APPENDIX-I

Table 1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Mncyclam. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*Y*	*z*	U(eq)
Cl3	3574.3(16)	5411.2(5)	557(2)	88.6(8)
O9	3547(6)	5413(3)	-803(6)	143(3)
O8	4590(9)	3754(3)	6164(12)	218(6)
O10	3400(4)	4980.2(17)	999(6)	89.6(17)
O11	4092(4)	5623(2)	1422(8)	110(2)
O12	2771(5)	5624(2)	997(10)	135(3)
Mn1	1572.7(5)	2500	5027.1(8)	17.4(3)
Cl1	3234.6(8)	3412.9(4)	1524.4(14)	43.4(4)
Cl2	4817.7(8)	3342.0(4)	6449.3(13)	40.4(4)
N4	441(3)	2500	5224(5)	28.1(11)
N3	2701(3)	2500	4781(5)	28.2(12)
N2	1638(2)	2972.3(13)	6399(4)	34.0(9)
C9	-215(4)	2500	5473(7)	29.7(14)
C7	3338(4)	2500	4405(7)	31.5(14)
N1	1508(2)	2974.0(13)	3657(4)	32.1(9)
C1	1977(4)	2500	8353(7)	50(2)
C2	2162(3)	2907(2)	7566(5)	44.5(13)
C5	972(3)	2909.4(19)	2491(5)	40.4(12)
C8	4131(4)	2500	3886(8)	48.5(19)
C6	1146(4)	2500	1713(7)	40.3(17)
C4	1325(4)	3380.4(16)	4409(6)	46.4(13)
C3	1817(3)	3378.4(16)	5690(6)	46.2(13)
C10	-1032(4)	2500	5816(8)	43.7(17)
O2	4051(3)	3334(2)	1448(7)	100(2)
O3	3126(8)	3730(7)	770(20)	415(18)
O7	5060(5)	3349(3)	7829(9)	149(4)
O1	3018(7)	3540(5)	2754(13)	240(8)
O5	4067(3)	3162(4)	6371(7)	149(4)
O6	5320(5)	3240(4)	5475(13)	209(6)
O4	2845(4)	3036(3)	1479(13)	196(6)
Mn2	0	5000	0	23.1(3)
N7	504(2)	5259.2(13)	1544(4)	35.0(9)
N5	267(3)	4403.9(13)	644(4)	39.4(10)
N6	993(2)	5053.8(14)	-1081(5)	40.2(10)
C16	753(3)	5447.4(16)	2455(5)	39.9(11)
C15	1088(4)	5515.2(19)	-1397(7)	55.0(15)
C17	1063(4)	5692(2)	3548(6)	60.4(17)
C11	-284(4)	4301.7(19)	1776(6)	50.9(14)
C14	1724(3)	4863(2)	-534(7)	54.5(15)
C12	1091(4)	4302(2)	971(6)	54.8(15)
C13	1627(4)	4396(2)	-211(7)	58.2(16)

