/05/2007	Time of Measurement 11:13:12.528 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.732

Figure C.16: The IR of the Cy_2-dien/Pb(II) Complex



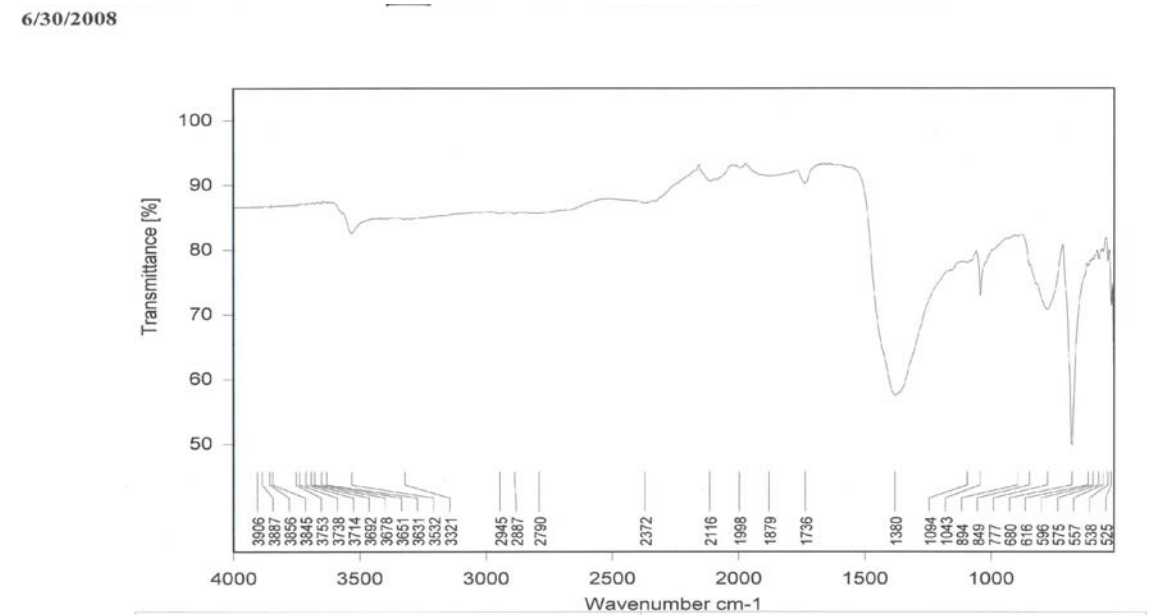
Path of File C:\WITS\SANDRA	Filename SAR012.0
Sample Name SAR012	Sample Form SOLID
Date of Measurement 23/04/2008	Time of Measurement 11:45:17.935 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.744

Figure C.17: The IR of the Cy_2-Otn/Pb(II) Complex



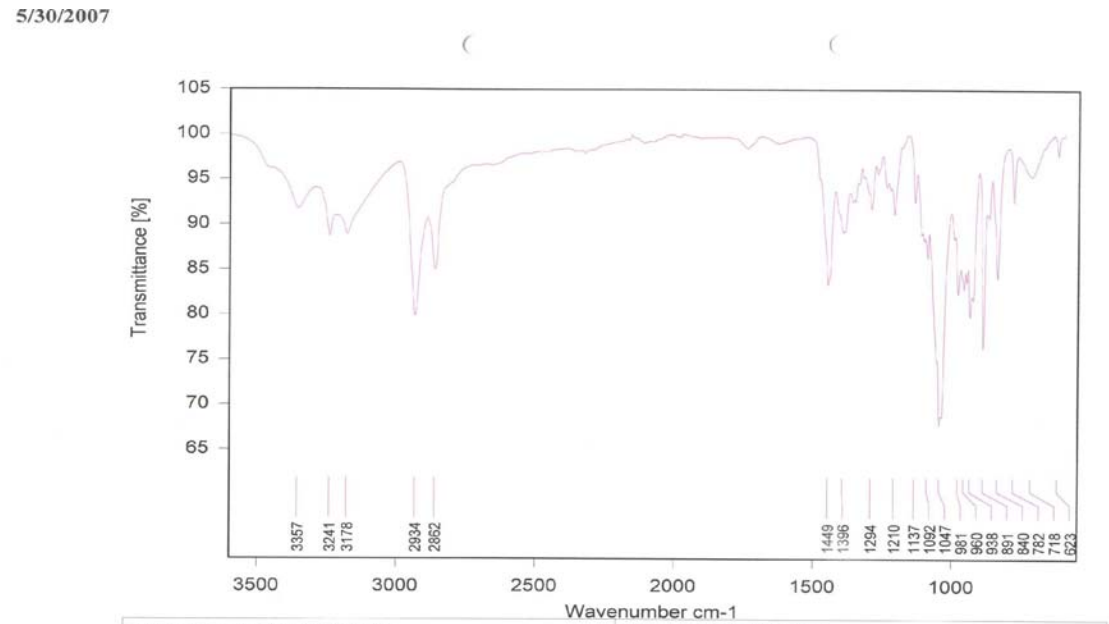
Path of File C:\WITS\SANDRA	Filename SAR042.0
Sample Name SAR042	Sample Form SOLID
Date of Measurement 26/06/2008	Time of Measurement 15:01:34.789 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.741

Figure C.18: The IR of the BHEEN/Pb(II) Complex



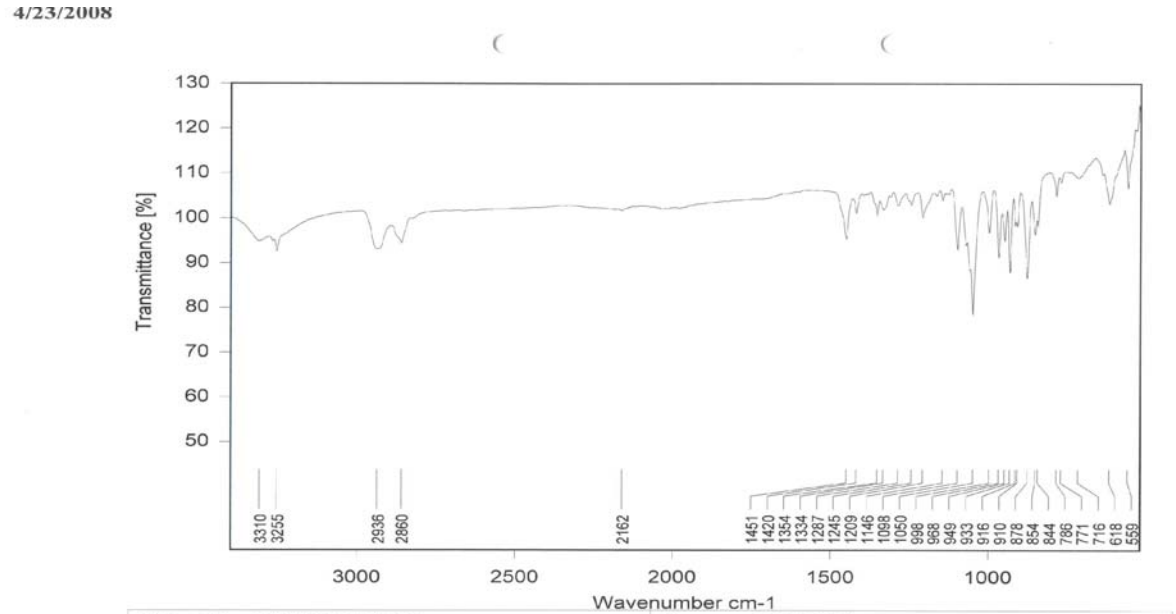
Path of File C:\WITS\SANDRA	Filename SAR031.1
Sample Name SAR031.1	Sample Form SOLID
Date of Measurement 02/06/2008	Time of Measurement 12:22:15.277 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.738

Figure C.19: The IR of the Cy_2-en/Cd(II) Complex



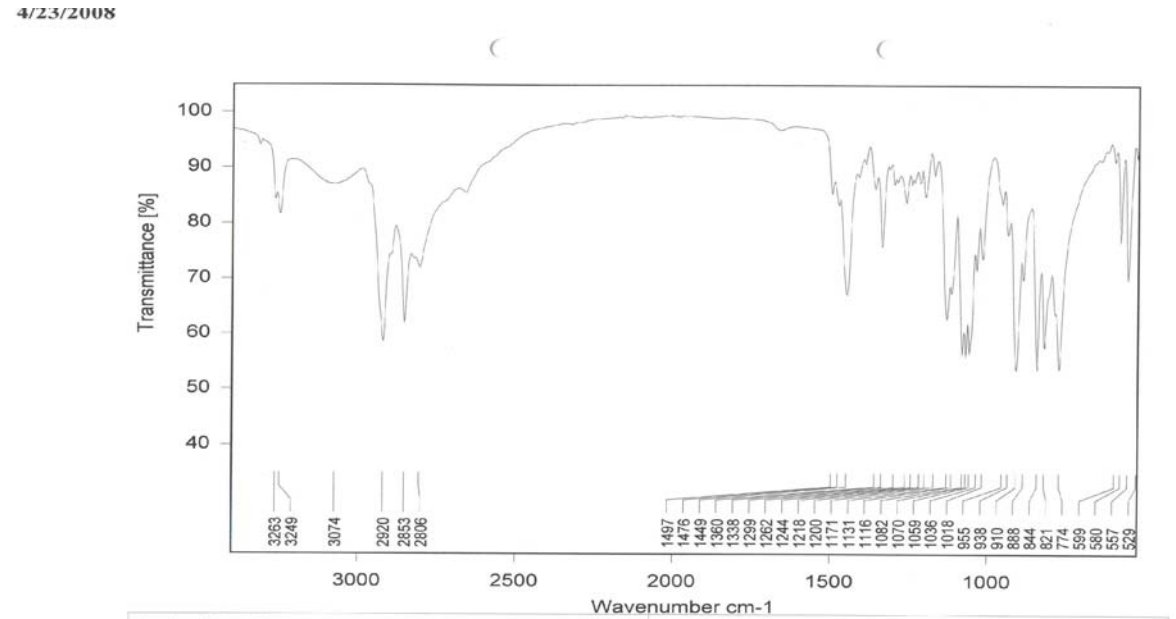
Path of File C:\WITS\SANDRA	Filename SANDRA.18
Sample Name SAR016	Sample Form SOLID ATR
Date of Measurement 30/05/2007	Time of Measurement 13:22:29.698 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.73

Figure C.20: The IR of the Cy_2-tn/Cd(II) Complex



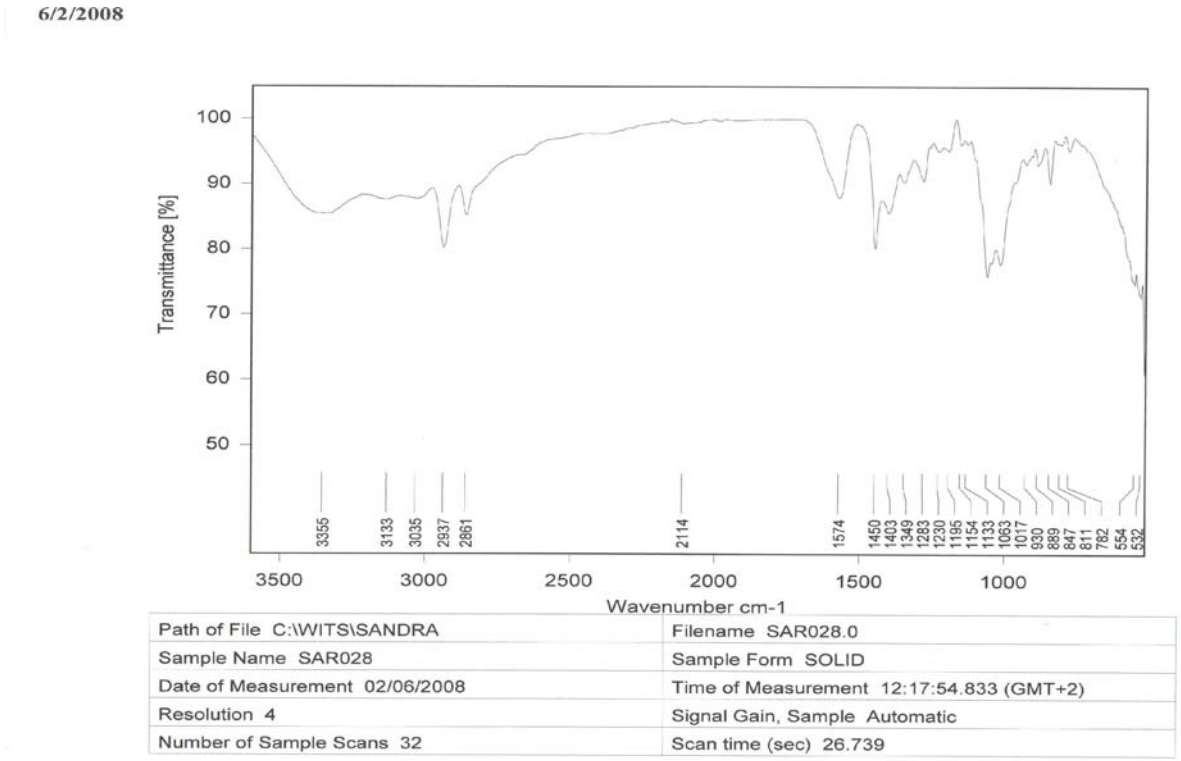
Path of File C:\WITS\SANDRA	Filename SAR018.1
Sample Name SAR018 FIRST POWDER	Sample Form SOLID
Date of Measurement 23/04/2008	Time of Measurement 11:53:53.586 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.744

Figure C.21: The IR of the Cy_2-dien/Cd(II) Complex



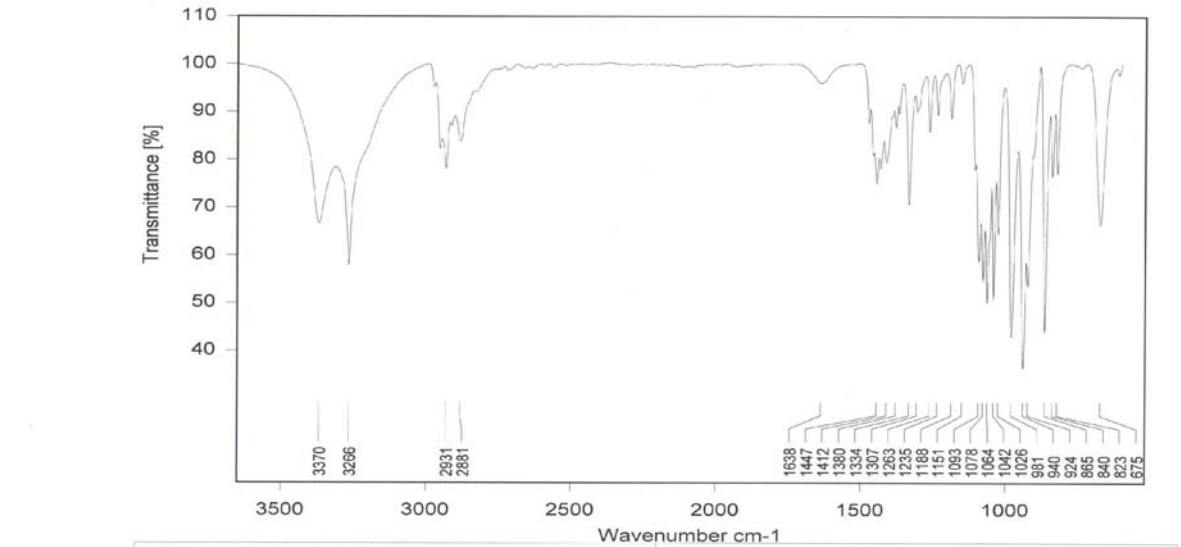
Path of File C:\WITS\SANDRA	Filename SAR019.1
Sample Name SAR019	Sample Form SOLID
Date of Measurement 23/04/2008	Time of Measurement 12:08:17.560 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.744

Figure C.22: The IR of the Cy_2-Otn/Cd(II) Complex



Path of File C:\WITS\SANDRA	Filename SAR028.0
Sample Name SAR028	Sample Form SOLID
Date of Measurement 02/06/2008	Time of Measurement 12:17:54.833 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.739

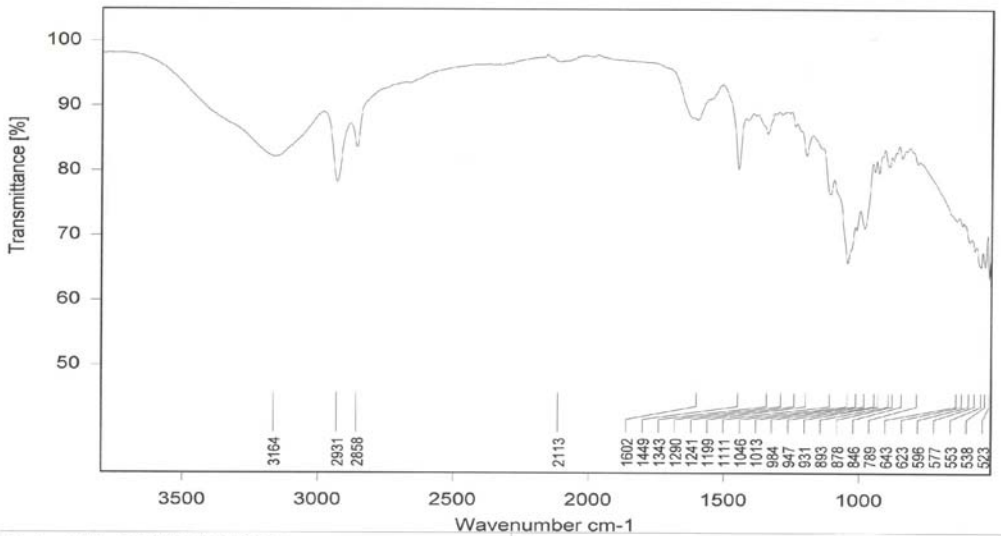
Figure C.23: The IR of the BHEEN/Cd(II) Complex



Path of File C:\WITS\SANDRA	Filename SAR041.0
Sample Name SAR041 - 2ND POWDER DMF	Sample Form ATR - SOLID
Date of Measurement 29/02/2008	Time of Measurement 09:55:55.836 (GMT+1)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.745

Figure C.24: The IR of the Cy_2-en/Ni(II) Complex

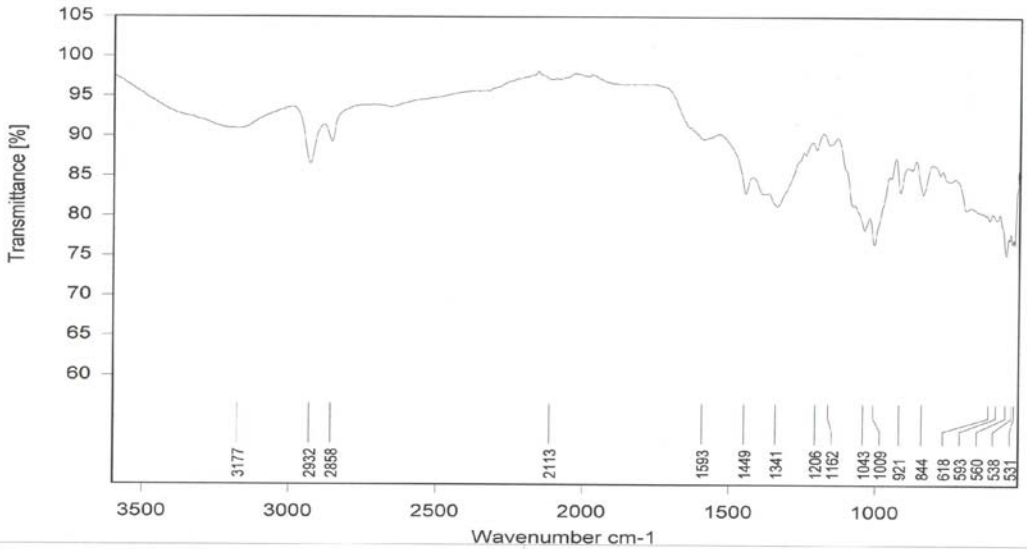
6/26/2008



Path of File C:\WITS\SANDRA	Filename SAR040.0
Sample Name SAR040	Sample Form SOLID
Date of Measurement 26/06/2008	Time of Measurement 14:57:16.566 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.741

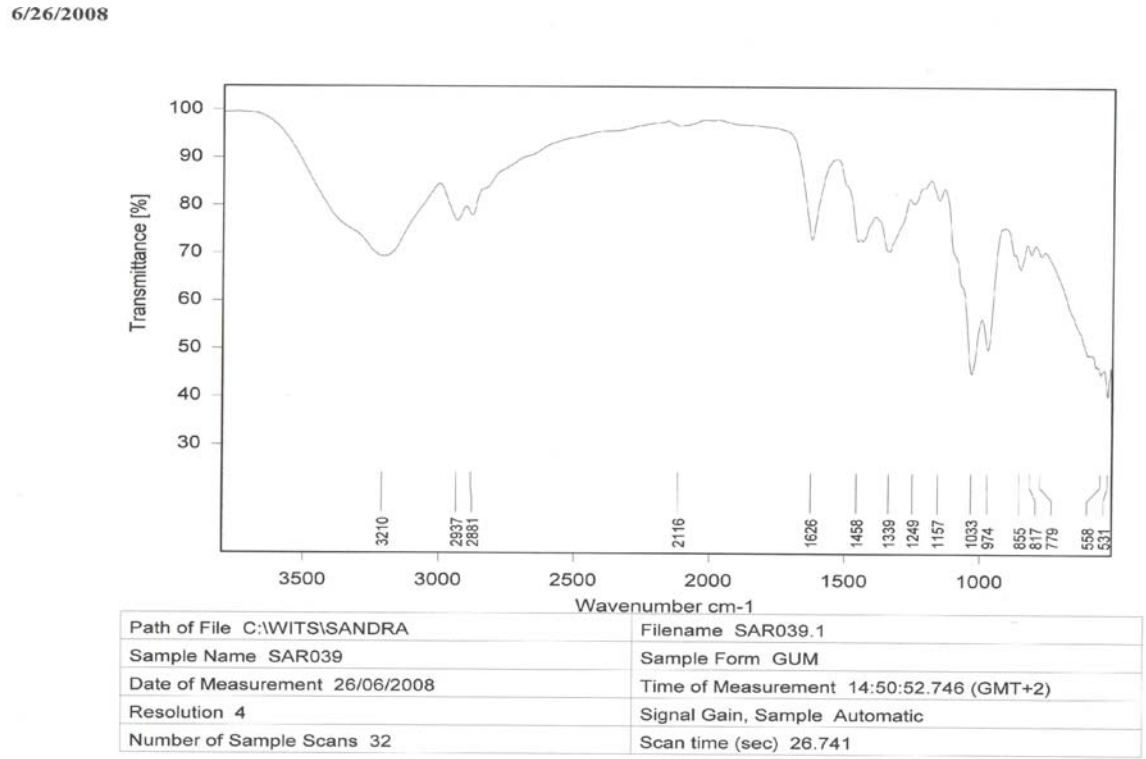
Figure C.25: The IR of the Cy_2-Otn/Ni(II) Complex

6/26/2008



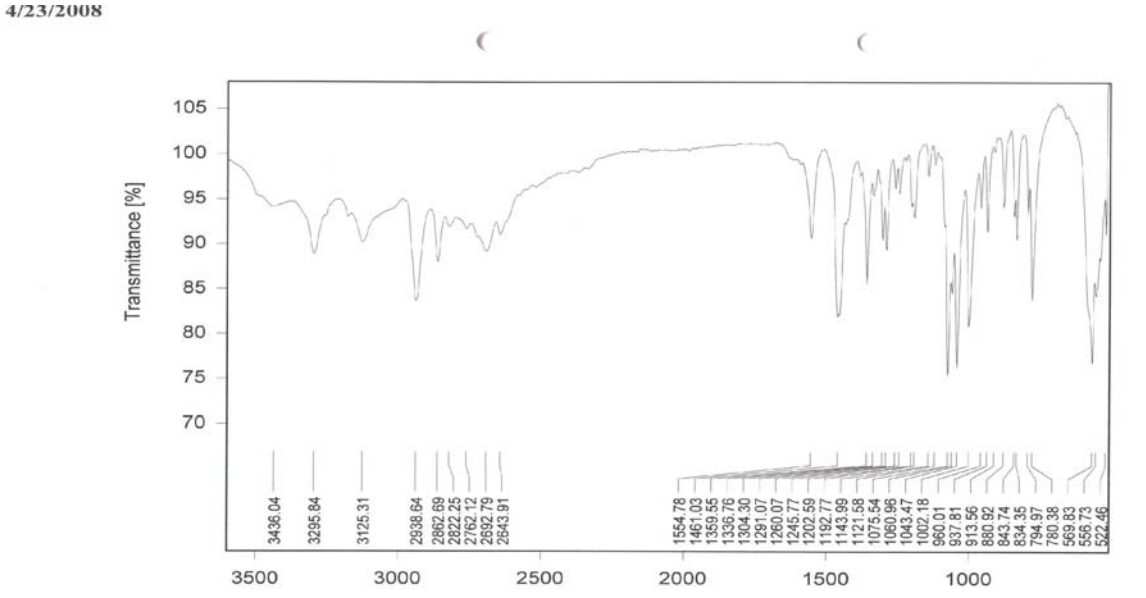
Path of File C:\WITS\SANDRA	Filename SAR037.0
Sample Name SAR037	Sample Form SOLID
Date of Measurement 26/06/2008	Time of Measurement 14:47:15.182 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.741

Figure C.26: The IR of the BHEEN/Ni(II) Complex



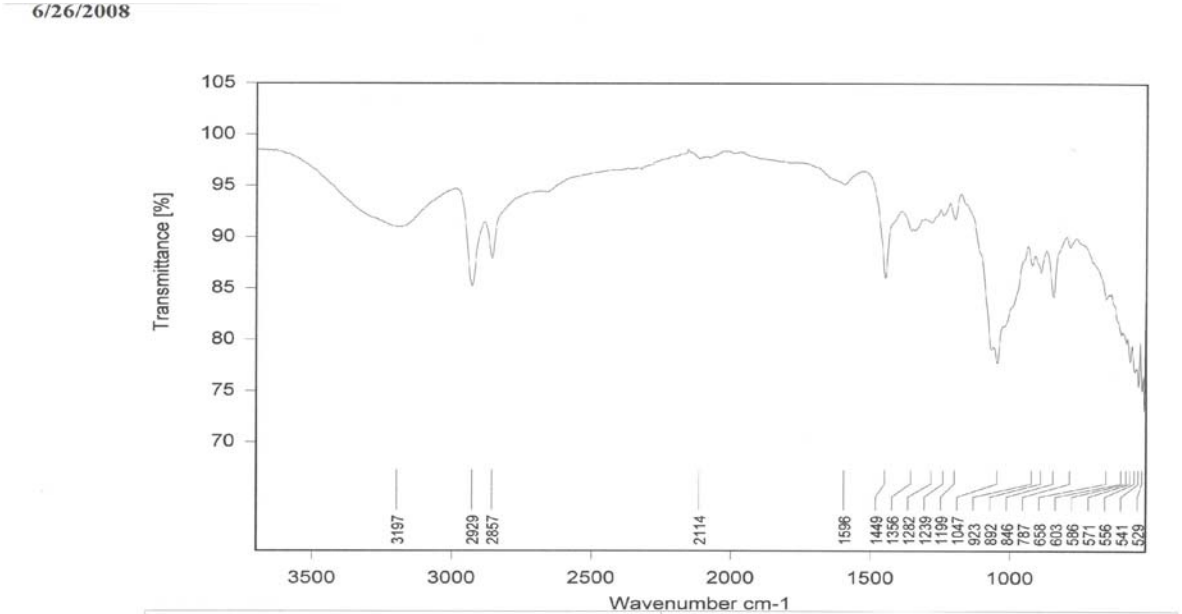
Path of File C:\WITS\SANDRA	Filename SAR039.1
Sample Name SAR039	Sample Form GUM
Date of Measurement 26/06/2008	Time of Measurement 14:50:52.746 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.741

Figure C.27: The IR of the Cy_2-en/Zn(II) Complex



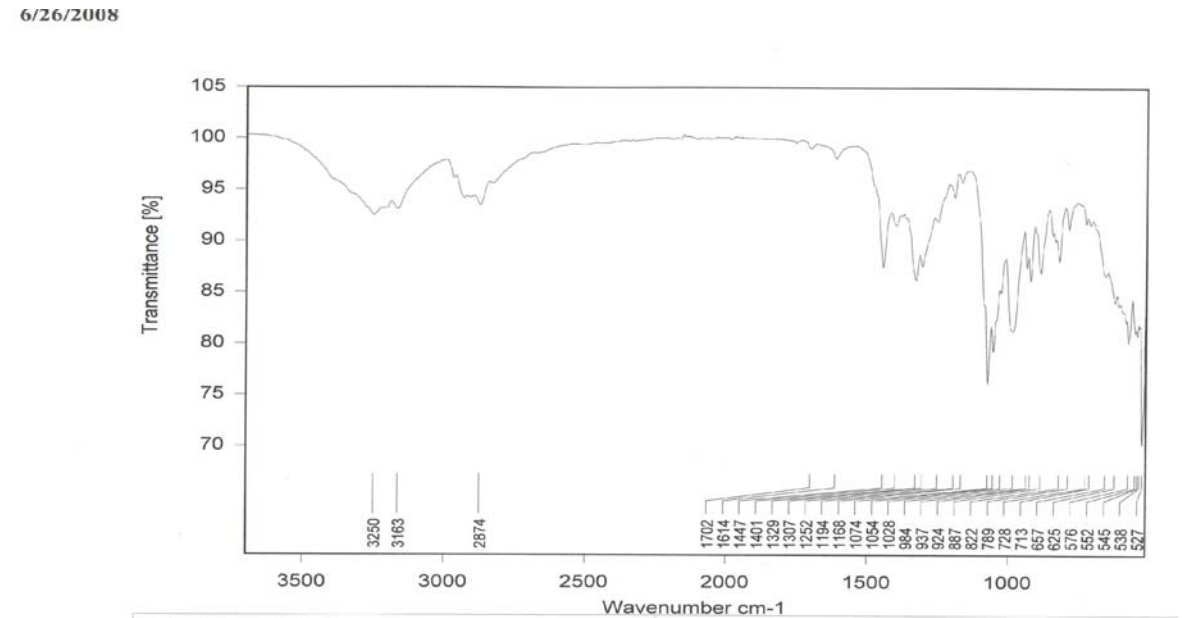
Path of File C:\WITS\SANDRA	Filename SAR023.0
Sample Name SAR023	Sample Form SOLID
Date of Measurement	Time of Measurement
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.744

Figure C.28: The IR of the Cy_2-Otn/Zn(II) Complex



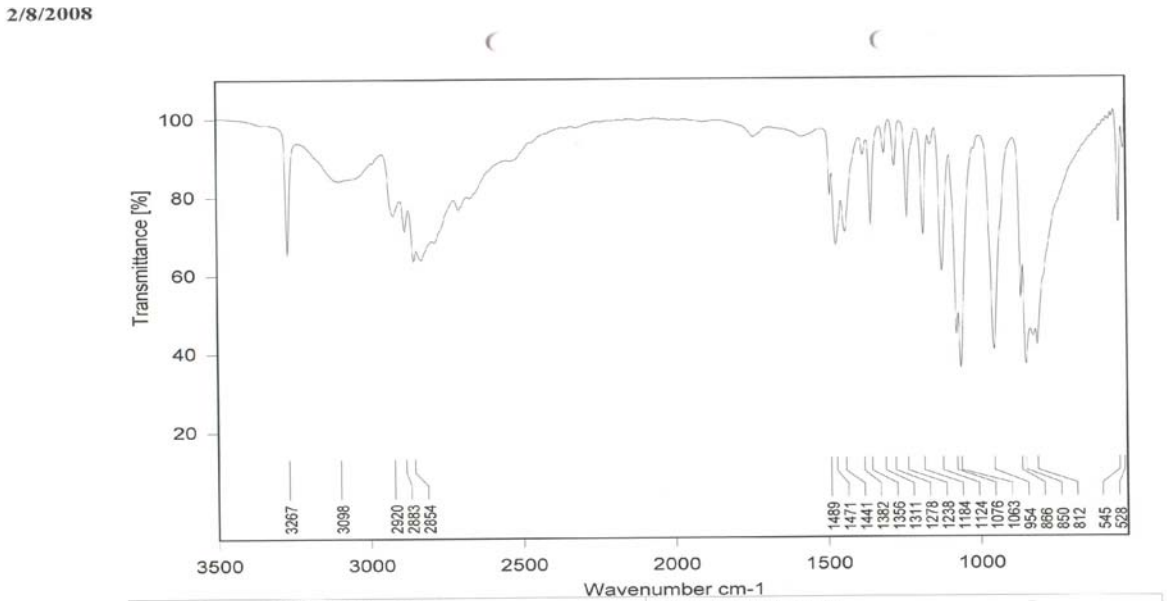
Path of File C:\WITS\SANDRA	Filename SAR045.0
Sample Name SAR045	Sample Form SOLID
Date of Measurement 26/06/2008	Time of Measurement 15:18:00.430 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.741

Figure C.29: The IR of the BHEEN/Zn(II) Complex



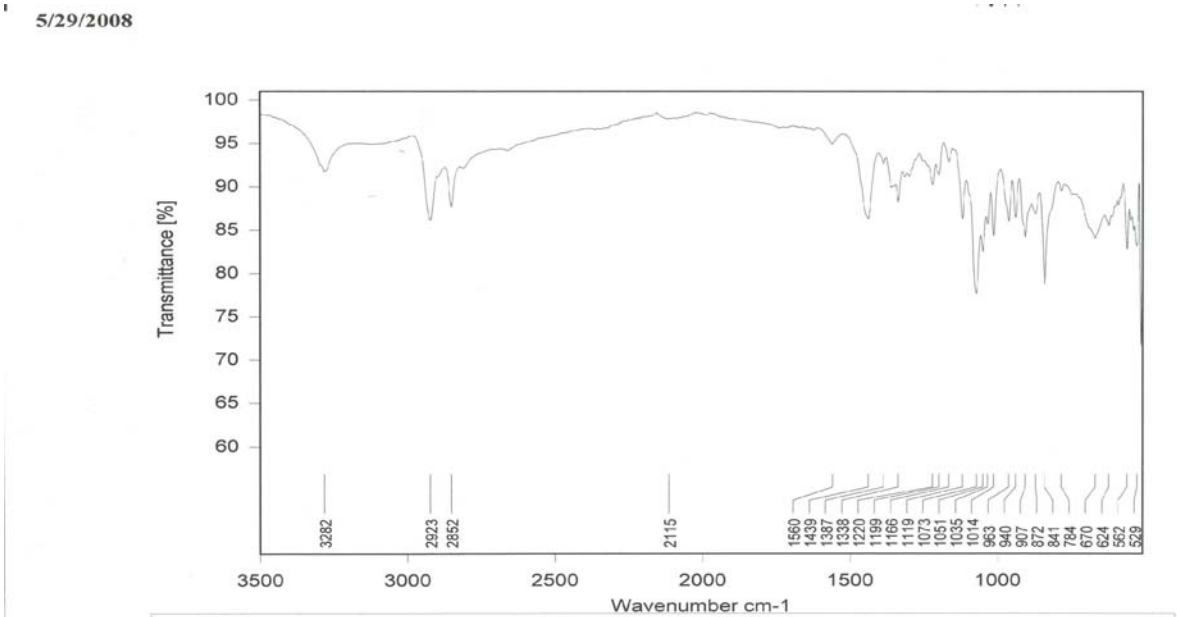
Path of File C:\WITS\SANDRA	Filename SAR048.0
Sample Name SAR048	Sample Form SOLID
Date of Measurement 26/06/2008	Time of Measurement 15:28:40.785 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.74

Figure C.30: The IR BHEEN (Sigma)



Path of File C:\WITS\SANDRA	Filename BHEEN.0
Sample Name BHEEN-SIGMA	Sample Form ATR - SOLID
Date of Measurement 08/02/2008	Time of Measurement 09:59:56.017 (GMT+1)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 16	Scan time (sec) 13.345

Figure C.31: The IR the Zwitterion **2**



Path of File C:\WITS\SAMANTHA	Filename L1.0
Sample Name L1	Sample Form SOLID
Date of Measurement 25/04/2008	Time of Measurement 11:35:23.248 (GMT+2)
Resolution 4	Signal Gain, Sample Automatic
Number of Sample Scans 32	Scan time (sec) 26.748

Appendix D – MS Data

All MS data was generated in the manner described in Chapter 2.

