

Exploration of catecholase-like activity of a series of magnetically coupled transition metal complexes of Mn, Co and Ni: new insights into solution state behavior of Mn complex

Abani Sarkar,^a Aratrika Chakraborty,^a Amit Adhikary,^a Suwendu Maity,^b Arnab Mandal,^a Debabrata Samanta,^c Prasanta Ghosh,^b and Debasis Das*^a

^aDepartment of Chemistry, University College of Science, University of Calcutta, 92 A. P. C. Road, Kolkata 700009, India

^bDepartment of Chemistry, R. K. Mission Residential College, Narendrapur, Kolkata 700 103, India

^cDepartment of Chemistry, Indian Institute of Technology, Kanpur, Kanpur-208016, India

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1. FT-IR plot

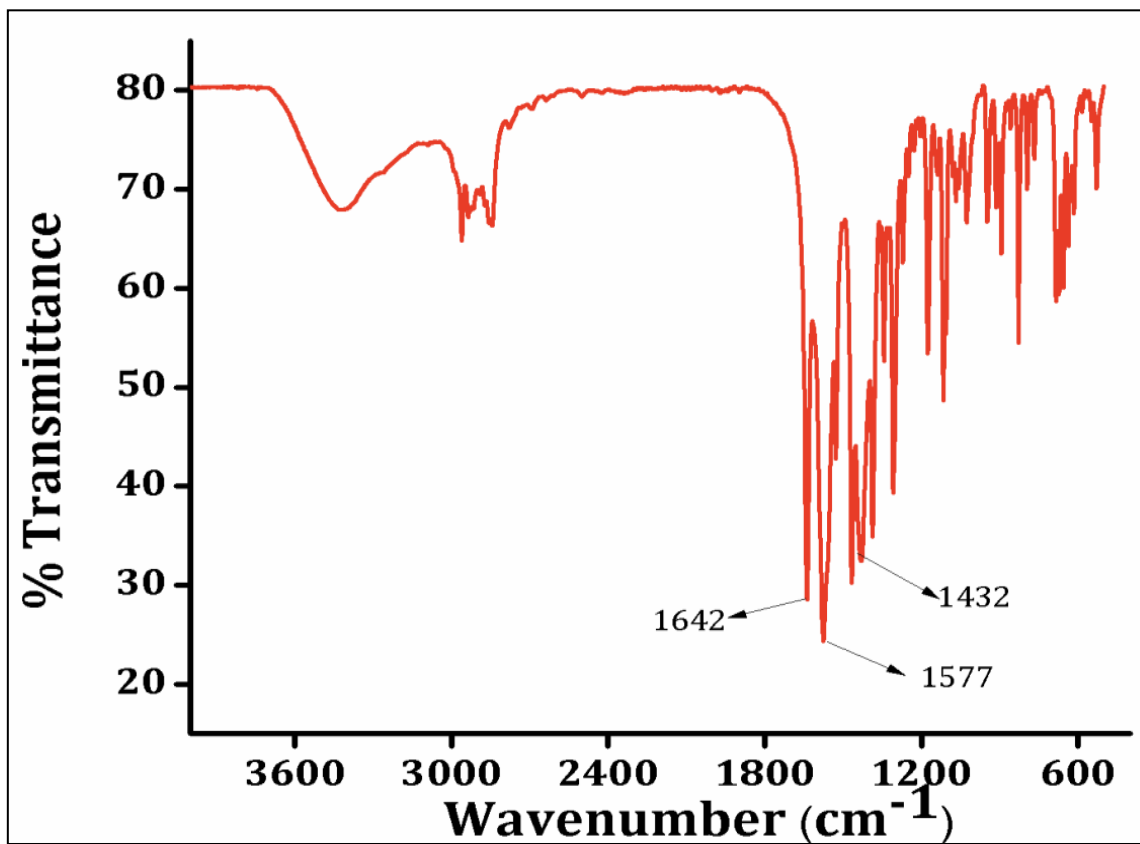


Fig. S1 FT-IR spectrum of complex 1.

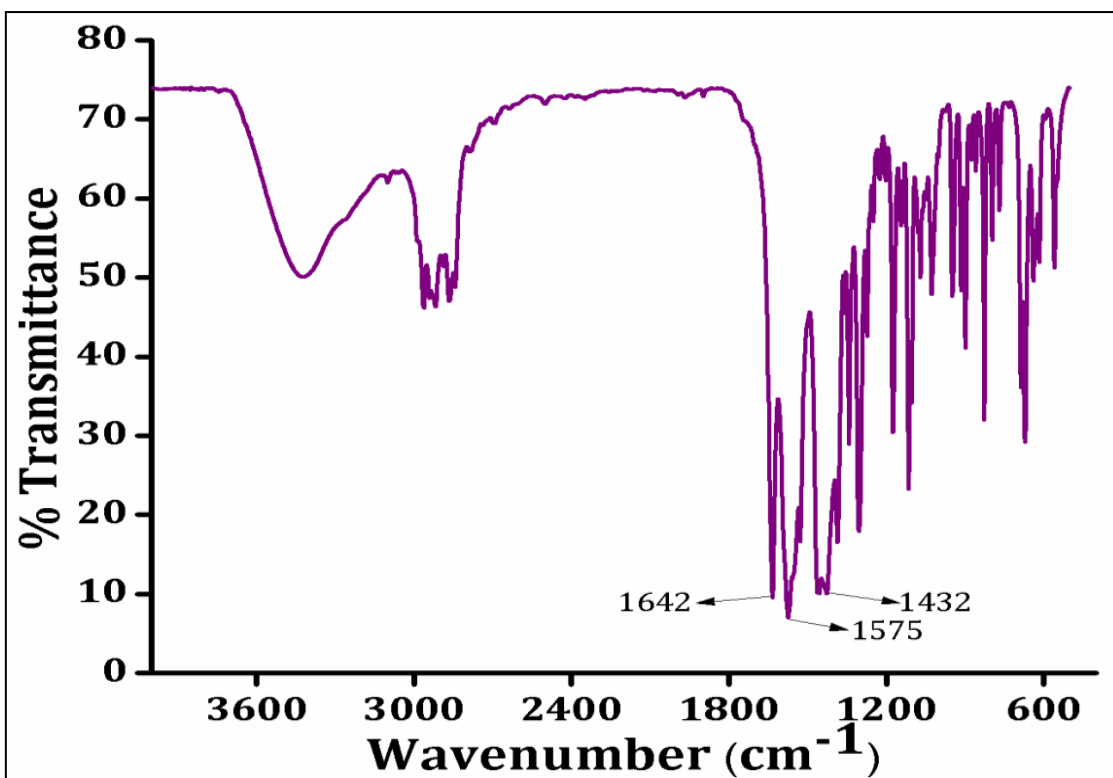


Fig. S2 FT-IR spectrum of complex 2.

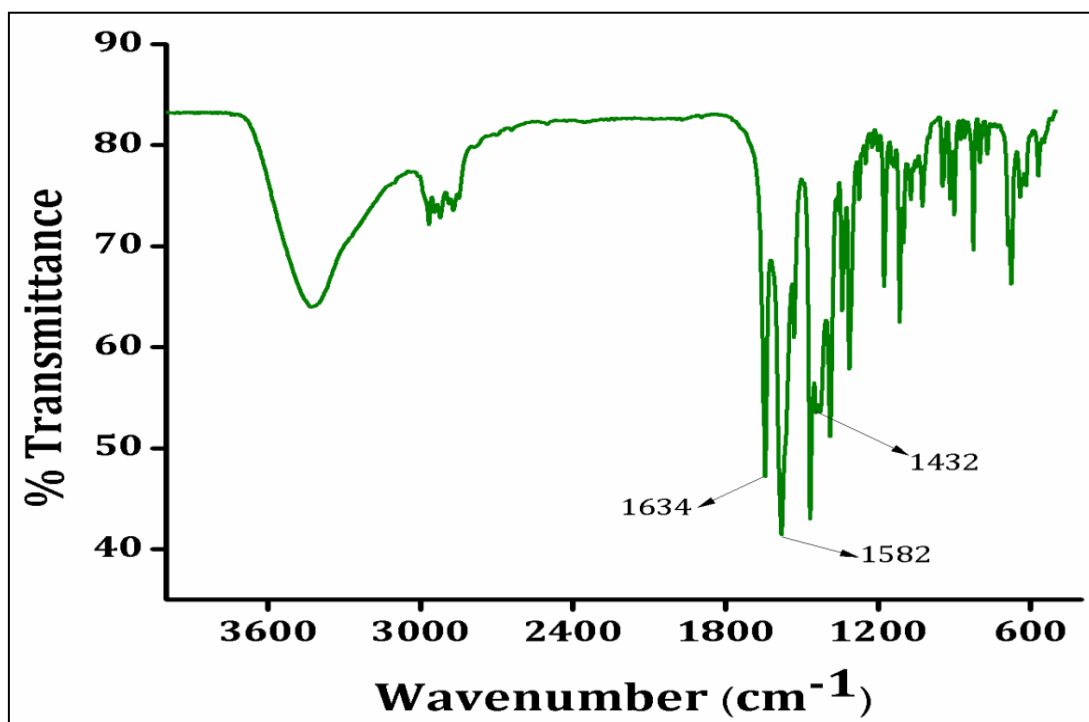


Fig. S3 FT-IR spectrum of complex 3.

2. UV-Vis spectral study

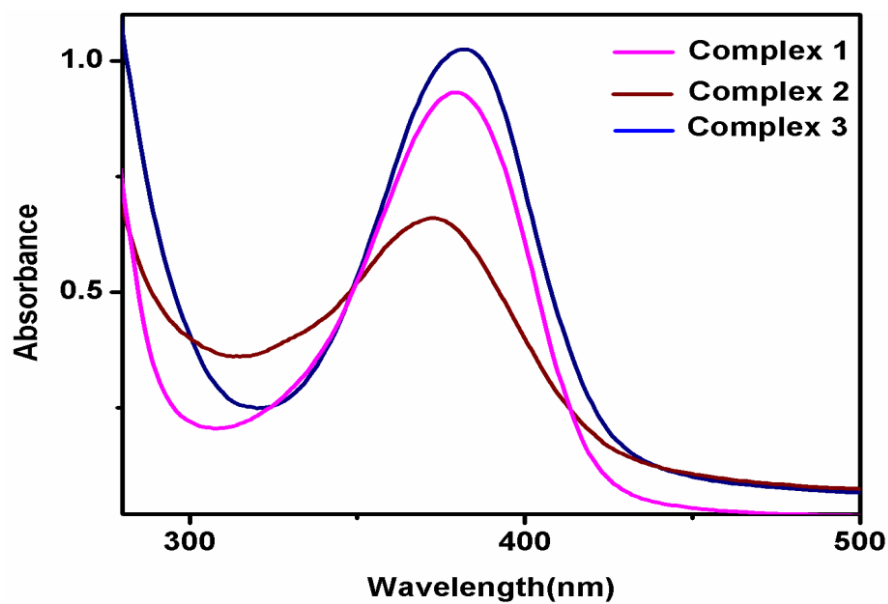


Fig. S4 UV-Vis spectra of complex 1 complex 2 and complex 3.