Table 2. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Mncyclam. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+...]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl3	157(2)	40.9(9)	68.0(12)	7.4(8)	-63.3(13)	-13.7(10)
O9	171(8)	209(9)	51(4)	47(5)	-1(4)	-12(6)
O8	380(16)	80(5)	193(9)	56(6)	154(11)	50(8)
O10	123(5)	65(3)	81(4)	12(3)	1(4)	11(3)
O11	94(4)	124(6)	112(5)	-11(4)	-37(4)	-18(4)
O12	124(6)	78(4)	202(9)	-49(5)	-26(6)	12(4)
Mn1	12.9(5)	23.9(5)	15.4(5)	0	0.1(3)	0
Cl1	44.7(7)	39.7(7)	46.0(7)	-0.4(5)	8.3(6)	-7.7(5)
Cl2	45.7(7)	33.7(6)	41.8(7)	-1.1(5)	-1.1(5)	4.5(5)
N4	22(3)	34(3)	29(3)	0	2(2)	0
N3	22(3)	39(3)	24(3)	0	-1(2)	0
N2	27.3(19)	40(2)	34(2)	-13.0(18)	-0.1(16)	0.2(16)
C9	29(4)	36(3)	24(3)	0	0(3)	0
C7	23(3)	43(4)	28(3)	0	-2(3)	0
N1	27.9(19)	36(2)	33(2)	7.0(17)	4.2(16)	-1.6(15)
C1	29(4)	98(7)	24(4)	0	-1(3)	0
C2	30(2)	72(4)	32(3)	-20(3)	-2(2)	-3(2)
C5	31(3)	62(3)	28(2)	16(2)	-1(2)	6(2)
C8	23(3)	75(6)	48(4)	0	9(3)	0
C6	25(3)	69(5)	28(3)	0	-2(3)	0
C4	49(3)	31(3)	59(4)	10(2)	7(3)	7(2)
C3	44(3)	36(3)	59(4)	-9(2)	2(3)	-6(2)
C10	28(3)	61(5)	42(4)	0	-6(3)	0
O2	48(3)	142(6)	111(5)	17(4)	2(3)	-21(3)
O3	196(12)	550(30)	490(30)	480(30)	189(15)	221(16)
O7	109(5)	236(11)	103(6)	-45(6)	-57(4)	64(6)
O1	172(9)	326(15)	223(11)	-200(12)	138(8)	-131(10)
O5	51(3)	306(12)	91(5)	17(6)	0(3)	-33(5)
O6	109(6)	275(13)	243(12)	-169(11)	100(7)	-80(8)
O4	90(5)	163(8)	336(14)	-169(9)	108(7)	-72(5)
Mn2	26.8(5)	23.7(5)	18.8(5)	0.3(3)	0.1(3)	-4.3(3)
N7	41(2)	36(2)	28(2)	-1.2(17)	-6.0(17)	-3.7(17)
N5	60(3)	30(2)	28(2)	1.4(17)	-2.1(19)	0.0(19)
N6	36(2)	48(3)	37(2)	-3.7(19)	5.6(19)	-8.9(18)
C16	44(3)	35(3)	40(3)	6(2)	-11(2)	-3(2)
C15	63(4)	45(3)	57(3)	0(3)	13(3)	-23(3)
C17	85(4)	48(3)	49(3)	-6(3)	-31(3)	-7(3)
C11	77(4)	37(3)	38(3)	7(2)	14(3)	-4(3)
C14	31(3)	67(4)	65(4)	-10(3)	5(3)	3(3)
C12	75(4)	46(3)	43(3)	-5(3)	-18(3)	21(3)
C13	44(3)	63(4)	67(4)	-1(3)	-3(3)	15(3)

Table 3. DFT Calculated Coordinates of 9-(4-hydroxyphenyl amino)-1-oxo phenalenone in neutral state (Singlet)

C	3.856601	1.810862	0.245346
C	2.750856	2.594673	0.253650
C	1.408938	2.040475	0.115139
C	1.297789	0.584450	-0.012498
C	3.769351	0.380410	0.100887
C	0.021612	-0.047566	-0.120146
C	-0.037714	-1.468787	-0.296185
C	1.102418	-2.220244	-0.322298
C	2.394489	-1.634786	-0.175754
C	3.570975	-2.410629	-0.187220
C	4.817765	-1.816608	-0.055813
C	4.909984	-0.427589	0.087716
C	2.476661	-0.217031	-0.029582
O	0.413221	2.808180	0.105002
N	-1.097594	0.719282	-0.091485
C	-2.448276	0.308629	-0.038016
C	-3.387967	0.988005	-0.829774
C	-4.738732	0.668968	-0.768826
C	-5.178479	-0.350538	0.083081
C	-4.253336	-1.028102	0.882860
C	-2.901726	-0.691503	0.832659
O	-6.515791	-0.631709	0.092808
H	4.844671	2.254716	0.345985
H	2.809954	3.673245	0.356714
H	-1.003052	-1.939156	-0.435098
H	1.032595	-3.295211	-0.469366
H	3.486774	-3.488317	-0.301705
H	5.717597	-2.423260	-0.064994
H	5.885191	0.041620	0.190954

H	-0.869302	1.729094	-0.056407
H	-3.045601	1.769957	-1.500739
H	-5.465544	1.193021	-1.380041
H	-4.589445	-1.807083	1.563844
H	-2.200642	-1.193543	1.490576
H	-6.686726	-1.340350	0.726833

Table 4. DFT Calculated Coordinates of 9-(4-hydroxyphenyl amino)-1-oxo phenalenone in anionic state (singlate)

C	3.773650	1.859783	0.272118
C	2.636679	2.611482	0.243978
C	1.320428	2.029235	0.060551
C	1.253661	0.580855	-0.048782
C	3.730075	0.436507	0.132595
C	-0.019053	-0.095000	-0.163409
C	-0.027478	-1.517480	-0.357281
C	1.129759	-2.236504	-0.365795
C	2.409173	-1.617834	-0.171195
C	3.598063	-2.360427	-0.148533
C	4.836882	-1.734499	0.013617
C	4.895658	-0.351947	0.152217
C	2.450313	-0.191548	-0.028055
O	0.296701	2.778148	-0.000778
N	-1.154082	0.632756	-0.125511
C	-2.495294	0.244216	-0.029569
C	-3.473475	1.106385	-0.584636
C	-4.815273	0.807863	-0.525486
C	-5.323940	-0.395533	0.116026