Figure D.1: The APCI Spectrum of Cy_2-en (Sample 1)

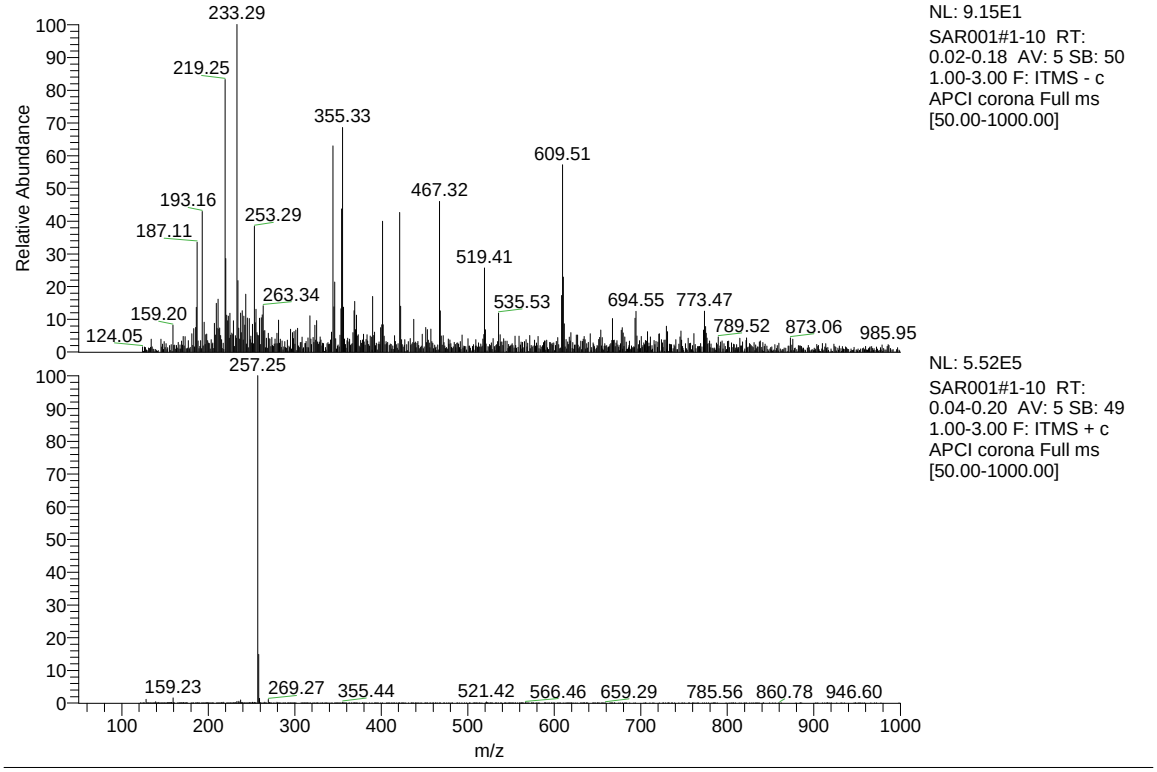


Figure D.2: The ESI+ Spectrum of Cy_2-en (Sample 2)

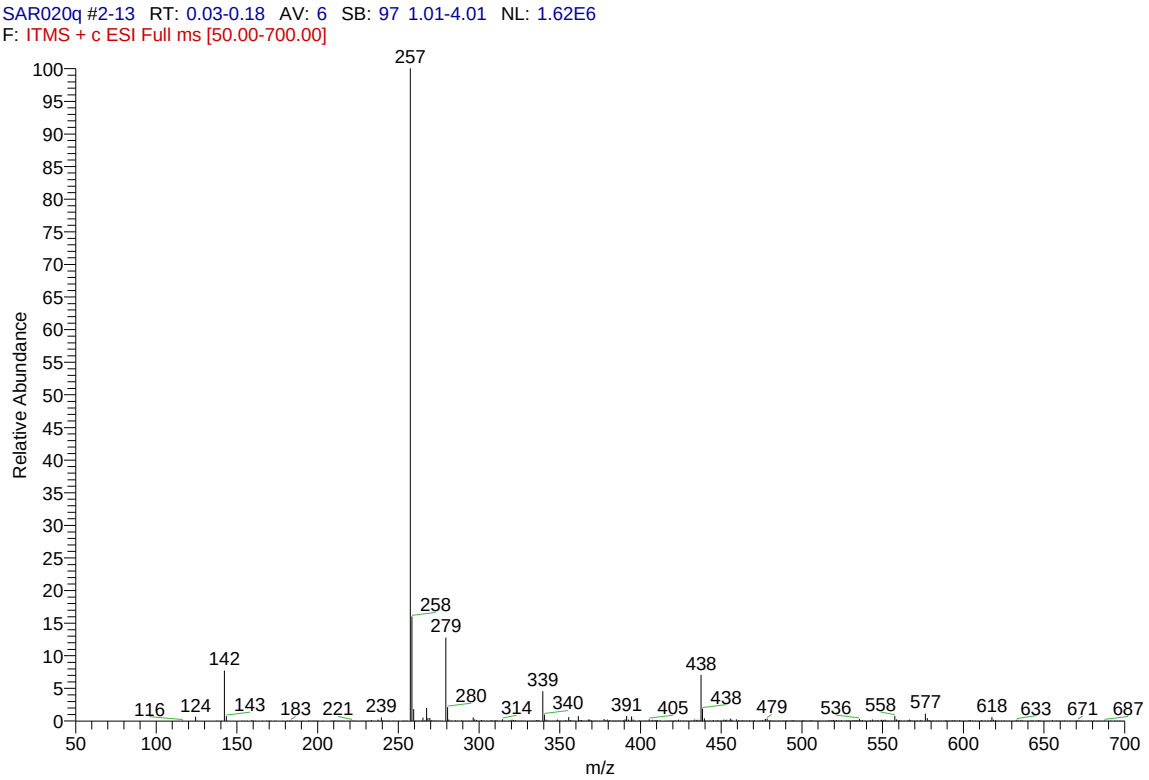


Figure D.3: The APCI Spectrum of Cy_2-en (Sample 3)

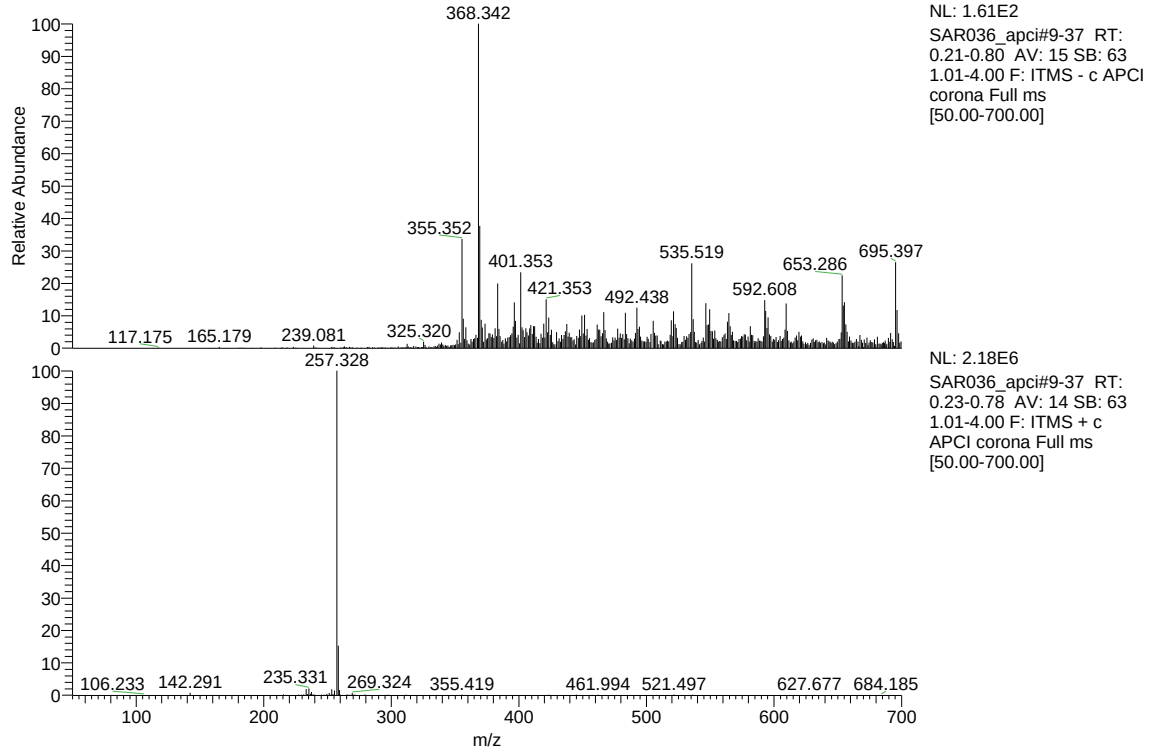


Figure D.4: The APCI Spectrum of Cy_2-tn (Sample 1)

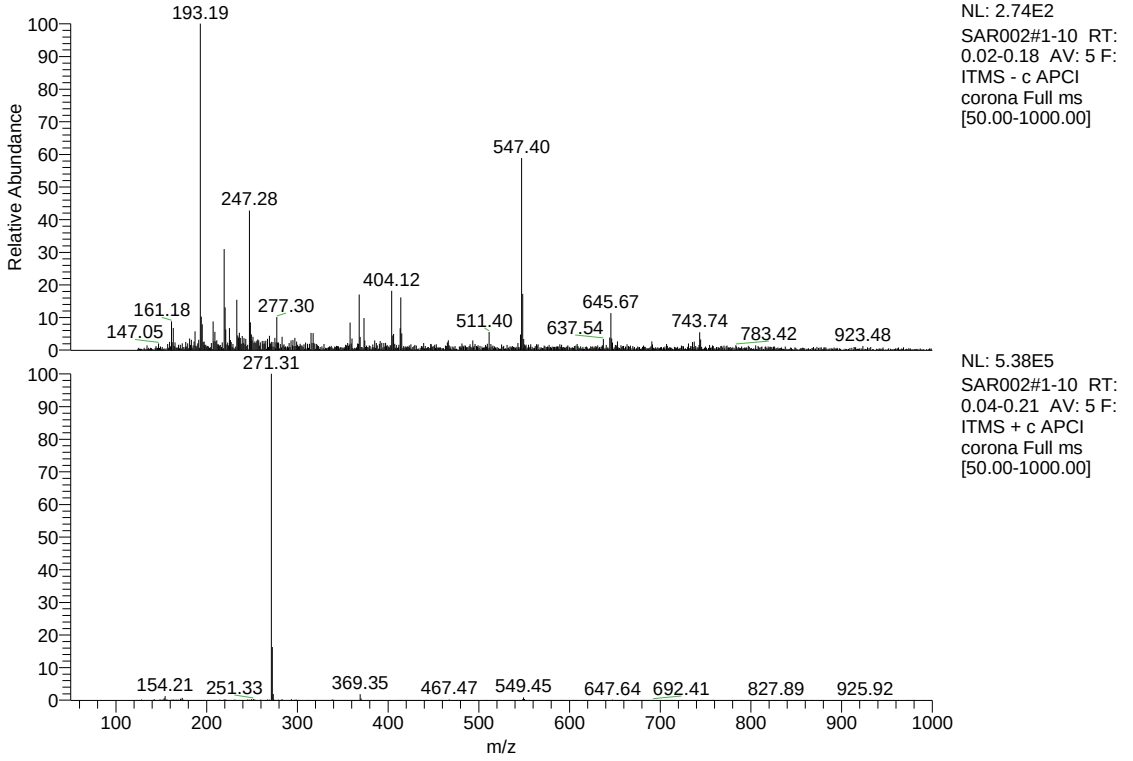


Figure D.5: The ESI Spectrum of Cy_2-tn (Sample 2)

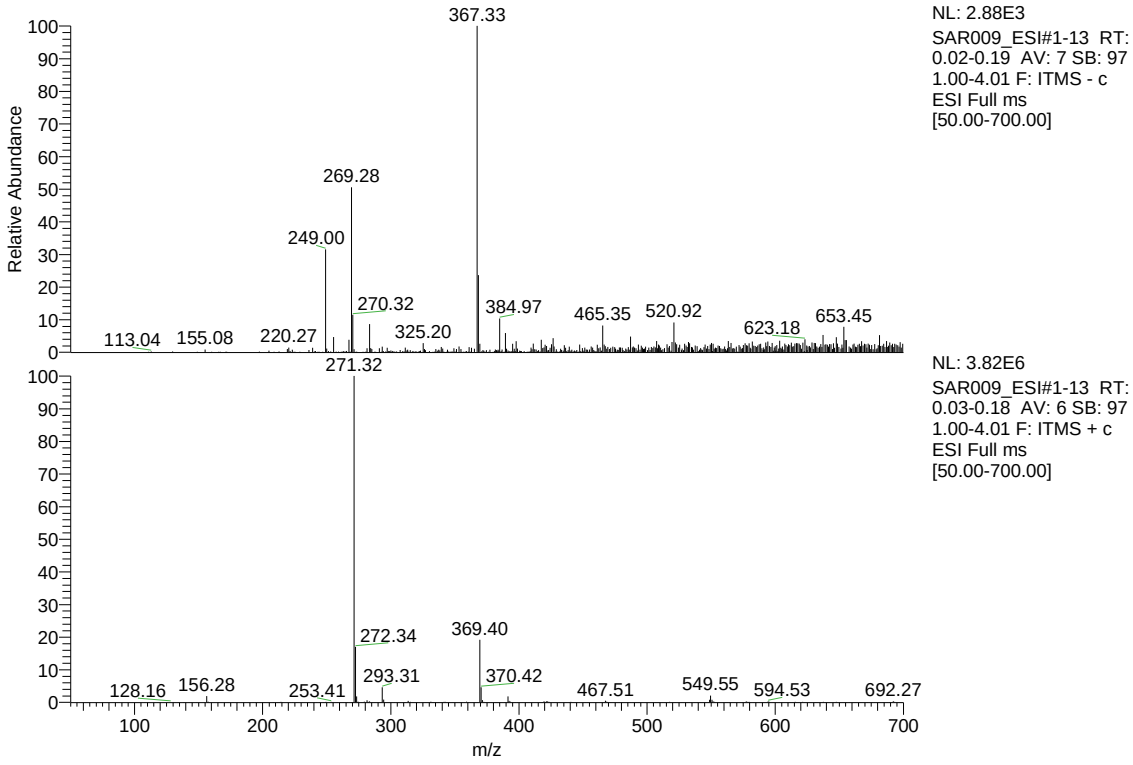


Figure D.6: The APCI Spectrum of Cy_2-dien (Sample 1)

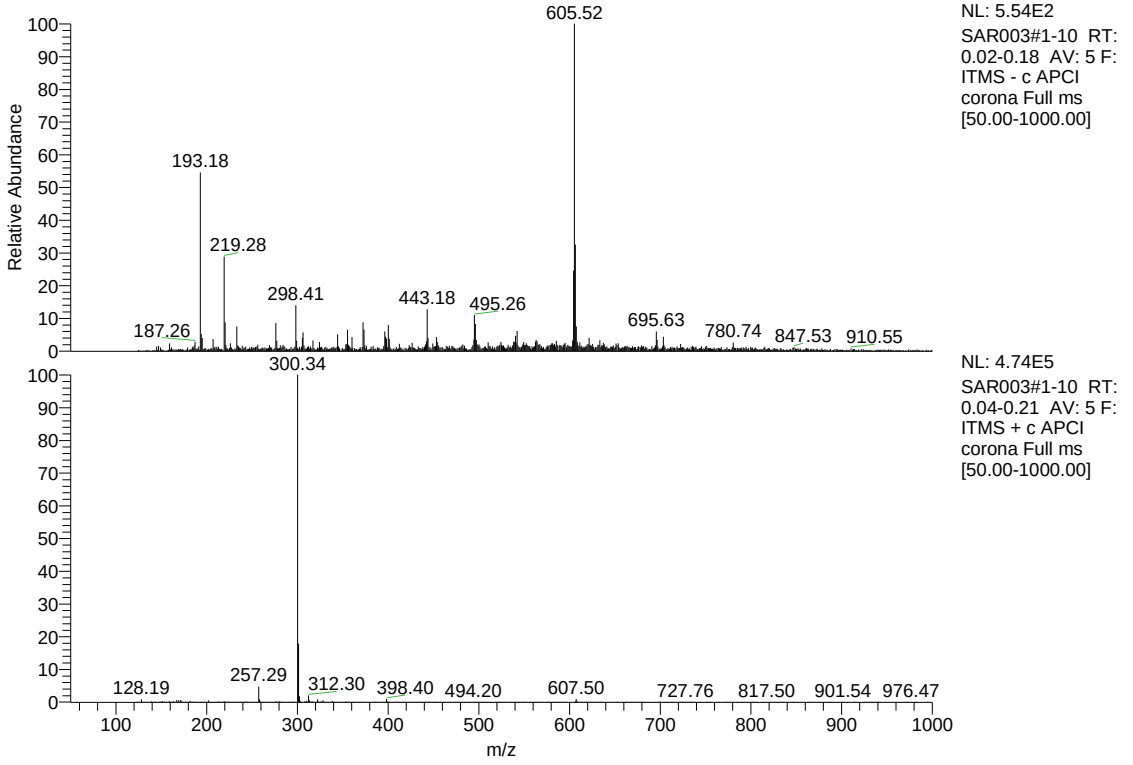


Figure D.7: The ESI Spectrum of Cy_2-dien (Sample 2)

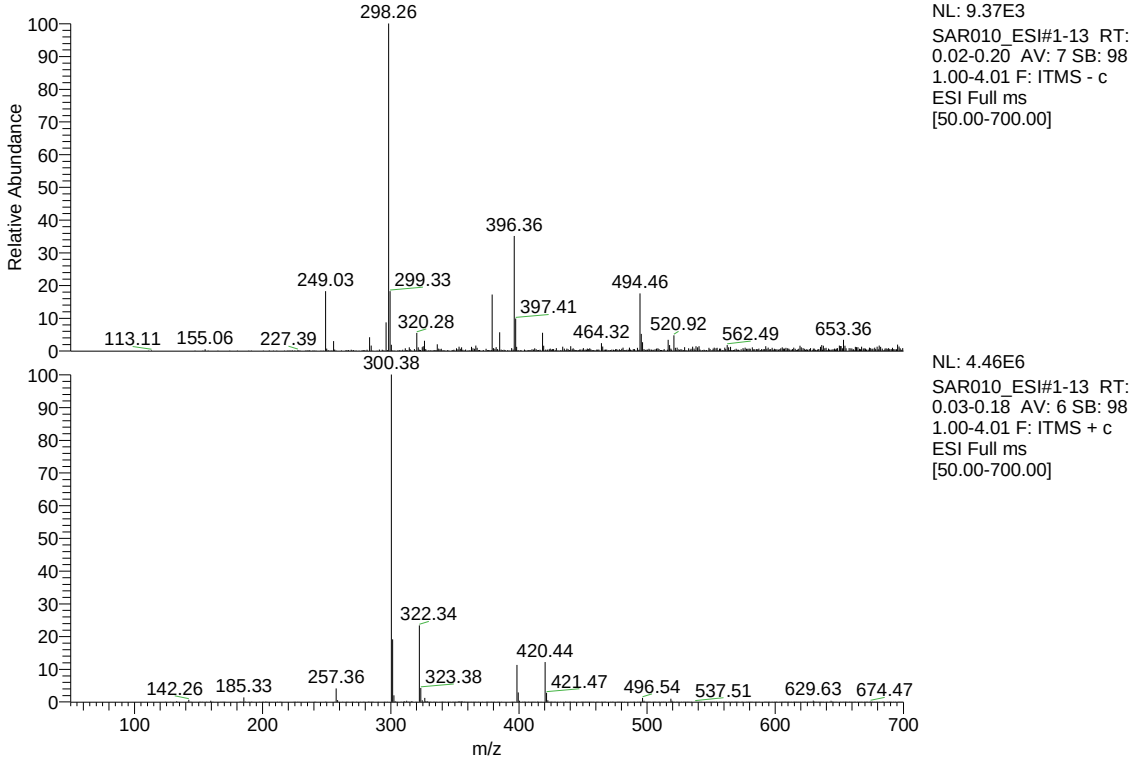


Figure D.8: The APCI Spectrum of Cy_2-Otn (Sample 1)

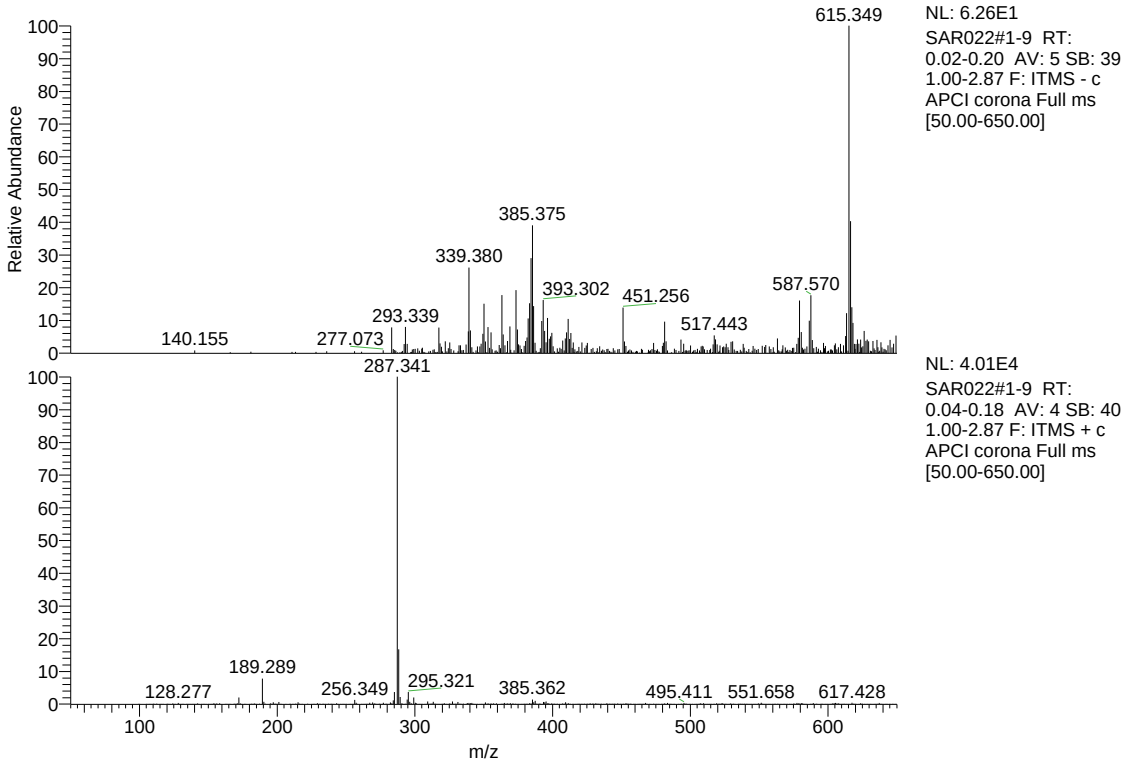


Figure D.9: The APCI Spectrum of Cy_2-Otn (Sample 2)

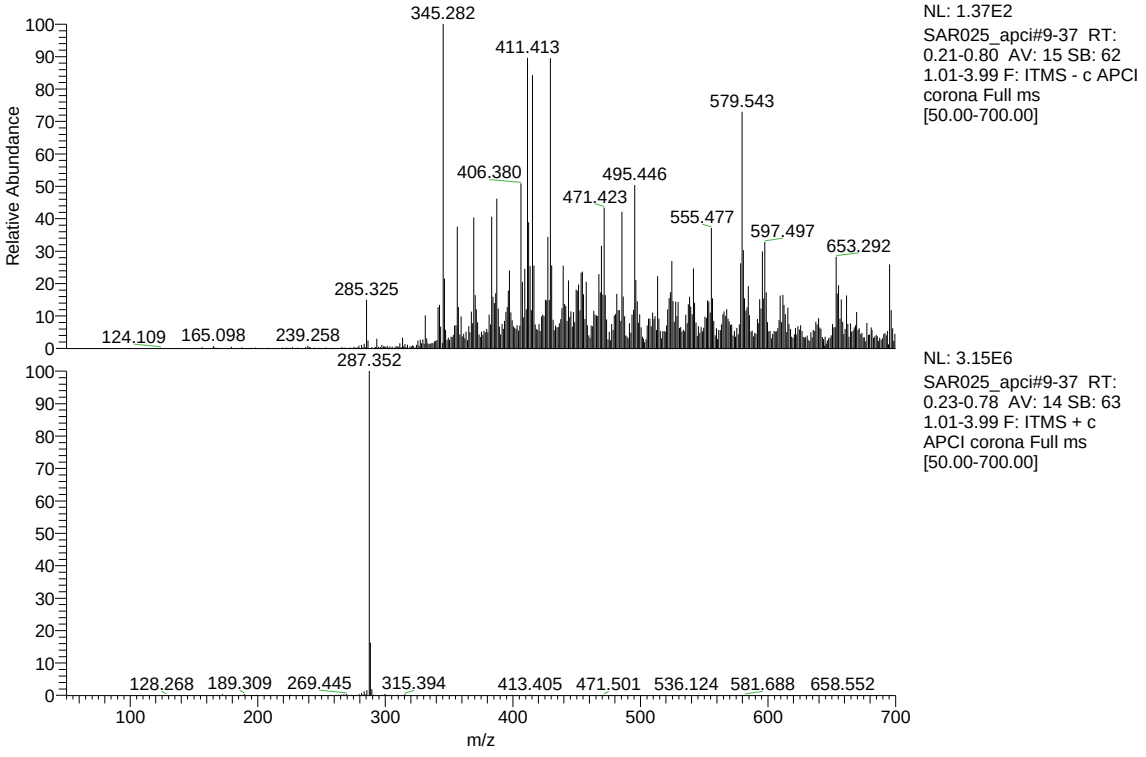


Figure D.10: The ESI Spectrum of Cy_2-Otn (Sample 3)

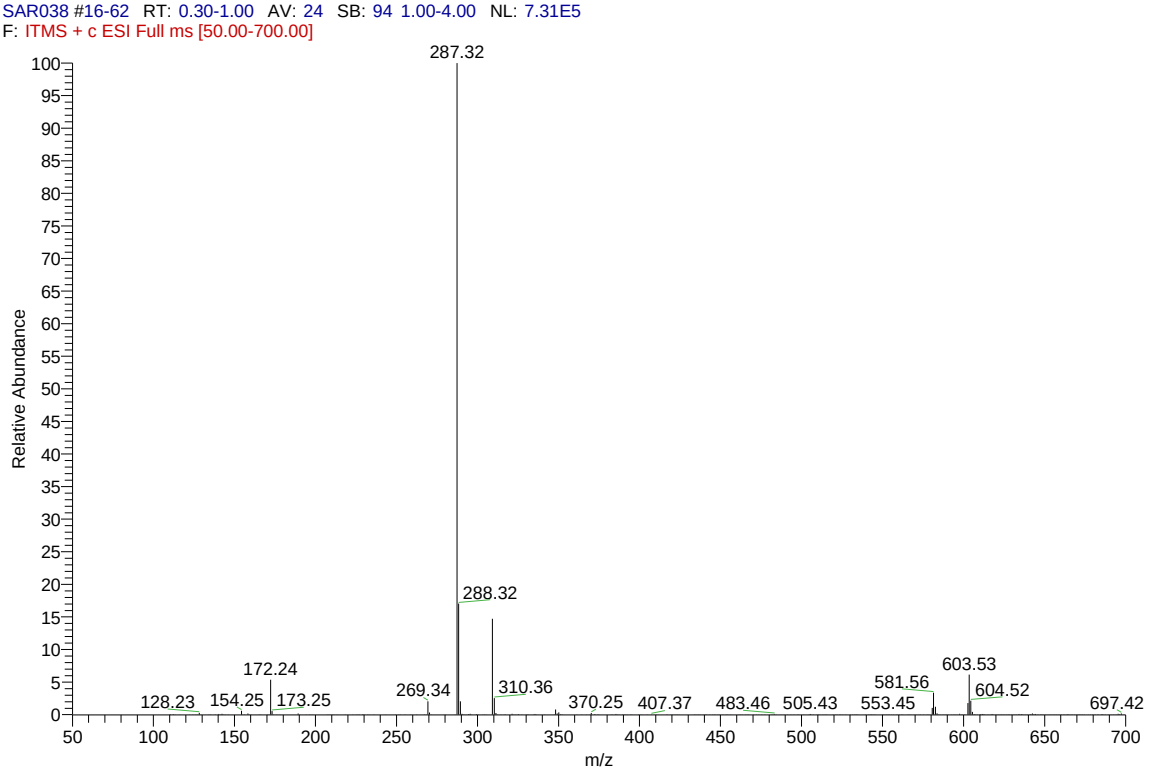


Figure D.11: The APCI Spectrum of the Imidazolinium Salt from the Attempted Cy_2-en/Pb(II) Reaction (Method 1)