3. ESI-MS mass spectra study

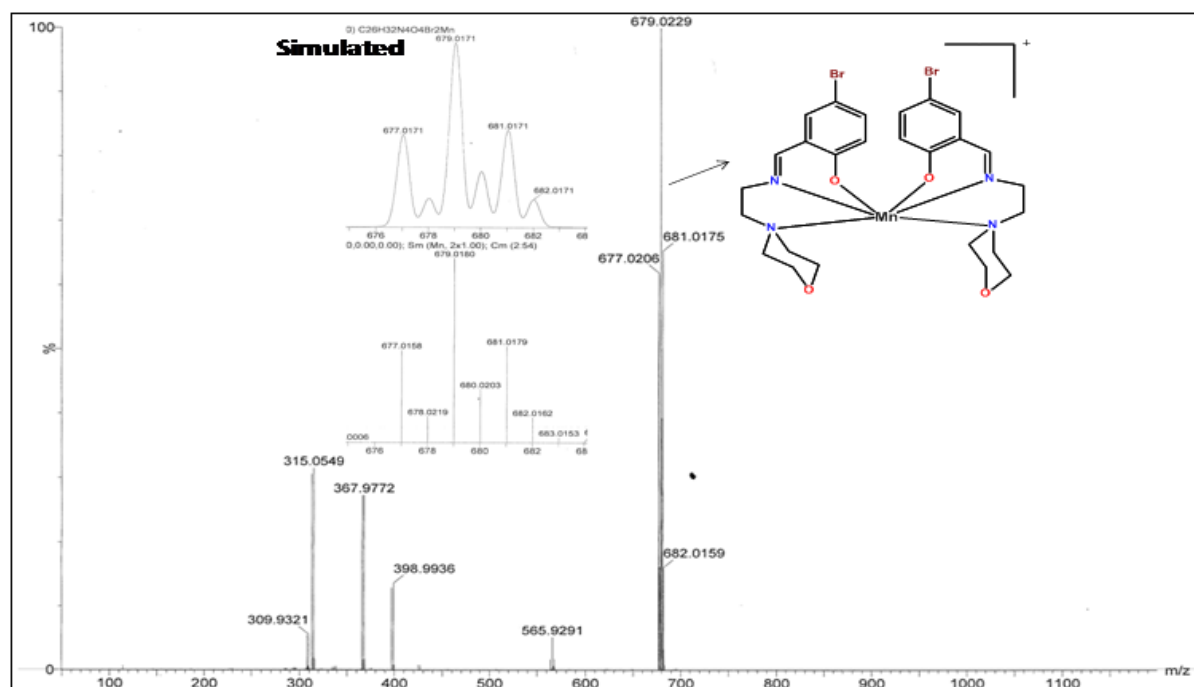


Fig. S5 ESI-MS spectra of complex 1

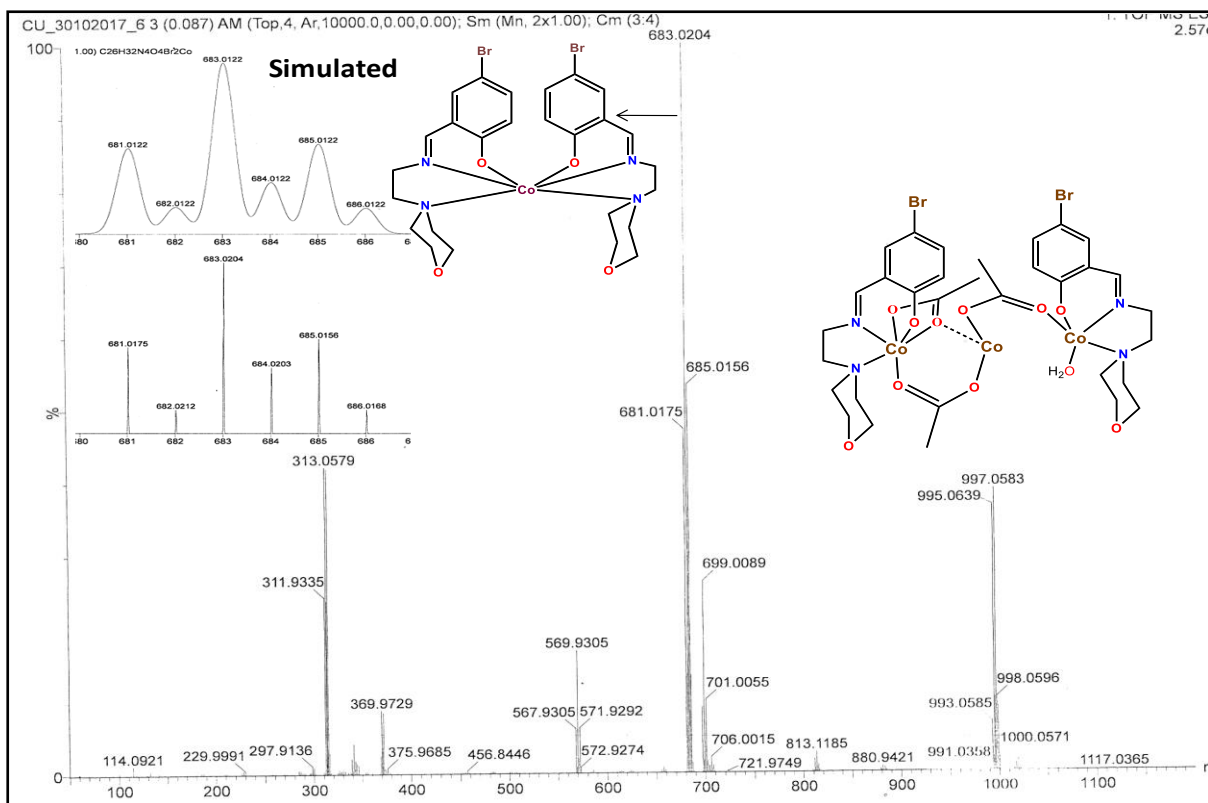


Fig. S6 ESI-MS spectra of complex 2.

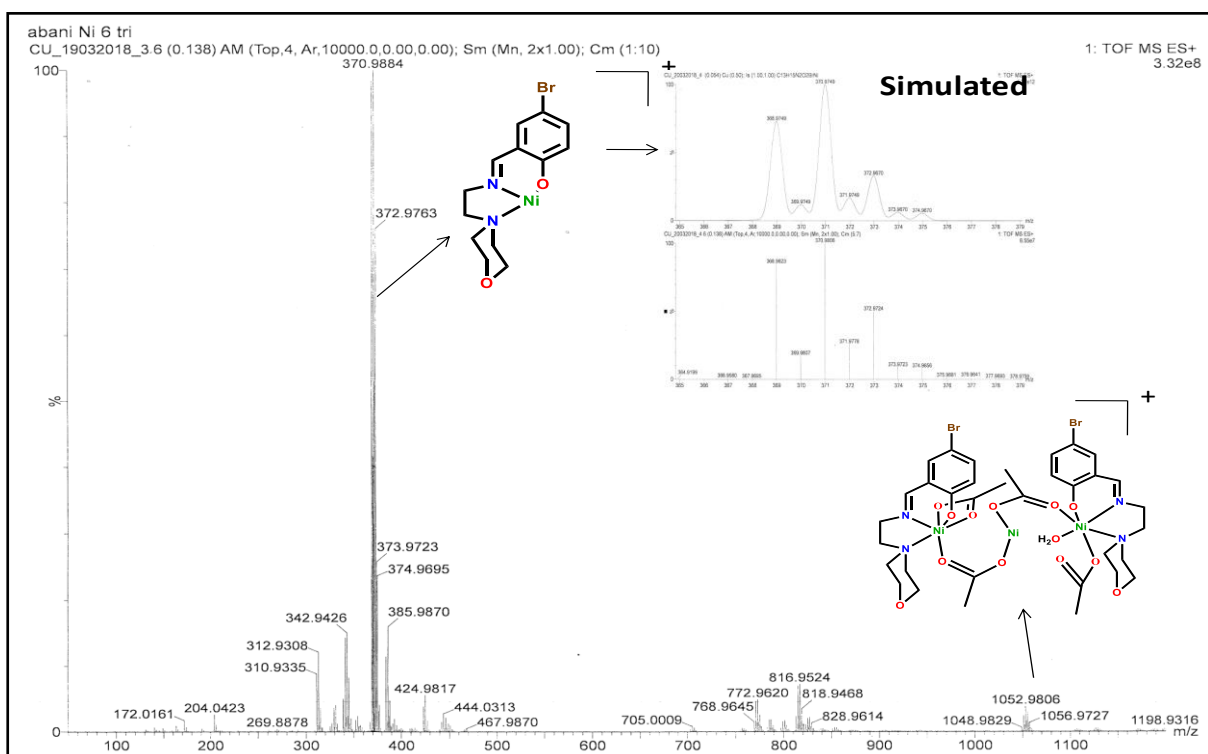


Fig. S7 ESI-MS spectra of complex 3.

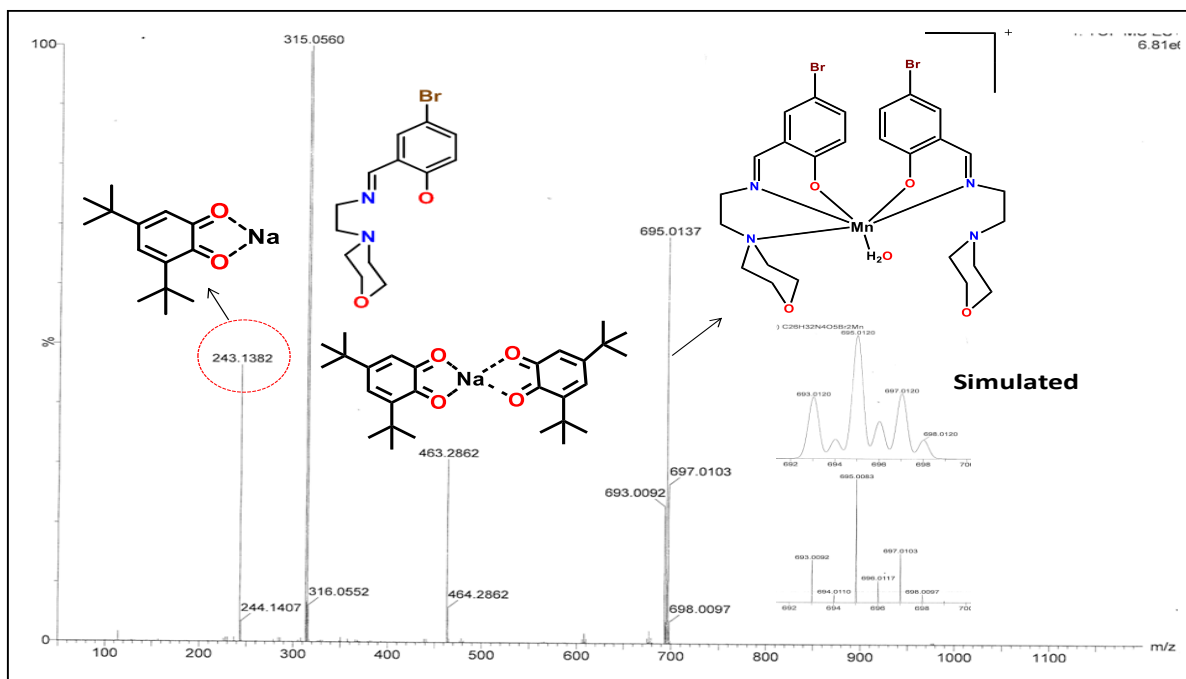


Fig. S9 ESI-MS spectra of complex **1** in presence of 3,5 DTBC at time 30 minutes.