C	-4.288734	-1.223532	0.715990
C	-2.947075	-0.915681	0.647263
O	-6.546413	-0.681554	0.168186
H	4.744976	2.335406	0.399602
H	2.665537	3.692970	0.342721
H	-0.976063	-2.006370	-0.540375
H	1.096655	-3.309073	-0.544597
H	3.542382	-3.441001	-0.261600
H	5.748784	-2.325294	0.029664
H	5.856236	0.143705	0.278148
H	-0.931898	1.649726	-0.123339
H	-3.135446	2.012059	-1.087114
H	-5.550082	1.475858	-0.968327
H	-4.621991	-2.103594	1.260939
H	-2.226940	-1.544482	1.163913

Table 5. Optimized coordinates of [(dpaq)Mn^{IV}(O)]$^{+}$ in quartet ground state.

Mn	4.371392000	5.062420000	1.711129000
O	6.129678000	5.792313000	5.356392000
O	3.890099000	5.235624000	0.104828000
N	3.469668000	3.322388000	2.079343000
N	4.918716000	4.808602000	3.629567000
N	5.445234000	6.779403000	1.853502000
N	2.893122000	6.286526000	2.371747000
N	6.184255000	4.326830000	1.170894000
C	2.741050000	2.632006000	1.205098000
H	2.643714000	3.073353000	0.216742000
C	2.138306000	1.406870000	1.548826000

H	1.552347000	0.877173000	0.802821000
C	2.304400000	0.902689000	2.827756000
H	1.847219000	-0.042871000	3.113373000
C	3.076883000	1.619002000	3.781142000
C	3.306888000	1.188470000	5.116546000
H	2.873425000	0.250451000	5.456479000
C	4.078170000	1.969844000	5.960743000
H	4.254953000	1.641550000	6.983387000
C	4.652343000	3.194415000	5.538363000
H	5.251557000	3.782971000	6.224660000
C	4.450642000	3.652053000	4.235165000
C	3.654499000	2.850043000	3.358129000
C	5.686957000	5.753661000	4.198169000
C	6.026543000	6.904176000	3.244571000
H	7.116482000	6.977094000	3.168218000
H	5.674061000	7.838566000	3.693688000
C	4.487533000	7.885170000	1.551006000
H	4.313874000	7.878394000	0.469089000
H	4.908309000	8.855916000	1.834489000
C	3.187884000	7.600113000	2.246182000
C	2.307551000	8.585742000	2.688914000
H	2.577645000	9.633558000	2.586639000
C	1.089651000	8.200793000	3.256313000
H	0.385826000	8.951838000	3.607159000
C	0.794732000	6.839746000	3.371531000
H	-0.138455000	6.494001000	3.807611000
C	1.728432000	5.908812000	2.922902000
H	1.545263000	4.842171000	3.002662000
C	6.512124000	6.679963000	0.812823000

H	6.036316000	6.854772000	-0.158715000
H	7.283973000	7.441274000	0.969453000
C	7.072015000	5.287108000	0.827488000
C	8.380195000	4.968926000	0.466933000
H	9.075370000	5.763379000	0.208077000
C	8.769096000	3.626657000	0.444589000
H	9.783784000	3.353933000	0.164144000
C	7.838244000	2.644446000	0.793183000
H	8.096097000	1.588969000	0.791205000
C	6.552668000	3.035654000	1.159182000
H	5.801272000	2.307448000	1.446584000

Table 6. Optimized coordinates of [(dpaq)Mn^{III}(OH)]$^{+}$ (1) in triplet ground state.

Mn	0.183765000	0.012825000	-0.249550000
O	1.343795000	-0.042483000	-4.144816000
O	0.276832000	0.066803000	1.586863000
N	-1.802093000	0.021408000	-0.423535000
N	0.066345000	-0.006429000	-2.202519000
N	2.188795000	0.006901000	-0.555891000
N	0.425132000	-1.999663000	-0.262821000
N	0.446267000	2.023937000	-0.276165000
C	-2.696601000	0.048269000	0.560859000
H	-2.295248000	0.075024000	1.570500000
C	-4.086233000	0.044827000	0.314996000
H	-4.770028000	0.067062000	1.159591000
C	-4.551243000	0.012936000	-0.986657000
H	-5.618548000	0.008622000	-1.199376000
C	-3.620874000	-0.012965000	-2.061800000
C	-3.981946000	-0.043646000	-3.437340000
H	-5.034937000	-0.050115000	-3.711577000