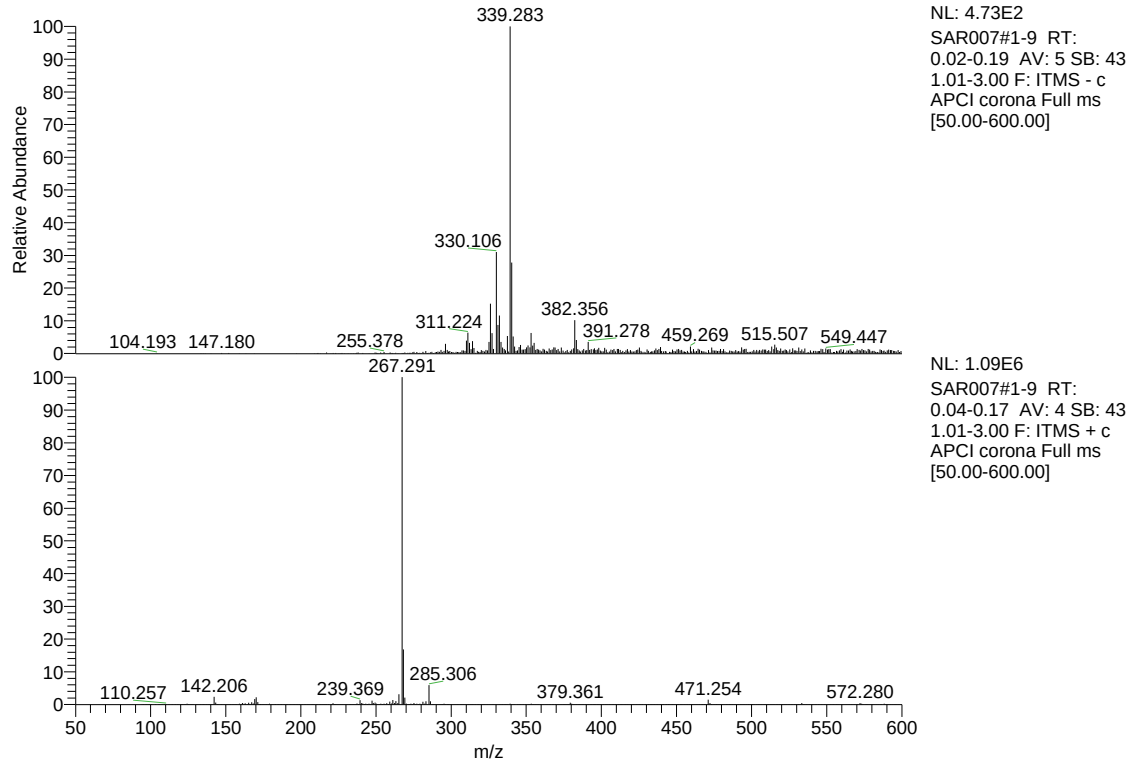


Figure D.12: The APCI Spectrum of the Attempted Cy_2-en/Pb(II) Reaction (Method 2)

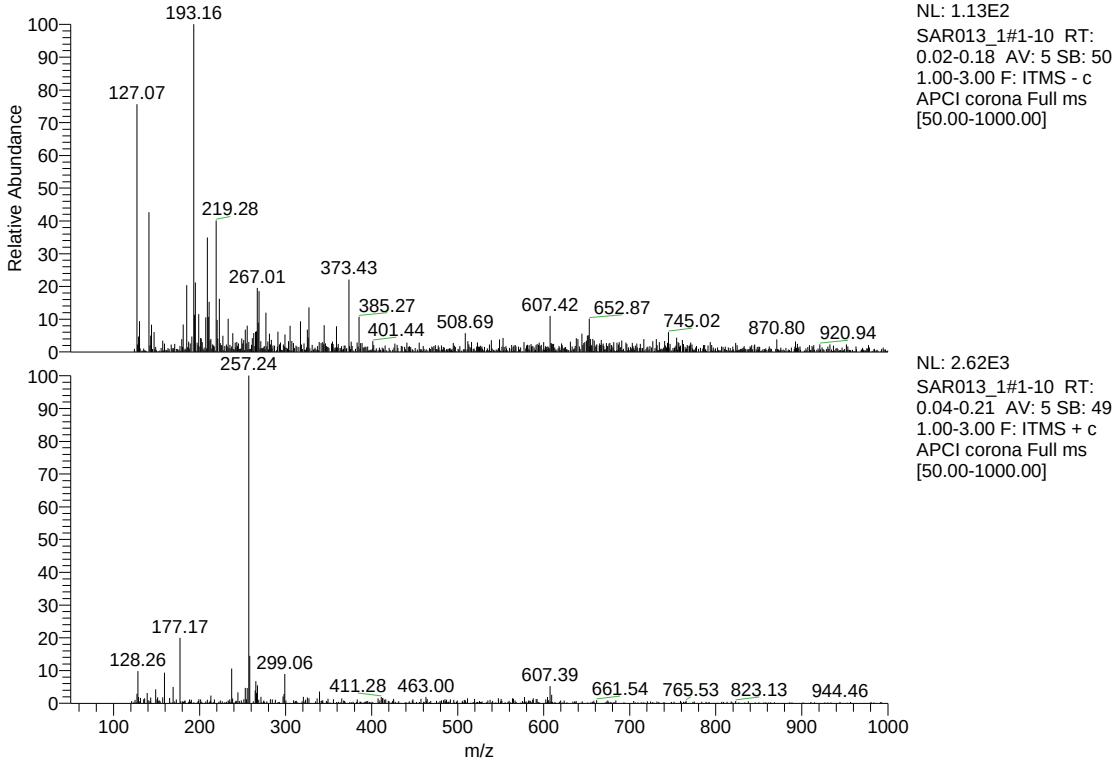


Figure D.13: The APCI Spectrum of the Attempted Cy_2-en/Pb(II) Reaction (Method 3)

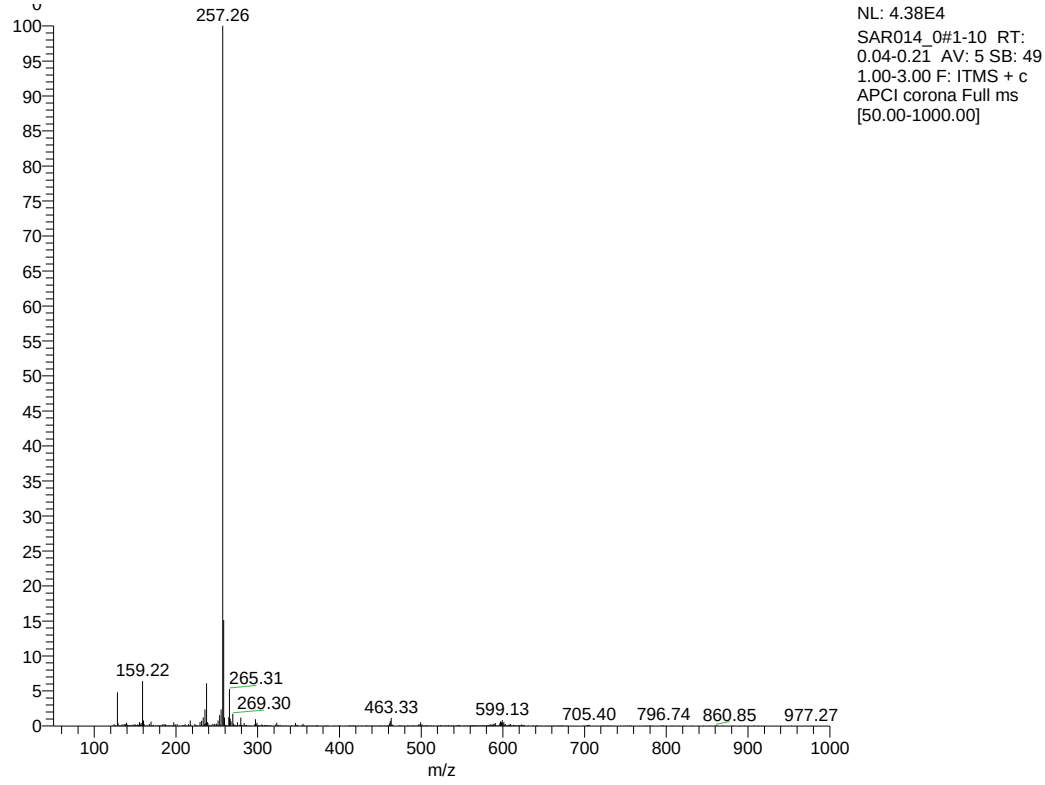


Figure D.14: The APCI Spectrum of the Attempted Cy_2-en/Pb(II) Reaction (Method 4)

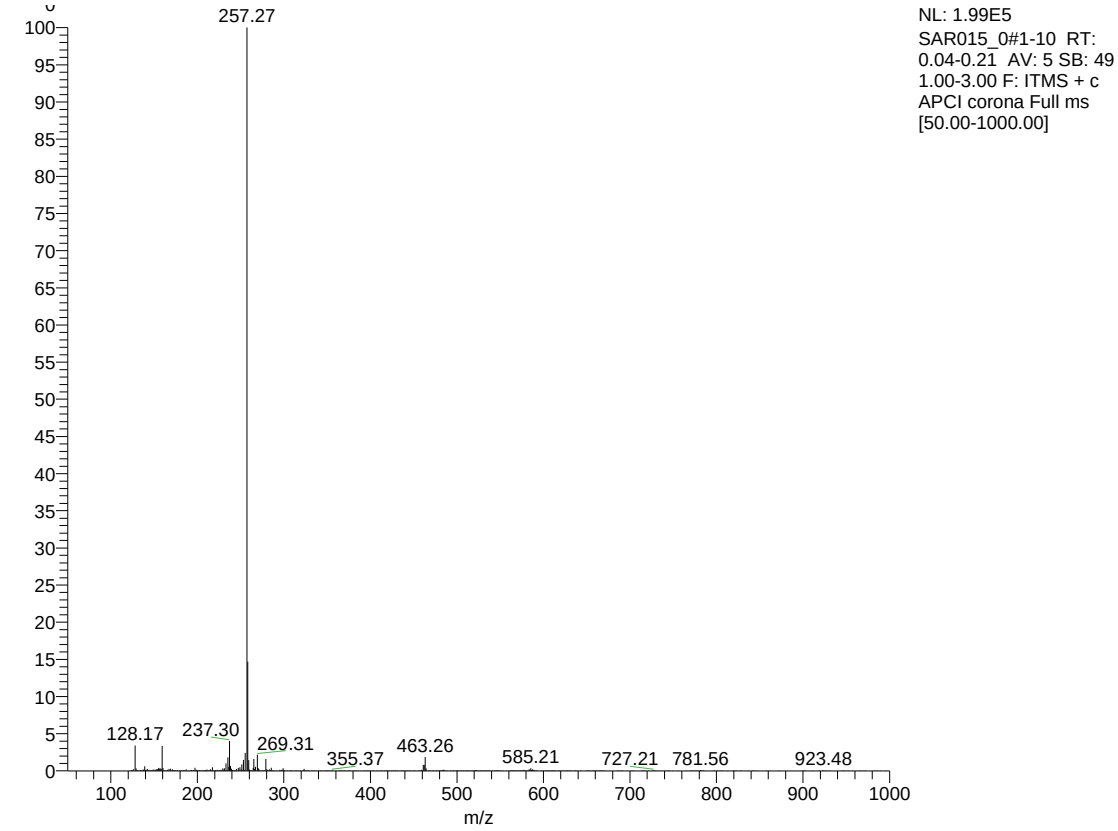


Figure D.15: The APCI Spectrum of the Successful Cy_2-en/Pb(II) Complex (Method 5)