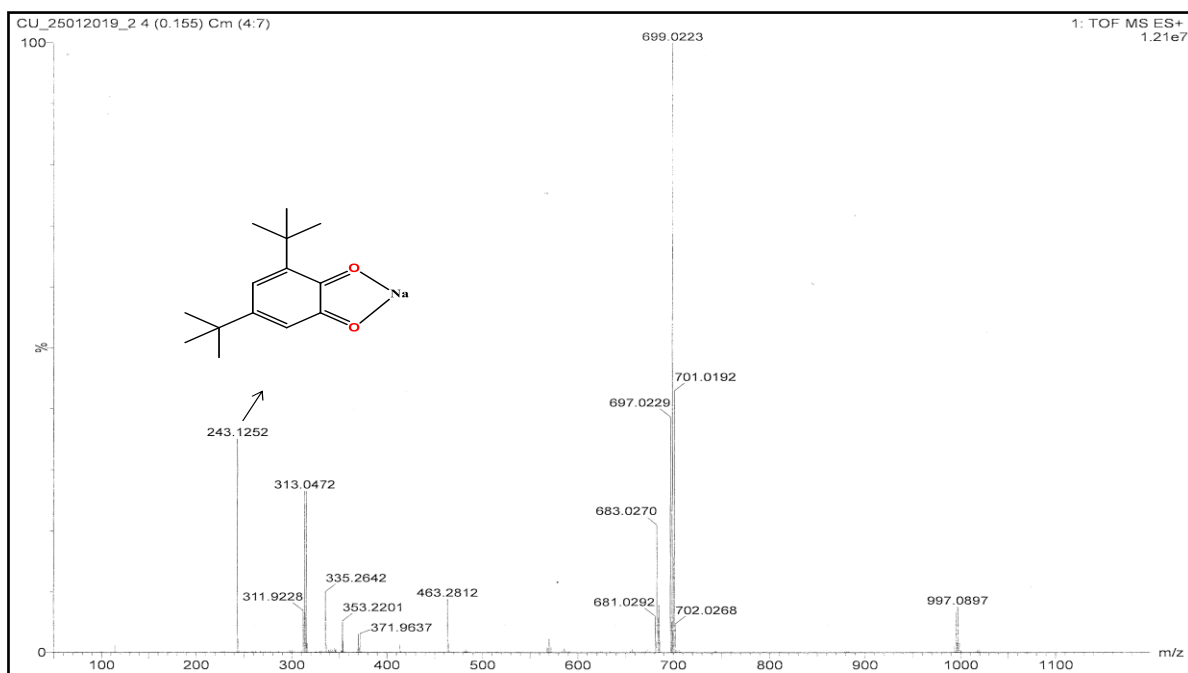


Fig. S10 ESI-MS spectra of complex **2** in presence of 3,5 DTBC at time 10 minutes.

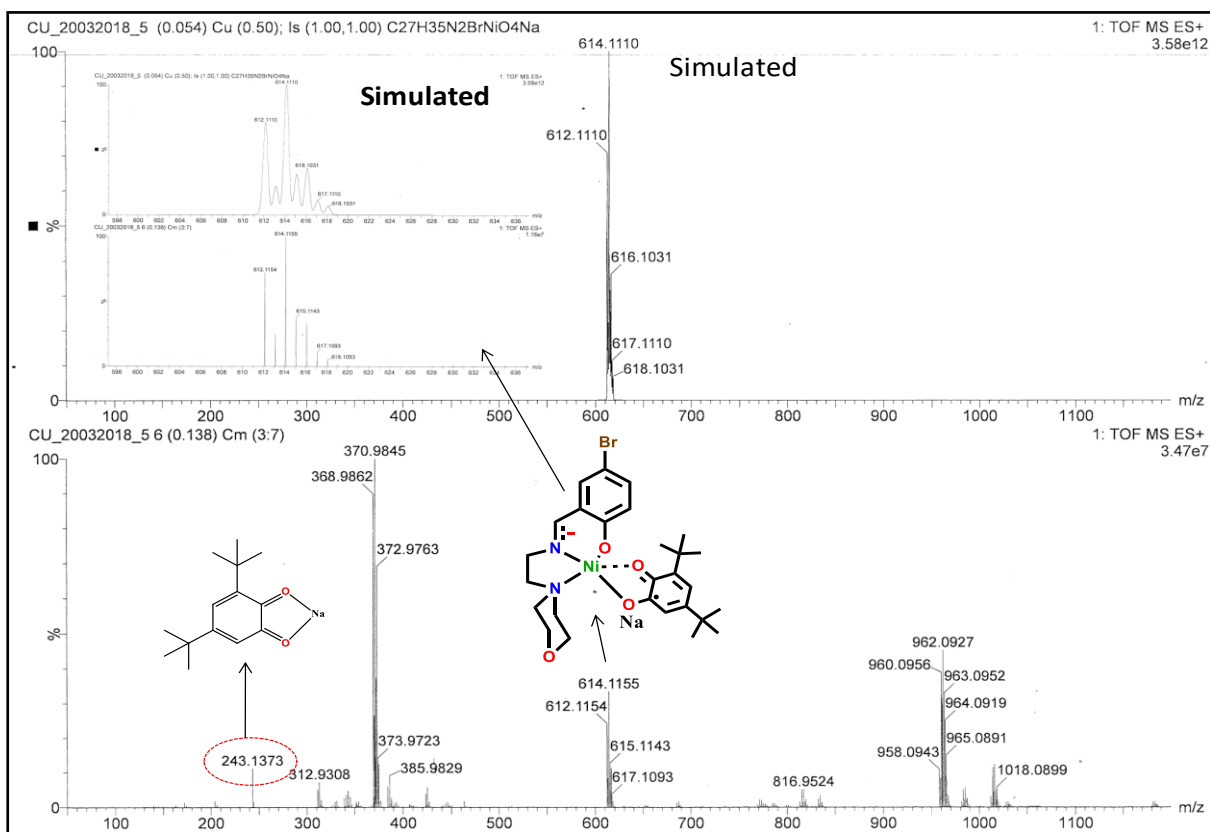


Fig. S11 ESI-MS spectra of complex **3** in presence of 3,5 DTBC at time 10 minutes.

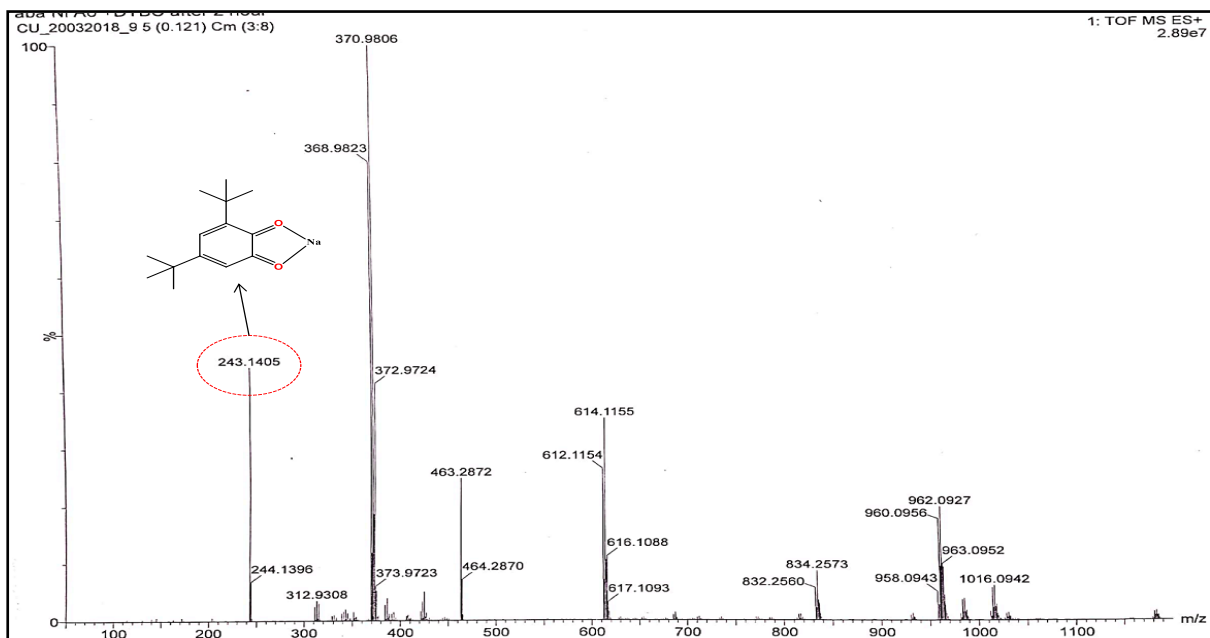


Fig. S12 ESI-MS spectra of complex **3** in presence of 3,5 DTBC at time 60 minutes.

Table 1 Crystallographic Data and Processing Parameters of Complexes **1-3**

	1	2	3
Formula	C ₃₄ H ₄₄ Br ₂ Mn ₃ N ₄ O ₁₂	C ₃₄ H ₄₄ Br ₂ Co ₃ N ₄ O ₁₂	C ₃₄ H ₄₂ Br ₂ N ₄ Ni ₃ O ₁₂
mol wt.	1025.35	1037.34	1034.59
cryst color	Light yellow	Brown	Green
cryst system	Monoclinic	Monoclinic	Monoclinic
space group	P2 _{1/n} (No. 14)	P2 _{1/c} (No. 14)	P2 _{1/c} (No. 4)
<i>a</i> (Å)	11.784(2)	11.4288(16)	11.1778(13)
<i>b</i> (Å)	9.5219(17)	9.4698(13)	9.5533(11)
<i>c</i> (Å)	19.786(4)	19.605(3)	19.611(2)
α (°)	90	90	90
β (°)	107.025(6)	105.643(3)	103.854(7)
γ (°)	90	90	90
<i>V</i> (Å ³)	2122.8(7)	2043.2(5)	2033.2(4)
<i>Z</i>	2	2	2
<i>T</i> (K)	296	291	300 K
ρ_{calcd} (g cm ⁻³)	1.604	1.686	1.693
Unique refl.	2153	2518	1800
reflection [<i>I</i> >2 σ (<i>I</i>)]	3635	3884	3571
μ (mm ⁻¹)	2.821	3.222	3.403
λ (Å)	0.71073	0.71073	0.71073
F(000)	1034	1046	1052
R ₁ ^a /GOF ^b	0.0678/1.04	0.0538/1.03	00.0832/1.041
wR ₂ ^c [<i>I</i> >2 σ (<i>I</i>)]	0.1661	0.1219	0.1773
residual density (eÅ ⁻³)	-0.35, 0.60	-0.47, 0.59	-0.61, 0.69
CCDC No.	1889042	1889043	1889359
^a R1 = $\Sigma F_o - F_c /\Sigma F_o $, ^b GOF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$. ^c wR2 = $\{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, $P = (F_o^2 + 2F_c^2)/3$			

5. Table S1. Selected bond length (Å) and bond angles (°) of Complex 1.

Mn(1)- O(4)	2.082(5)	O(1)-Mn(1)-N(1)	83.9(2)
Mn(1)- O(1)	2.130(4)	O(1)-Mn(1)-N(2)	161.83(18)
Mn(1)- N(1)	2.152(6)	O(2)-Mn(1)-O(3)	57.36(14)
Mn(1)- O(2)	2.266(4)	O(2)-Mn(1)-O(4)	93.00(18)
Mn(1)- O(3)	2.298(5)	O(2)-Mn(1)-N(1)	157.19(19)
Mn(1)- N(2)	2.365(6)	O(2)-Mn(1)-N(2)	115.30(19)
Mn(2)- O(5)	2.126(5)	O(3)-Mn(1)-O(4)	146.36(18)
Mn(2)- O(5)	2.126(5)	O(3)-Mn(1)-N(1)	108.84(19)
Mn(2)- O(2)	2.179(4)	O(3)-Mn(1)-N(2)	85.73(19)
Mn(2)- O(2)	2.179(4)	O(4)-Mn(1)-N(1)	104.2(2)
Mn(2)- O(1)	2.206(4)	O(4)-Mn(1)-N(2)	94.7(2)
Mn(2)- O(1)	2.206(4)	N(1)-Mn(1)-N(2)	78.6(2)
O(1)- C(1)	1.310(7)	O(1)-Mn(2)-O(2)	80.20(16)
C(2)- C(1)	1.395(8)	O(1)-Mn(2)-O(5)	88.99(15)
C(4)- C(5)	1.347(10)	O(1)-Mn(2)-O(1a)	180.00
C(4)- C(3)	1.374(10)	O(1)-Mn(2)-O(2a)	99.80(16)
C(3)- C(2)	1.372(8)	O(1)-Mn(2)-O(5a)	91.01(15)
C(1)- C(6)	1.414(9)	O(2)-Mn(2)-O(5)	90.65(16)
C(6)- C(5)	1.418(9)	O(1a)-Mn(2)-O(2)	99.80(16)
C(6)- C(7)	1.427(9)	O(2)-Mn(2)-O(2a)	180.00
C(7)- N(1)	1.260(9)	O(2)-Mn(2)-O(5a)	89.35(16)
N(1)- C(8)	1.461(9)	O(1a)-Mn(2)-O(5)	91.01(15)
C(8)- C(9)	1.465(12)	O(2a)-Mn(2)-O(5)	89.35(16)
C(1)- C(6)	1.414(9)	O(5)-Mn(2)-O(5a)	180.00
O(1)-Mn(1)-O(2)	79.94(16)	O(1a)-Mn(2)-O(2a)	80.20(16)
O(1)-Mn(1)-O(3)	95.45(16)	O(1a)-Mn(2)-O(5a)	88.99(15)
O(1)-Mn(1)-O(4)	94.24(18)	O(2a)-Mn(2)-O(5a)	90.65(16)

Table. S2 Selected bond length (Å) and bond angles (°) of Complex **2**.