C	-2.991749000	-0.064242000	-4.404834000
H	-3.269055000	-0.087777000	-5.457303000
C	-1.614088000	-0.054530000	-4.071661000
H	-0.862314000	-0.069256000	-4.852763000
C	-1.221720000	-0.024894000	-2.733703000
C	-2.237287000	-0.006135000	-1.727957000
C	1.214275000	-0.014826000	-2.912246000
C	2.464576000	0.031333000	-2.035757000
H	3.017197000	0.943967000	-2.284946000
H	3.109151000	-0.813064000	-2.302485000
C	2.695507000	-1.241750000	0.082165000
H	2.738373000	-1.061804000	1.162534000
H	3.705438000	-1.488849000	-0.264459000
C	1.726272000	-2.365995000	-0.175384000
C	2.113085000	-3.703081000	-0.264009000
H	3.166240000	-3.965555000	-0.202500000
C	1.130898000	-4.683498000	-0.430992000
H	1.409396000	-5.732490000	-0.502666000
C	-0.209553000	-4.295521000	-0.510585000
H	-1.005718000	-5.023418000	-0.641277000
C	-0.520225000	-2.940304000	-0.427795000
H	-1.545893000	-2.590353000	-0.493168000
C	2.696964000	1.235743000	0.120463000
H	2.704472000	1.033742000	1.197317000
H	3.718536000	1.475093000	-0.196572000
C	1.746824000	2.374563000	-0.143984000
C	2.150114000	3.708809000	-0.203333000
H	3.203383000	3.959729000	-0.106255000
C	1.183636000	4.701227000	-0.389513000
H	1.474601000	5.748093000	-0.439891000

C	-0.157303000	4.328045000	-0.517810000
H	-0.941253000	5.065782000	-0.666343000
C	-0.483621000	2.975022000	-0.460346000
H	-1.510053000	2.636312000	-0.563198000
H	0.190572000	-0.807511000	1.995007000

APPENDIX II

LIST OF PUBLICATION(S)

1. Amritaa Mitra, Anand Pariyar, Suranjana Bose, Pinaki Bandyopadhyay, Arindam Sarkar,. "*First phenalenone based receptor for selective iodide ion sensing*", Sensors and Actuators B 210 (2015) 712–718, doi.org/10.1016/j.snb.2015.01.032.

2. Amritaa Mitra, Suranjana Bose, Sachidulal Biswas, Pinaki Bandyopadhyay and Arindam Sarkar, "*Phenalenone based colorimetric pH indicators and fluorometric pH sensors for alkaline solution" communicated*.

3. Amritaa Mitra, Sachidulal Biswas, Achintesh N. Biswas, Pinaki Bandyopadhyay, "*Manganese (IV)-oxo Compound of Non-heme Anionic Ligand: Generation, Characterisation and Reactivity towards Weak C-H Bonds*", manuscript under preparation.

APPENDIX-III

LIST OF SEMINAR AND SYMPOSIUM ATTENDED

1. Presented the work "*Manganese (IV)-oxo Compound of Non-heme Anionic Ligand: Generation, Characterisation and Reactivity towards Weak C-H Bonds*" in **5th Symposium on Advanced Biological Inorganic Chemistry** held Kolkata, 2017.

2. Presented the work "*Phenalenone based colorimetric and fluorimetric pH sensor for alkaline solution*" in **19th CRSI National Symposium in Chemistry (NSC-19)** held at University of North Bengal, Siliguri, 2016.

3. Presented the work "*Nonheme Diiron (III) Complexes As Bio-Inspered Fnctional Models Of Methane Monooxygenase: Synthesis, Structure And Reactivity*" in **16th Symposium on Modern Trends in Inorganic Chemistry** held at Jadavpur University, Kolkata, 2015.

4. Presented the work "*The First Phenalenone Based Receptor for Selective Iodide Ion Sensing*" in **16th CRSI (Chemical Research Society of India) National Symposium in Chemistry**, held in Indian Institute of Technology Bombay, Mumbai, Maharashtra, 2014.

5. Presented the work "*Ligand Non-Innocent Behaviour of Cu(II)-Dipyrromethene Complex in Redox Reactions and Its Use as an Oxidation Catalyst: C-H Activation at Room Temperature*" in **15th CRSI (Chemical Research Society of India) National Symposium in Chemistry** held in Benaras Hindu University, Varanasi, India, 2013.

LIST OF ORAL PRESENTATIONS

1. **Seminar on Frontiers in Chemistry** 2015 (March, 2015) held in Department of Chemistry, University of North Bengal, Darjeeling.

LIST OF WORKSHOP ATTENDED

1. "**Winter school on Computational Chemistry**". During December 29, 2014 to January 10, 2015 held at School of Chemistry, University of Hyderabad.
2. "**Workshop on Mass and NMR Technique**" from January 28-29, 2013 at SAIF CDRI Lucknow.

SPECIAL ACHIEVEMENT

1. Received '***Financial Support***' to participate in the 7th CRSI-RSC symposium held at Banaras Hindu University, Varanasi, India, 2013.