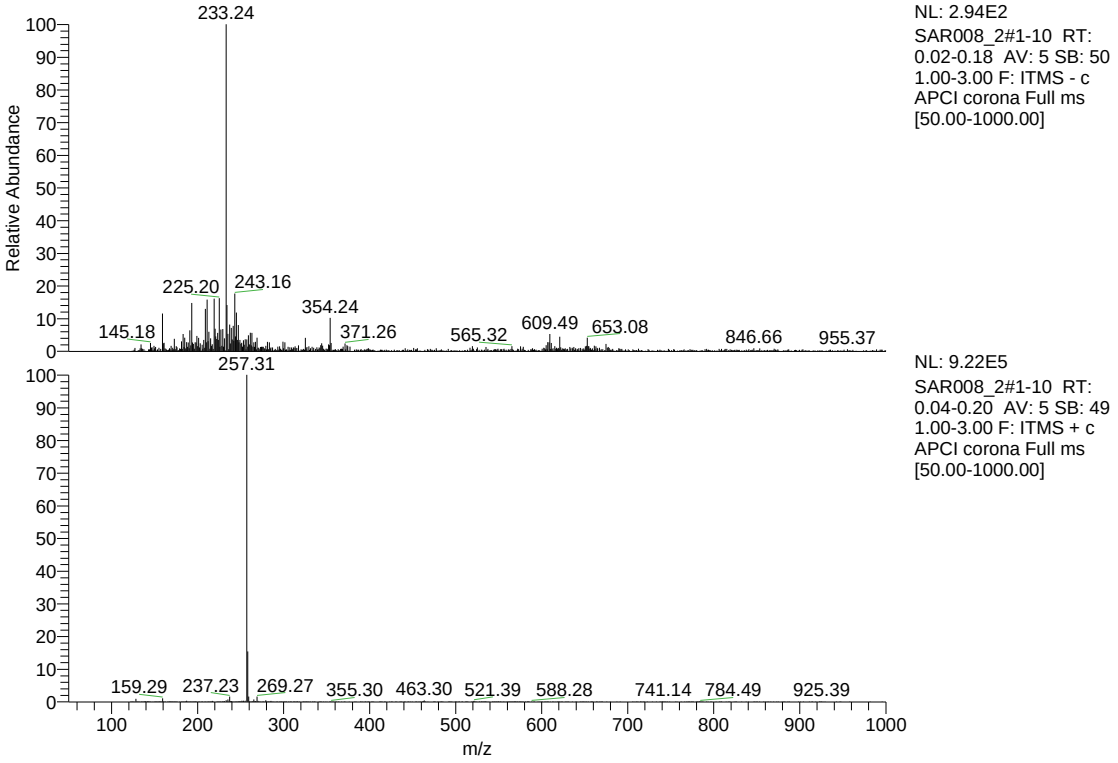


Figure D.16: The APCI Spectrum of the Attempted Cy_2-tn/Pb(II) Complex

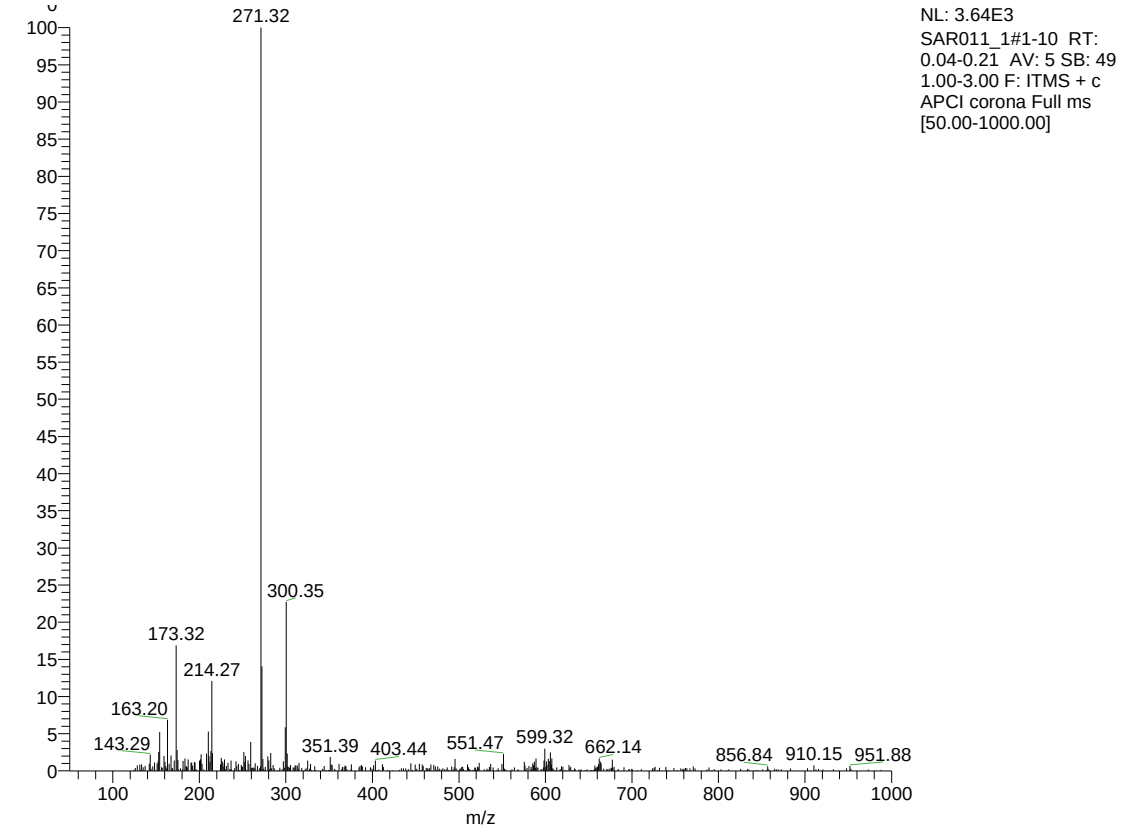


Figure D.17: The APCI Spectrum of the Cy_2-dien/Pb(II) Complex

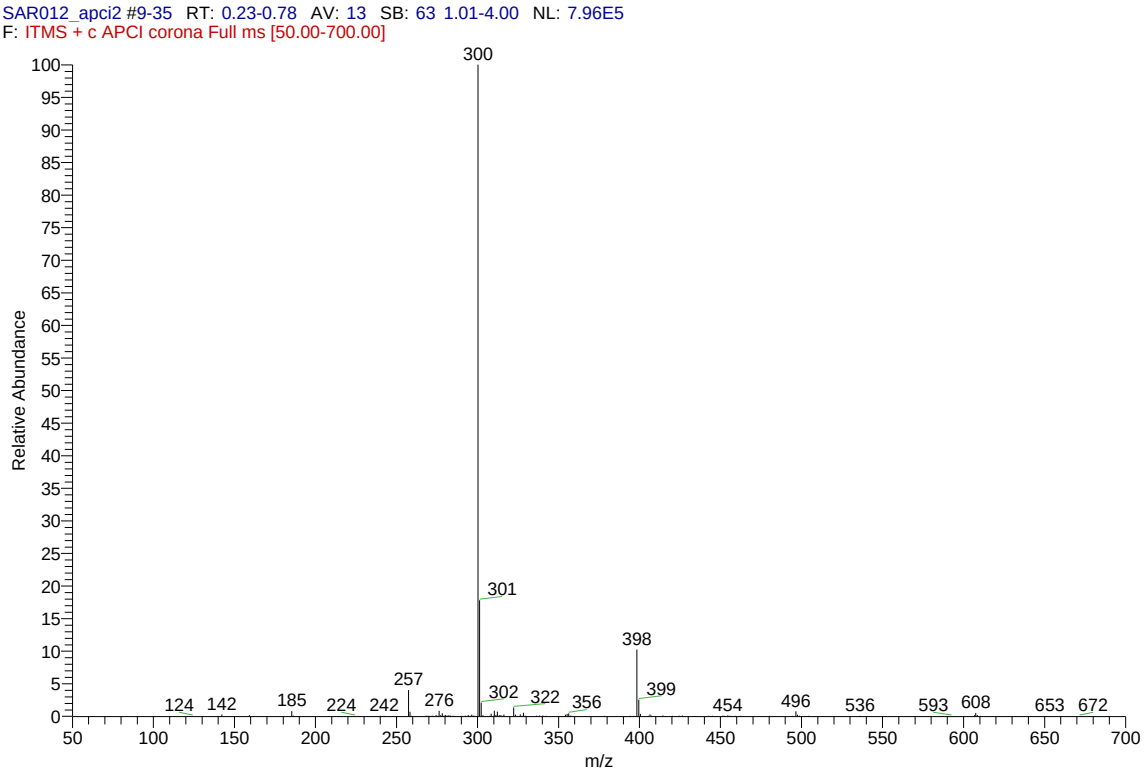


Figure D.18: The APCI Spectrum of the BHEEN/Pb(II) Complex

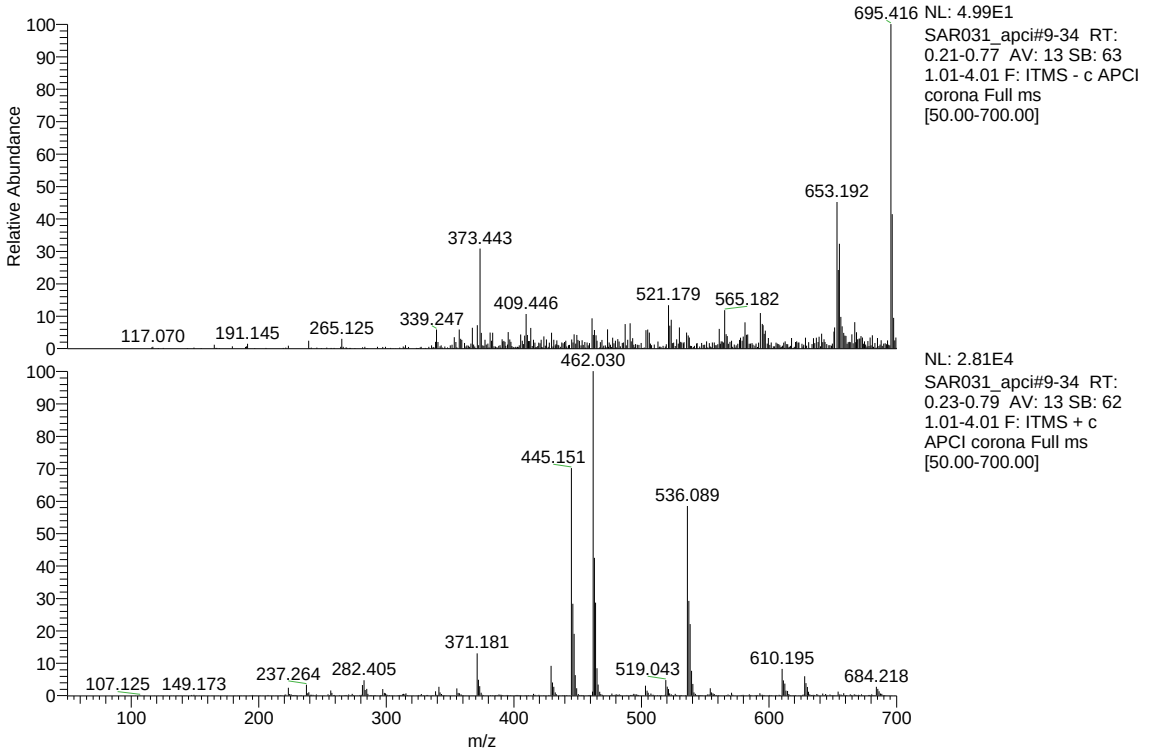


Figure D.19: The APCI Spectrum of the Cy_2-en/Cd(II) Complex

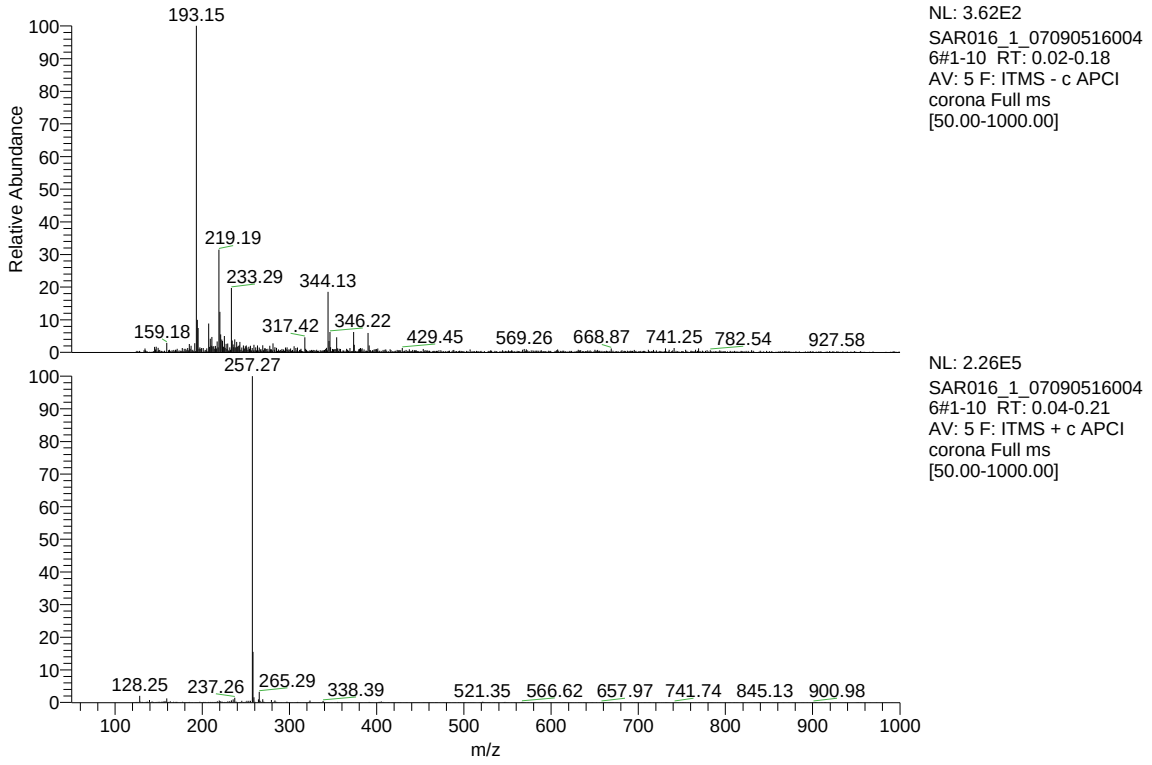


Figure D.20: The APCI Spectrum of the Cy_2-tn/Cd(II) Complex

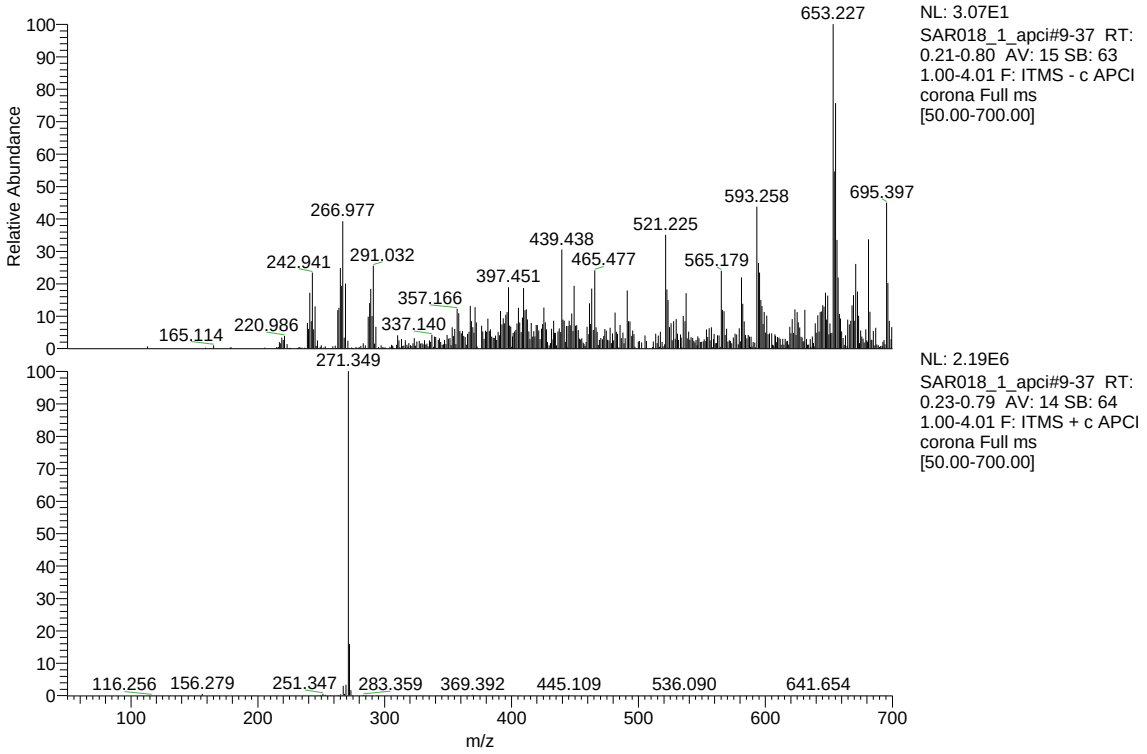


Figure D.21: The ESI Spectrum of the Cy_2-tn/Cd(II) Complex

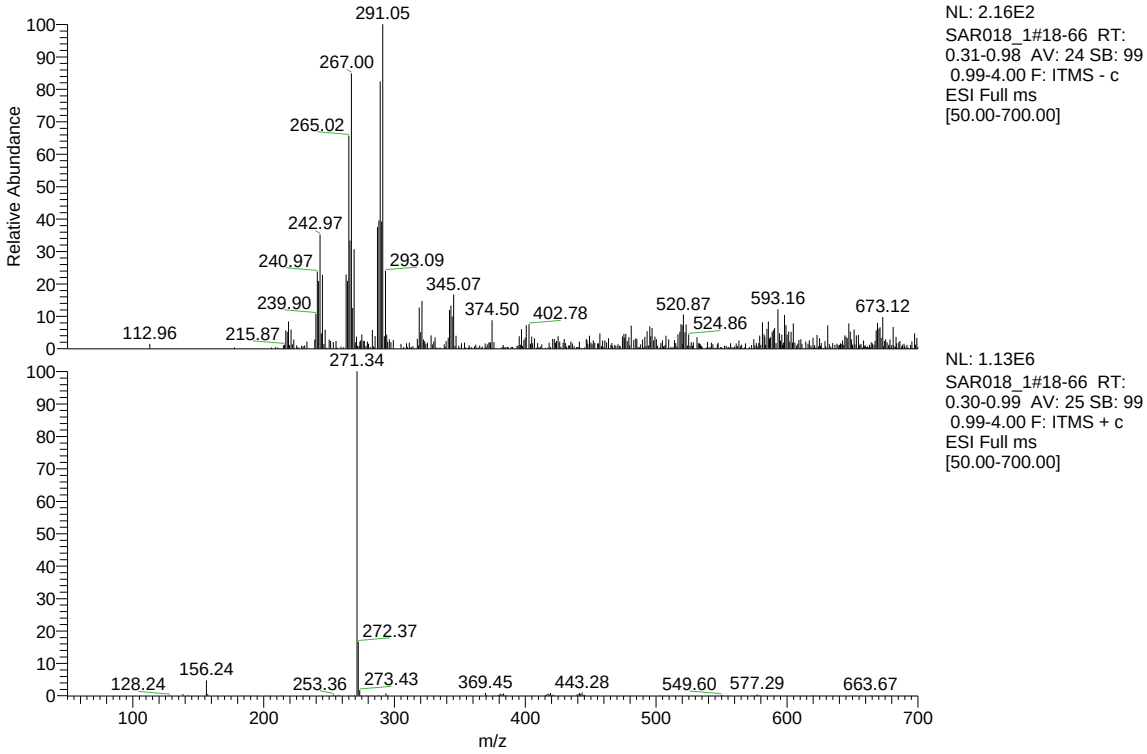


Figure D.22: The APCI Spectrum of the Cy_2-dien/Cd(II) Complex

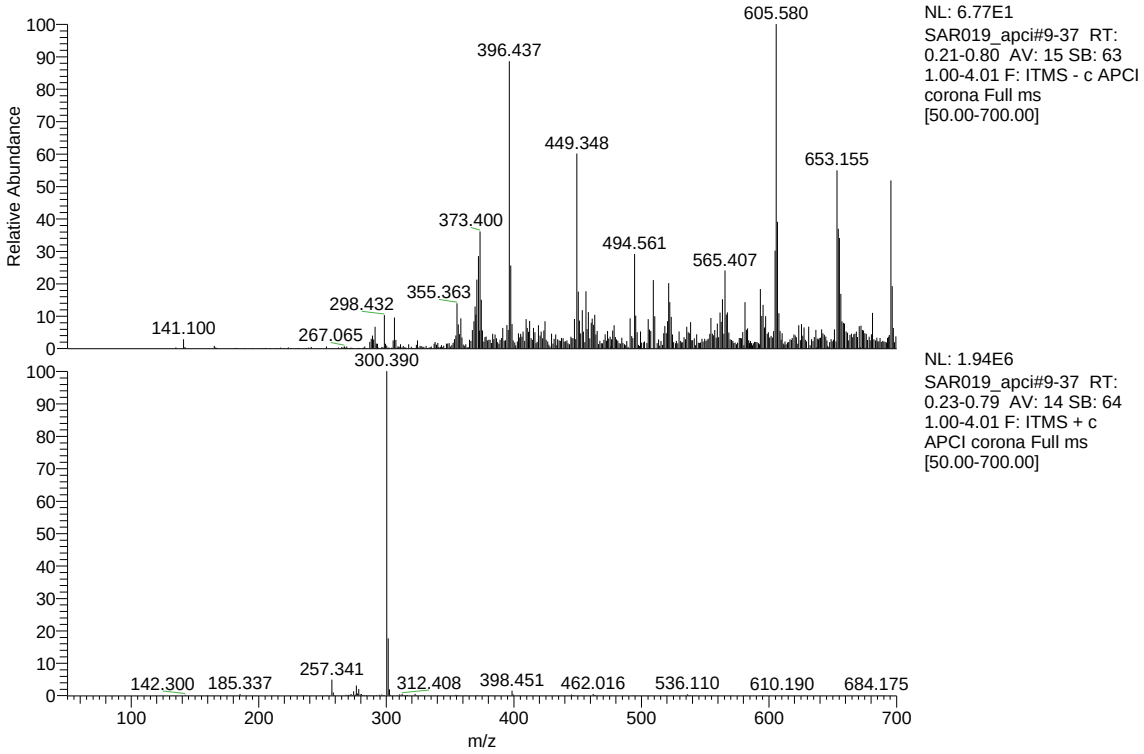


Figure D.23: The APCI Spectrum of the Cy_2-Otn/Cd(II) Complex

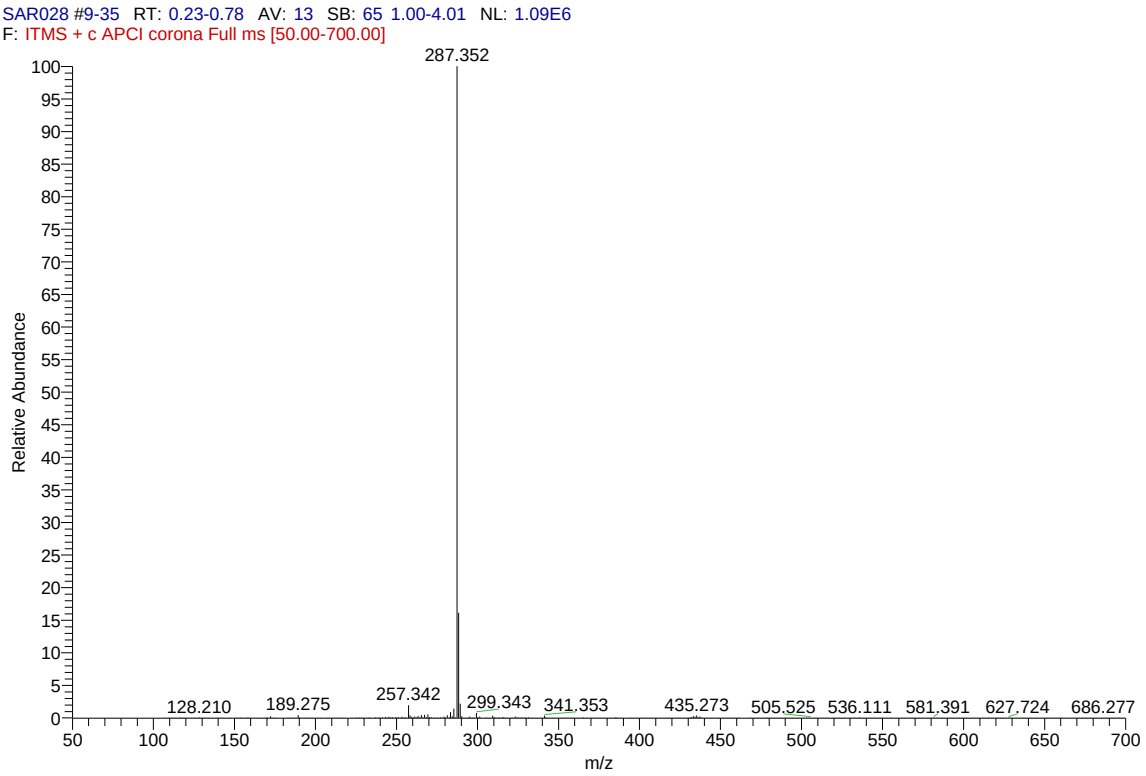


Figure D.24: The APCI Spectrum of the BHEEN/Cd(II) Complex

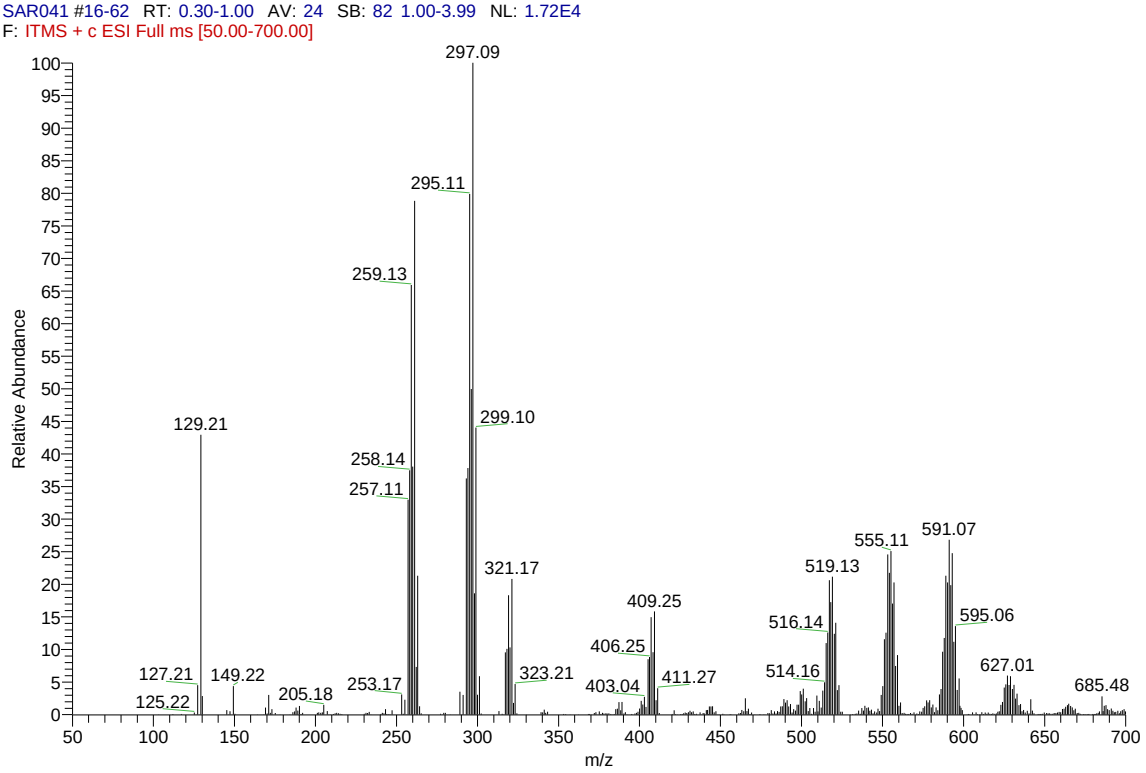


Figure D.25: The APCI Spectrum of the Cy_2-en/Ni(II) Complex

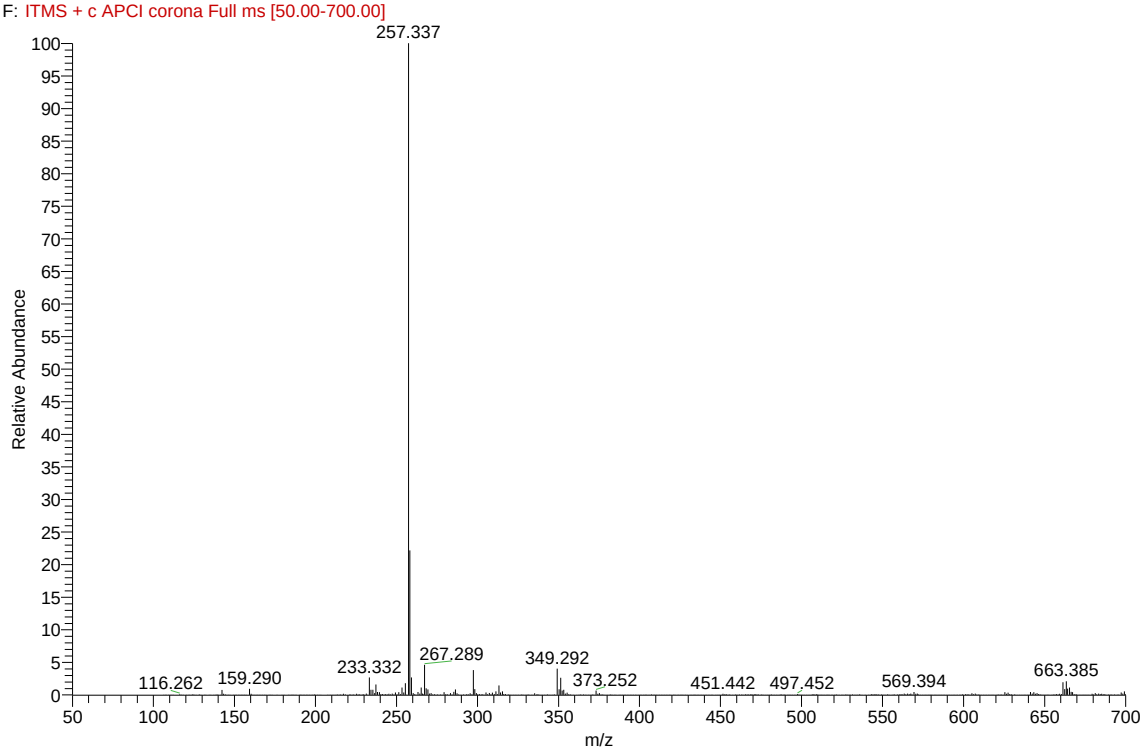


Figure D.26: The APCI Spectrum of the Cy_2-Otn/Ni(II) Complex

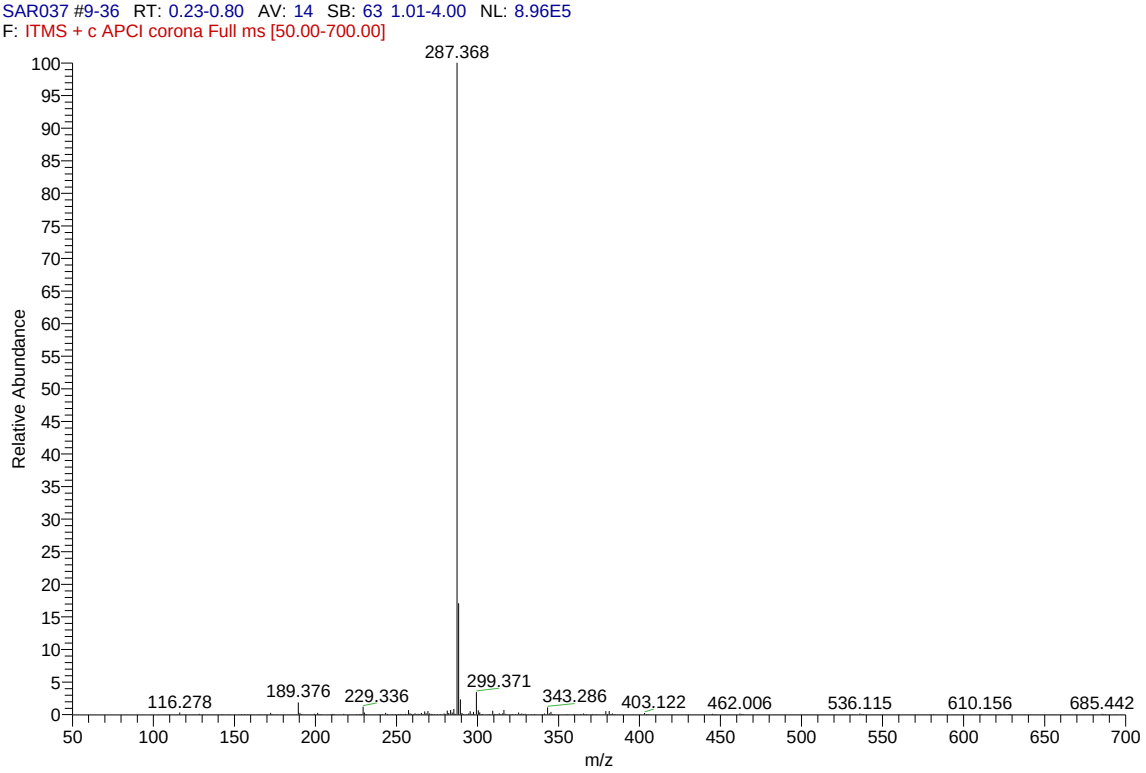


Figure D.27: The APCI Spectrum of the BHEEN/Ni(II) Complex

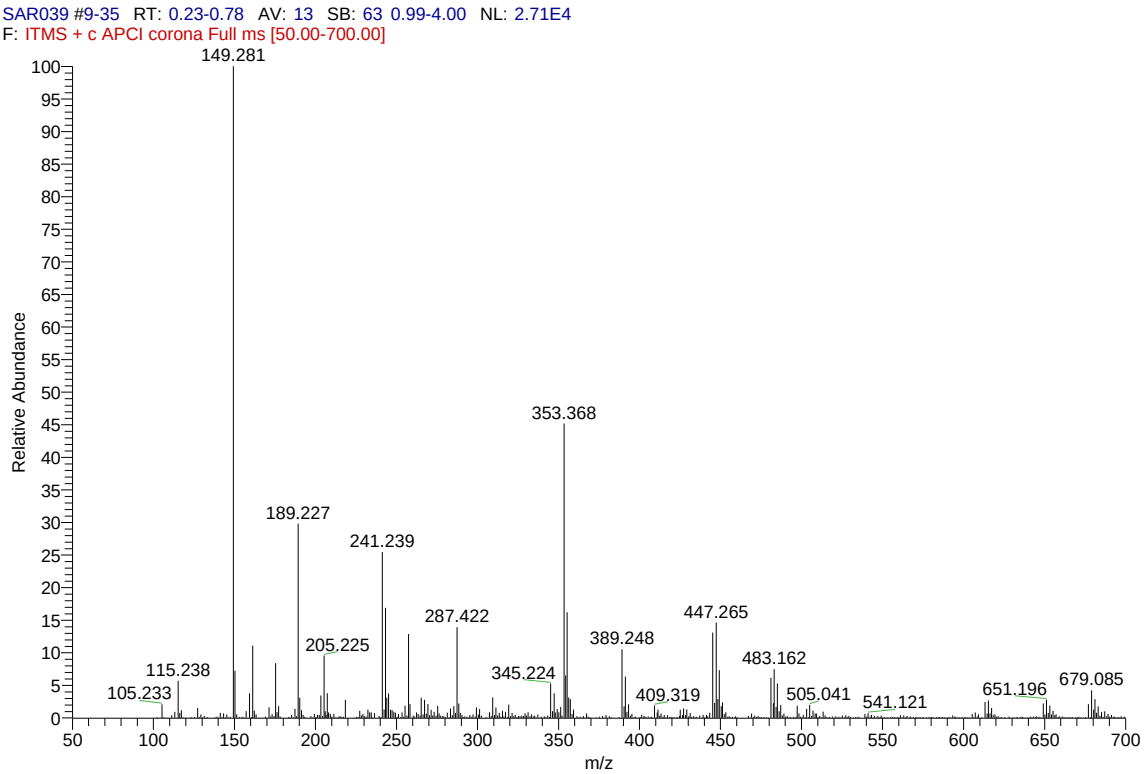


Figure D.28: The ESI Spectrum of the Cy_2-en/Zn(II) Complex

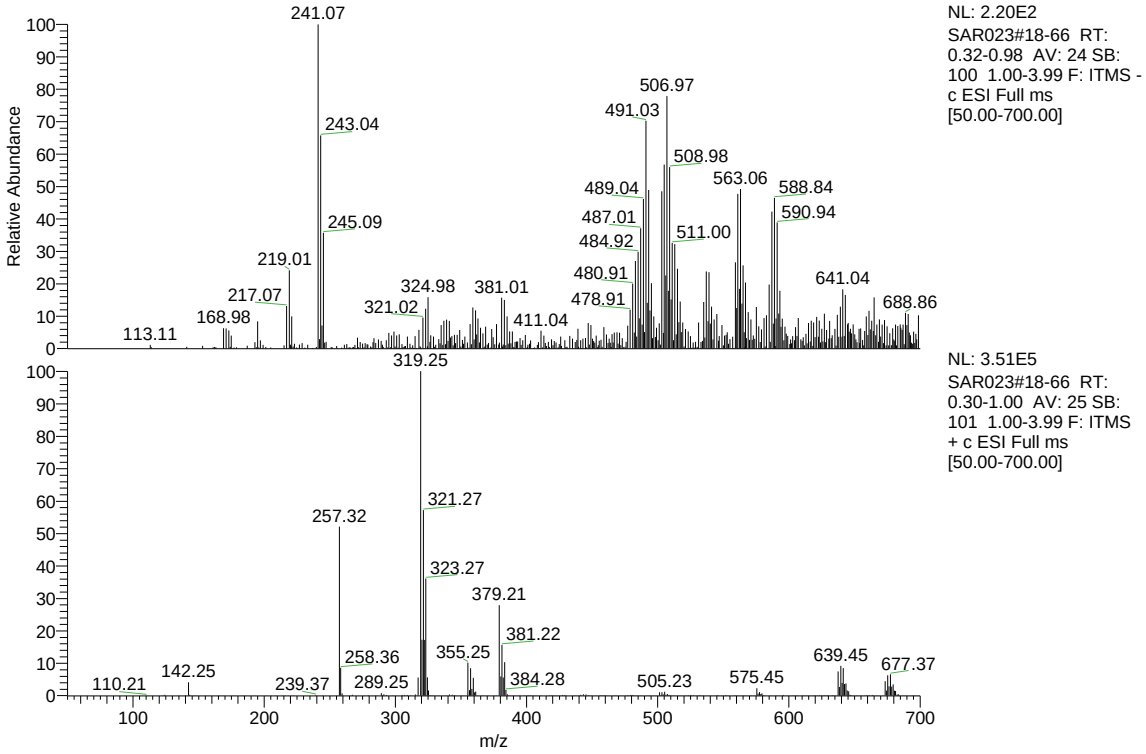


Figure D.29: The APCI Spectrum of the Cy_2-Otn/Zn(II) Complex

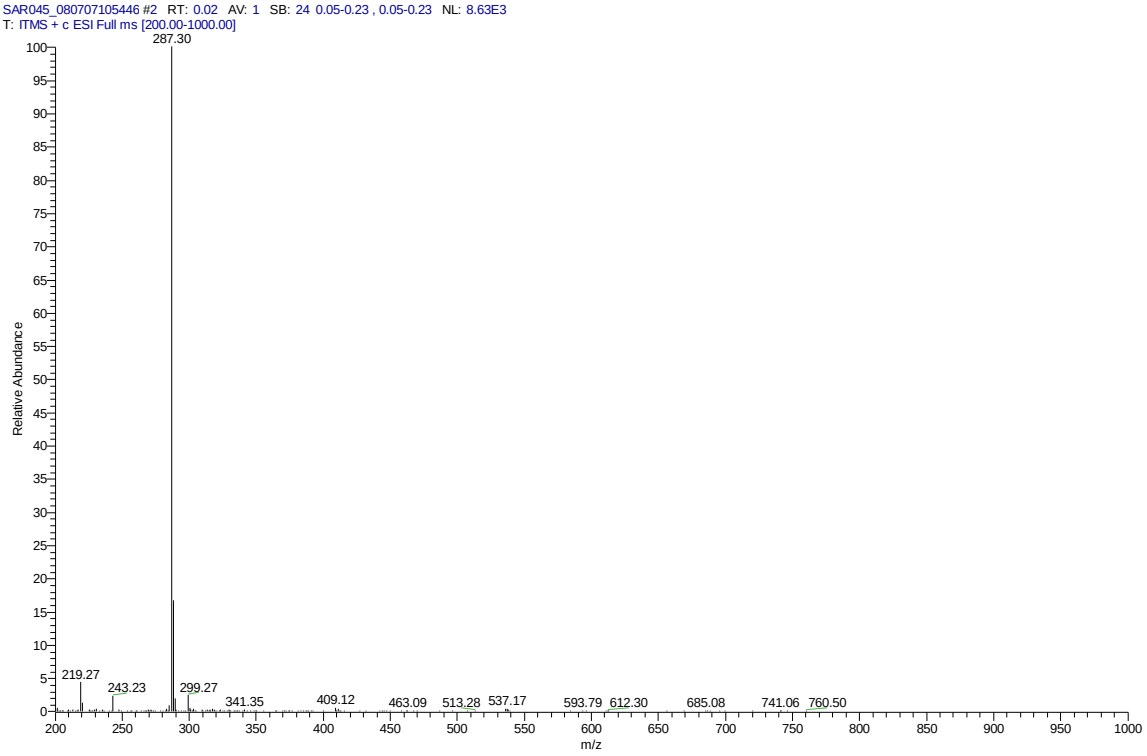


Figure D.30: The APCI Spectrum of the BHEEN/Zn(II) Complex

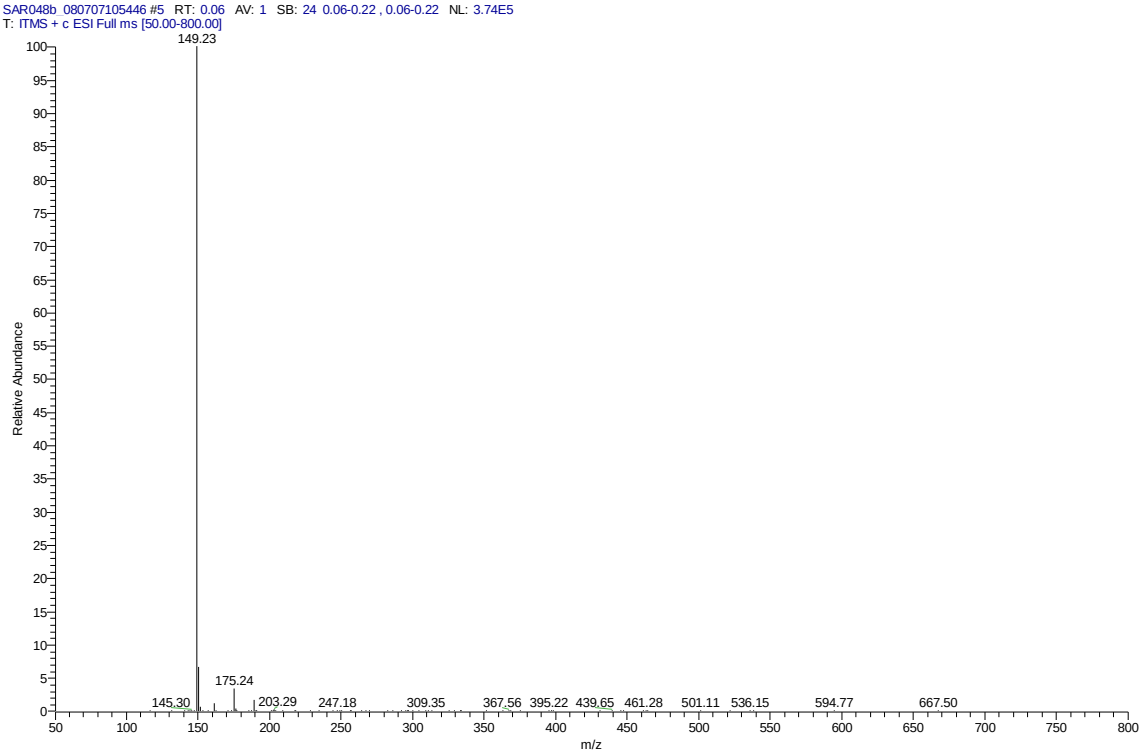
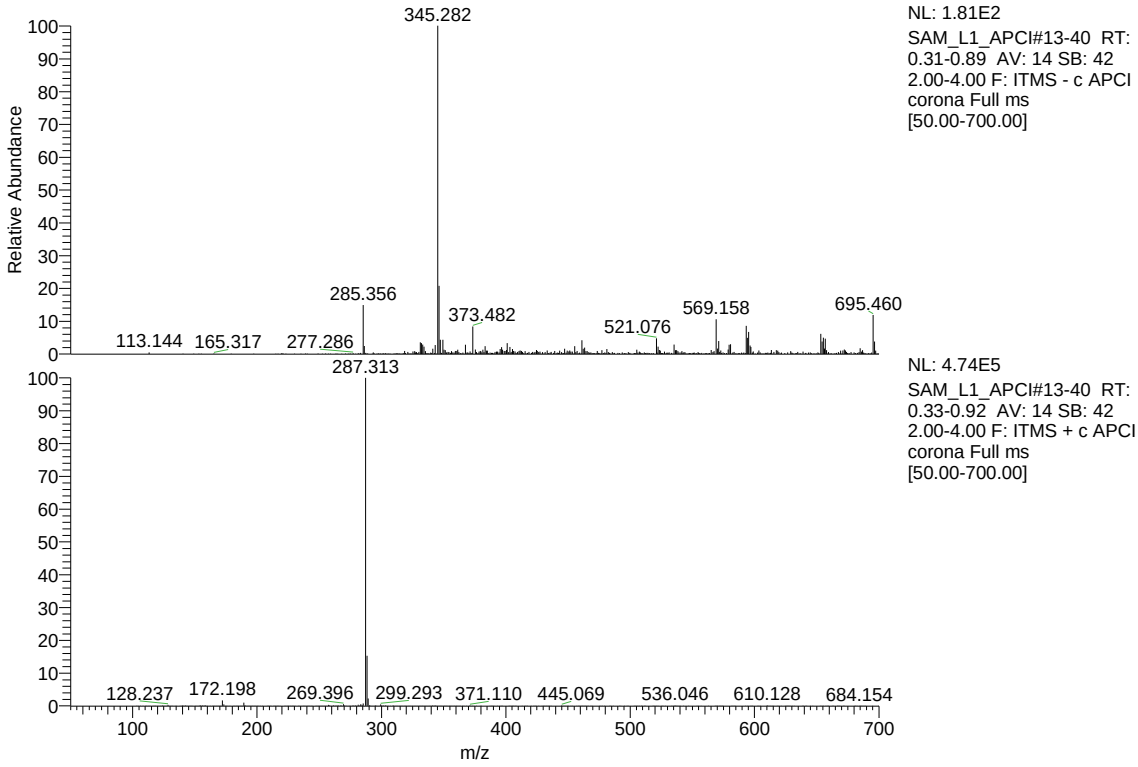


Figure D.31: The APCI Spectrum of the Zwitterion **2**



Appendix E

XRD Data

Cy_2-en Data

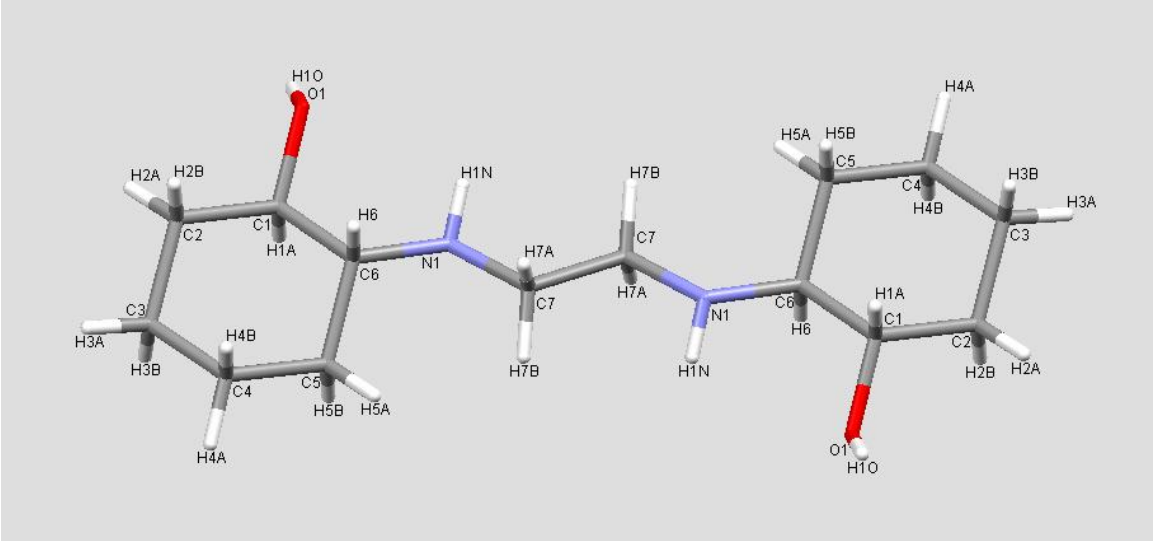


Figure E.1: XRD structure of Cy_2-en and the labelling scheme used

Table E.1: Crystal data and structure refinement for 7m_al3_0s.

Identification code	7m_al3_0s	
Empirical formula	C32 H4 N4 O4	
Formula weight	508.39	
Temperature	293(2) K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.281(5) Å	α = 90°.
	b = 8.110(5) Å	β = 102.776(5)°.
	c = 7.123(5) Å	γ = 90°.
Volume	691.9(7) $Å^3$	
Z	1	
Density (calculated)	1.220 Mg/m^3	
Absorption coefficient	0.084 mm^{-1}	
F(000)	256	
Crystal size	0.42 x 0.38 x 0.10 mm^3	
Theta range for data collection	1.70 to 28.31°.	

Index ranges	-16<=h<=16, -10<=k<=10, -9<=l<=9
Reflections collected	9394
Independent reflections	1721 [R(int) = 0.1057]
Completeness to theta = 28.31°	99.7 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1721 / 0 / 87
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0584, wR2 = 0.1399
R indices (all data)	R1 = 0.0784, wR2 = 0.1520
Largest diff. peak and hole	0.378 and -0.251 e.Å^{-3}

Table E.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 7m_al3_0s. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2939(1)	4047(2)	9017(2)	16(1)
C(2)	1983(2)	4769(2)	9797(2)	23(1)
C(3)	936(2)	5027(2)	8225(3)	28(1)
C(4)	1193(2)	6074(2)	6600(2)	23(1)
C(5)	2140(1)	5326(2)	5817(2)	20(1)
C(6)	3186(1)	5119(2)	7405(2)	15(1)
C(7)	4468(1)	5351(2)	5208(2)	18(1)
O(1)	3913(1)	3906(1)	10509(2)	20(1)
N(1)	4113(1)	4372(2)	6704(2)	16(1)

Table E.3: Bond lengths [Å] and angles [°] for 7m_al3_0s.