Co(1)- O(3)	2.041(4)	O(3)-Co(1)-O(4a)	90.71(14)
Co(2)- O(2)	2.017(4)	O(1a)-Co(1)-O(4)	99.68(13)
Co(1)- O(1)	2.086(3)	O(3a)-Co(1)-O(4)	90.71(14)
Co(1)- O(4)	2.159(3)	O(4)-Co(1)-O(4a)	180.00
Co(2)-N(1)	2.018(4)	O(1a)-Co(1)-O(3a)	91.38(14)
Co(2)- O(1)	2.044(4)	O(1a)-Co(1)-O(4a)	80.32(13)
Co(2)- O(4)	2.184(4)	O(3a)-Co(1)-O(4a)	89.29(14)
Co(2)- O(5)	2.186(4)	O(1)-Co(2)-O(2)	94.30(15)
Co(2)- N(2)	2.304(4)	O(1)-Co(2)-O(4)	80.62(14)
N(1)- C(8)	1.469(7)	O(1)-Co(2)-O(5)	94.01(16)
O(1)- C(1)	1.301(6)	O(1)-Co(2)-N(1)	88.94(17)
C(1)-C(2)	1.395(7)	O(1)-Co(2)-N(2)	169.46(14)
C(1)- C(6)	1.416(7)	O(2)-Co(2)-O(4)	94.22(15)
C(2)- C(3)	1.369(7)	O(2)-Co(2)-O(5)	150.90(15)
C(3)- C(4)	1.377(8)	O(2)-Co(2)-N(1)	101.11(17)
C(5)- C(4)	1.357(8)	O(2)-Co(2)-N(2)	91.13(15)
C(6)- C(5)	1.402(7)	O(2)-Co(2)-C(14)	123.80(17)
C(6)- C(7)	1.445(8)	O(4)-Co(2)-O(5)	59.82(13)
N(1)- C(7)	1.276(7)	O(4)-Co(2)-N(1)	162.07(16)
N(2)- C(9)	1.475(7)	O(4)-Co(2)-N(2)	108.02(15)
O(1)-Co(1)-O(3)	91.38(14)	O(4)-Co(2)-C(14)	30.26(16)
O(1)-Co(1)-O(4)	80.32(13)	O(5)-Co(2)-N(1)	106.89(16)
O(1)-Co(1)-O(1a)	180.00	O(5)-Co(2)-N(2)	85.54(17)
O(1)-Co(1)-O(3a)	88.62(14)	O(5)-Co(2)-C(14)	29.62(16)
O(1)-Co(1)-O(4a)	99.68(13)	N(1)-Co(2)-N(2)	81.14(17)
O(3)-Co(1)-O(4)	89.29(14)	N(1)-Co(2)-C(14)	135.03(18)
O(1a)-Co(1)-O(3)	88.62(14)	N(2)-Co(2)-C(14)	98.76(18)
O(3)-Co(1)-O(3a)	180.00		

Table. S3 Selected bond length (Å) and bond angles (°) of Complex **3**.

Ni(1)-O(1)	2.0212(2)	O(3)-Ni(1)-N(1)	99.08(1)
Ni(1)-O(3)	2.0010(2)	O(3)-Ni(1)-N(2)	91.99(1)
Ni(1)-O(4)	2.2184(3)	O(4)-Ni(1)-O(5)	61.20(1)
Ni(1)-O(5)	2.1294(2)	O(4)-Ni(1)-N(1)	104.33(1)
Ni(1)-N(1)	1.9869(2)	O(4)-Ni(1)-N(2)	88.47(1)
Ni(1)-N(2)	2.2050(3)	O(5)-Ni(1)-N(1)	162.31(1)
Ni(2)-O(1)	2.0775(2)	O(5)-Ni(1)-N(2)	105.36(1)
Ni(2)-O(2)	2.0103(2)	N(1)-Ni(1)-N(2)	83.12(1)
Ni(2)-O(5)	2.1248(2)	O(1)-Ni(2)-O(2)	91.34(1)
Ni(2)-O(1_a)	2.0775(2)	O(1)-Ni(2)-O(5)	80.59(1)
Ni(2)-O(2_a)	2.0103(2)	O(1)-Ni(2)-O(1_a)	180.00
Ni(2)-O(5_a)	2.1248(2)	O(1)-Ni(2)-O(2_a)	88.66(1)
O(1)-C(1)	1.2918(2)	O(1)-Ni(2)-O(5_a)	99.41(1)
O(2)-C(16)	1.2638(1)	O(2)-Ni(2)-O(5)	89.33(1)
O(3)-C(16)	1.2644(1)	O(1_a)-Ni(2)-O(2)	88.66(1)
O(4)-C(14)	1.2712(1)	O(2)-Ni(2)-O(2_a)	180.00
O(5)-C(14)	1.2880(1)	O(2)-Ni(2)-O(5_a)	90.67(1)
O(11)-C(11)	1.4038(2)	O(1_a)-Ni(2)-O(5)	99.41(1)
O(11)-C(12)	1.4377(2)	O(2_a)-Ni(2)-O(5)	90.67(1)
N(1)-C(7)	1.2720(1)	O(5)-Ni(2)-O(5_a)	180.00
N(1)-C(8)	1.4659(2)	O(1_a)-Ni(2)-O(2_a)	91.34(1)
N(2)-C(9)	1.4963(2)	O(1_a)-Ni(2)-O(5_a)	80.59(1)
N(2)-C(10)	1.4909(2)	O(2_a)-Ni(2)-O(5_a)	89.33(1)
N(2)-C(13)	1.4971(2)	O(1)-Ni(1)-N(1)	88.89(1)
O(1)-Ni(1)-O(3)	91.40(1)	O(1)-Ni(1)-N(2)	171.72(1)
O(1)-Ni(1)-O(4)	91.43(1)	O(3)-Ni(1)-O(4)	156.46(1)
O(1)-Ni(1)-O(5)	81.77(1)	O(3)-Ni(1)-O(5)	96.15(1)

6. PXRD

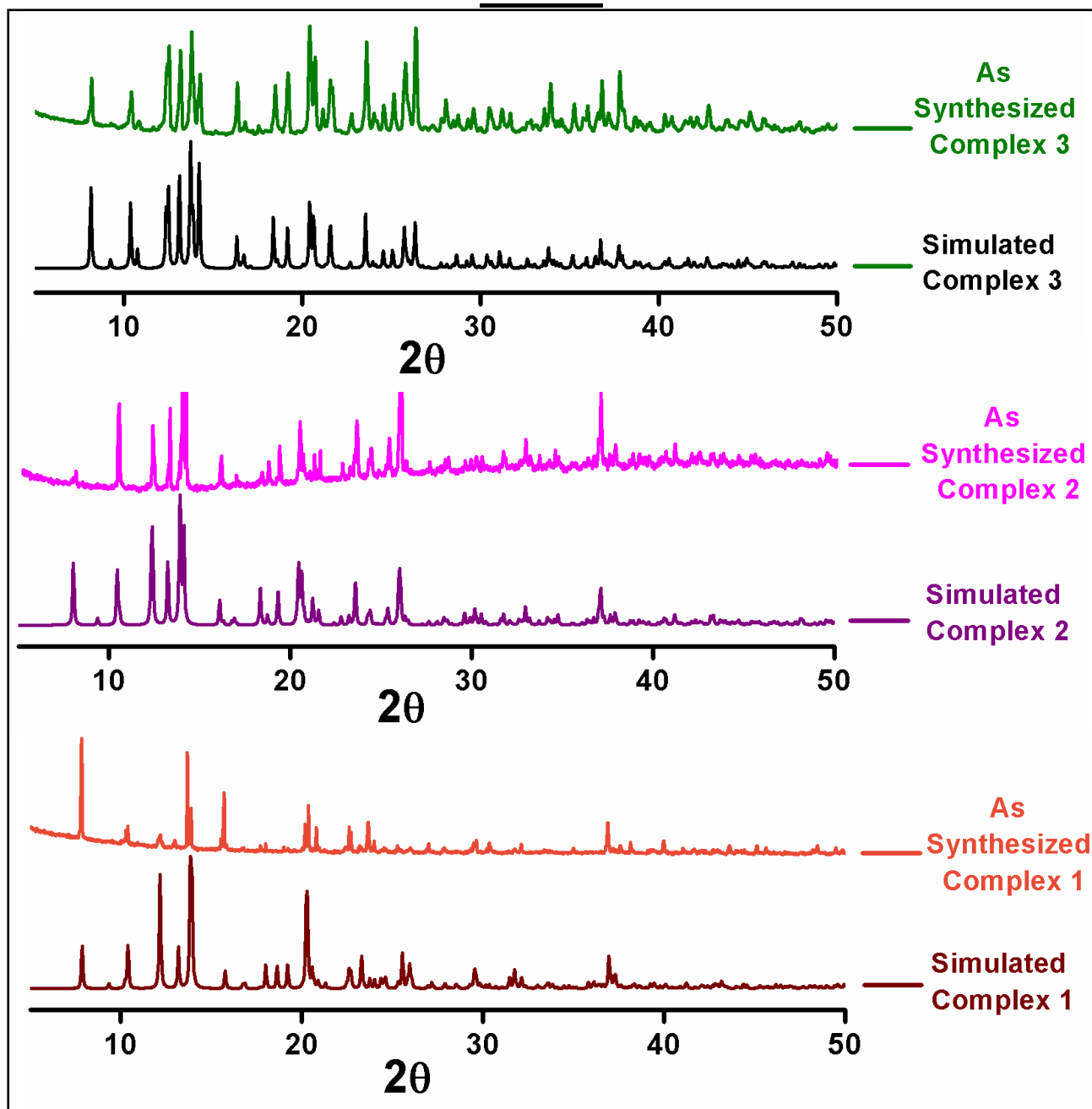


Fig. S13 PXRD patterns of Complex 1, 2 and 3.