C(1)-O(1)	1.418(2)
C(1)-C(2)	1.522(2)
C(1)-C(6)	1.523(2)
C(1)-H(1A)	0.9800
C(2)-C(3)	1.521(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.524(2)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.523(2)
C(4)-H(4A)	0.9700

C(4)-H(4B)	0.9700
C(5)-C(6)	1.522(2)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-N(1)	1.470(2)
C(6)-H(6)	0.9800
C(7)-N(1)	1.471(2)
C(7)-C(7)#1	1.514(3)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
O(1)-H(1O)	0.8200
N(1)-H(1N)	0.83(2)

O(1)-C(1)-C(2)	110.37(13)
O(1)-C(1)-C(6)	109.56(13)
C(2)-C(1)-C(6)	110.77(13)
O(1)-C(1)-H(1A)	108.7
C(2)-C(1)-H(1A)	108.7
C(6)-C(1)-H(1A)	108.7
C(3)-C(2)-C(1)	112.22(14)
C(3)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2A)	109.2
C(3)-C(2)-H(2B)	109.2
C(1)-C(2)-H(2B)	109.2
H(2A)-C(2)-H(2B)	107.9
C(2)-C(3)-C(4)	110.67(15)
C(2)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
C(5)-C(4)-C(3)	111.03(14)
C(5)-C(4)-H(4A)	109.4
C(3)-C(4)-H(4A)	109.4
C(5)-C(4)-H(4B)	109.4
C(3)-C(4)-H(4B)	109.4
H(4A)-C(4)-H(4B)	108.0
C(4)-C(5)-C(6)	111.08(14)
C(4)-C(5)-H(5A)	109.4
C(6)-C(5)-H(5A)	109.4
C(4)-C(5)-H(5B)	109.4
C(6)-C(5)-H(5B)	109.4
H(5A)-C(5)-H(5B)	108.0
N(1)-C(6)-C(5)	112.49(13)
N(1)-C(6)-C(1)	108.63(13)
C(5)-C(6)-C(1)	110.28(14)

N(1)-C(6)-H(6)	108.4
C(5)-C(6)-H(6)	108.4
C(1)-C(6)-H(6)	108.4
N(1)-C(7)-C(7)#1	110.22(16)
N(1)-C(7)-H(7A)	109.6
C(7)#1-C(7)-H(7A)	109.6
N(1)-C(7)-H(7B)	109.6
C(7)#1-C(7)-H(7B)	109.6
H(7A)-C(7)-H(7B)	108.1
C(1)-O(1)-H(1O)	109.5
C(6)-N(1)-C(7)	113.54(13)
C(6)-N(1)-H(1N)	107.9(14)
C(7)-N(1)-H(1N)	102.9(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table E.4: Anisotropic displacement parameters ($Å^2$x 10^3)for 7m_al3_0s. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	21(1)	14(1)	13(1)	1(1)	4(1)	-1(1)
C(2)	30(1)	24(1)	17(1)	3(1)	12(1)	2(1)
C(3)	25(1)	33(1)	29(1)	9(1)	12(1)	3(1)
C(4)	24(1)	22(1)	22(1)	2(1)	5(1)	2(1)
C(5)	26(1)	19(1)	15(1)	1(1)	6(1)	2(1)
C(6)	22(1)	11(1)	14(1)	-1(1)	6(1)	-1(1)
C(7)	25(1)	16(1)	15(1)	2(1)	7(1)	-1(1)
O(1)	28(1)	17(1)	14(1)	3(1)	2(1)	-1(1)
N(1)	21(1)	15(1)	11(1)	0(1)	5(1)	0(1)

Table E.5: Torsion angles [°] for 7m_al3_0s.

O(1)-C(1)-C(2)-C(3)	177.01(13)
C(6)-C(1)-C(2)-C(3)	55.48(19)
C(1)-C(2)-C(3)-C(4)	-54.6(2)
C(2)-C(3)-C(4)-C(5)	55.0(2)
C(3)-C(4)-C(5)-C(6)	-57.13(19)
C(4)-C(5)-C(6)-N(1)	179.04(13)
C(4)-C(5)-C(6)-C(1)	57.59(17)
O(1)-C(1)-C(6)-N(1)	57.96(16)
C(2)-C(1)-C(6)-N(1)	179.96(13)
O(1)-C(1)-C(6)-C(5)	-178.33(12)

C(2)-C(1)-C(6)-C(5)	-56.32(17)
C(5)-C(6)-N(1)-C(7)	60.74(18)
C(1)-C(6)-N(1)-C(7)	-176.88(13)
C(7)#1-C(7)-N(1)-C(6)	171.04(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table E.6: Hydrogen bonds for 7m_al3_0s [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...N(1)#2	0.82	1.97	2.785(2)	175.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 x,-y+1/2,z+1/2

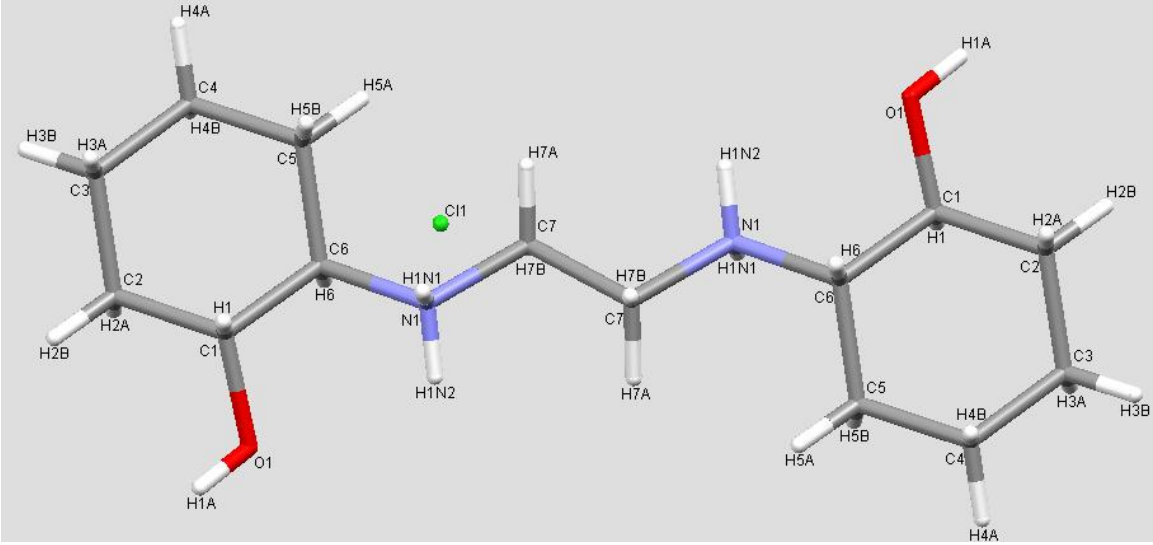


Figure E.2: XRD structure of the protonated Cy_2-en and the labelling scheme used

Table E.7: Crystal data and structure refinement for 7m_al6_0s.

Identification code	7m_al6_0s
Empirical formula	C14 H30 Cl2 N2 O2
Formula weight	329.30

Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 5.8557(3) Å	α = 97.885(3)°.
	b = 6.9089(3) Å	β = 98.174(4)°.
	c = 11.1223(7) Å	γ = 107.415(3)°.
Volume	417.21(4) Å3	
Z	1	
Density (calculated)	1.311 Mg/m3	
Absorption coefficient	0.393 mm-1	
F(000)	178	
Crystal size	0.35 x 0.31 x 0.07 mm3	
Theta range for data collection	1.88 to 25.49°.	
Index ranges	-7<=h<=7, -8<=k<=8, -13<=l<=12	
Reflections collected	5128	
Independent reflections	1533 [R(int) = 0.0476]	
Completeness to theta = 25.49°	98.8 %	
Absorption correction	Multiscan	
Max. and min. transmission	0.9730 and 0.8747	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	1533 / 0 / 92	
Goodness-of-fit on F^2	1.306	
Final R indices [I>2sigma(I)]	R1 = 0.0586, wR2 = 0.1699	
R indices (all data)	R1 = 0.0615, wR2 = 0.1708	
Largest diff. peak and hole	0.713 and -0.334 e.$Å^{-3}$	

Table E.8: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 7m_al6_0s. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3106(9)	1363(7)	2173(4)	31(1)
C(2)	2827(10)	284(8)	3266(4)	38(1)
C(3)	3016(11)	1793(8)	4425(5)	45(1)
C(4)	1127(12)	2868(9)	4243(5)	50(1)
C(5)	1329(10)	3933(8)	3134(4)	37(1)
C(6)	1211(8)	2433(6)	1975(4)	26(1)
C(7)	-182(8)	4604(7)	595(4)	27(1)
Cl(1)	6262(2)	7355(2)	1634(1)	35(1)
N(1)	1609(7)	3526(5)	909(3)	24(1)
O(1)	2792(8)	-28(6)	1035(3)	47(1)

Table E.9: Bond lengths [Å] and angles [°] for 7m_al6_0s.

C(1)-O(1)	1.433(5)
C(1)-C(2)	1.514(6)
C(1)-C(6)	1.514(6)
C(1)-H(1)	0.9800
C(2)-C(3)	1.510(7)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.512(8)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.521(7)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.518(6)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-N(1)	1.500(5)
C(6)-H(6)	0.9800
C(7)-N(1)	1.487(5)
C(7)-C(7)#1	1.517(8)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
N(1)-H(1N1)	0.9000
N(1)-H(1N2)	0.9000
O(1)-H(1A)	0.8200
O(1)-C(1)-C(2)	113.0(4)
O(1)-C(1)-C(6)	106.4(4)
C(2)-C(1)-C(6)	110.6(4)
O(1)-C(1)-H(1)	108.9
C(2)-C(1)-H(1)	108.9
C(6)-C(1)-H(1)	108.9
C(3)-C(2)-C(1)	110.9(4)
C(3)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.0
C(2)-C(3)-C(4)	110.9(4)
C(2)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
C(3)-C(4)-C(5)	111.4(4)

C(3)-C(4)-H(4A)	109.3
C(5)-C(4)-H(4A)	109.3
C(3)-C(4)-H(4B)	109.3
C(5)-C(4)-H(4B)	109.3
H(4A)-C(4)-H(4B)	108.0
C(6)-C(5)-C(4)	111.2(4)
C(6)-C(5)-H(5A)	109.4
C(4)-C(5)-H(5A)	109.4
C(6)-C(5)-H(5B)	109.4
C(4)-C(5)-H(5B)	109.4
H(5A)-C(5)-H(5B)	108.0
N(1)-C(6)-C(1)	108.6(3)
N(1)-C(6)-C(5)	110.9(3)
C(1)-C(6)-C(5)	111.4(4)
N(1)-C(6)-H(6)	108.6
C(1)-C(6)-H(6)	108.6
C(5)-C(6)-H(6)	108.6
N(1)-C(7)-C(7)#1	109.3(4)
N(1)-C(7)-H(7A)	109.8
C(7)#1-C(7)-H(7A)	109.8
N(1)-C(7)-H(7B)	109.8
C(7)#1-C(7)-H(7B)	109.8
H(7A)-C(7)-H(7B)	108.3
C(7)-N(1)-C(6)	114.1(3)
C(7)-N(1)-H(1N1)	108.7
C(6)-N(1)-H(1N1)	108.7
C(7)-N(1)-H(1N2)	108.7
C(6)-N(1)-H(1N2)	108.7
H(1N1)-N(1)-H(1N2)	107.6
C(1)-O(1)-H(1A)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z

Table E.10: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 7m_al6_0s. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U11	U22	U33	U23	U13	U12
C(1)	37(3)	30(2)	29(2)	6(2)	1(2)	18(2)
C(2)	49(3)	35(3)	35(3)	12(2)	1(2)	21(2)
C(3)	63(4)	44(3)	32(3)	18(2)	7(2)	21(3)
C(4)	73(4)	55(3)	39(3)	22(3)	26(3)	32(3)
C(5)	53(3)	34(3)	34(3)	10(2)	15(2)	23(2)

C(6)	30(2)	23(2)	27(2)	10(2)	6(2)	10(2)
C(7)	28(2)	27(2)	30(2)	9(2)	5(2)	16(2)
Cl(1)	28(1)	32(1)	46(1)	5(1)	10(1)	11(1)
N(1)	31(2)	21(2)	24(2)	6(1)	5(2)	14(2)
O(1)	74(3)	46(2)	36(2)	5(2)	5(2)	42(2)

Table E.11: Torsion angles [°] for 7m_al6_0s.

O(1)-C(1)-C(2)-C(3)	-176.4(4)
C(6)-C(1)-C(2)-C(3)	-57.3(6)
C(1)-C(2)-C(3)-C(4)	57.3(6)
C(2)-C(3)-C(4)-C(5)	-55.7(7)
C(3)-C(4)-C(5)-C(6)	54.3(6)
O(1)-C(1)-C(6)-N(1)	-58.5(5)
C(2)-C(1)-C(6)-N(1)	178.4(4)
O(1)-C(1)-C(6)-C(5)	179.0(4)
C(2)-C(1)-C(6)-C(5)	55.9(5)
C(4)-C(5)-C(6)-N(1)	-175.5(4)
C(4)-C(5)-C(6)-C(1)	-54.4(6)
C(7)#1-C(7)-N(1)-C(6)	-172.3(4)
C(1)-C(6)-N(1)-C(7)	178.6(4)
C(5)-C(6)-N(1)-C(7)	-58.7(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z

Table E.12: Hydrogen bonds for 7m_al6_0s [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N1)...Cl(1)	0.90	2.22	3.090(4)	163.9
N(1)-H(1N2)...Cl(1)#2	0.90	2.60	3.303(4)	135.3
O(1)-H(1A)...Cl(1)#3	0.82	2.35	3.160(4)	168.4

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z #2 -x+1,-y+1,-z #3 x,y-1,z

Cy_2-Otn Data

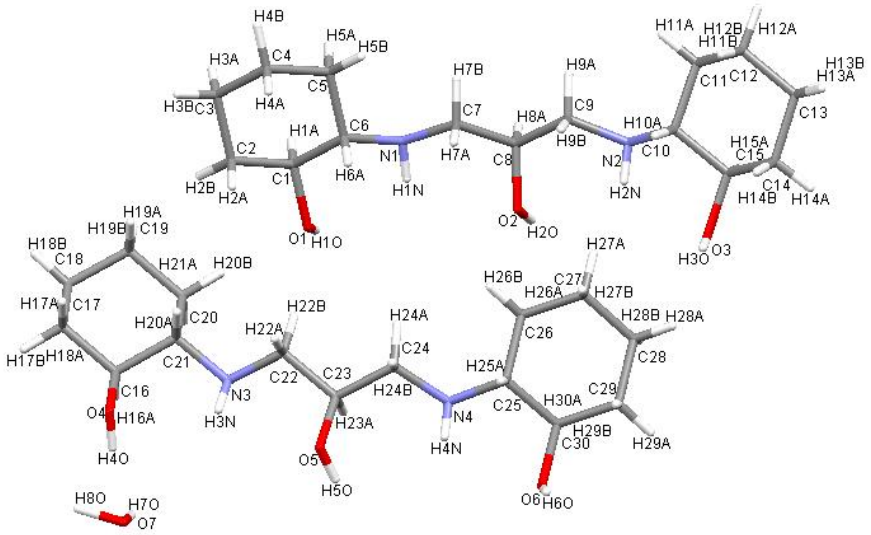


Figure E.3: XRD structure of Cy_2-Otn and the labelling scheme used

Table E.13: Crystal data and structure refinement for 7m_al19_0s.

Identification code	7m_al19_0s	
Empirical formula	C30 H62 N4 O7	
Formula weight	590.84	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.0830(2) Å	α = 104.5330(10)°.
	b = 10.6966(3) Å	β = 104.7020(10)°.
	c = 16.6006(4) Å	γ = 90.5310(10)°.
Volume	1671.31(7) $Å^3$	
Z	2	
Density (calculated)	1.174 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	652	
Crystal size	0.42 x 0.22 x 0.16 mm^3	
Theta range for data collection	1.31 to 28.00°.	
Index ranges	-13<=h<=13, -14<=k<=14, -21<=l<=21	
Reflections collected	29863	
Independent reflections	8075 [R(int) = 0.0548]	
Completeness to theta = 28.00°	100.0 %	
Absorption correction	None	
Max. and min. transmission	0.9869 and 0.9662	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8075 / 0 / 397
Goodness-of-fit on F^2	1.002
Final R indices [I>2sigma(I)]	R1 = 0.0504, wR2 = 0.1196
R indices (all data)	R1 = 0.0868, wR2 = 0.1338
Largest diff. peak and hole	0.397 and -0.226 e.Å^{-3}

Table E.14: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 7m_al19_0s. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-1447(2)	5680(2)	3207(1)	28(1)
C(2)	-2250(2)	6857(2)	3151(1)	36(1)
C(3)	-3660(2)	6681(2)	3294(1)	39(1)
C(4)	-4453(2)	5476(2)	2657(1)	38(1)
C(5)	-3657(2)	4283(2)	2714(1)	35(1)
C(6)	-2239(2)	4462(2)	2577(1)	26(1)
C(7)	-1984(2)	2142(2)	2045(1)	31(1)
C(8)	-955(2)	1119(2)	2019(1)	27(1)
C(9)	-1687(2)	-116(2)	1390(1)	35(1)
C(10)	-1480(2)	-2161(2)	432(1)	32(1)
C(11)	-2417(2)	-3078(2)	647(1)	39(1)
C(12)	-3182(2)	-4090(2)	-169(1)	53(1)
C(13)	-2190(2)	-4828(2)	-608(1)	53(1)
C(14)	-1166(2)	-3941(2)	-776(1)	40(1)
C(15)	-452(2)	-2906(2)	29(1)	35(1)
N(1)	-1419(1)	3353(1)	2684(1)	27(1)
N(2)	-774(1)	-1126(1)	1195(1)	30(1)
O(1)	-150(1)	5846(1)	3029(1)	33(1)
O(2)	165(1)	1554(1)	1754(1)	31(1)
O(3)	496(1)	-2064(1)	-126(1)	40(1)
C(16)	6725(2)	10880(2)	7888(1)	32(1)
C(17)	5788(2)	11611(2)	8394(1)	38(1)
C(18)	5927(2)	11229(2)	9231(1)	38(1)
C(19)	5648(2)	9785(2)	9061(1)	32(1)
C(20)	6552(2)	9050(2)	8527(1)	29(1)
C(21)	6396(2)	9438(2)	7691(1)	27(1)
C(22)	6691(2)	7409(2)	6722(1)	37(1)
C(23)	7632(2)	6675(2)	6239(1)	33(1)
C(24)	7059(2)	5297(2)	5791(1)	39(1)
C(25)	7607(2)	3175(2)	5005(1)	27(1)
C(26)	6897(2)	2411(2)	5459(1)	37(1)

C(27)	6490(2)	1022(2)	4942(1)	45(1)
C(28)	7688(2)	354(2)	4687(1)	53(1)
C(29)	8351(2)	1109(2)	4207(1)	43(1)
C(30)	8802(2)	2474(2)	4760(1)	29(1)
N(3)	7290(1)	8712(1)	7198(1)	30(1)
N(4)	8123(1)	4476(1)	5561(1)	28(1)
O(4)	6596(1)	11252(1)	7111(1)	46(1)
O(5)	7833(1)	7341(1)	5631(1)	42(1)
O(6)	9534(1)	3217(1)	4382(1)	31(1)
O(7)	9337(1)	11798(1)	7277(1)	70(1)

Table E.15: Bond lengths [Å] and angles [°] for 7m_al19_0s.

C(1)-O(1)	1.4304(17)
C(1)-C(2)	1.514(2)
C(1)-C(6)	1.517(2)
C(1)-H(1A)	0.9800
C(2)-C(3)	1.517(2)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.513(2)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.524(2)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.521(2)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-N(1)	1.474(2)
C(6)-H(6A)	0.9800
C(7)-N(1)	1.456(2)
C(7)-C(8)	1.515(2)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-O(2)	1.4250(17)
C(8)-C(9)	1.509(2)
C(8)-H(8A)	0.9800
C(9)-N(2)	1.455(2)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-N(2)	1.470(2)
C(10)-C(15)	1.503(2)
C(10)-C(11)	1.520(2)
C(10)-H(10A)	0.9800

C(11)-C(12)	1.523(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.501(3)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.518(3)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-C(15)	1.512(2)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-O(3)	1.420(2)
C(15)-H(15A)	0.9800
N(1)-H(1N)	0.848(17)
N(2)-H(2N)	0.836(18)
O(1)-H(1O)	0.8200
O(2)-H(2O)	0.8200
O(3)-H(3O)	0.8200
C(16)-O(4)	1.4184(18)
C(16)-C(21)	1.510(2)
C(16)-C(17)	1.516(2)
C(16)-H(16A)	0.9800
C(17)-C(18)	1.518(2)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.509(2)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-C(20)	1.519(2)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-C(21)	1.518(2)
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-N(3)	1.468(2)
C(21)-H(21A)	0.9800
C(22)-N(3)	1.456(2)
C(22)-C(23)	1.498(2)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-O(5)	1.424(2)
C(23)-C(24)	1.508(2)
C(23)-H(23A)	0.9800
C(24)-N(4)	1.458(2)
C(24)-H(24A)	0.9700

C(24)-H(24B)	0.9700
C(25)-N(4)	1.469(2)
C(25)-C(30)	1.515(2)
C(25)-C(26)	1.523(2)
C(25)-H(25A)	0.9800
C(26)-C(27)	1.511(2)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(27)-C(28)	1.508(3)
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(28)-C(29)	1.522(3)
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(29)-C(30)	1.512(2)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700
C(30)-O(6)	1.4293(17)
C(30)-H(30A)	0.9800
N(3)-H(3N)	0.816(17)
N(4)-H(4N)	0.794(17)
O(4)-H(4O)	0.8200
O(5)-H(5O)	0.8200
O(6)-H(6O)	0.8200
O(7)-H(7O)	1.21(4)
O(7)-H(8O)	1.074(12)

O(1)-C(1)-C(2)	110.36(13)
O(1)-C(1)-C(6)	109.18(12)
C(2)-C(1)-C(6)	111.21(13)
O(1)-C(1)-H(1A)	108.7
C(2)-C(1)-H(1A)	108.7
C(6)-C(1)-H(1A)	108.7
C(1)-C(2)-C(3)	111.50(14)
C(1)-C(2)-H(2A)	109.3
C(3)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2B)	109.3
C(3)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	108.0
C(4)-C(3)-C(2)	110.52(14)
C(4)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
C(3)-C(4)-C(5)	111.07(14)

C(3)-C(4)-H(4A)	109.4
C(5)-C(4)-H(4A)	109.4
C(3)-C(4)-H(4B)	109.4
C(5)-C(4)-H(4B)	109.4
H(4A)-C(4)-H(4B)	108.0
C(6)-C(5)-C(4)	111.00(14)
C(6)-C(5)-H(5A)	109.4
C(4)-C(5)-H(5A)	109.4
C(6)-C(5)-H(5B)	109.4
C(4)-C(5)-H(5B)	109.4
H(5A)-C(5)-H(5B)	108.0
N(1)-C(6)-C(1)	108.28(12)
N(1)-C(6)-C(5)	111.82(13)
C(1)-C(6)-C(5)	110.96(13)
N(1)-C(6)-H(6A)	108.6
C(1)-C(6)-H(6A)	108.6
C(5)-C(6)-H(6A)	108.6
N(1)-C(7)-C(8)	112.57(12)
N(1)-C(7)-H(7A)	109.1
C(8)-C(7)-H(7A)	109.1
N(1)-C(7)-H(7B)	109.1
C(8)-C(7)-H(7B)	109.1
H(7A)-C(7)-H(7B)	107.8
O(2)-C(8)-C(9)	111.27(13)
O(2)-C(8)-C(7)	108.91(13)
C(9)-C(8)-C(7)	107.70(12)
O(2)-C(8)-H(8A)	109.6
C(9)-C(8)-H(8A)	109.6
C(7)-C(8)-H(8A)	109.6
N(2)-C(9)-C(8)	113.71(13)
N(2)-C(9)-H(9A)	108.8
C(8)-C(9)-H(9A)	108.8
N(2)-C(9)-H(9B)	108.8
C(8)-C(9)-H(9B)	108.8
H(9A)-C(9)-H(9B)	107.7
N(2)-C(10)-C(15)	110.39(13)
N(2)-C(10)-C(11)	112.04(14)
C(15)-C(10)-C(11)	109.98(14)
N(2)-C(10)-H(10A)	108.1
C(15)-C(10)-H(10A)	108.1
C(11)-C(10)-H(10A)	108.1
C(10)-C(11)-C(12)	110.22(15)
C(10)-C(11)-H(11A)	109.6
C(12)-C(11)-H(11A)	109.6
C(10)-C(11)-H(11B)	109.6
C(12)-C(11)-H(11B)	109.6

H(11A)-C(11)-H(11B)	108.1
C(13)-C(12)-C(11)	110.74(16)
C(13)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12A)	109.5
C(13)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1
C(12)-C(13)-C(14)	112.32(16)
C(12)-C(13)-H(13A)	109.1
C(14)-C(13)-H(13A)	109.1
C(12)-C(13)-H(13B)	109.1
C(14)-C(13)-H(13B)	109.1
H(13A)-C(13)-H(13B)	107.9
C(15)-C(14)-C(13)	112.13(15)
C(15)-C(14)-H(14A)	109.2
C(13)-C(14)-H(14A)	109.2
C(15)-C(14)-H(14B)	109.2
C(13)-C(14)-H(14B)	109.2
H(14A)-C(14)-H(14B)	107.9
O(3)-C(15)-C(10)	111.23(14)
O(3)-C(15)-C(14)	112.45(14)
C(10)-C(15)-C(14)	110.92(14)
O(3)-C(15)-H(15A)	107.3
C(10)-C(15)-H(15A)	107.3
C(14)-C(15)-H(15A)	107.3
C(7)-N(1)-C(6)	113.95(12)
C(7)-N(1)-H(1N)	107.7(11)
C(6)-N(1)-H(1N)	106.6(12)
C(9)-N(2)-C(10)	110.72(12)
C(9)-N(2)-H(2N)	104.0(12)
C(10)-N(2)-H(2N)	104.8(12)
C(1)-O(1)-H(1O)	109.5
C(8)-O(2)-H(2O)	109.5
C(15)-O(3)-H(3O)	109.5
O(4)-C(16)-C(21)	110.10(14)
O(4)-C(16)-C(17)	110.60(13)
C(21)-C(16)-C(17)	110.38(13)
O(4)-C(16)-H(16A)	108.6
C(21)-C(16)-H(16A)	108.6
C(17)-C(16)-H(16A)	108.6
C(16)-C(17)-C(18)	111.04(14)
C(16)-C(17)-H(17A)	109.4
C(18)-C(17)-H(17A)	109.4
C(16)-C(17)-H(17B)	109.4
C(18)-C(17)-H(17B)	109.4
H(17A)-C(17)-H(17B)	108.0

C(19)-C(18)-C(17)	110.99(14)
C(19)-C(18)-H(18A)	109.4
C(17)-C(18)-H(18A)	109.4
C(19)-C(18)-H(18B)	109.4
C(17)-C(18)-H(18B)	109.4
H(18A)-C(18)-H(18B)	108.0
C(18)-C(19)-C(20)	111.02(13)
C(18)-C(19)-H(19A)	109.4
C(20)-C(19)-H(19A)	109.4
C(18)-C(19)-H(19B)	109.4
C(20)-C(19)-H(19B)	109.4
H(19A)-C(19)-H(19B)	108.0
C(21)-C(20)-C(19)	111.89(13)
C(21)-C(20)-H(20A)	109.2
C(19)-C(20)-H(20A)	109.2
C(21)-C(20)-H(20B)	109.2
C(19)-C(20)-H(20B)	109.2
H(20A)-C(20)-H(20B)	107.9
N(3)-C(21)-C(16)	111.20(13)
N(3)-C(21)-C(20)	110.13(13)
C(16)-C(21)-C(20)	109.60(13)
N(3)-C(21)-H(21A)	108.6
C(16)-C(21)-H(21A)	108.6
C(20)-C(21)-H(21A)	108.6
N(3)-C(22)-C(23)	111.37(13)
N(3)-C(22)-H(22A)	109.4
C(23)-C(22)-H(22A)	109.4
N(3)-C(22)-H(22B)	109.4
C(23)-C(22)-H(22B)	109.4
H(22A)-C(22)-H(22B)	108.0
O(5)-C(23)-C(22)	108.15(14)
O(5)-C(23)-C(24)	110.77(14)
C(22)-C(23)-C(24)	111.62(14)
O(5)-C(23)-H(23A)	108.7
C(22)-C(23)-H(23A)	108.7
C(24)-C(23)-H(23A)	108.7
N(4)-C(24)-C(23)	111.62(13)
N(4)-C(24)-H(24A)	109.3
C(23)-C(24)-H(24A)	109.3
N(4)-C(24)-H(24B)	109.3
C(23)-C(24)-H(24B)	109.3
H(24A)-C(24)-H(24B)	108.0
N(4)-C(25)-C(30)	108.75(12)
N(4)-C(25)-C(26)	111.19(13)
C(30)-C(25)-C(26)	110.26(14)
N(4)-C(25)-H(25A)	108.9

C(30)-C(25)-H(25A)	108.9
C(26)-C(25)-H(25A)	108.9
C(27)-C(26)-C(25)	112.36(14)
C(27)-C(26)-H(26A)	109.1
C(25)-C(26)-H(26A)	109.1
C(27)-C(26)-H(26B)	109.1
C(25)-C(26)-H(26B)	109.1
H(26A)-C(26)-H(26B)	107.9
C(28)-C(27)-C(26)	111.94(15)
C(28)-C(27)-H(27A)	109.2
C(26)-C(27)-H(27A)	109.2
C(28)-C(27)-H(27B)	109.2
C(26)-C(27)-H(27B)	109.2
H(27A)-C(27)-H(27B)	107.9
C(27)-C(28)-C(29)	111.02(17)
C(27)-C(28)-H(28A)	109.4
C(29)-C(28)-H(28A)	109.4
C(27)-C(28)-H(28B)	109.4
C(29)-C(28)-H(28B)	109.4
H(28A)-C(28)-H(28B)	108.0
C(30)-C(29)-C(28)	109.84(15)
C(30)-C(29)-H(29A)	109.7
C(28)-C(29)-H(29A)	109.7
C(30)-C(29)-H(29B)	109.7
C(28)-C(29)-H(29B)	109.7
H(29A)-C(29)-H(29B)	108.2
O(6)-C(30)-C(29)	113.25(13)
O(6)-C(30)-C(25)	111.05(13)
C(29)-C(30)-C(25)	111.67(13)
O(6)-C(30)-H(30A)	106.8
C(29)-C(30)-H(30A)	106.8
C(25)-C(30)-H(30A)	106.8
C(22)-N(3)-C(21)	112.18(13)
C(22)-N(3)-H(3N)	107.9(12)
C(21)-N(3)-H(3N)	108.3(12)
C(24)-N(4)-C(25)	114.56(12)
C(24)-N(4)-H(4N)	110.0(12)
C(25)-N(4)-H(4N)	106.3(12)
C(16)-O(4)-H(4O)	109.5
C(23)-O(5)-H(5O)	109.5
C(30)-O(6)-H(6O)	109.5
H(7O)-O(7)-H(8O)	81.3(16)

Symmetry transformations used to generate equivalent atoms:

Table E.16: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 7m_al19_0s. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	24(1)	33(1)	27(1)	10(1)	7(1)	-1(1)
C(2)	36(1)	30(1)	38(1)	9(1)	6(1)	2(1)
C(3)	37(1)	43(1)	38(1)	13(1)	12(1)	17(1)
C(4)	24(1)	46(1)	46(1)	17(1)	10(1)	9(1)
C(5)	23(1)	36(1)	46(1)	12(1)	9(1)	0(1)
C(6)	22(1)	31(1)	27(1)	10(1)	6(1)	2(1)
C(7)	22(1)	34(1)	34(1)	6(1)	4(1)	1(1)
C(8)	21(1)	33(1)	28(1)	8(1)	7(1)	1(1)
C(9)	24(1)	36(1)	40(1)	5(1)	6(1)	3(1)
C(10)	29(1)	31(1)	35(1)	12(1)	6(1)	3(1)
C(11)	32(1)	35(1)	54(1)	13(1)	18(1)	2(1)
C(12)	38(1)	40(1)	77(2)	11(1)	14(1)	-7(1)
C(13)	45(1)	35(1)	69(1)	3(1)	7(1)	-2(1)
C(14)	37(1)	38(1)	40(1)	3(1)	8(1)	6(1)
C(15)	31(1)	39(1)	37(1)	11(1)	10(1)	3(1)
N(1)	19(1)	28(1)	32(1)	7(1)	5(1)	0(1)
N(2)	25(1)	31(1)	34(1)	7(1)	11(1)	1(1)
O(1)	24(1)	40(1)	35(1)	14(1)	5(1)	-4(1)
O(2)	23(1)	42(1)	31(1)	13(1)	8(1)	2(1)
O(3)	33(1)	54(1)	33(1)	11(1)	9(1)	-6(1)
C(16)	25(1)	40(1)	34(1)	19(1)	5(1)	0(1)
C(17)	33(1)	33(1)	50(1)	15(1)	12(1)	6(1)
C(18)	30(1)	44(1)	38(1)	7(1)	13(1)	6(1)
C(19)	23(1)	45(1)	32(1)	13(1)	11(1)	4(1)
C(20)	26(1)	34(1)	30(1)	13(1)	10(1)	4(1)
C(21)	19(1)	37(1)	26(1)	11(1)	6(1)	2(1)
C(22)	26(1)	47(1)	37(1)	3(1)	11(1)	0(1)
C(23)	23(1)	44(1)	32(1)	8(1)	10(1)	3(1)
C(24)	25(1)	47(1)	43(1)	1(1)	15(1)	0(1)
C(25)	22(1)	35(1)	24(1)	8(1)	6(1)	-4(1)
C(26)	33(1)	47(1)	33(1)	12(1)	12(1)	-12(1)
C(27)	46(1)	49(1)	40(1)	12(1)	10(1)	-21(1)
C(28)	70(1)	32(1)	59(1)	10(1)	22(1)	-12(1)
C(29)	48(1)	34(1)	49(1)	4(1)	21(1)	-3(1)
C(30)	29(1)	33(1)	28(1)	11(1)	10(1)	-2(1)
N(3)	28(1)	39(1)	26(1)	10(1)	11(1)	0(1)
N(4)	23(1)	35(1)	28(1)	7(1)	13(1)	-2(1)
O(4)	40(1)	65(1)	48(1)	39(1)	12(1)	4(1)
O(5)	40(1)	57(1)	40(1)	19(1)	21(1)	11(1)
O(6)	28(1)	38(1)	29(1)	8(1)	12(1)	-4(1)
O(7)	49(1)	90(1)	75(1)	49(1)	-1(1)	-18(1)

Table E.17: Torsion angles [°] for 7m_al19_0s.