7. Catechol Oxidation Kinetic study

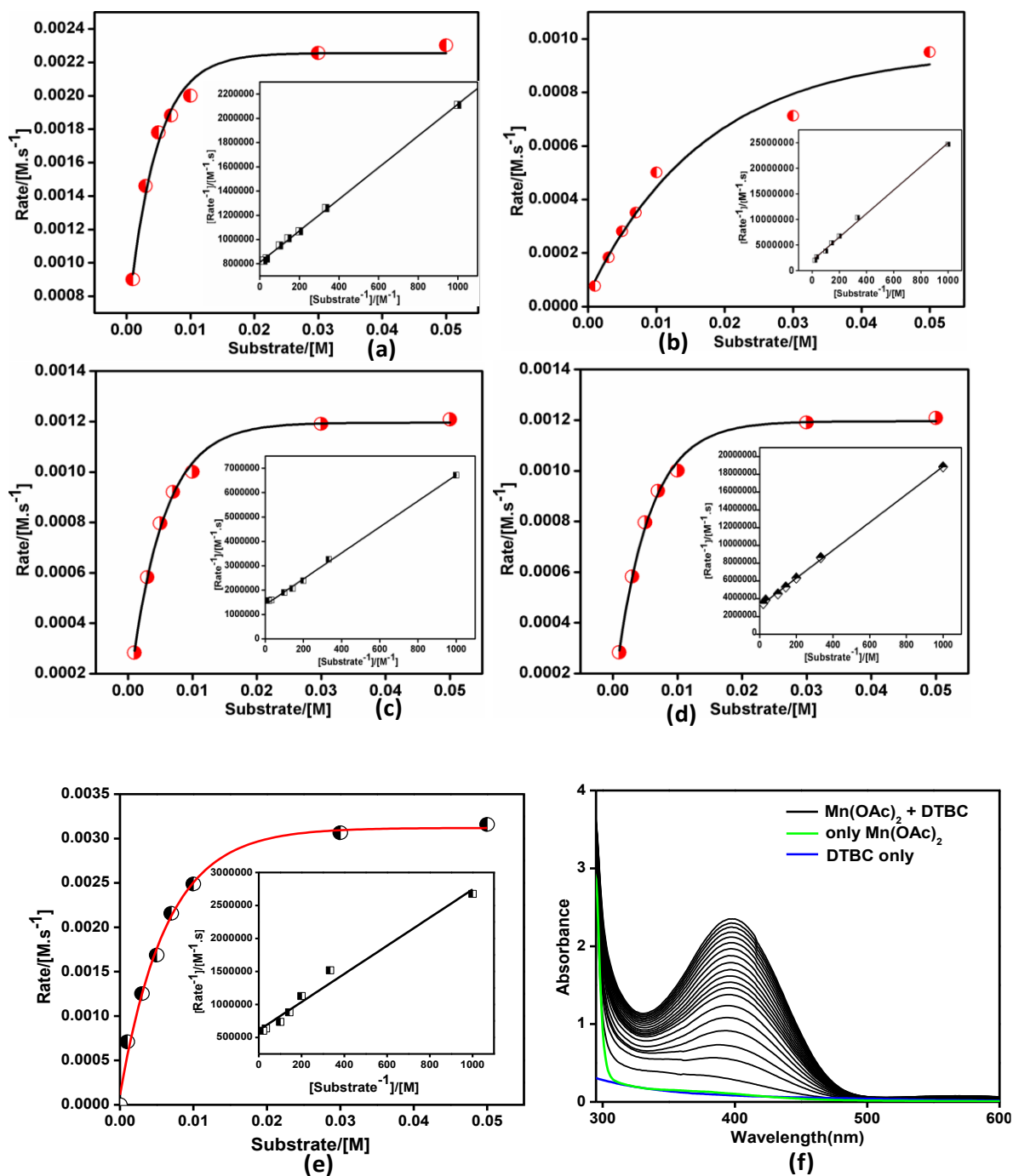


Fig. S14 Dependence of the rate of reaction on the substrate concentration (insets: Lineweaver Burk plot) for (a) Mn(II) and (b) Mn(III) of complex 1 (c), (d) for complex 2 and complex 3 respectively and (e) represent only Mn(OAc)₂ salt and (f) represent UV-Vis study of Mn(OAc)₂ in presence of 3,5 DTBC.

Table. S4 Measurement of Conductance of complex (1-3) and the only acetate salt of Mn, Co, and Ni with time.

Time	0 minute	10 minute	30 minute	60 minute	120 minute	180 minute	After 1day
Only Mn(OAc) ₂ .2H ₂ O	10.00	9.26	7.45	6.01	4.52	3.09	3.00
Only Co(OAc) ₂ .2H ₂ O	12.13	12.10	11.28	11.20	10.50	10.48	10.46
Only Ni(OAc) ₂ .2H ₂ O	11.80	11.78	11.80	11.75	11.76	11.75	11.70
Only complex 1	4.10	6.20	10.06	14.24	20.00	26.20	25.02
Only complex 2	3.58	5.02	6.70	7.05	7.01	7.03	7.52
Only complex 3	3.25	3.32	3.33	3.33	3.33	3.34	3.33
Compound	Conductance (μS)						

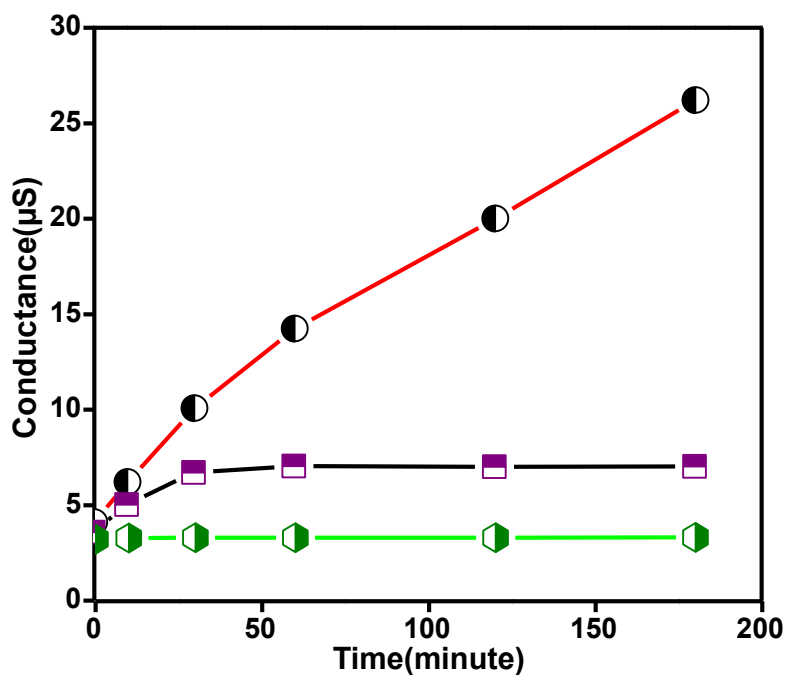


Fig. S15 Measurement of Conductance with time of complex (1-3)

8. Catalytic Cycle of Catechol Oxidation for complex 2.

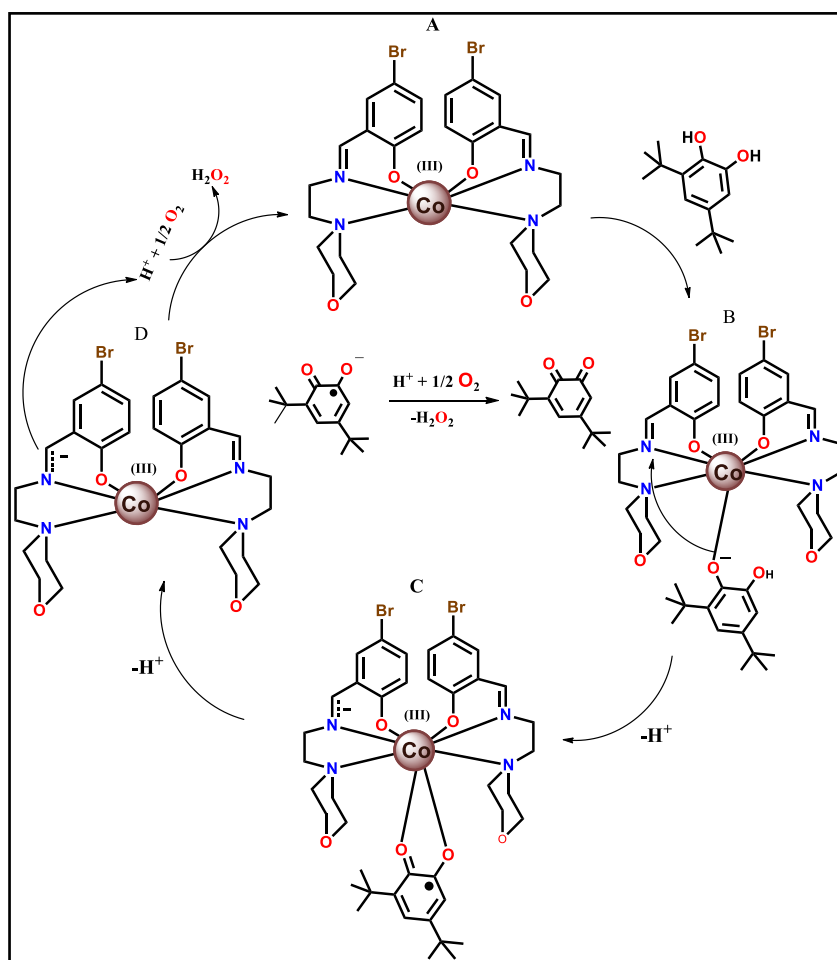


Fig. S16 Probable mechanistic pathway for oxidation of 3,5 DTBC to 3,5 DTBQ in presence of complex 2.

For $[\text{Co}_3\text{L}_2(\text{OAc})_4]$ ESI-MS generates a peak m/z at 683.02 which corresponds to two Schiff base coordinated to a single cobalt centre i.e complex 2 exists as a mononuclear species in solution phase. From the EPR study it was observed that Complex 2 was EPR silent, which proved that Complex 2 exists as Cobalt(III) species in solution state. And after addition of 3,5 DTBC eight line spectrum was observed. From the simulation data g value of approximate 2 was obtained for the eight line spectrum and Lw value is also very low. That represent a radical species is generated during this reaction but if there is generation a imine radical there must be a single line soectrum in EPR study. But here we observe eight line spectrum due to the coupling between the centran metal Co^{59} and the imine radical. From the above point of view we try to give a probable mechanistic

path way for oxidation of 3,5 DTBC to 3,5 DTBQ by complex **2**. In first step 3,5 DTBC form a adduct with complex **2** by release of a proton(Supporting Information, B, Fig. S14). During the course of oxidation 3,5 DTBC moiety gives a electron from oxygen centre to the cobalt(III) center and during this reaction radical species is generated but if there is generation a imine radical and observe eight line spectrum due to the coupling between the centran metal Co^{59} and the imine radical. EPR spectrum of complex **2** in presence and in absence of catechol are given in Fig.9.

10. Catalytic Cycle of Catechol Oxidation for complex **2**.

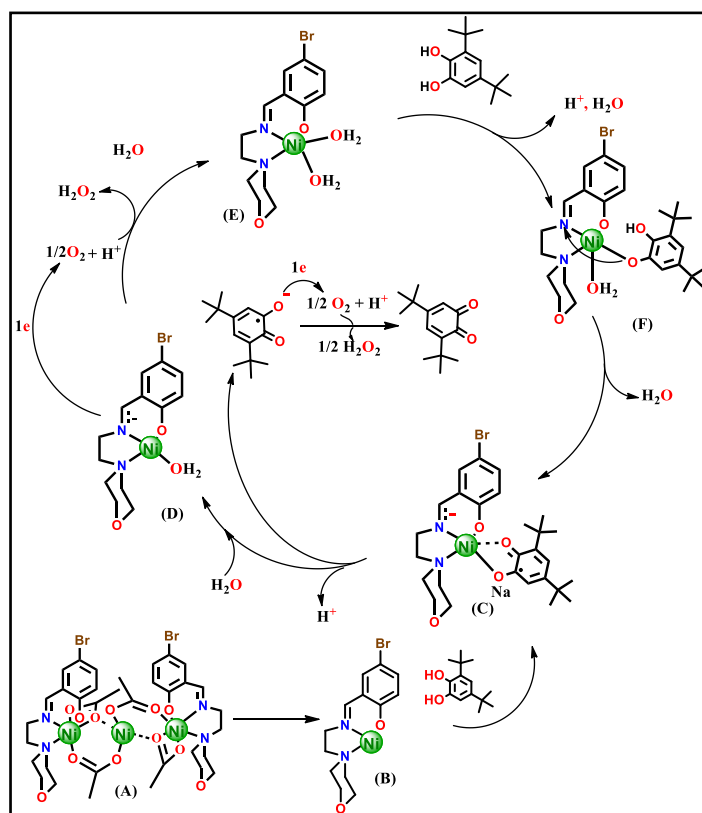


Fig. S17 Probable mechanistic pathway for oxidation of 3,5 DTBC to 3,5 DTBQ in presence of complex **3**.