O(1)-C(1)-C(2)-C(3)	177.27(13)
C(6)-C(1)-C(2)-C(3)	55.95(18)
C(1)-C(2)-C(3)-C(4)	-56.38(19)
C(2)-C(3)-C(4)-C(5)	56.39(19)
C(3)-C(4)-C(5)-C(6)	-56.25(19)
O(1)-C(1)-C(6)-N(1)	59.69(16)
C(2)-C(1)-C(6)-N(1)	-178.30(13)
O(1)-C(1)-C(6)-C(5)	-177.24(12)
C(2)-C(1)-C(6)-C(5)	-55.23(17)
C(4)-C(5)-C(6)-N(1)	176.37(13)
C(4)-C(5)-C(6)-C(1)	55.36(18)
N(1)-C(7)-C(8)-O(2)	-63.77(17)
N(1)-C(7)-C(8)-C(9)	175.45(13)
O(2)-C(8)-C(9)-N(2)	51.38(19)
C(7)-C(8)-C(9)-N(2)	170.67(14)
N(2)-C(10)-C(11)-C(12)	177.08(14)
C(15)-C(10)-C(11)-C(12)	-59.75(18)
C(10)-C(11)-C(12)-C(13)	57.3(2)
C(11)-C(12)-C(13)-C(14)	-53.4(2)
C(12)-C(13)-C(14)-C(15)	52.0(2)
N(2)-C(10)-C(15)-O(3)	-51.94(18)
C(11)-C(10)-C(15)-O(3)	-176.07(14)
N(2)-C(10)-C(15)-C(14)	-177.88(14)
C(11)-C(10)-C(15)-C(14)	57.98(19)
C(13)-C(14)-C(15)-O(3)	-179.34(15)
C(13)-C(14)-C(15)-C(10)	-54.1(2)
C(8)-C(7)-N(1)-C(6)	164.80(13)
C(1)-C(6)-N(1)-C(7)	-172.91(13)
C(5)-C(6)-N(1)-C(7)	64.54(17)
C(8)-C(9)-N(2)-C(10)	-165.84(14)
C(15)-C(10)-N(2)-C(9)	158.02(14)
C(11)-C(10)-N(2)-C(9)	-79.04(17)
O(4)-C(16)-C(17)-C(18)	-179.54(14)
C(21)-C(16)-C(17)-C(18)	58.37(18)
C(16)-C(17)-C(18)-C(19)	-56.08(19)
C(17)-C(18)-C(19)-C(20)	54.06(18)
C(18)-C(19)-C(20)-C(21)	-55.23(18)
O(4)-C(16)-C(21)-N(3)	57.42(16)
C(17)-C(16)-C(21)-N(3)	179.81(13)
O(4)-C(16)-C(21)-C(20)	179.43(12)
C(17)-C(16)-C(21)-C(20)	-58.19(16)
C(19)-C(20)-C(21)-N(3)	179.68(13)
C(19)-C(20)-C(21)-C(16)	57.04(17)
N(3)-C(22)-C(23)-O(5)	-61.64(18)
N(3)-C(22)-C(23)-C(24)	176.27(14)

O(5)-C(23)-C(24)-N(4)	77.77(18)
C(22)-C(23)-C(24)-N(4)	-161.66(14)
N(4)-C(25)-C(26)-C(27)	-173.86(14)
C(30)-C(25)-C(26)-C(27)	-53.16(18)
C(25)-C(26)-C(27)-C(28)	53.2(2)
C(26)-C(27)-C(28)-C(29)	-54.9(2)
C(27)-C(28)-C(29)-C(30)	57.1(2)
C(28)-C(29)-C(30)-O(6)	175.32(15)
C(28)-C(29)-C(30)-C(25)	-58.4(2)
N(4)-C(25)-C(30)-O(6)	-54.17(16)
C(26)-C(25)-C(30)-O(6)	-176.32(12)
N(4)-C(25)-C(30)-C(29)	178.38(13)
C(26)-C(25)-C(30)-C(29)	56.23(17)
C(23)-C(22)-N(3)-C(21)	-178.77(13)
C(16)-C(21)-N(3)-C(22)	-157.87(13)
C(20)-C(21)-N(3)-C(22)	80.44(17)
C(23)-C(24)-N(4)-C(25)	-170.91(14)
C(30)-C(25)-N(4)-C(24)	175.43(13)
C(26)-C(25)-N(4)-C(24)	-62.98(18)

Symmetry transformations used to generate equivalent atoms:

Table E.18: Hydrogen bonds for 7m_al19_0s [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(1)	0.848(17)	2.400(17)	2.8057(17)	110.1(13)
N(2)-H(2N)...O(3)	0.836(18)	2.335(17)	2.7926(18)	114.9(14)
N(2)-H(2N)...O(2)	0.836(18)	2.450(17)	2.8543(18)	110.7(14)
N(3)-H(3N)...O(4)	0.816(17)	2.424(17)	2.842(2)	112.8(14)
N(4)-H(4N)...O(6)	0.794(17)	2.398(16)	2.7912(16)	111.7(14)

Symmetry transformations used to generate equivalent atoms:

BHEEN Data

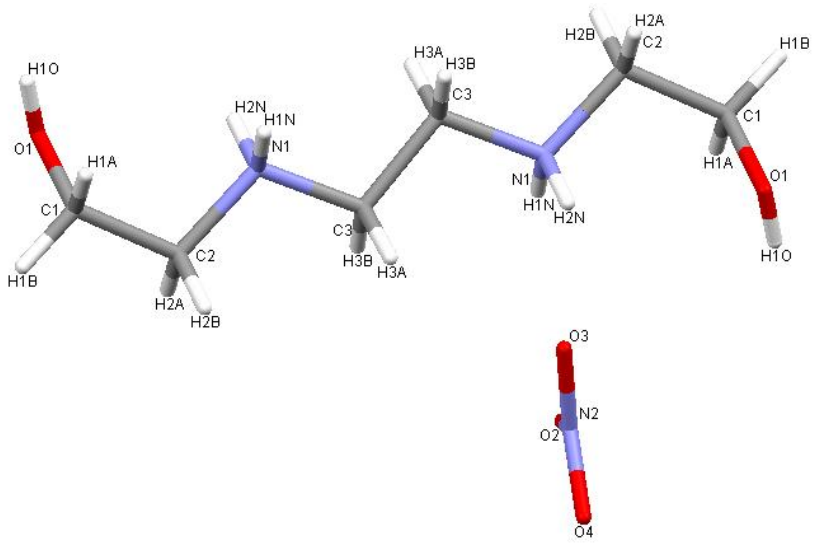


Figure E.4: XRD structure of the nitrate salt of BHEEN and the labelling scheme used

Table E.19: Crystal data and structure refinement for 8m_alv11_0s.

Identification code	8m_alv11_0s
Empirical formula	C6 H18 N4 O8
Formula weight	274.24
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 7.6230(3) Å α = 90°
	b = 10.0645(5) Å β = 90°
	c = 15.6002(9) Å γ = 90°
Volume	1196.87(10) $Å^3$
Z	4
Density (calculated)	1.522 Mg/m^3
Absorption coefficient	0.140 mm^{-1}
F(000)	584
Crystal size	0.43 x 0.36 x 0.09 mm^3
Theta range for data collection	2.61 to 27.98°.
Index ranges	-8≤h≤10, -12≤k≤13, -20≤l≤10
Reflections collected	6852
Independent reflections	1437 [R(int) = 0.0373]
Completeness to theta = 27.98°	99.8 %
Absorption correction	None
Max. and min. transmission	0.9875 and 0.9423
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	1437 / 0 / 86
Goodness-of-fit on F^2	1.069
Final R indices [I>2σ(I)]	$R_1 = 0.0327$, $wR_2 = 0.0842$
R indices (all data)	$R_1 = 0.0425$, $wR_2 = 0.0877$
Largest diff. peak and hole	0.323 and -0.210 e.Å^{-3}

Table E.20: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 8m_alv11_0s. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	172(2)	2700(1)	7147(1)	27(1)
C(2)	394(2)	1312(1)	6798(1)	24(1)
C(3)	163(2)	-42(1)	5479(1)	22(1)
N(1)	62(1)	1307(1)	5857(1)	19(1)
N(2)	616(1)	3791(1)	4251(1)	24(1)
O(1)	1369(1)	3568(1)	6738(1)	31(1)
O(2)	-931(1)	3803(1)	4466(1)	40(1)
O(3)	1655(1)	2949(1)	4571(1)	29(1)
O(4)	1210(1)	4589(1)	3713(1)	34(1)

Table E.21: Bond lengths [Å] and angles [°] for 8m_alv11_0s.

C(1)-O(1)	1.4152(15)
C(1)-C(2)	1.5083(15)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-N(1)	1.4888(15)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-N(1)	1.4823(13)
C(3)-C(3)#1	1.517(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
N(1)-H(1N)	0.9200
N(1)-H(2N)	0.9200
N(2)-O(2)	1.2260(13)
N(2)-O(4)	1.2459(13)
N(2)-O(3)	1.2630(12)
O(1)-H(1O)	0.788(17)

O(1)-C(1)-C(2)	109.67(10)
O(1)-C(1)-H(1A)	109.7
C(2)-C(1)-H(1A)	109.7
O(1)-C(1)-H(1B)	109.7
C(2)-C(1)-H(1B)	109.7
H(1A)-C(1)-H(1B)	108.2
N(1)-C(2)-C(1)	109.87(9)
N(1)-C(2)-H(2A)	109.7
C(1)-C(2)-H(2A)	109.7
N(1)-C(2)-H(2B)	109.7
C(1)-C(2)-H(2B)	109.7
H(2A)-C(2)-H(2B)	108.2
N(1)-C(3)-C(3)#1	109.45(11)
N(1)-C(3)-H(3A)	109.8
C(3)#1-C(3)-H(3A)	109.8
N(1)-C(3)-H(3B)	109.8
C(3)#1-C(3)-H(3B)	109.8
H(3A)-C(3)-H(3B)	108.2
C(3)-N(1)-C(2)	112.74(8)
C(3)-N(1)-H(1N)	109.0
C(2)-N(1)-H(1N)	109.0
C(3)-N(1)-H(2N)	109.0
C(2)-N(1)-H(2N)	109.0
H(1N)-N(1)-H(2N)	107.8
O(2)-N(2)-O(4)	121.82(10)
O(2)-N(2)-O(3)	120.05(10)
O(4)-N(2)-O(3)	118.13(9)
C(1)-O(1)-H(1O)	104.4(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1

Table E.22: Anisotropic displacement parameters ($Å^2$ x 10^3)for 8m_alv11_0s. The anisotropic displacement factor exponent takes the form: -2p2[h2a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13
C(1)	34(1)	25(1)	23(1)	-1(1)	1(1)
C(2)	29(1)	22(1)	21(1)	1(1)	-3(1)
C(3)	25(1)	17(1)	22(1)	0(1)	-1(1)
N(1)	19(1)	18(1)	21(1)	2(1)	-1(1)
N(2)	24(1)	22(1)	24(1)	-3(1)	-2(1)
O(1)	31(1)	23(1)	41(1)	2(1)	-4(1)
O(2)	19(1)	46(1)	56(1)	0(1)	3(1)
O(3)	25(1)	26(1)	36(1)	10(1)	1(1)
O(4)	39(1)	32(1)	31(1)	12(1)	2(1)

Table E.23: Torsion angles [°] for 8m_alv11_0s.

C(3)#1-C(3)-N(1)-C(2)	-179.16(11)
C(1)-C(2)-N(1)-C(3)	-176.90(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1

Table E.24: Hydrogen bonds for 8m_alv11_0s [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(3)#2	0.92	1.88	2.7843(12)	168.8
O(1)-H(1O)...O(4)#3	0.788(17)	2.022(16)	2.7924(13)	165.5(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1 #2 x-1/2,-y+1/2,-z+1 #3 -x,-y+1,-z+1

Cy_2-en/Pb complex

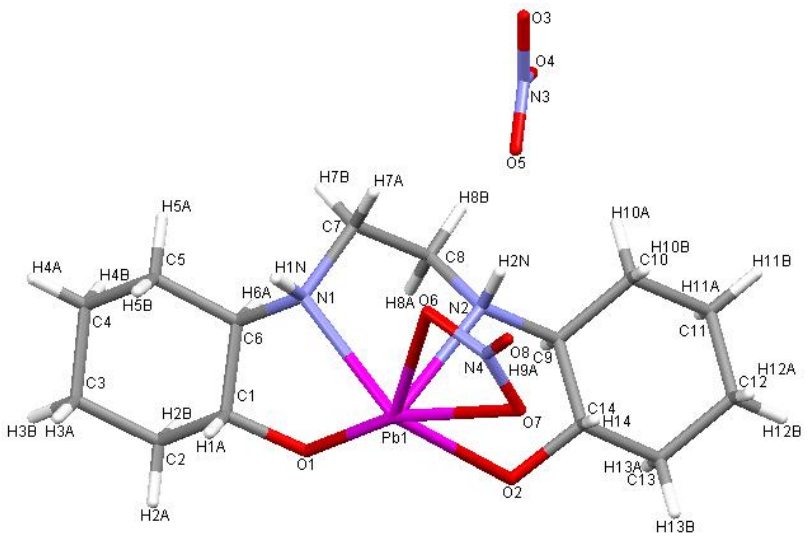


Figure E.5: XRD structure of the lead(II) complex of Cy_2-en and the labelling scheme used

Table E.25: Crystal data and structure refinement for 7m_al10_0a.

Identification code	7m_al10_0a	
Empirical formula	C14 H26 N4 O8 Pb	
Formula weight	585.58	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.0573(2) Å	α = 90°.
	b = 9.7265(2) Å	β = 107.4940(10)°.
	c = 11.4533(2) Å	γ = 90°.
Volume	962.32(3) $Å^3$	
Z	2	
Density (calculated)	2.021 Mg/m^3	
Absorption coefficient	8.815 mm^{-1}	
F(000)	568	
Crystal size	0.31 x 0.14 x 0.13 mm^3	
Theta range for data collection	1.86 to 28.00°.	
Index ranges	-11<=h<=11, -12<=k<=12, -14<=l<=15	
Reflections collected	16110	
Independent reflections	4640 [R(int) = 0.0608]	

Completeness to theta = 28.00°	100.0 %
Absorption correction	Integration
Max. and min. transmission	0.3936 and 0.1708
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4640 / 1 / 244
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0196, wR2 = 0.0441
R indices (all data)	R1 = 0.0212, wR2 = 0.0444
Absolute structure parameter	-0.012(5)
Largest diff. peak and hole	0.793 and -0.731 e.Å^{-3}

Table E.26: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 7m_al10_0a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3432(3)	2217(7)	2714(2)	24(1)
C(2)	2981(5)	1728(4)	3815(3)	28(1)
C(3)	3886(4)	2513(4)	4956(3)	33(1)
C(4)	3566(5)	4051(4)	4767(3)	34(1)
C(5)	3987(5)	4543(4)	3632(3)	31(1)
C(6)	3121(4)	3727(4)	2494(3)	24(1)
C(7)	2509(5)	5252(4)	684(3)	30(1)
C(8)	1182(4)	4591(4)	-288(3)	27(1)
C(9)	572(5)	3142(4)	-2133(3)	22(1)
C(10)	39(5)	4099(4)	-3257(4)	34(1)
C(11)	-1243(5)	3404(4)	-4286(4)	35(1)
C(12)	-706(5)	2038(6)	-4637(3)	37(1)
C(13)	-164(6)	1090(5)	-3511(4)	37(1)
C(14)	1112(5)	1799(4)	-2497(3)	29(1)
N(1)	3552(4)	4187(3)	1413(2)	26(1)
N(2)	1796(4)	3818(4)	-1129(3)	23(1)
N(3)	2368(5)	7621(4)	-2032(3)	36(1)
N(4)	5723(4)	3466(3)	-1619(3)	30(1)
O(1)	2535(3)	1517(3)	1606(2)	27(1)
O(2)	1578(5)	941(3)	-1414(3)	44(1)
O(3)	2975(4)	8751(4)	-2151(4)	51(1)
O(4)	1032(4)	7600(4)	-2003(4)	74(1)
O(5)	3125(5)	6558(4)	-1937(3)	45(1)
O(6)	5540(4)	4147(3)	-728(3)	44(1)
O(7)	4901(4)	2454(4)	-1996(2)	35(1)
O(8)	6744(4)	3821(3)	-2077(3)	43(1)
Pb(1)	3832(1)	2229(1)	69(1)	27(1)

Table E.27: Bond lengths [Å] and angles [°] for 7m_al10_0a.

C(1)-O(1)	1.454(4)
C(1)-C(6)	1.502(8)
C(1)-C(2)	1.514(5)
C(1)-H(1A)	0.9800
C(2)-C(3)	1.523(5)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.527(6)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.536(5)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.526(5)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-N(1)	1.476(4)
C(6)-H(6A)	0.9800
C(7)-N(1)	1.479(5)
C(7)-C(8)	1.514(5)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-N(2)	1.458(5)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-N(2)	1.489(5)
C(9)-C(14)	1.497(5)
C(9)-C(10)	1.544(5)
C(9)-H(9A)	0.9800
C(10)-C(11)	1.540(5)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.510(7)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.540(6)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.534(5)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-O(2)	1.448(5)
C(14)-H(14)	0.9800
N(1)-Pb(1)	2.509(3)
N(1)-H(1N)	0.9100

N(2)-Pb(1)	2.480(4)
N(2)-H(2N)	0.9100
N(3)-O(4)	1.221(5)
N(3)-O(5)	1.227(5)
N(3)-O(3)	1.254(5)
N(4)-O(7)	1.231(5)
N(4)-O(8)	1.241(5)
N(4)-O(6)	1.269(4)
O(1)-Pb(1)	2.491(3)
O(2)-Pb(1)	2.557(4)
O(6)-Pb(1)	2.748(3)

O(1)-C(1)-C(6)	106.5(3)
O(1)-C(1)-C(2)	111.1(4)
C(6)-C(1)-C(2)	111.3(3)
O(1)-C(1)-H(1A)	109.3
C(6)-C(1)-H(1A)	109.3
C(2)-C(1)-H(1A)	109.3
C(1)-C(2)-C(3)	110.3(3)
C(1)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2A)	109.6
C(1)-C(2)-H(2B)	109.6
C(3)-C(2)-H(2B)	109.6
H(2A)-C(2)-H(2B)	108.1
C(2)-C(3)-C(4)	109.8(3)
C(2)-C(3)-H(3A)	109.7
C(4)-C(3)-H(3A)	109.7
C(2)-C(3)-H(3B)	109.7
C(4)-C(3)-H(3B)	109.7
H(3A)-C(3)-H(3B)	108.2
C(3)-C(4)-C(5)	109.9(3)
C(3)-C(4)-H(4A)	109.7
C(5)-C(4)-H(4A)	109.7
C(3)-C(4)-H(4B)	109.7
C(5)-C(4)-H(4B)	109.7
H(4A)-C(4)-H(4B)	108.2
C(6)-C(5)-C(4)	111.5(3)
C(6)-C(5)-H(5A)	109.3
C(4)-C(5)-H(5A)	109.3
C(6)-C(5)-H(5B)	109.3
C(4)-C(5)-H(5B)	109.3
H(5A)-C(5)-H(5B)	108.0
N(1)-C(6)-C(1)	110.7(3)
N(1)-C(6)-C(5)	111.2(3)
C(1)-C(6)-C(5)	110.1(3)
N(1)-C(6)-H(6A)	108.2

C(1)-C(6)-H(6A)	108.2
C(5)-C(6)-H(6A)	108.2
N(1)-C(7)-C(8)	110.4(3)
N(1)-C(7)-H(7A)	109.6
C(8)-C(7)-H(7A)	109.6
N(1)-C(7)-H(7B)	109.6
C(8)-C(7)-H(7B)	109.6
H(7A)-C(7)-H(7B)	108.1
N(2)-C(8)-C(7)	109.1(3)
N(2)-C(8)-H(8A)	109.9
C(7)-C(8)-H(8A)	109.9
N(2)-C(8)-H(8B)	109.9
C(7)-C(8)-H(8B)	109.9
H(8A)-C(8)-H(8B)	108.3
N(2)-C(9)-C(14)	111.8(3)
N(2)-C(9)-C(10)	110.5(3)
C(14)-C(9)-C(10)	109.9(3)
N(2)-C(9)-H(9A)	108.2
C(14)-C(9)-H(9A)	108.2
C(10)-C(9)-H(9A)	108.2
C(11)-C(10)-C(9)	110.4(3)
C(11)-C(10)-H(10A)	109.6
C(9)-C(10)-H(10A)	109.6
C(11)-C(10)-H(10B)	109.6
C(9)-C(10)-H(10B)	109.6
H(10A)-C(10)-H(10B)	108.1
C(12)-C(11)-C(10)	111.1(4)
C(12)-C(11)-H(11A)	109.4
C(10)-C(11)-H(11A)	109.4
C(12)-C(11)-H(11B)	109.4
C(10)-C(11)-H(11B)	109.4
H(11A)-C(11)-H(11B)	108.0
C(11)-C(12)-C(13)	110.6(3)
C(11)-C(12)-H(12A)	109.5
C(13)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
C(13)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1
C(14)-C(13)-C(12)	110.0(4)
C(14)-C(13)-H(13A)	109.7
C(12)-C(13)-H(13A)	109.7
C(14)-C(13)-H(13B)	109.7
C(12)-C(13)-H(13B)	109.7
H(13A)-C(13)-H(13B)	108.2
O(2)-C(14)-C(9)	107.4(3)
O(2)-C(14)-C(13)	110.4(3)

C(9)-C(14)-C(13)	111.6(3)
O(2)-C(14)-H(14)	109.1
C(9)-C(14)-H(14)	109.1
C(13)-C(14)-H(14)	109.1
C(6)-N(1)-C(7)	113.6(3)
C(6)-N(1)-Pb(1)	112.7(2)
C(7)-N(1)-Pb(1)	110.5(2)
C(6)-N(1)-H(1N)	106.5
C(7)-N(1)-H(1N)	106.5
Pb(1)-N(1)-H(1N)	106.5
C(8)-N(2)-C(9)	113.2(3)
C(8)-N(2)-Pb(1)	108.9(2)
C(9)-N(2)-Pb(1)	114.1(2)
C(8)-N(2)-H(2N)	106.7
C(9)-N(2)-H(2N)	106.7
Pb(1)-N(2)-H(2N)	106.7
O(4)-N(3)-O(5)	121.0(4)
O(4)-N(3)-O(3)	119.2(4)
O(5)-N(3)-O(3)	119.8(4)
O(7)-N(4)-O(8)	121.6(4)
O(7)-N(4)-O(6)	119.1(4)
O(8)-N(4)-O(6)	119.3(4)
C(1)-O(1)-Pb(1)	103.2(2)
C(14)-O(2)-Pb(1)	104.8(2)
N(4)-O(6)-Pb(1)	97.8(2)
N(2)-Pb(1)-O(1)	97.73(11)
N(2)-Pb(1)-N(1)	70.80(10)
O(1)-Pb(1)-N(1)	67.76(9)
N(2)-Pb(1)-O(2)	68.01(11)
O(1)-Pb(1)-O(2)	83.18(10)
N(1)-Pb(1)-O(2)	124.89(11)
N(2)-Pb(1)-O(6)	78.02(11)
O(1)-Pb(1)-O(6)	148.84(8)
N(1)-Pb(1)-O(6)	81.91(9)
O(2)-Pb(1)-O(6)	121.91(10)

Table E.28: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 7m_al10_0a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(1)	28(1)	21(1)	-1(3)	6(1)	-2(2)
C(2)	29(2)	29(2)	29(2)	3(1)	12(2)	1(1)
C(3)	35(2)	44(4)	21(2)	6(2)	6(2)	4(2)
C(4)	41(2)	37(2)	20(2)	-3(2)	6(2)	0(2)
C(5)	39(2)	28(2)	22(2)	-3(1)	4(2)	-5(2)
C(6)	25(2)	25(2)	21(2)	-1(1)	8(1)	-4(1)
C(7)	41(2)	25(2)	22(2)	-2(1)	7(2)	-8(2)
C(8)	29(2)	26(2)	23(2)	-1(1)	5(2)	4(1)
C(9)	20(2)	24(2)	22(2)	1(1)	4(2)	-1(1)
C(10)	37(2)	28(2)	30(2)	3(2)	0(2)	1(2)
C(11)	36(2)	41(2)	23(2)	-3(2)	0(2)	-1(2)
C(12)	36(2)	54(4)	21(1)	-8(2)	6(1)	-4(2)
C(13)	43(3)	34(2)	33(2)	-12(2)	10(2)	-7(2)
C(14)	34(2)	26(2)	23(2)	0(1)	3(2)	1(1)
N(1)	23(2)	34(2)	21(1)	1(1)	6(1)	-8(1)
N(2)	23(2)	24(2)	20(2)	-2(1)	5(1)	-2(1)
N(3)	28(2)	48(3)	29(2)	4(1)	6(2)	-6(2)
N(4)	31(2)	33(2)	28(2)	12(1)	11(2)	6(1)
O(1)	30(1)	28(1)	24(1)	-7(1)	10(1)	-6(1)
O(2)	67(3)	23(2)	30(2)	1(1)	-1(2)	2(2)
O(3)	44(2)	40(2)	73(2)	-12(2)	24(2)	-13(2)
O(4)	34(2)	75(4)	116(3)	24(2)	29(2)	5(2)
O(5)	42(2)	36(2)	55(2)	12(2)	16(2)	10(2)
O(6)	52(2)	38(2)	51(2)	-16(1)	33(2)	-7(1)
O(7)	44(2)	35(2)	26(1)	-5(1)	10(1)	-13(2)
O(8)	50(2)	41(2)	51(2)	3(1)	35(2)	-1(1)
Pb(1)	26(1)	35(1)	21(1)	5(1)	10(1)	9(1)

Table E.29: Torsion angles [°] for 7m_al10_0a.

O(1)-C(1)-C(2)-C(3)	-177.8(4)
C(6)-C(1)-C(2)-C(3)	-59.2(4)
C(1)-C(2)-C(3)-C(4)	58.9(4)
C(2)-C(3)-C(4)-C(5)	-57.2(4)
C(3)-C(4)-C(5)-C(6)	56.3(4)
O(1)-C(1)-C(6)-N(1)	-58.3(3)
C(2)-C(1)-C(6)-N(1)	-179.5(3)
O(1)-C(1)-C(6)-C(5)	178.4(3)
C(2)-C(1)-C(6)-C(5)	57.2(4)

C(4)-C(5)-C(6)-N(1)	-179.0(3)
C(4)-C(5)-C(6)-C(1)	-55.9(4)
N(1)-C(7)-C(8)-N(2)	-62.5(4)
N(2)-C(9)-C(10)-C(11)	-179.2(4)
C(14)-C(9)-C(10)-C(11)	57.0(5)
C(9)-C(10)-C(11)-C(12)	-56.7(5)
C(10)-C(11)-C(12)-C(13)	56.5(5)
C(11)-C(12)-C(13)-C(14)	-56.3(5)
N(2)-C(9)-C(14)-O(2)	57.6(4)
C(10)-C(9)-C(14)-O(2)	-179.3(3)
N(2)-C(9)-C(14)-C(13)	178.7(3)
C(10)-C(9)-C(14)-C(13)	-58.2(5)
C(12)-C(13)-C(14)-O(2)	177.3(4)
C(12)-C(13)-C(14)-C(9)	57.9(5)
C(1)-C(6)-N(1)-C(7)	143.9(3)
C(5)-C(6)-N(1)-C(7)	-93.3(4)
C(1)-C(6)-N(1)-Pb(1)	17.3(3)
C(5)-C(6)-N(1)-Pb(1)	140.0(3)
C(8)-C(7)-N(1)-C(6)	-89.8(4)
C(8)-C(7)-N(1)-Pb(1)	38.1(4)
C(7)-C(8)-N(2)-C(9)	-179.3(3)
C(7)-C(8)-N(2)-Pb(1)	52.6(3)
C(14)-C(9)-N(2)-C(8)	-146.2(3)
C(10)-C(9)-N(2)-C(8)	91.0(4)
C(14)-C(9)-N(2)-Pb(1)	-20.9(4)
C(10)-C(9)-N(2)-Pb(1)	-143.6(3)
C(6)-C(1)-O(1)-Pb(1)	67.9(2)
C(2)-C(1)-O(1)-Pb(1)	-170.7(3)
C(9)-C(14)-O(2)-Pb(1)	-62.5(3)
C(13)-C(14)-O(2)-Pb(1)	175.7(3)
O(7)-N(4)-O(6)-Pb(1)	15.4(4)
O(8)-N(4)-O(6)-Pb(1)	-163.3(3)
C(8)-N(2)-Pb(1)-O(1)	39.7(3)
C(9)-N(2)-Pb(1)-O(1)	-88.0(3)
C(8)-N(2)-Pb(1)-N(1)	-23.5(2)
C(9)-N(2)-Pb(1)-N(1)	-151.1(3)
C(8)-N(2)-Pb(1)-O(2)	119.1(3)
C(9)-N(2)-Pb(1)-O(2)	-8.6(2)
C(8)-N(2)-Pb(1)-O(6)	-109.0(3)
C(9)-N(2)-Pb(1)-O(6)	123.4(3)
C(1)-O(1)-Pb(1)-N(2)	-107.3(3)
C(1)-O(1)-Pb(1)-N(1)	-41.8(3)
C(1)-O(1)-Pb(1)-O(2)	-174.0(3)
C(1)-O(1)-Pb(1)-O(6)	-27.7(3)
C(6)-N(1)-Pb(1)-N(2)	120.3(3)
C(7)-N(1)-Pb(1)-N(2)	-8.0(2)

C(6)-N(1)-Pb(1)-O(1)	13.1(2)
C(7)-N(1)-Pb(1)-O(1)	-115.2(3)
C(6)-N(1)-Pb(1)-O(2)	76.9(2)
C(7)-N(1)-Pb(1)-O(2)	-51.4(3)
C(6)-N(1)-Pb(1)-O(6)	-159.6(2)
C(7)-N(1)-Pb(1)-O(6)	72.1(2)
C(14)-O(2)-Pb(1)-N(2)	37.2(2)
C(14)-O(2)-Pb(1)-O(1)	138.4(3)
C(14)-O(2)-Pb(1)-N(1)	81.6(3)
C(14)-O(2)-Pb(1)-O(6)	-21.8(3)
N(4)-O(6)-Pb(1)-N(2)	-99.7(2)
N(4)-O(6)-Pb(1)-O(1)	175.2(2)
N(4)-O(6)-Pb(1)-N(1)	-171.7(2)
N(4)-O(6)-Pb(1)-O(2)	-45.4(3)

Symmetry transformations used to generate equivalent atoms:

Table E.30: Hydrogen bonds for 7m_al10_0a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(3)#1	0.91	2.33	3.031(5)	133.8
N(2)-H(2N)...O(5)	0.91	2.31	3.174(5)	157.9

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z

Cy_2-en/Cd Data

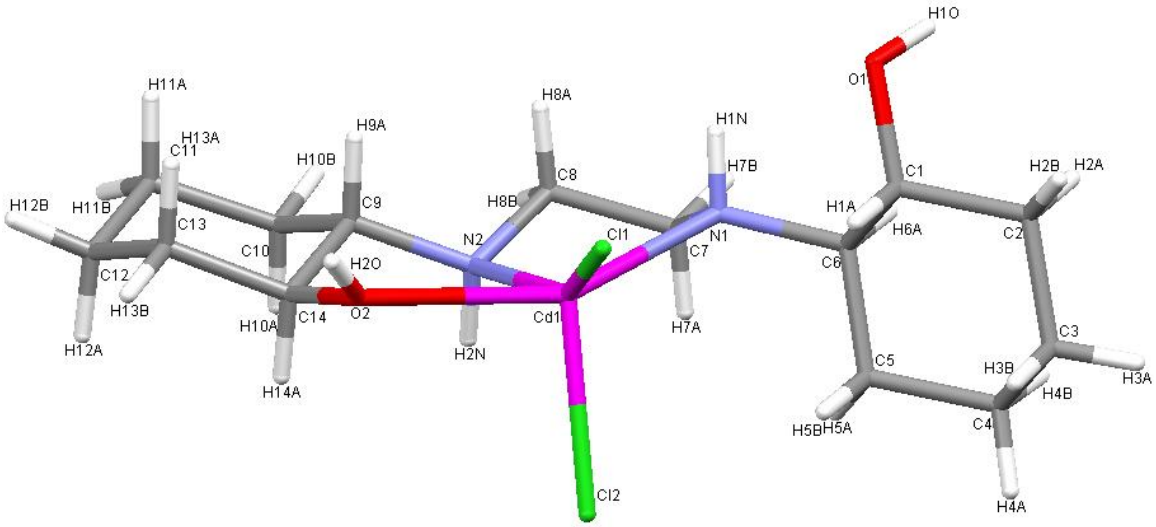


Figure E.6: The XRD structure of the cadmium(II) complex of Cy_2-en and the labelling scheme used

Table E.31: Crystal data and structure refinement for 7m_al7_a.