Complex **3** i.e. $[\text{Ni}_3\text{L}_2(\text{OAc})_4]$, also exists as a mononuclear species in solution phase. It generates a peak at m/z at 368.97 consisted with the formula $[(\text{C}_{13}\text{H}_{16}\text{BrN}_2\text{O}_2\text{Ni}(\text{II}))]$. In solution phase complex **3** remained EPR silent. With addition of 3,5 DTBC to complex **3**, a sharp signal is generated at $g = 2.009$ which is indicative of formation of a radical during the course of the oxidation reaction. With the help of ESI-MS and EPR study we proposed a plausible mechanism for oxidation of 3, 5 DTBC to 3,5 DTBQ by complex **3**.

In first step $[(C_{13}H_{16}BrN_2O_2Ni(II))]$ forms an adduct with 3,5 DTBC through the release of two protons (Supporting Information d, Figure S16) During the course of the oxidation of 3,5 DTBC to 3,5 DTBQ a imine radical is duly generated, which was responsible for generation a peak at $g = 2.009$ (Supporting Information E, Fig. S17). In the final step, the imine species gives up an electron to form H_2O_2 .

11. UV-Vis spectra of the reaction mixture of 3,5 DTBC and complex 1,2 and 3 and KI.

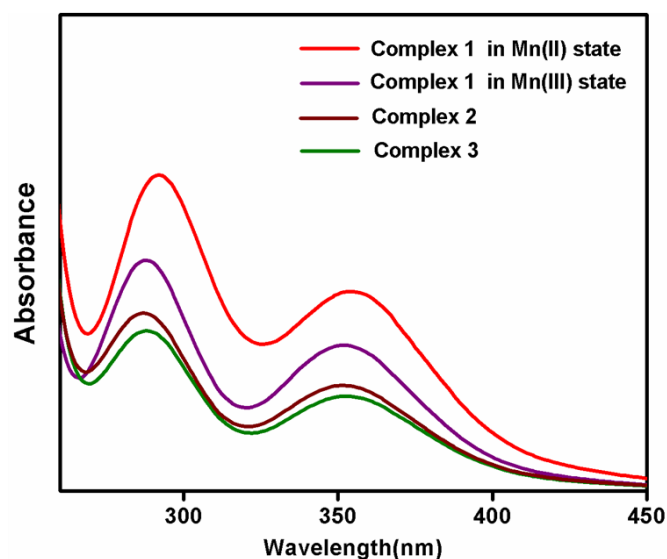


Fig. S18. UV-Vis spectra of the reaction mixture of 3,5 DTBC and complex 1,2 and 3 and KI.

Table. S5 Experimental and simulated EPR data of all complexes(1-3).

Complex	Conditions	A(G)	Line width (Lw)	g
Complex 1 Mn(II)	DMF Solution at Room Temperature	^{55}Mn , 85.8	7.5	2.011
Complex 1 Mn(III)	DMF Solution at Room Temperature in presence of catechol	$^{55}Mn(I=5/2)$, 82.85 Imine Radical	8 0.8	1.998 2.001
Complex 2	DMF Solution at Room Temperature in presence of catechol	$^{59}Co(I=7/2)$, 9.24	0.5	2.005
Complex 3	DMF Solution at Room Temperature in presence of catechol	Imine Radical	0.5	2.009

12. Coordinates and Energies of the Optimized Structures

Intermediate A

Mn	0.008941000	-0.631679000	0.019638000
O	1.061654000	0.781058000	-0.988183000
C	4.049041000	3.340131000	0.337343000
C	3.411259000	3.513907000	-0.907870000
H	3.709158000	4.338399000	-1.550619000
C	2.415942000	2.661713000	-1.323936000
H	1.921551000	2.795195000	-2.281048000
C	1.971890000	1.564567000	-0.524572000
C	2.623420000	1.399764000	0.745272000
C	2.286451000	0.367521000	1.688061000
H	2.875138000	0.382489000	2.616660000
N	1.377481000	-0.536752000	1.563468000
C	1.115370000	-1.409423000	2.699882000
H	0.563904000	-0.850227000	3.465993000
H	2.044453000	-1.766634000	3.164944000
C	0.293649000	-2.605945000	2.236466000
H	-0.008764000	-3.220329000	3.101181000
H	0.914914000	-3.228099000	1.582473000
N	-0.881635000	-2.181513000	1.455731000
C	-1.544121000	-3.345776000	0.862809000
H	-2.042504000	-3.956053000	1.632614000
H	-0.815976000	-3.973606000	0.350876000
C	-1.864839000	-1.509735000	2.323596000
H	-1.454075000	-0.589340000	2.732074000
H	-2.182860000	-2.190940000	3.129382000
C	3.646751000	2.294725000	1.134244000
H	4.117169000	2.141435000	2.104185000
O	-1.111140000	0.763678000	0.938008000
C	-4.452454000	2.857532000	-0.352808000
C	-3.858934000	3.091039000	0.904586000
H	-4.280788000	3.845527000	1.563890000
C	-2.751923000	2.386064000	1.311734000
H	-2.285462000	2.571607000	2.274414000
C	-2.144081000	1.384315000	0.493441000
C	-2.764956000	1.144018000	-0.780604000
C	-2.288894000	0.166431000	-1.722598000

H	-2.816957000	0.155164000	-2.686872000
N	-1.330655000	-0.676532000	-1.548314000
C	-0.943303000	-1.546451000	-2.646865000
H	-1.358147000	-2.550567000	-2.480763000
H	-1.336781000	-1.187186000	-3.607392000
C	0.581960000	-1.598957000	-2.704308000
H	0.921953000	-2.220088000	-3.549466000
H	0.954695000	-0.579556000	-2.828956000
N	1.135149000	-2.111014000	-1.431059000
C	2.568004000	-1.792090000	-1.333933000
H	3.135147000	-2.292909000	-2.134664000
H	2.704835000	-0.714573000	-1.404124000
C	1.006310000	-3.569579000	-1.396886000
H	-0.029701000	-3.873126000	-1.552290000
H	1.621840000	-4.033879000	-2.184261000
C	-3.896756000	1.898479000	-1.166612000
H	-4.333622000	1.699560000	-2.144180000
H	4.832210000	4.017253000	0.659242000
H	-5.322064000	3.422576000	-0.669094000
H	-2.731971000	-1.230175000	1.720504000
H	-2.293599000	-3.002427000	0.143428000
H	2.942121000	-2.135247000	-0.364729000
H	1.345431000	-3.952978000	-0.430379000

Intermediate B

Mn	0.202108000	-0.371068000	-0.454600000
O	2.043659000	-0.356415000	-1.294793000
C	5.745932000	-1.226859000	0.358032000
C	5.615312000	-0.520717000	-0.857107000
H	6.508809000	-0.200894000	-1.387481000
C	4.380968000	-0.233126000	-1.385356000
H	4.276728000	0.305545000	-2.321985000
C	3.166617000	-0.620271000	-0.735462000
C	3.309624000	-1.329002000	0.506363000
C	2.203096000	-1.815365000	1.281715000
H	2.497449000	-2.463615000	2.121776000
N	0.940009000	-1.590117000	1.114794000
C	0.029583000	-2.257336000	2.039036000
H	0.583352000	-2.979049000	2.654756000

H	-0.719044000	-2.796548000	1.451700000
C	-0.768400000	-1.300082000	2.962608000
H	-0.673355000	-1.591911000	4.014712000
H	-1.813818000	-1.318919000	2.667223000
N	-0.308212000	0.117744000	2.877762000
C	-1.395801000	1.076640000	3.191071000
H	-1.746964000	0.908267000	4.212156000
H	-2.194619000	0.916802000	2.465823000
C	0.897759000	0.364676000	3.699712000
H	1.649836000	-0.386291000	3.457204000
H	0.629355000	0.307947000	4.757534000
C	4.601567000	-1.621867000	1.006599000
H	4.673697000	-2.175876000	1.941702000
O	0.628274000	1.285089000	0.680309000
C	0.522980000	5.311281000	-0.365415000
C	0.890649000	4.888257000	0.918939000
H	1.170791000	5.621623000	1.670814000
C	0.913637000	3.546507000	1.240431000
H	1.231228000	3.225086000	2.228858000
C	0.568447000	2.529803000	0.309138000
C	0.190070000	2.972104000	-1.000091000
C	-0.235554000	2.093533000	-2.076719000
H	-0.472843000	2.602769000	-3.021516000
N	-0.389958000	0.826539000	-2.008671000
C	-0.894849000	0.088164000	-3.153594000
H	-1.977028000	-0.043386000	-3.020492000
H	-0.736699000	0.632422000	-4.094831000
C	-0.182780000	-1.261803000	-3.203927000
H	-0.567893000	-1.874594000	-4.035749000
H	0.885226000	-1.080770000	-3.356098000
N	-0.319866000	-1.974824000	-1.920065000
C	0.661127000	-3.060742000	-1.838084000
H	0.510726000	-3.796254000	-2.644731000
H	1.667278000	-2.642464000	-1.900554000
C	-1.667325000	-2.530580000	-1.761268000
H	-2.422032000	-1.752311000	-1.883160000
H	-1.847739000	-3.326558000	-2.501939000
C	0.184702000	4.348900000	-1.295119000
H	-0.105164000	4.651831000	-2.299580000

H	6.724991000	-1.454769000	0.764364000
H	0.507379000	6.364261000	-0.622993000
H	1.288322000	1.351305000	3.451056000
H	-0.998274000	2.088004000	3.082309000
H	0.546799000	-3.566757000	-0.874911000
H	-1.778671000	-2.930187000	-0.750636000
O	-1.585020000	-0.547560000	0.517533000
C	-2.832378000	-0.319467000	0.198797000
C	-3.820590000	-1.288661000	0.526256000
C	-3.291027000	0.849799000	-0.434747000
C	-5.156112000	-1.104706000	0.211580000
C	-4.638724000	1.035086000	-0.749840000
H	-2.552423000	1.615304000	-0.657010000
C	-5.577744000	0.061293000	-0.437065000
H	-5.878279000	-1.877637000	0.473181000
H	-4.950379000	1.953479000	-1.239474000
H	-6.626284000	0.197454000	-0.679247000
O	-3.358056000	-2.416765000	1.176292000
H	-4.115035000	-2.999391000	1.331391000
H	-0.037520000	0.369827000	1.890482000

Intermediate C

Mn	0.118324000	-0.376046000	-0.278627000
O	2.262375000	0.270932000	-1.307187000
C	5.960977000	-1.061728000	0.061648000
C	5.827178000	-0.475632000	-1.197952000
H	6.688672000	-0.354045000	-1.846493000
C	4.575945000	-0.034380000	-1.610989000
H	4.432911000	0.442327000	-2.575475000
C	3.454299000	-0.177136000	-0.798371000
C	3.554322000	-0.801868000	0.466842000
C	2.483864000	-1.099263000	1.405499000
H	2.861816000	-1.521242000	2.341750000
N	1.175424000	-1.011138000	1.272335000
C	0.445758000	-1.502917000	2.450873000
H	1.144648000	-1.957930000	3.162970000
H	-0.272169000	-2.263620000	2.131538000
C	-0.405563000	-0.433308000	3.170325000
H	-0.287434000	-0.502424000	4.257012000

H	-1.445853000	-0.588133000	2.892936000
N	-0.050266000	0.969702000	2.792724000
C	-1.170189000	1.899647000	3.086401000
H	-1.400976000	1.850236000	4.153659000
H	-2.018691000	1.583466000	2.480415000
C	1.213413000	1.422655000	3.416822000
H	1.996290000	0.696967000	3.194387000
H	1.065625000	1.510392000	4.496120000
C	4.845839000	-1.213713000	0.866105000
H	4.952619000	-1.686519000	1.839570000
O	0.613449000	1.629244000	0.229588000
C	-1.178741000	5.117166000	-1.173851000
C	-0.386374000	5.112590000	-0.021757000
H	-0.216792000	6.035849000	0.525443000
C	0.200776000	3.939230000	0.419169000
H	0.848412000	3.939581000	1.292639000
C	0.015745000	2.706200000	-0.246061000
C	-0.785819000	2.717415000	-1.424196000
C	-1.049173000	1.547746000	-2.252595000
H	-1.534754000	1.762670000	-3.213754000
N	-0.790764000	0.329276000	-1.950008000
C	-1.162769000	-0.716668000	-2.894348000
H	-2.153757000	-1.094389000	-2.609041000
H	-1.230612000	-0.337029000	-3.922746000
C	-0.113246000	-1.818368000	-2.810743000
H	-0.370632000	-2.661543000	-3.472697000
H	0.849463000	-1.404121000	-3.128605000
N	0.046415000	-2.273795000	-1.417550000
C	1.298969000	-3.020917000	-1.269239000
H	1.308841000	-3.913455000	-1.915672000
H	2.143944000	-2.378159000	-1.529610000
C	-1.079528000	-3.125323000	-1.011141000
H	-2.026739000	-2.602207000	-1.158889000
H	-1.091773000	-4.059987000	-1.594621000
C	-1.352458000	3.928301000	-1.859044000
H	-1.953480000	3.914649000	-2.766108000
H	6.929456000	-1.406049000	0.409577000
H	-1.636819000	6.033130000	-1.530173000
H	1.486446000	2.388110000	2.989299000

H	-0.868248000	2.909944000	2.804192000
H	1.408011000	-3.333251000	-0.227630000
H	-0.998793000	-3.359547000	0.053378000
O	-1.797700000	0.038503000	0.803422000
C	-2.873295000	-0.550691000	0.447724000
C	-3.228563000	-1.850017000	1.075187000
C	-3.750702000	-0.012219000	-0.543769000
C	-4.430891000	-2.500304000	0.611159000
C	-4.881129000	-0.687535000	-0.938833000
H	-3.484551000	0.953260000	-0.966962000
C	-5.218752000	-1.944101000	-0.359721000
H	-4.674666000	-3.454188000	1.070128000
H	-5.532691000	-0.259943000	-1.695696000
H	-6.117325000	-2.456534000	-0.691871000
O	-2.486821000	-2.354931000	1.952337000
H	0.105067000	1.028951000	1.751375000
H	1.880962000	0.988436000	-0.733324000

Intermediate D

Mn	0.038377000	0.101330000	0.688130000
O	1.978134000	-0.345435000	1.651280000
C	5.577203000	1.364306000	0.325296000
C	5.577114000	0.066664000	0.852776000
H	6.496552000	-0.497318000	0.942315000
C	4.367412000	-0.492282000	1.272490000
H	4.347488000	-1.486984000	1.706638000
C	3.182671000	0.216837000	1.149392000
C	3.134050000	1.509991000	0.579906000
C	1.954756000	2.303807000	0.367552000
H	2.171104000	3.344313000	0.114136000
N	0.666568000	1.928951000	0.383382000
C	-0.288225000	3.054096000	0.107118000
H	0.249198000	4.010298000	0.196387000
H	-1.061172000	3.025592000	0.877591000
C	-1.073023000	3.005093000	-1.213951000
H	-1.697305000	3.904298000	-1.261930000
H	-1.698965000	2.118108000	-1.254444000
N	-0.247304000	3.005859000	-2.509458000
C	0.601362000	1.730319000	-2.651865000

H	-0.152134000	0.923851000	-2.563644000
H	1.331149000	1.678928000	-1.857465000
C	-1.241353000	3.005639000	-3.686714000
H	-1.948078000	3.826565000	-3.551125000
H	-1.713546000	1.991499000	-3.610752000
C	4.387459000	2.065258000	0.199299000
H	4.393474000	3.064326000	-0.224289000
O	0.957988000	-0.494804000	-0.869563000
C	1.878499000	-4.301907000	-2.309712000
C	2.279432000	-3.129902000	-2.989386000
H	2.846457000	-3.214213000	-3.909959000
C	1.954601000	-1.882028000	-2.499664000
H	2.250494000	-0.976235000	-3.012406000
C	1.211159000	-1.722820000	-1.299782000
C	0.802916000	-2.914413000	-0.615161000
C	0.033970000	-2.865774000	0.592776000
H	-0.242870000	-3.834127000	1.021567000
N	-0.368010000	-1.774464000	1.194687000
C	-1.184435000	-1.884899000	2.432269000
H	-2.219531000	-1.663304000	2.162089000
H	-1.133077000	-2.894941000	2.860613000
C	-0.626381000	-0.850454000	3.419114000
H	-1.193010000	-0.840176000	4.360539000
H	0.422102000	-1.082208000	3.625811000
N	-0.657350000	0.508371000	2.762699000
C	0.275973000	1.454014000	3.462088000
H	0.006793000	1.553672000	4.523126000
H	1.290460000	1.074003000	3.354258000
C	-2.056982000	1.060307000	2.803673000
H	-2.755494000	0.289042000	2.492619000
H	-2.294882000	1.394384000	3.823002000
C	1.150901000	-4.183047000	-1.143969000
H	0.825310000	-5.072949000	-0.612181000
H	6.506949000	1.820010000	0.006197000
H	2.134271000	-5.276910000	-2.705025000
H	-0.664959000	3.129426000	-4.606481000
H	1.064061000	1.764988000	-3.641863000
H	0.206642000	2.422451000	2.966780000
H	-2.153924000	1.866020000	2.083116000

O	-1.604145000	0.566108000	0.037492000
C	-2.721723000	-0.009161000	-0.643173000
C	-3.919961000	0.392950000	0.243075000
C	-2.577141000	-1.468487000	-0.922660000
C	-4.669405000	-0.696592000	0.868592000
C	-3.338886000	-2.395967000	-0.316566000
H	-1.838166000	-1.676781000	-1.684375000
C	-4.384086000	-1.998209000	0.614323000
H	-5.471560000	-0.405485000	1.536964000
H	-3.221648000	-3.450824000	-0.541834000
H	-4.970926000	-2.781511000	1.086665000
O	-4.145484000	1.593086000	0.494406000
H	2.022671000	-1.338550000	1.648373000
O	-2.955819000	0.684751000	-1.897772000
O	-1.847036000	0.325561000	-2.892967000
H	0.352935000	3.842301000	-2.539247000

Intermediate E

Mn	0.118371000	-0.165817000	0.942471000
O	2.034908000	-1.047198000	1.640726000
C	5.555872000	-0.304215000	-0.451702000
C	5.243110000	-1.598034000	-0.045491000
H	5.919743000	-2.419696000	-0.256239000
C	4.060737000	-1.844660000	0.643719000
H	3.817103000	-2.849124000	0.980328000
C	3.178597000	-0.804732000	0.908738000
C	3.457838000	0.502500000	0.492165000
C	2.565365000	1.664692000	0.636105000
H	3.060339000	2.630358000	0.502895000
N	1.300877000	1.629325000	0.806139000
C	0.609310000	2.905773000	0.666320000
H	1.230923000	3.719101000	1.066313000
H	-0.342892000	2.854209000	1.197724000
C	0.323278000	3.154029000	-0.826647000
H	-0.182174000	4.123135000	-0.914763000
H	-0.386430000	2.400029000	-1.174103000
N	1.557081000	3.128195000	-1.608870000
C	1.584747000	2.010358000	-2.543199000

H	1.382436000	1.077042000	-2.007123000
H	2.577354000	1.946518000	-3.005374000
C	1.842250000	4.388307000	-2.266072000
H	1.870850000	5.196043000	-1.526979000
H	1.094156000	4.651448000	-3.035290000
C	4.669071000	0.727117000	-0.172837000
H	4.890677000	1.739415000	-0.500503000
O	0.750393000	-0.885030000	-0.841537000
C	-0.844789000	-3.969018000	-3.111856000
C	-0.209880000	-2.855336000	-3.703189000
H	-0.118860000	-2.805477000	-4.785321000
C	0.297254000	-1.829410000	-2.939133000
H	0.786890000	-0.973005000	-3.392211000
C	0.210492000	-1.835025000	-1.510789000
C	-0.491044000	-2.948972000	-0.922913000
C	-0.827094000	-3.013802000	0.473612000
H	-1.342803000	-3.931102000	0.793769000
N	-0.654782000	-2.072366000	1.340588000
C	-1.239148000	-2.203326000	2.668286000
H	-2.297662000	-1.917985000	2.609639000
H	-1.193364000	-3.236471000	3.040157000
C	-0.494044000	-1.273632000	3.620806000
H	-0.943520000	-1.308764000	4.626736000
H	0.545838000	-1.610866000	3.706386000
N	-0.466454000	0.108440000	3.108571000
C	0.538098000	0.886996000	3.839954000
H	0.323730000	0.904168000	4.920376000
H	1.527973000	0.454318000	3.672021000
C	-1.783975000	0.744668000	3.257958000
H	-2.529013000	0.222728000	2.657317000
H	-2.079572000	0.761690000	4.319286000
C	-0.974049000	-3.995967000	-1.743875000
H	-1.485177000	-4.828596000	-1.263325000
H	6.478369000	-0.101969000	-0.984343000
H	-1.233916000	-4.773527000	-3.725202000
H	2.823437000	4.337357000	-2.750938000
H	0.830463000	2.115158000	-3.343149000
H	0.537239000	1.912662000	3.462598000

H	-1.733862000	1.760654000	2.865946000
O	-1.528203000	0.884429000	0.475233000
C	-2.388220000	0.660570000	-0.534922000
C	-3.297131000	1.914608000	-0.574442000
C	-3.168649000	-0.624750000	-0.334429000
C	-4.590253000	1.823616000	0.138931000
C	-4.389125000	-0.628861000	0.216469000
H	-2.649731000	-1.546360000	-0.587448000
C	-5.092284000	0.627664000	0.492408000
H	-5.129252000	2.753109000	0.295131000
H	-4.901081000	-1.561355000	0.439302000
H	-6.065725000	0.569739000	0.974598000
O	-2.907103000	2.955165000	-1.062088000
H	1.776937000	-1.979452000	1.533137000
O	-1.612598000	0.574575000	-1.744134000
O	-2.483126000	0.180628000	-2.807510000
H	-2.087911000	-0.682357000	-3.027499000

Intermediate F

Mn	0.576178000	-0.319113000	0.031577000
O	-0.097924000	1.094198000	-0.998448000
C	-1.174201000	4.910089000	0.232947000
C	-1.631738000	4.358479000	-0.976180000
H	-2.279850000	4.944765000	-1.620507000
C	-1.275209000	3.081523000	-1.361740000
H	-1.627486000	2.653225000	-2.293938000
C	-0.441977000	2.283322000	-0.550376000
C	0.020452000	2.837915000	0.675986000
C	0.850396000	2.114948000	1.596332000
H	1.138821000	2.657422000	2.503962000
N	1.256682000	0.896701000	1.468703000
C	1.963984000	0.263681000	2.585531000
H	1.281175000	0.171345000	3.437413000
H	2.815543000	0.873474000	2.908182000
C	2.454604000	-1.105501000	2.137069000
H	2.800786000	-1.696206000	2.996509000
H	3.297489000	-0.985256000	1.453268000
N	1.384911000	-1.828876000	1.4084870003