Identification code	7m_al7_a
Empirical formula	C15 H28 Cd Cl2 N2 O3
Formula weight	467.69
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 7.6698(7) Å α = 75.694(4)° b = 11.0270(10) Å β = 80.960(4)° c = 12.4807(13) Å γ = 81.170(4).
Volume	1002.84(17) Å3
Z	2
Density (calculated)	1.549 Mg/m^3
Absorption coefficient	1.369 mm^{-1}
F(000)	476
Crystal size	0.44 x 0.26 x 0.06 mm^3
Theta range for data collection	1.70 to 23.90°.
Index ranges	-7≤h≤8, -12≤k≤11, -13≤l≤13
Reflections collected	8065
Independent reflections	2523 [R(int) = 0.0385]
Completeness to theta = 23.90°	80.9 %

Absorption correction	Integration
Max. and min. transmission	0.9224 and 0.5842
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2523 / 0 / 214
Goodness-of-fit on F^2	1.068
Final R indices [I>2σ(I)]	$R_1 = 0.0280$, $wR_2 = 0.0697$
R indices (all data)	$R_1 = 0.0304$, $wR_2 = 0.0713$
Largest diff. peak and hole	1.029 and -0.682 e.Å^{-3}

Table E.32: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 7m_al7_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	-4381(6)	847(4)	7002(3)	32(1)
C(2)	-5694(6)	716(4)	8070(4)	40(1)
C(3)	-5241(7)	1463(5)	8841(4)	51(1)
C(4)	-5175(8)	2835(5)	8249(4)	59(2)
C(5)	-3855(7)	2957(4)	7178(4)	50(1)
C(6)	-4349(6)	2223(4)	6415(3)	33(1)
C(7)	-3476(6)	3549(4)	4569(3)	36(1)
C(8)	-2273(6)	3630(4)	3480(3)	35(1)
C(9)	902(5)	3319(4)	2703(3)	29(1)
C(10)	888(6)	4437(4)	1697(3)	41(1)
C(11)	2319(7)	4189(5)	740(4)	47(1)
C(12)	4138(6)	3824(4)	1132(4)	44(1)
C(13)	4115(6)	2698(4)	2134(3)	36(1)
C(14)	2745(5)	2994(4)	3075(3)	30(1)
C(15)	-710(20)	1728(17)	-220(30)	410(20)
N(1)	-3099(4)	2322(3)	5356(3)	29(1)
N(2)	-411(4)	3524(3)	3664(3)	28(1)
O(1)	-4790(4)	146(3)	6257(2)	34(1)
O(2)	2750(4)	1993(3)	4060(2)	36(1)
O(3)	350(20)	1208(12)	813(12)	314(9)
Cl(1)	1024(1)	-214(1)	6295(1)	36(1)
Cl(2)	833(2)	3398(1)	6350(1)	47(1)
Cd(1)	29(1)	1971(1)	5281(1)	31(1)

Table E.33: Bond lengths [Å] and angles [°] for 7m_al7_a.

C(1)-O(1)	1.441(5)
C(1)-C(6)	1.516(6)
C(1)-C(2)	1.530(6)
C(1)-H(1A)	0.9900
C(2)-C(3)	1.520(7)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(3)-C(4)	1.515(7)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(4)-C(5)	1.535(7)
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(5)-C(6)	1.514(6)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(6)-N(1)	1.497(5)
C(6)-H(6A)	0.9900
C(7)-N(1)	1.481(5)
C(7)-C(8)	1.509(6)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(8)-N(2)	1.464(5)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(9)-N(2)	1.480(5)
C(9)-C(14)	1.519(6)
C(9)-C(10)	1.527(6)
C(9)-H(9A)	0.9900
C(10)-C(11)	1.537(6)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(11)-C(12)	1.514(7)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(12)-C(13)	1.529(6)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(13)-C(14)	1.512(6)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(14)-O(2)	1.436(5)
C(14)-H(14A)	0.9900
C(15)-O(3)	1.58(3)
N(1)-Cd(1)	2.361(3)

N(1)-H(1N)	0.9200
N(2)-Cd(1)	2.334(3)
N(2)-H(2N)	0.9200
O(1)-H(1O)	0.8300
O(2)-Cd(1)	2.383(3)
O(2)-H(2O)	0.75(4)
Cl(1)-Cd(1)	2.4935(10)
Cl(2)-Cd(1)	2.4955(11)
O(1)-C(1)-C(6)	110.1(3)
O(1)-C(1)-C(2)	112.0(3)
C(6)-C(1)-C(2)	110.4(3)
O(1)-C(1)-H(1A)	108.1
C(6)-C(1)-H(1A)	108.1
C(2)-C(1)-H(1A)	108.1
C(3)-C(2)-C(1)	111.1(4)
C(3)-C(2)-H(2A)	109.4
C(1)-C(2)-H(2A)	109.4
C(3)-C(2)-H(2B)	109.4
C(1)-C(2)-H(2B)	109.4
H(2A)-C(2)-H(2B)	108.0
C(4)-C(3)-C(2)	110.8(4)
C(4)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
C(3)-C(4)-C(5)	110.8(4)
C(3)-C(4)-H(4A)	109.5
C(5)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
C(5)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	108.1
C(6)-C(5)-C(4)	110.4(4)
C(6)-C(5)-H(5A)	109.6
C(4)-C(5)-H(5A)	109.6
C(6)-C(5)-H(5B)	109.6
C(4)-C(5)-H(5B)	109.6
H(5A)-C(5)-H(5B)	108.1
N(1)-C(6)-C(5)	112.2(3)
N(1)-C(6)-C(1)	109.3(3)
C(5)-C(6)-C(1)	110.5(4)
N(1)-C(6)-H(6A)	108.3
C(5)-C(6)-H(6A)	108.3
C(1)-C(6)-H(6A)	108.3
N(1)-C(7)-C(8)	111.5(3)

N(1)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7A)	109.3
N(1)-C(7)-H(7B)	109.3
C(8)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	108.0
N(2)-C(8)-C(7)	110.4(3)
N(2)-C(8)-H(8A)	109.6
C(7)-C(8)-H(8A)	109.6
N(2)-C(8)-H(8B)	109.6
C(7)-C(8)-H(8B)	109.6
H(8A)-C(8)-H(8B)	108.1
N(2)-C(9)-C(14)	109.0(3)
N(2)-C(9)-C(10)	113.9(3)
C(14)-C(9)-C(10)	110.2(3)
N(2)-C(9)-H(9A)	107.9
C(14)-C(9)-H(9A)	107.9
C(10)-C(9)-H(9A)	107.9
C(9)-C(10)-C(11)	111.7(4)
C(9)-C(10)-H(10A)	109.3
C(11)-C(10)-H(10A)	109.3
C(9)-C(10)-H(10B)	109.3
C(11)-C(10)-H(10B)	109.3
H(10A)-C(10)-H(10B)	108.0
C(12)-C(11)-C(10)	111.2(4)
C(12)-C(11)-H(11A)	109.4
C(10)-C(11)-H(11A)	109.4
C(12)-C(11)-H(11B)	109.4
C(10)-C(11)-H(11B)	109.4
H(11A)-C(11)-H(11B)	108.0
C(11)-C(12)-C(13)	110.7(4)
C(11)-C(12)-H(12A)	109.5
C(13)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
C(13)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1
C(14)-C(13)-C(12)	110.6(4)
C(14)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	108.1
O(2)-C(14)-C(13)	112.6(3)
O(2)-C(14)-C(9)	110.7(3)
C(13)-C(14)-C(9)	110.7(3)
O(2)-C(14)-H(14A)	107.6
C(13)-C(14)-H(14A)	107.6

C(9)-C(14)-H(14A)	107.6
C(7)-N(1)-C(6)	111.3(3)
C(7)-N(1)-Cd(1)	105.2(2)
C(6)-N(1)-Cd(1)	124.0(3)
C(7)-N(1)-H(1N)	104.9
C(6)-N(1)-H(1N)	104.9
Cd(1)-N(1)-H(1N)	104.9
C(8)-N(2)-C(9)	114.9(3)
C(8)-N(2)-Cd(1)	108.3(2)
C(9)-N(2)-Cd(1)	112.5(2)
C(8)-N(2)-H(2N)	106.9
C(9)-N(2)-H(2N)	106.9
Cd(1)-N(2)-H(2N)	106.9
C(1)-O(1)-H(1O)	109.5
C(14)-O(2)-Cd(1)	114.5(2)
C(14)-O(2)-H(2O)	111(3)
Cd(1)-O(2)-H(2O)	122(3)
N(2)-Cd(1)-N(1)	77.02(11)
N(2)-Cd(1)-O(2)	71.97(11)
N(1)-Cd(1)-O(2)	144.21(11)
N(2)-Cd(1)-Cl(1)	152.95(8)
N(1)-Cd(1)-Cl(1)	111.03(8)
O(2)-Cd(1)-Cl(1)	90.16(8)
N(2)-Cd(1)-Cl(2)	96.02(8)
N(1)-Cd(1)-Cl(2)	105.94(8)
O(2)-Cd(1)-Cl(2)	94.79(9)
Cl(1)-Cd(1)-Cl(2)	105.81(4)

Symmetry transformations used to generate equivalent atoms:

Table E.34: Anisotropic displacement parameters ($Å^2$ x 10^3)for 7m_al7_a. The anisotropic displacement factor exponent takes the form: -2p2[h2a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13
C(1)	31(2)	33(2)	34(2)	-12(2)	-1(2)
C(2)	42(3)	35(2)	37(2)	-7(2)	6(2)
C(3)	63(3)	55(3)	32(3)	-12(2)	4(2)
C(4)	87(4)	50(3)	44(3)	-24(3)	14(3)
C(5)	72(4)	43(3)	41(3)	-21(2)	10(3)
C(6)	32(2)	32(2)	32(2)	-9(2)	6(2)
C(7)	30(2)	34(2)	40(3)	-7(2)	-7(2)
C(8)	40(3)	31(2)	32(2)	-1(2)	-10(2)
C(9)	33(2)	27(2)	27(2)	-10(2)	-2(2)
C(10)	51(3)	39(3)	29(2)	-2(2)	-4(2)
C(11)	60(3)	47(3)	29(2)	-1(2)	0(2)

C(12)	52(3)	42(3)	34(3)	-5(2)	10(2)
C(13)	34(2)	39(2)	36(2)	-9(2)	2(2)
C(14)	37(2)	26(2)	26(2)	-4(2)	-1(2)
C(15)	129(11)	180(14)	840(60)	170(20)	-230(20)
N(1)	28(2)	28(2)	31(2)	-11(2)	-1(2)
N(2)	31(2)	23(2)	29(2)	-6(2)	-3(2)
O(1)	30(2)	31(2)	43(2)	-15(1)	0(1)
O(2)	37(2)	32(2)	32(2)	-2(2)	1(1)
O(3)	361(17)	293(14)	340(16)	-227(13)	221(14)
Cl(1)	38(1)	25(1)	40(1)	-3(1)	-4(1)
Cl(2)	47(1)	39(1)	60(1)	-23(1)	-13(1)
Cd(1)	30(1)	28(1)	28(1)	-2(1)	-1(1)

Table E.35: Torsion angles [°] for 7m_al7_a.

O(1)-C(1)-C(2)-C(3)	-179.9(4)
C(6)-C(1)-C(2)-C(3)	-56.8(5)
C(1)-C(2)-C(3)-C(4)	55.9(5)
C(2)-C(3)-C(4)-C(5)	-55.9(6)
C(3)-C(4)-C(5)-C(6)	57.2(6)
C(4)-C(5)-C(6)-N(1)	179.8(4)
C(4)-C(5)-C(6)-C(1)	-58.0(5)
O(1)-C(1)-C(6)-N(1)	-54.1(4)
C(2)-C(1)-C(6)-N(1)	-178.3(3)
O(1)-C(1)-C(6)-C(5)	-177.9(3)
C(2)-C(1)-C(6)-C(5)	57.9(5)
N(1)-C(7)-C(8)-N(2)	-61.7(4)
N(2)-C(9)-C(10)-C(11)	178.1(3)
C(14)-C(9)-C(10)-C(11)	55.3(5)
C(9)-C(10)-C(11)-C(12)	-54.2(5)
C(10)-C(11)-C(12)-C(13)	54.8(5)
C(11)-C(12)-C(13)-C(14)	-57.6(5)
C(12)-C(13)-C(14)-O(2)	-176.4(3)
C(12)-C(13)-C(14)-C(9)	59.2(4)
N(2)-C(9)-C(14)-O(2)	51.0(4)
C(10)-C(9)-C(14)-O(2)	176.6(3)
N(2)-C(9)-C(14)-C(13)	176.5(3)
C(10)-C(9)-C(14)-C(13)	-57.9(4)
C(8)-C(7)-N(1)-C(6)	-177.4(3)
C(8)-C(7)-N(1)-Cd(1)	45.9(4)
C(5)-C(6)-N(1)-C(7)	-77.4(4)
C(1)-C(6)-N(1)-C(7)	159.7(3)
C(5)-C(6)-N(1)-Cd(1)	49.6(4)
C(1)-C(6)-N(1)-Cd(1)	-73.3(4)
C(7)-C(8)-N(2)-C(9)	167.6(3)

C(7)-C(8)-N(2)-Cd(1)	41.0(4)
C(14)-C(9)-N(2)-C(8)	-169.9(3)
C(10)-C(9)-N(2)-C(8)	66.6(4)
C(14)-C(9)-N(2)-Cd(1)	-45.4(3)
C(10)-C(9)-N(2)-Cd(1)	-168.9(3)
C(13)-C(14)-O(2)-Cd(1)	-156.7(3)
C(9)-C(14)-O(2)-Cd(1)	-32.3(4)
C(8)-N(2)-Cd(1)-N(1)	-12.4(2)
C(9)-N(2)-Cd(1)-N(1)	-140.5(3)
C(8)-N(2)-Cd(1)-O(2)	149.5(3)
C(9)-N(2)-Cd(1)-O(2)	21.4(2)
C(8)-N(2)-Cd(1)-Cl(1)	98.6(3)
C(9)-N(2)-Cd(1)-Cl(1)	-29.4(4)
C(8)-N(2)-Cd(1)-Cl(2)	-117.4(2)
C(9)-N(2)-Cd(1)-Cl(2)	114.5(2)
C(7)-N(1)-Cd(1)-N(2)	-17.4(2)
C(6)-N(1)-Cd(1)-N(2)	-147.0(3)
C(7)-N(1)-Cd(1)-O(2)	-47.8(3)
C(6)-N(1)-Cd(1)-O(2)	-177.3(2)
C(7)-N(1)-Cd(1)-Cl(1)	-170.4(2)
C(6)-N(1)-Cd(1)-Cl(1)	60.1(3)
C(7)-N(1)-Cd(1)-Cl(2)	75.2(2)
C(6)-N(1)-Cd(1)-Cl(2)	-54.3(3)
C(14)-O(2)-Cd(1)-N(2)	6.4(2)
C(14)-O(2)-Cd(1)-N(1)	37.5(4)
C(14)-O(2)-Cd(1)-Cl(1)	165.7(3)
C(14)-O(2)-Cd(1)-Cl(2)	-88.4(3)

Symmetry transformations used to generate equivalent atoms:

Table E.36: Hydrogen bonds for 7m_al7_a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(1)#1	0.75(4)	1.95(5)	2.702(4)	172(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z+1

BHEEN/Cd Data

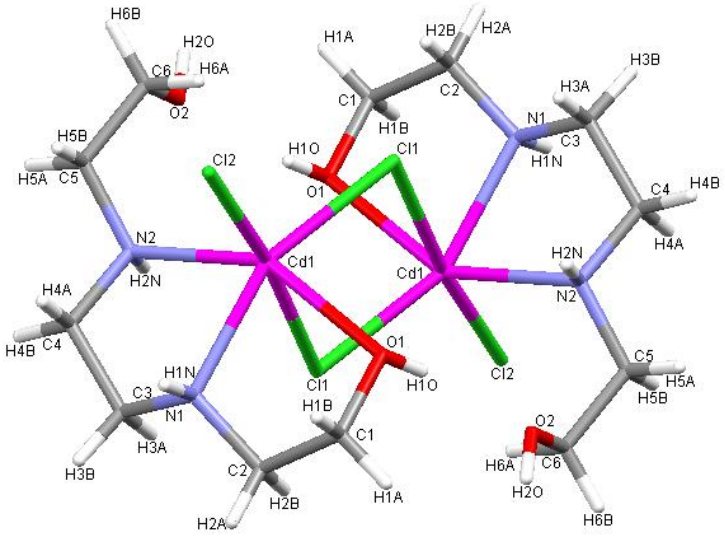


Figure E.7: The cadmium(II) complex of BHEEN and the labelling scheme used

Table E.37: Crystal data and structure refinement for 8m_alv4_0a.

Identification code	8m_alv4_0a	
Empirical formula	C12 H32 Cd2 Cl4 N4 O4	
Formula weight	663.02	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 11.0918(3) Å	α = 90°.
	b = 12.4205(3) Å	β = 90°.
	c = 15.9911(4) Å	γ = 90°.
Volume	2203.03(10) $Å^3$	
Z	4	
Density (calculated)	1.999 Mg/m^3	
Absorption coefficient	2.440 mm^{-1}	
F(000)	1312	
Crystal size	0.28 x 0.18 x 0.04 mm^3	
Theta range for data collection	2.55 to 27.99°.	
Index ranges	-13<=h<=14, -14<=k<=16, -20<=l<=21	
Reflections collected	25373	
Independent reflections	2659 [R(int) = 0.0626]	
Completeness to theta = 27.99°	100.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.9087 and 0.5482	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	2659 / 0 / 126
Goodness-of-fit on F^2	0.956
Final R indices [I>2σ(I)]	$R_1 = 0.0222$, $wR_2 = 0.0498$
R indices (all data)	$R_1 = 0.0301$, $wR_2 = 0.0521$
Largest diff. peak and hole	1.206 and -0.406 e.Å^{-3}

Table E.38: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 8m_alv4_0a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8634(2)	2592(2)	-1204(1)	22(1)
C(2)	7515(2)	1918(2)	-1080(1)	20(1)
C(3)	6392(2)	957(2)	44(1)	19(1)
C(4)	6449(2)	743(2)	974(1)	21(1)
C(5)	7749(2)	272(2)	2145(1)	20(1)
C(6)	8989(2)	-62(2)	2422(1)	23(1)
N(1)	7300(1)	1777(2)	-182(1)	16(1)
N(2)	7634(1)	296(2)	1226(1)	16(1)
O(1)	9664(1)	2114(1)	-810(1)	20(1)
O(2)	9244(2)	-1134(2)	2146(1)	28(1)
Cd(1)	9070(1)	1272(1)	479(1)	16(1)
Cl(1)	11172(1)	617(1)	611(1)	21(1)
Cl(2)	9058(1)	2912(1)	1437(1)	23(1)

Table E.39: Bond lengths [Å] and angles [°] for 8m_alv4_0a.

C(1)-O(1)	1.433(3)
C(1)-C(2)	1.510(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-N(1)	1.466(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-N(1)	1.477(3)
C(3)-C(4)	1.511(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-N(2)	1.482(2)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-N(2)	1.476(2)

C(5)-C(6)	1.503(3)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-O(2)	1.431(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
N(1)-Cd(1)	2.3172(16)
N(1)-H(1N)	0.9300
N(2)-Cd(1)	2.3312(16)
N(2)-H(2N)	0.9300
O(1)-Cd(1)	2.4030(16)
O(1)-H(1O)	0.76(3)
O(2)-H(2O)	0.77(3)
Cd(1)-Cl(1)	2.4782(5)
Cd(1)-Cl(2)	2.5486(6)
Cd(1)-Cl(1)#1	2.9353(6)
Cl(1)-Cd(1)#1	2.9353(6)

O(1)-C(1)-C(2)	111.63(18)
O(1)-C(1)-H(1A)	109.3
C(2)-C(1)-H(1A)	109.3
O(1)-C(1)-H(1B)	109.3
C(2)-C(1)-H(1B)	109.3
H(1A)-C(1)-H(1B)	108.0
N(1)-C(2)-C(1)	109.15(17)
N(1)-C(2)-H(2A)	109.9
C(1)-C(2)-H(2A)	109.9
N(1)-C(2)-H(2B)	109.9
C(1)-C(2)-H(2B)	109.9
H(2A)-C(2)-H(2B)	108.3
N(1)-C(3)-C(4)	109.49(16)
N(1)-C(3)-H(3A)	109.8
C(4)-C(3)-H(3A)	109.8
N(1)-C(3)-H(3B)	109.8
C(4)-C(3)-H(3B)	109.8
H(3A)-C(3)-H(3B)	108.2
N(2)-C(4)-C(3)	111.73(16)
N(2)-C(4)-H(4A)	109.3
C(3)-C(4)-H(4A)	109.3
N(2)-C(4)-H(4B)	109.3
C(3)-C(4)-H(4B)	109.3
H(4A)-C(4)-H(4B)	107.9
N(2)-C(5)-C(6)	112.22(16)
N(2)-C(5)-H(5A)	109.2
C(6)-C(5)-H(5A)	109.2
N(2)-C(5)-H(5B)	109.2

C(6)-C(5)-H(5B)	109.2
H(5A)-C(5)-H(5B)	107.9
O(2)-C(6)-C(5)	110.30(18)
O(2)-C(6)-H(6A)	109.6
C(5)-C(6)-H(6A)	109.6
O(2)-C(6)-H(6B)	109.6
C(5)-C(6)-H(6B)	109.6
H(6A)-C(6)-H(6B)	108.1
C(2)-N(1)-C(3)	115.67(16)
C(2)-N(1)-Cd(1)	109.97(12)
C(3)-N(1)-Cd(1)	106.20(12)
C(2)-N(1)-H(1N)	108.3
C(3)-N(1)-H(1N)	108.3
Cd(1)-N(1)-H(1N)	108.3
C(5)-N(2)-C(4)	110.81(15)
C(5)-N(2)-Cd(1)	117.50(12)
C(4)-N(2)-Cd(1)	105.78(12)
C(5)-N(2)-H(2N)	107.4
C(4)-N(2)-H(2N)	107.4
Cd(1)-N(2)-H(2N)	107.4
C(1)-O(1)-Cd(1)	109.81(12)
C(1)-O(1)-H(1O)	108.4(19)
Cd(1)-O(1)-H(1O)	116(2)
C(6)-O(2)-H(2O)	112(2)
N(1)-Cd(1)-N(2)	78.17(6)
N(1)-Cd(1)-O(1)	73.92(6)
N(2)-Cd(1)-O(1)	148.52(5)
N(1)-Cd(1)-Cl(1)	157.67(4)
N(2)-Cd(1)-Cl(1)	115.41(4)
O(1)-Cd(1)-Cl(1)	87.59(4)
N(1)-Cd(1)-Cl(2)	93.07(5)
N(2)-Cd(1)-Cl(2)	95.96(4)
O(1)-Cd(1)-Cl(2)	99.74(4)
Cl(1)-Cd(1)-Cl(2)	102.493(18)
N(1)-Cd(1)-Cl(1)#1	82.39(5)
N(2)-Cd(1)-Cl(1)#1	79.96(4)
O(1)-Cd(1)-Cl(1)#1	82.19(4)
Cl(1)-Cd(1)-Cl(1)#1	82.786(17)
Cl(2)-Cd(1)-Cl(1)#1	174.407(15)
Cd(1)-Cl(1)-Cd(1)#1	97.214(17)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z

Table E.40: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 8m_alv4_0a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	28(1)	16(1)	23(1)	4(1)	1(1)	5(1)
C(2)	23(1)	19(1)	18(1)	-1(1)	-4(1)	4(1)
C(3)	14(1)	19(1)	23(1)	-1(1)	-5(1)	2(1)
C(4)	13(1)	23(1)	26(1)	2(1)	0(1)	2(1)
C(5)	20(1)	23(1)	18(1)	0(1)	1(1)	1(1)
C(6)	22(1)	28(1)	19(1)	2(1)	-1(1)	0(1)
N(1)	18(1)	14(1)	17(1)	-2(1)	-2(1)	1(1)
N(2)	14(1)	15(1)	18(1)	-1(1)	1(1)	2(1)
O(1)	22(1)	19(1)	20(1)	0(1)	1(1)	3(1)
O(2)	29(1)	32(1)	23(1)	2(1)	-3(1)	11(1)
Cd(1)	13(1)	18(1)	17(1)	1(1)	-1(1)	0(1)
Cl(1)	15(1)	19(1)	29(1)	-4(1)	-2(1)	2(1)
Cl(2)	25(1)	21(1)	23(1)	-6(1)	0(1)	-2(1)

Table E.41: Torsion angles [°] for 8m_alv4_0a.

O(1)-C(1)-C(2)-N(1)	57.5(2)
N(1)-C(3)-C(4)-N(2)	-62.6(2)
N(2)-C(5)-C(6)-O(2)	-62.4(2)
C(1)-C(2)-N(1)-C(3)	-167.83(18)
C(1)-C(2)-N(1)-Cd(1)	-47.6(2)
C(4)-C(3)-N(1)-C(2)	168.63(17)
C(4)-C(3)-N(1)-Cd(1)	46.34(18)
C(6)-C(5)-N(2)-C(4)	-173.70(18)
C(6)-C(5)-N(2)-Cd(1)	-52.0(2)
C(3)-C(4)-N(2)-C(5)	170.11(18)
C(3)-C(4)-N(2)-Cd(1)	41.7(2)
C(2)-C(1)-O(1)-Cd(1)	-36.4(2)
C(2)-N(1)-Cd(1)-N(2)	-144.06(15)
C(3)-N(1)-Cd(1)-N(2)	-18.22(12)
C(2)-N(1)-Cd(1)-O(1)	21.23(13)
C(3)-N(1)-Cd(1)-O(1)	147.07(14)
C(2)-N(1)-Cd(1)-Cl(1)	-14.0(2)
C(3)-N(1)-Cd(1)-Cl(1)	111.86(14)
C(2)-N(1)-Cd(1)-Cl(2)	120.49(13)
C(3)-N(1)-Cd(1)-Cl(2)	-113.67(12)
C(2)-N(1)-Cd(1)-Cl(1)#1	-62.79(13)
C(3)-N(1)-Cd(1)-Cl(1)#1	63.05(12)
C(5)-N(2)-Cd(1)-N(1)	-136.35(15)
C(4)-N(2)-Cd(1)-N(1)	-12.07(13)

C(5)-N(2)-Cd(1)-O(1)	-164.21(13)
C(4)-N(2)-Cd(1)-O(1)	-39.93(19)
C(5)-N(2)-Cd(1)-Cl(1)	62.42(15)
C(4)-N(2)-Cd(1)-Cl(1)	-173.30(12)
C(5)-N(2)-Cd(1)-Cl(2)	-44.46(14)
C(4)-N(2)-Cd(1)-Cl(2)	79.82(13)
C(5)-N(2)-Cd(1)-Cl(1)#1	139.40(14)
C(4)-N(2)-Cd(1)-Cl(1)#1	-96.32(13)
C(1)-O(1)-Cd(1)-N(1)	8.30(13)
C(1)-O(1)-Cd(1)-N(2)	36.7(2)
C(1)-O(1)-Cd(1)-Cl(1)	175.64(14)
C(1)-O(1)-Cd(1)-Cl(2)	-82.10(13)
C(1)-O(1)-Cd(1)-Cl(1)#1	92.59(13)
N(1)-Cd(1)-Cl(1)-Cd(1)#1	-48.75(13)
N(2)-Cd(1)-Cl(1)-Cd(1)#1	75.24(5)
O(1)-Cd(1)-Cl(1)-Cd(1)#1	-82.43(4)
Cl(2)-Cd(1)-Cl(1)-Cd(1)#1	178.122(18)
Cl(1)#1-Cd(1)-Cl(1)-Cd(1)#1	0.0

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z

Table E.42: Hydrogen bonds for 8m_alv4_0a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...O(2)#1	0.76(3)	2.00(3)	2.741(2)	165(3)
O(2)-H(2O)...Cl(2)#2	0.77(3)	2.41(3)	3.1756(18)	169(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z #2 -x+2,y-1/2,-z+1/2

BHEEN/Zn Data

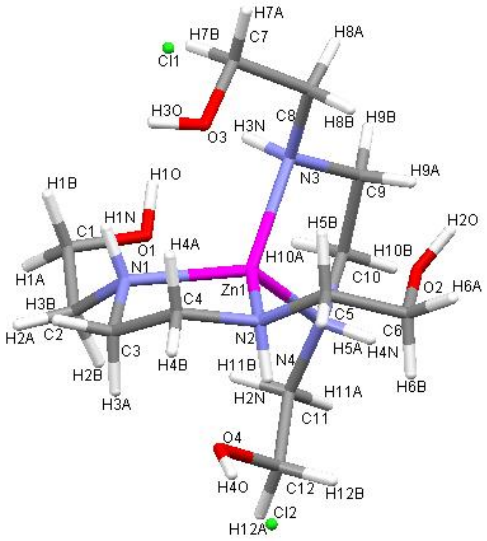


Figure E.8: The Zinc complex of BHEEN and the labelling scheme used

Table E.43: Crystal data and structure refinement for 8m_alv22_0a.

Identification code	8m_alv22_0a	
Empirical formula	C12 H32 Cl2 N4 O4 Zn	
Formula weight	432.69	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 15.3169(2) Å	α = 90°.
	b = 8.98000(10) Å	β = 105.2260(10)°.
	c = 14.3231(2) Å	γ = 90°.
Volume	1900.93(4) $Å^3$	
Z	4	
Density (calculated)	1.512 Mg/m^3	
Absorption coefficient	1.596 mm^{-1}	
F(000)	912	
Crystal size	0.33 x 0.28 x 0.22 mm^3	
Theta range for data collection	1.38 to 28.00°.	
Index ranges	-20<=h<=20, -11<=k<=11, -18<=l<=18	
Reflections collected	39686	
Independent reflections	4588 [R(int) = 0.0422]	
Completeness to theta = 28.00°	100.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.7204 and 0.6210	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4588 / 0 / 212
Goodness-of-fit on F^2	1.042
Final R indices [I>2σ(I)]	$R_1 = 0.0211$, $wR_2 = 0.0546$
R indices (all data)	$R_1 = 0.0247$, $wR_2 = 0.0556$
Largest diff. peak and hole	0.321 and -0.440 e.Å^{-3}

Table E.44: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 8m_alv22_0a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9151(1)	6684(2)	9108(1)	25(1)
C(2)	8776(1)	5199(2)	9296(1)	24(1)
C(3)	8449(1)	2681(1)	8648(1)	27(1)
C(4)	8039(1)	1799(1)	7745(1)	30(1)
C(5)	6807(1)	1859(2)	6240(1)	33(1)
C(6)	5908(1)	2559(2)	5786(1)	35(1)
C(7)	8951(1)	4943(1)	5752(1)	26(1)
C(8)	8036(1)	5658(2)	5422(1)	23(1)
C(9)	6942(1)	7224(1)	5946(1)	23(1)
C(10)	6576(1)	7603(1)	6803(1)	22(1)
C(11)	6234(1)	6605(1)	8244(1)	22(1)
C(12)	5933(1)	5249(1)	8695(1)	24(1)
N(1)	8565(1)	4268(1)	8410(1)	21(1)
N(2)	7195(1)	2547(1)	7198(1)	22(1)
N(3)	7746(1)	6246(1)	6263(1)	18(1)
N(4)	6414(1)	6229(1)	7305(1)	18(1)
O(1)	8469(1)	7510(1)	8446(1)	28(1)
O(2)	6002(1)	4106(1)	5632(1)	36(1)
O(3)	8882(1)	3653(1)	6303(1)	35(1)
O(4)	6645(1)	4188(1)	8899(1)	26(1)
Zn(1)	7465(1)	4796(1)	7271(1)	18(1)
Cl(1)	9388(1)	8792(1)	6950(1)	30(1)
Cl(2)	5882(1)	1011(1)	8455(1)	28(1)

Table E.45: Bond lengths [Å] and angles [°] for 8m_alv22_0a.

C(1)-O(1)	1.4226(15)
C(1)-C(2)	1.5041(18)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-N(1)	1.4822(16)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-N(1)	1.4861(15)
C(3)-C(4)	1.5060(19)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-N(2)	1.4839(17)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-N(2)	1.4799(16)
C(5)-C(6)	1.498(2)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-O(2)	1.4198(17)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-O(3)	1.4210(16)
C(7)-C(8)	1.5006(19)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-N(3)	1.4854(15)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-N(3)	1.4840(15)
C(9)-C(10)	1.5152(17)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-N(4)	1.4814(14)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-N(4)	1.4811(15)
C(11)-C(12)	1.5061(17)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-O(4)	1.4195(15)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
N(1)-Zn(1)	2.0683(10)
N(1)-H(1N)	0.9300
N(2)-Zn(1)	2.0584(10)

N(2)-H(2N)	0.9300
N(3)-Zn(1)	2.0711(10)
N(3)-H(3N)	0.9300
N(4)-Zn(1)	2.0719(10)
N(4)-H(4N)	0.9300
O(1)-H(1O)	0.8400
O(2)-H(2O)	0.8400
O(3)-H(3O)	0.8400
O(4)-H(4O)	0.8400

O(1)-C(1)-C(2)	109.44(10)
O(1)-C(1)-H(1A)	109.8
C(2)-C(1)-H(1A)	109.8
O(1)-C(1)-H(1B)	109.8
C(2)-C(1)-H(1B)	109.8
H(1A)-C(1)-H(1B)	108.2
N(1)-C(2)-C(1)	110.81(10)
N(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.1
N(1)-C(3)-C(4)	110.82(11)
N(1)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
N(1)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
N(2)-C(4)-C(3)	108.91(10)
N(2)-C(4)-H(4A)	109.9
C(3)-C(4)-H(4A)	109.9
N(2)-C(4)-H(4B)	109.9
C(3)-C(4)-H(4B)	109.9
H(4A)-C(4)-H(4B)	108.3
N(2)-C(5)-C(6)	109.09(11)
N(2)-C(5)-H(5A)	109.9
C(6)-C(5)-H(5A)	109.9
N(2)-C(5)-H(5B)	109.9
C(6)-C(5)-H(5B)	109.9
H(5A)-C(5)-H(5B)	108.3
O(2)-C(6)-C(5)	111.07(11)
O(2)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6A)	109.4
O(2)-C(6)-H(6B)	109.4
C(5)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0

O(3)-C(7)-C(8)	108.88(11)
O(3)-C(7)-H(7A)	109.9
C(8)-C(7)-H(7A)	109.9
O(3)-C(7)-H(7B)	109.9
C(8)-C(7)-H(7B)	109.9
H(7A)-C(7)-H(7B)	108.3
N(3)-C(8)-C(7)	110.49(10)
N(3)-C(8)-H(8A)	109.6
C(7)-C(8)-H(8A)	109.6
N(3)-C(8)-H(8B)	109.6
C(7)-C(8)-H(8B)	109.6
H(8A)-C(8)-H(8B)	108.1
N(3)-C(9)-C(10)	109.85(10)
N(3)-C(9)-H(9A)	109.7
C(10)-C(9)-H(9A)	109.7
N(3)-C(9)-H(9B)	109.7
C(10)-C(9)-H(9B)	109.7
H(9A)-C(9)-H(9B)	108.2
N(4)-C(10)-C(9)	110.52(10)
N(4)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10A)	109.5
N(4)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1
N(4)-C(11)-C(12)	110.85(10)
N(4)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11A)	109.5
N(4)-C(11)-H(11B)	109.5
C(12)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.1
O(4)-C(12)-C(11)	109.00(10)
O(4)-C(12)-H(12A)	109.9
C(11)-C(12)-H(12A)	109.9
O(4)-C(12)-H(12B)	109.9
C(11)-C(12)-H(12B)	109.9
H(12A)-C(12)-H(12B)	108.3
C(2)-N(1)-C(3)	110.91(10)
C(2)-N(1)-Zn(1)	119.67(8)
C(3)-N(1)-Zn(1)	106.23(8)
C(2)-N(1)-H(1N)	106.4
C(3)-N(1)-H(1N)	106.4
Zn(1)-N(1)-H(1N)	106.4
C(5)-N(2)-C(4)	112.48(10)
C(5)-N(2)-Zn(1)	118.88(8)
C(4)-N(2)-Zn(1)	106.38(8)
C(5)-N(2)-H(2N)	106.1

C(4)-N(2)-H(2N)	106.1
Zn(1)-N(2)-H(2N)	106.1
C(9)-N(3)-C(8)	111.28(9)
C(9)-N(3)-Zn(1)	106.09(7)
C(8)-N(3)-Zn(1)	120.16(8)
C(9)-N(3)-H(3N)	106.1
C(8)-N(3)-H(3N)	106.1
Zn(1)-N(3)-H(3N)	106.1
C(11)-N(4)-C(10)	110.21(9)
C(11)-N(4)-Zn(1)	119.59(8)
C(10)-N(4)-Zn(1)	105.99(7)
C(11)-N(4)-H(4N)	106.8
C(10)-N(4)-H(4N)	106.8
Zn(1)-N(4)-H(4N)	106.8
C(1)-O(1)-H(1O)	109.5
C(6)-O(2)-H(2O)	109.5
C(7)-O(3)-H(3O)	109.5
C(12)-O(4)-H(4O)	109.5
N(2)-Zn(1)-N(1)	85.76(4)
N(2)-Zn(1)-N(3)	131.09(4)
N(1)-Zn(1)-N(3)	114.76(4)
N(2)-Zn(1)-N(4)	117.60(4)
N(1)-Zn(1)-N(4)	126.92(4)
N(3)-Zn(1)-N(4)	86.05(4)

Symmetry transformations used to generate equivalent atoms:

Table E.46: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 8m_alv22_0a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(1)	34(1)	23(1)	-3(1)	2(1)	0(1)
C(2)	18(1)	36(1)	17(1)	2(1)	3(1)	1(1)
C(3)	24(1)	26(1)	32(1)	13(1)	8(1)	7(1)
C(4)	35(1)	17(1)	41(1)	5(1)	18(1)	5(1)
C(5)	53(1)	23(1)	27(1)	-9(1)	16(1)	-10(1)
C(6)	37(1)	47(1)	24(1)	-10(1)	13(1)	-22(1)
C(7)	25(1)	30(1)	26(1)	-4(1)	14(1)	-4(1)
C(8)	25(1)	30(1)	16(1)	0(1)	9(1)	-3(1)
C(9)	23(1)	24(1)	21(1)	7(1)	5(1)	3(1)
C(10)	22(1)	18(1)	26(1)	5(1)	8(1)	4(1)
C(11)	21(1)	24(1)	23(1)	-2(1)	10(1)	2(1)
C(12)	20(1)	29(1)	24(1)	3(1)	10(1)	3(1)
N(1)	19(1)	23(1)	22(1)	4(1)	8(1)	2(1)

N(2)	27(1)	21(1)	22(1)	-2(1)	12(1)	-2(1)
N(3)	18(1)	21(1)	15(1)	0(1)	5(1)	0(1)
N(4)	17(1)	20(1)	18(1)	0(1)	5(1)	-1(1)
O(1)	22(1)	37(1)	25(1)	4(1)	6(1)	4(1)
O(2)	45(1)	37(1)	25(1)	-8(1)	8(1)	-1(1)
O(3)	32(1)	31(1)	42(1)	7(1)	9(1)	2(1)
O(4)	22(1)	25(1)	33(1)	4(1)	9(1)	3(1)
Zn(1)	22(1)	16(1)	17(1)	2(1)	6(1)	3(1)
Cl(1)	25(1)	32(1)	33(1)	-2(1)	11(1)	-7(1)
Cl(2)	26(1)	32(1)	25(1)	2(1)	7(1)	-5(1)

Table E.47: Torsion angles [°] for 8m_alv22_0a.

O(1)-C(1)-C(2)-N(1)	66.45(13)
N(1)-C(3)-C(4)-N(2)	-53.10(14)
N(2)-C(5)-C(6)-O(2)	61.98(14)
O(3)-C(7)-C(8)-N(3)	66.35(13)
N(3)-C(9)-C(10)-N(4)	-53.11(13)
N(4)-C(11)-C(12)-O(4)	63.23(14)
C(1)-C(2)-N(1)-C(3)	163.69(10)
C(1)-C(2)-N(1)-Zn(1)	-72.11(12)
C(4)-C(3)-N(1)-C(2)	167.57(10)
C(4)-C(3)-N(1)-Zn(1)	36.03(12)
C(6)-C(5)-N(2)-C(4)	173.53(11)
C(6)-C(5)-N(2)-Zn(1)	-61.24(13)
C(3)-C(4)-N(2)-C(5)	172.89(10)
C(3)-C(4)-N(2)-Zn(1)	41.10(11)
C(10)-C(9)-N(3)-C(8)	170.99(10)
C(10)-C(9)-N(3)-Zn(1)	38.65(11)
C(7)-C(8)-N(3)-C(9)	168.18(10)
C(7)-C(8)-N(3)-Zn(1)	-67.04(12)
C(12)-C(11)-N(4)-C(10)	171.58(10)
C(12)-C(11)-N(4)-Zn(1)	-65.29(12)
C(9)-C(10)-N(4)-C(11)	168.68(10)
C(9)-C(10)-N(4)-Zn(1)	37.93(11)
C(5)-N(2)-Zn(1)-N(1)	-145.20(10)
C(4)-N(2)-Zn(1)-N(1)	-17.08(8)
C(5)-N(2)-Zn(1)-N(3)	-25.70(12)
C(4)-N(2)-Zn(1)-N(3)	102.42(8)
C(5)-N(2)-Zn(1)-N(4)	84.95(10)
C(4)-N(2)-Zn(1)-N(4)	-146.93(7)
C(2)-N(1)-Zn(1)-N(2)	-136.55(9)
C(3)-N(1)-Zn(1)-N(2)	-10.12(8)
C(2)-N(1)-Zn(1)-N(3)	89.71(9)

C(3)-N(1)-Zn(1)-N(3)	-143.87(7)
C(2)-N(1)-Zn(1)-N(4)	-14.86(10)
C(3)-N(1)-Zn(1)-N(4)	111.56(8)
C(9)-N(3)-Zn(1)-N(2)	109.62(8)
C(8)-N(3)-Zn(1)-N(2)	-17.57(11)
C(9)-N(3)-Zn(1)-N(1)	-143.28(7)
C(8)-N(3)-Zn(1)-N(1)	89.52(9)
C(9)-N(3)-Zn(1)-N(4)	-14.15(8)
C(8)-N(3)-Zn(1)-N(4)	-141.34(9)
C(11)-N(4)-Zn(1)-N(2)	86.90(9)
C(10)-N(4)-Zn(1)-N(2)	-147.93(7)
C(11)-N(4)-Zn(1)-N(1)	-19.85(10)
C(10)-N(4)-Zn(1)-N(1)	105.31(8)
C(11)-N(4)-Zn(1)-N(3)	-138.09(9)
C(10)-N(4)-Zn(1)-N(3)	-12.92(7)

Symmetry transformations used to generate equivalent atoms:

Table E.48: Hydrogen bonds for 8m_alv22_0a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4N)...O(2)	0.93	2.44	2.9961(13)	119
O(1)-H(1O)...Cl(1)	0.84	2.25	3.0789(10)	167
O(2)-H(2O)...Cl(2)#1	0.84	2.26	3.0775(10)	164
O(3)-H(3O)...Cl(1)#2	0.84	2.32	3.1330(11)	164
O(4)-H(4O)...Cl(2)	0.84	2.25	3.0846(10)	171

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z-1/2 #2 -x+2,y-1/2,-z+3/2

Imidazolinium Salt (1) Data

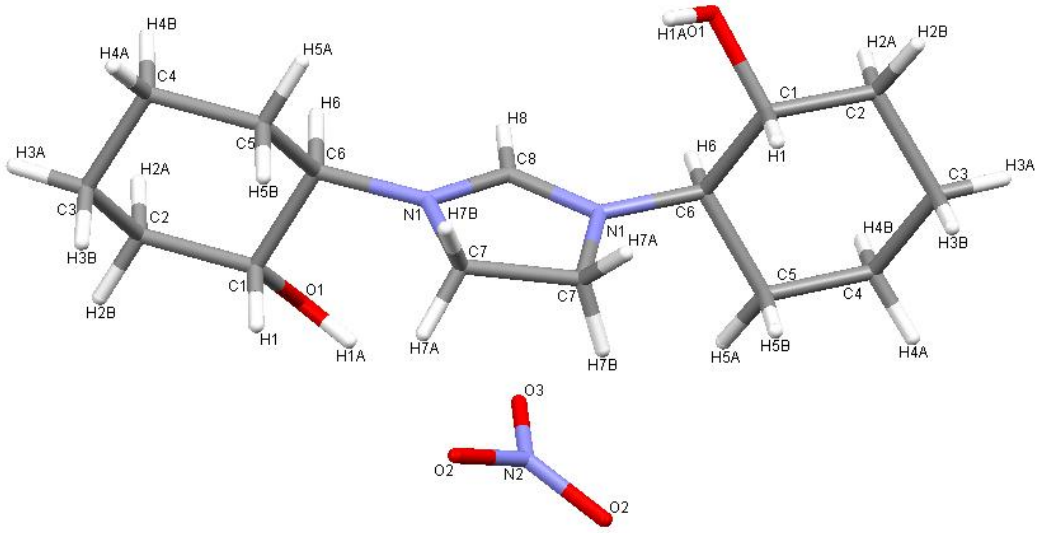


Figure E.9: The Imidazolinium Salt **1** and the labelling scheme used

Table E.49: Crystal data and structure refinement for 7m_al11_0s.

Identification code	7m_al11_0s
Empirical formula	C15 H27 N3 O5
Formula weight	329.40
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C222(1)
Unit cell dimensions	a = 7.0296(2) Å α = 90°. b = 9.8263(2) Å β = 90°. c = 25.1764(6) Å γ = 90°.
Volume	1739.06(7) $Å^3$
Z	4
Density (calculated)	1.258 Mg/m^3
Absorption coefficient	0.094 mm^{-1}
F(000)	712
Crystal size	0.45 x 0.29 x 0.16 mm^3
Theta range for data collection	1.62 to 28.29°.
Index ranges	-9≤h≤9, -13≤k≤11, -31≤l≤33
Reflections collected	10862
Independent reflections	1244 [R(int) = 0.0418]
Completeness to theta = 28.29°	100.0 %
Absorption correction	None
Max. and min. transmission	0.9850 and 0.9587
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1244 / 0 / 120
Goodness-of-fit on F^2	1.142

Final R indices [I>2σ(I)]	$R_1 = 0.0370$, $wR_2 = 0.0981$
R indices (all data)	$R_1 = 0.0400$, $wR_2 = 0.1000$
Absolute structure parameter	-10(10)
Largest diff. peak and hole	0.215 and -0.186 e.Å^{-3}

Table E.50: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 7m_al11_0s. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	282(2)	2933(1)	2928(1)	24(1)
N(2)	5000	2398(2)	2500	27(1)
O(1)	-2815(2)	4016(2)	3559(1)	48(1)
O(2)	5816(2)	1769(2)	2863(1)	36(1)
O(3)	5000	3651(2)	2500	62(1)
C(1)	-1273(3)	3304(2)	3792(1)	29(1)
C(2)	-971(3)	3888(2)	4348(1)	39(1)
C(3)	753(4)	3264(3)	4617(1)	47(1)
C(4)	2525(3)	3461(3)	4287(1)	52(1)
C(5)	2259(3)	2858(3)	3732(1)	43(1)
C(6)	531(2)	3490(2)	3464(1)	25(1)
C(7)	235(2)	1464(2)	2799(1)	25(1)
C(8)	0	3650(2)	2500	24(1)

Table E.51: Bond lengths [Å] and angles [°] for 7m_al11_0s.

N(1)-C(8)	1.3026(17)
N(1)-C(6)	1.4671(18)
N(1)-C(7)	1.4796(19)
N(2)-O(3)	1.231(3)
N(2)-O(2)#1	1.2443(16)
N(2)-O(2)	1.2443(16)
O(1)-C(1)	1.418(2)
O(1)-H(1A)	0.80(3)
C(1)-C(6)	1.524(2)
C(1)-C(2)	1.529(2)
C(1)-H(1)	0.9800
C(2)-C(3)	1.516(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.509(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.530(3)

C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.521(2)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-H(6)	0.9800
C(7)-C(7)#2	1.541(3)
C(7)-H(7A)	0.97(2)
C(7)-H(7B)	0.94(3)
C(8)-N(1)#2	1.3026(16)
C(8)-H(8)	0.93(3)

C(8)-N(1)-C(6)	125.25(13)
C(8)-N(1)-C(7)	110.05(13)
C(6)-N(1)-C(7)	124.65(12)
O(3)-N(2)-O(2)#1	119.78(10)
O(3)-N(2)-O(2)	119.78(10)
O(2)#1-N(2)-O(2)	120.4(2)
C(1)-O(1)-H(1A)	106(3)
O(1)-C(1)-C(6)	110.66(14)
O(1)-C(1)-C(2)	107.49(16)
C(6)-C(1)-C(2)	109.61(14)
O(1)-C(1)-H(1)	109.7
C(6)-C(1)-H(1)	109.7
C(2)-C(1)-H(1)	109.7
C(3)-C(2)-C(1)	111.57(16)
C(3)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2A)	109.3
C(3)-C(2)-H(2B)	109.3
C(1)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	108.0
C(4)-C(3)-C(2)	111.26(16)
C(4)-C(3)-H(3A)	109.4
C(2)-C(3)-H(3A)	109.4
C(4)-C(3)-H(3B)	109.4
C(2)-C(3)-H(3B)	109.4
H(3A)-C(3)-H(3B)	108.0
C(3)-C(4)-C(5)	110.61(19)
C(3)-C(4)-H(4A)	109.5
C(5)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
C(5)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	108.1
C(6)-C(5)-C(4)	110.14(17)
C(6)-C(5)-H(5A)	109.6
C(4)-C(5)-H(5A)	109.6

C(6)-C(5)-H(5B)	109.6
C(4)-C(5)-H(5B)	109.6
H(5A)-C(5)-H(5B)	108.1
N(1)-C(6)-C(5)	110.50(14)
N(1)-C(6)-C(1)	110.74(13)
C(5)-C(6)-C(1)	112.08(13)
N(1)-C(6)-H(6)	107.8
C(5)-C(6)-H(6)	107.8
C(1)-C(6)-H(6)	107.8
N(1)-C(7)-C(7)#2	102.66(8)
N(1)-C(7)-H(7A)	110.5(12)
C(7)#2-C(7)-H(7A)	113.4(12)
N(1)-C(7)-H(7B)	107.8(14)
C(7)#2-C(7)-H(7B)	113.5(14)
H(7A)-C(7)-H(7B)	108.7(17)
N(1)#2-C(8)-N(1)	114.48(19)
N(1)#2-C(8)-H(8)	122.76(9)
N(1)-C(8)-H(8)	122.76(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+1/2 #2 -x,y,-z+1/2

Table E.52: Anisotropic displacement parameters ($Å^2$x 10^3)for 7m_al11_0s. The anisotropic displacement factor exponent takes the form: -2p2[h2a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13
N(1)	34(1)	22(1)	16(1)	-1(1)	-1(1)
N(2)	25(1)	24(1)	32(1)	0	5(1)
O(1)	36(1)	63(1)	46(1)	-21(1)	-11(1)
O(2)	35(1)	37(1)	36(1)	0(1)	-7(1)
O(3)	106(2)	20(1)	60(1)	0	4(2)
C(1)	31(1)	33(1)	24(1)	-3(1)	2(1)
C(2)	44(1)	51(1)	21(1)	-6(1)	5(1)
C(3)	66(1)	59(1)	16(1)	-1(1)	-2(1)
C(4)	42(1)	89(2)	26(1)	-11(1)	-14(1)
C(5)	32(1)	73(1)	23(1)	-9(1)	-5(1)
C(6)	32(1)	28(1)	15(1)	-1(1)	-1(1)
C(7)	31(1)	22(1)	23(1)	1(1)	0(1)
C(8)	29(1)	23(1)	19(1)	0	0(1)

Table E.53: Torsion angles [°] for 7m_al11_0s.

O(1)-C(1)-C(2)-C(3)	-175.64(17)
C(6)-C(1)-C(2)-C(3)	-55.3(2)
C(1)-C(2)-C(3)-C(4)	56.8(3)
C(2)-C(3)-C(4)-C(5)	-56.9(3)
C(3)-C(4)-C(5)-C(6)	56.5(3)
C(8)-N(1)-C(6)-C(5)	-131.43(16)
C(7)-N(1)-C(6)-C(5)	51.3(2)
C(8)-N(1)-C(6)-C(1)	103.77(17)
C(7)-N(1)-C(6)-C(1)	-73.5(2)
C(4)-C(5)-C(6)-N(1)	179.13(17)
C(4)-C(5)-C(6)-C(1)	-56.8(2)
O(1)-C(1)-C(6)-N(1)	-61.85(19)
C(2)-C(1)-C(6)-N(1)	179.77(15)
O(1)-C(1)-C(6)-C(5)	174.24(16)
C(2)-C(1)-C(6)-C(5)	55.9(2)
C(8)-N(1)-C(7)-C(7)#2	-2.6(2)
C(6)-N(1)-C(7)-C(7)#2	175.03(16)
C(6)-N(1)-C(8)-N(1)#2	-176.56(18)
C(7)-N(1)-C(8)-N(1)#2	1.10(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+1/2 #2 -x,y,-z+1/2

Table E.54: Hydrogen bonds for 7m_al11_0s [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...O(2)#3	0.80(3)	2.19(3)	2.977(2)	165(3)
O(1)-H(1A)...O(3)#3	0.80(3)	2.44(3)	3.0969(16)	140(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+1/2 #2 -x,y,-z+1/2 #3 x-1,y,z

Zwitterion (2) Data

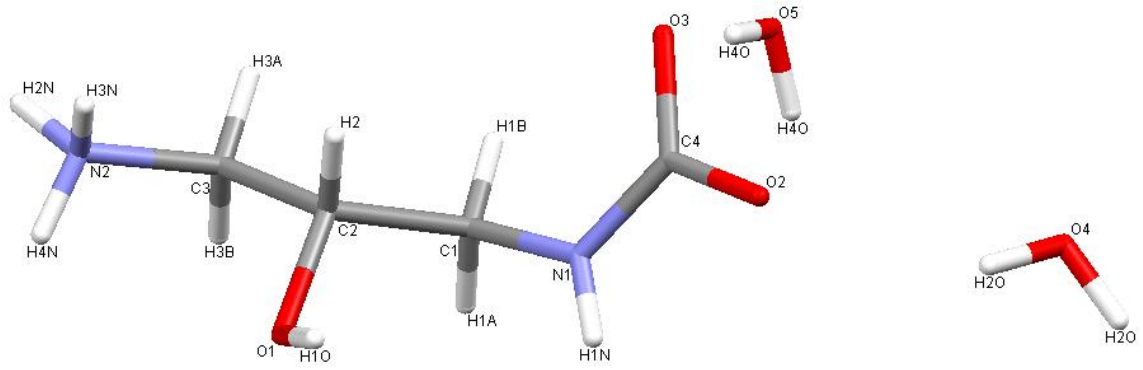


Figure E.10: The Zwitterion **2** and the labelling scheme used

Table E.55: Crystal data and structure refinement for 8m_alv8_0ff.

Identification code	8m_alv8_0ff
Empirical formula	C4 H12 N2 O4
Formula weight	152.16
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2/c
Unit cell dimensions	a = 8.4164(3) Å α = 90°. b = 5.9335(2) Å β = 116.764(2)°. c = 15.6461(6) Å γ = 90°.
Volume	697.64(4) $Å^3$
Z	4
Density (calculated)	1.449 Mg/m^3
Absorption coefficient	0.128 mm^{-1}
F(000)	328
Crystal size	0.47 x 0.11 x 0.09 mm^3
Theta range for data collection	2.71 to 28.33°.
Index ranges	-10≤h≤11, -7≤k≤7, -20≤l≤20
Reflections collected	9150
Independent reflections	1748 [R(int) = 0.0579]
Completeness to theta = 28.33°	100.0 %
Absorption correction	None
Max. and min. transmission	0.9886 and 0.9424
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1748 / 0 / 120
Goodness-of-fit on F^2	1.027

Final R indices [I>2σ(I)]	$R_1 = 0.0458$, $wR_2 = 0.1207$
R indices (all data)	$R_1 = 0.0682$, $wR_2 = 0.1296$
Largest diff. peak and hole	0.591 and -0.203 e.Å^{-3}

Table E.56: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 8m_alv8_0ff. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6350(2)	7346(3)	1400(1)	23(1)
C(2)	7659(2)	8056(3)	1027(1)	23(1)
C(3)	7215(2)	6873(3)	94(1)	24(1)
C(4)	7663(2)	7100(3)	3165(1)	19(1)
N(1)	6823(2)	8256(3)	2344(1)	23(1)
N(2)	8430(2)	7582(3)	-311(1)	21(1)
O(1)	7611(2)	10400(2)	871(1)	33(1)
O(2)	8031(2)	8078(2)	3949(1)	25(1)
O(3)	8045(2)	5030(2)	3128(1)	23(1)
O(4)	0	2601(3)	2500	27(1)
O(5)	5000	2482(3)	2500	35(1)

Table E.57: Bond lengths [Å] and angles [°] for 8m_alv8_0ff.

C(1)-N(1)	1.450(2)
C(1)-C(2)	1.521(2)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-O(1)	1.410(2)
C(2)-C(3)	1.507(2)
C(2)-H(2)	0.9800
C(3)-N(2)	1.485(2)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-O(2)	1.262(2)
C(4)-O(3)	1.2779(19)
C(4)-N(1)	1.342(2)
N(1)-H(1N)	0.83(2)
N(2)-H(2N)	0.93(2)
N(2)-H(3N)	0.90(3)
N(2)-H(4N)	0.88(2)
O(1)-H(1O)	1.03(4)
O(4)-H(2O)	0.90(2)
O(5)-H(4O)	0.85(2)

N(1)-C(1)-C(2)	112.00(14)
N(1)-C(1)-H(1A)	109.2
C(2)-C(1)-H(1A)	109.2
N(1)-C(1)-H(1B)	109.2
C(2)-C(1)-H(1B)	109.2
H(1A)-C(1)-H(1B)	107.9
O(1)-C(2)-C(3)	108.47(14)
O(1)-C(2)-C(1)	111.74(15)
C(3)-C(2)-C(1)	109.67(14)
O(1)-C(2)-H(2)	109.0
C(3)-C(2)-H(2)	109.0
C(1)-C(2)-H(2)	109.0
N(2)-C(3)-C(2)	111.24(14)
N(2)-C(3)-H(3A)	109.4
C(2)-C(3)-H(3A)	109.4
N(2)-C(3)-H(3B)	109.4
C(2)-C(3)-H(3B)	109.4
H(3A)-C(3)-H(3B)	108.0
O(2)-C(4)-O(3)	122.02(15)
O(2)-C(4)-N(1)	119.19(15)
O(3)-C(4)-N(1)	118.79(15)
C(4)-N(1)-C(1)	124.72(16)
C(4)-N(1)-H(1N)	115.6(14)
C(1)-N(1)-H(1N)	119.5(14)
C(3)-N(2)-H(2N)	110.7(12)
C(3)-N(2)-H(3N)	110.8(14)
H(2N)-N(2)-H(3N)	109.4(17)
C(3)-N(2)-H(4N)	111.2(13)
H(2N)-N(2)-H(4N)	105.6(18)
H(3N)-N(2)-H(4N)	108.9(19)
C(2)-O(1)-H(1O)	110.1(19)

Symmetry transformations used to generate equivalent atoms:

Table E.58: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 8m_alv8_0ff. The anisotropic displacement factor exponent takes the form: -2p2[h2a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13
C(1)	22(1)	26(1)	17(1)	1(1)	7(1)
C(2)	26(1)	23(1)	17(1)	-1(1)	9(1)
C(3)	28(1)	25(1)	21(1)	-2(1)	12(1)
C(4)	17(1)	22(1)	20(1)	0(1)	10(1)
N(1)	30(1)	21(1)	21(1)	1(1)	13(1)
N(2)	27(1)	20(1)	17(1)	-2(1)	10(1)

O(1)	51(1)	24(1)	27(1)	1(1)	18(1)
O(2)	29(1)	27(1)	19(1)	-5(1)	10(1)
O(3)	27(1)	19(1)	22(1)	2(1)	12(1)
O(4)	33(1)	21(1)	34(1)	0	22(1)
O(5)	28(1)	19(1)	53(1)	0	14(1)

Table E.59: Torsion angles [°] for 8m_alv8_0ff.

N(1)-C(1)-C(2)-O(1)	-65.54(19)
N(1)-C(1)-C(2)-C(3)	174.14(15)
O(1)-C(2)-C(3)-N(2)	55.83(19)
C(1)-C(2)-C(3)-N(2)	178.12(15)
O(2)-C(4)-N(1)-C(1)	178.96(15)
O(3)-C(4)-N(1)-C(1)	-1.9(3)
C(2)-C(1)-N(1)-C(4)	-100.2(2)

Symmetry transformations used to generate equivalent atoms:

Table E.60: Hydrogen bonds for 8m_alv8_0ff [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...O(4)#1	1.03(4)	1.74(4)	2.7620(17)	178(3)
N(2)-H(2N)...O(3)#2	0.93(2)	1.86(2)	2.7867(19)	172.9(18)
N(2)-H(3N)...O(2)#3	0.90(3)	1.90(3)	2.790(2)	172(2)
N(2)-H(4N)...O(2)#4	0.88(2)	1.92(2)	2.782(2)	168.2(19)
O(4)-H(2O)...O(3)#5	0.90(2)	1.79(2)	2.6837(15)	171(2)
O(5)-H(4O)...O(3)	0.85(2)	1.90(2)	2.7482(17)	174(2)

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y+1,z #2 x,-y+1,z-1/2 #3 -x+2,y,-z+1/2
#4 x,-y+2,z-1/2 #5 x-1,y,z