C	1.930647000	-3.045125000	0.780652000
H	2.269812000	-3.756628000	1.544832000
H	2.777420000	-2.792363000	0.146447000
C	0.345844000	-2.271173000	2.369888000
H	-0.121862000	-1.417659000	2.854559000
H	0.804467000	-2.933503000	3.115542000
C	-0.358541000	4.150705000	1.039474000
H	0.005833000	4.553223000	1.981516000
O	-1.034133000	-0.470360000	0.945136000
C	-4.696775000	-1.967812000	-0.304282000
C	-4.552710000	-1.242778000	0.891247000
H	-5.421247000	-1.064682000	1.518134000
C	-3.326765000	-0.743906000	1.283248000
H	-3.213312000	-0.177526000	2.201395000
C	-2.174104000	-0.947887000	0.495373000
C	-2.316027000	-1.683358000	-0.712482000
C	-1.219477000	-1.928511000	-1.605350000
H	-1.467799000	-2.452213000	-2.534992000
N	0.007173000	-1.574220000	-1.423243000
C	0.987397000	-1.759030000	-2.488508000
H	1.664574000	-2.579030000	-2.218070000
H	0.500328000	-2.029235000	-3.432117000
C	1.747947000	-0.446576000	-2.640329000
H	2.499783000	-0.513541000	-3.438300000
H	1.038433000	0.347579000	-2.879960000
N	2.399399000	-0.095894000	-1.348840000
C	2.786090000	1.335032000	-1.352881000
H	3.490779000	1.531891000	-2.171248000
H	1.904773000	1.959310000	-1.475275000
C	3.662277000	-0.857329000	-1.253577000
H	3.494506000	-1.923083000	-1.401271000
H	4.357869000	-0.518039000	-2.032215000
C	-3.586212000	-2.175861000	-1.088934000
H	-3.671630000	-2.728926000	-2.021261000
H	-1.461381000	5.913663000	0.523594000
H	-5.665297000	-2.350690000	-0.603336000
H	-0.431595000	-2.813248000	1.829065000
H	1.149061000	-3.515715000	0.179296000

H	3.271359000	1.572252000	-0.402630000
H	4.138091000	-0.692541000	-0.285908000

Intermediate G

Mn	0.158023000	-0.481009000	-0.517266000
O	1.880949000	-0.514826000	-1.285168000
C	5.583382000	-0.900277000	0.535057000
C	5.426703000	-0.231306000	-0.692591000
H	6.299072000	0.180532000	-1.191211000
C	4.185881000	-0.092860000	-1.279654000
H	4.061920000	0.412331000	-2.231513000
C	3.028057000	-0.612481000	-0.661356000
C	3.180718000	-1.274240000	0.586623000
C	2.075196000	-1.837285000	1.309522000
H	2.358687000	-2.458772000	2.168154000
N	0.811946000	-1.680087000	1.075837000
C	-0.124761000	-2.343430000	1.984870000
H	0.430998000	-3.028561000	2.635363000
H	-0.834121000	-2.931171000	1.393821000
C	-0.980296000	-1.378583000	2.842746000
H	-1.038182000	-1.728759000	3.878021000
H	-1.980137000	-1.313909000	2.421814000
N	-0.426594000	0.013353000	2.892166000
C	-1.487700000	1.011576000	3.197568000
H	-1.920625000	0.790250000	4.175237000
H	-2.246483000	0.953445000	2.415509000
C	0.713348000	0.129894000	3.837888000
H	1.455447000	-0.631858000	3.600449000
H	0.342869000	-0.007764000	4.855523000
C	4.468719000	-1.417938000	1.152721000
H	4.564430000	-1.943889000	2.100218000
O	0.648832000	1.025168000	0.607612000
C	0.926110000	5.050832000	-0.408358000
C	1.237699000	4.583684000	0.876624000
H	1.579721000	5.281719000	1.634775000
C	1.128926000	3.242983000	1.190201000
H	1.406617000	2.880703000	2.175773000
C	0.703100000	2.288464000	0.240601000

C	0.380667000	2.765279000	-1.062024000
C	-0.120363000	1.926002000	-2.126308000
H	-0.328067000	2.432632000	-3.075388000
N	-0.376998000	0.672208000	-2.044751000
C	-0.914700000	-0.073136000	-3.177134000
H	-1.996250000	-0.183897000	-3.031256000
H	-0.753470000	0.460166000	-4.120619000
C	-0.217823000	-1.430789000	-3.203536000
H	-0.648120000	-2.085025000	-3.973840000
H	0.843995000	-1.280018000	-3.411565000
N	-0.315715000	-2.075280000	-1.868336000
C	0.665227000	-3.173342000	-1.772525000
H	0.483061000	-3.918811000	-2.557562000
H	1.671646000	-2.766416000	-1.871348000
C	-1.667880000	-2.632705000	-1.665191000
H	-2.426149000	-1.856543000	-1.768174000
H	-1.853467000	-3.425249000	-2.402352000
C	0.506245000	4.140740000	-1.353388000
H	0.256846000	4.476958000	-2.356945000
H	6.565078000	-1.009148000	0.980821000
H	1.017011000	6.102699000	-0.651603000
H	1.161809000	1.117197000	3.726309000
H	-1.033756000	2.004498000	3.198197000
H	0.560099000	-3.653640000	-0.796866000
H	-1.751971000	-3.035252000	-0.656177000
O	-1.519786000	-0.577529000	0.307932000

Intermediate H

Mn	-0.217941000	0.418413000	-0.400276000
O	1.886590000	0.654682000	-1.633172000
C	4.887887000	-2.123292000	-0.882863000
C	5.176875000	-0.759754000	-0.875944000
H	6.192081000	-0.416277000	-0.707647000
C	4.171962000	0.172924000	-1.103855000
H	4.397935000	1.236294000	-1.113397000
C	2.865107000	-0.247898000	-1.322108000
C	2.536864000	-1.611009000	-1.270285000
C	1.187197000	-2.177447000	-1.322523000
H	1.175326000	-3.235390000	-1.625876000

N	0.074700000	-1.629219000	-0.995256000
C	-1.106346000	-2.492578000	-1.005813000
H	-0.915278000	-3.398192000	-1.600885000
H	-1.958486000	-1.955830000	-1.430528000
C	-1.569379000	-2.862658000	0.397937000
H	-2.432473000	-3.524695000	0.323545000
H	-1.851583000	-1.961908000	0.941871000
N	-0.485353000	-3.571312000	1.195739000
C	0.200461000	-2.632400000	2.144875000
H	-0.548596000	-2.286628000	2.858962000
H	0.608019000	-1.771873000	1.603628000
C	-1.031778000	-4.756476000	1.918736000
H	-1.449186000	-5.456668000	1.194872000
H	-1.815875000	-4.404529000	2.590684000
C	3.579631000	-2.533082000	-1.086768000
H	3.342661000	-3.594437000	-1.086287000
O	1.137802000	0.098776000	1.021230000
C	4.048402000	2.666280000	2.506656000
C	4.085897000	1.277608000	2.734836000
H	4.901658000	0.851164000	3.311916000
C	3.106105000	0.447693000	2.237444000
H	3.141983000	-0.625102000	2.403594000
C	2.013638000	0.942581000	1.474960000
C	1.987328000	2.356646000	1.236229000
C	0.958537000	3.018918000	0.470064000
H	1.025284000	4.113868000	0.428080000
N	0.019318000	2.436075000	-0.189263000
C	-0.892839000	3.188588000	-1.036325000
H	-1.895412000	3.152987000	-0.591960000
H	-0.598900000	4.241722000	-1.132957000
C	-0.881120000	2.500700000	-2.401038000
H	-1.561773000	2.997709000	-3.106831000
H	0.133287000	2.556990000	-2.812687000
N	-1.233642000	1.065843000	-2.264086000
C	-0.760525000	0.325156000	-3.445699000
H	-1.176312000	0.751571000	-4.369500000
H	0.330344000	0.354821000	-3.488030000
C	-2.702347000	0.929969000	-2.186214000

H	-3.102193000	1.561510000	-1.390804000
H	-3.158957000	1.226813000	-3.140838000
C	3.006318000	3.180827000	1.771820000
H	2.949365000	4.251905000	1.588929000
H	5.673060000	-2.854672000	-0.730986000
H	4.818765000	3.314673000	2.906989000
H	-0.232380000	-5.228771000	2.490682000
H	0.989257000	-3.182497000	2.661301000
H	-1.087939000	-0.715008000	-3.367718000
H	-2.972949000	-0.102195000	-1.954261000
O	-1.940845000	0.044245000	0.685161000
C	-3.169063000	0.377532000	0.862458000
C	-4.228578000	-0.519514000	0.346224000
C	-3.542692000	1.579473000	1.519859000
C	-5.596693000	-0.123033000	0.571226000
C	-4.868641000	1.903738000	1.690121000

Intermediate I

Mn	0.292233000	-0.334942000	-0.523674000
O	2.598767000	0.029562000	-0.879496000
C	5.990700000	-1.446943000	1.014405000
C	6.112325000	-0.692397000	-0.150514000
H	7.090043000	-0.502311000	-0.580565000
C	4.979750000	-0.185046000	-0.777108000
H	5.066729000	0.389237000	-1.695616000
C	3.718817000	-0.423040000	-0.240817000
C	3.566876000	-1.165248000	0.942819000
C	2.311439000	-1.401995000	1.664104000
H	2.477698000	-1.858670000	2.649128000
N	1.108338000	-1.129421000	1.324212000
C	0.067211000	-1.426083000	2.318288000
H	0.501050000	-1.846628000	3.237273000
H	-0.614470000	-2.161612000	1.878378000
C	-0.841532000	-0.237864000	2.583312000
H	-1.798934000	-0.594671000	2.966597000
H	-1.025540000	0.290494000	1.653746000
N	-0.355759000	0.825369000	3.542317000
C	1.073597000	1.212342000	3.348867000

H	1.203312000	1.432552000	2.284870000
H	1.710709000	0.383566000	3.657762000
C	-1.252813000	2.016141000	3.372295000
H	-2.292758000	1.687421000	3.412767000
H	-1.049782000	2.426336000	2.380587000
C	4.730652000	-1.667814000	1.548072000
H	4.630439000	-2.240337000	2.466543000
O	0.354858000	1.497574000	0.304363000
C	0.030940000	5.263290000	-1.446043000
C	0.336476000	5.095129000	-0.085907000
H	0.491301000	5.967989000	0.542108000
C	0.448466000	3.836714000	0.467716000
H	0.702488000	3.721178000	1.517912000
C	0.253363000	2.652784000	-0.292457000
C	-0.027759000	2.834147000	-1.684898000
C	-0.193013000	1.746949000	-2.616620000
H	-0.429088000	2.040538000	-3.647738000
N	-0.070753000	0.493411000	-2.352594000
C	-0.275210000	-0.506040000	-3.393663000
H	-1.308959000	-0.869023000	-3.330453000
H	-0.124951000	-0.090419000	-4.398148000
C	0.704087000	-1.645946000	-3.139114000
H	0.579250000	-2.446587000	-3.883136000
H	1.724388000	-1.255883000	-3.225921000
N	0.549054000	-2.179491000	-1.766270000
C	1.722073000	-2.999208000	-1.428754000
H	1.816404000	-3.852889000	-2.115611000
H	2.630703000	-2.397881000	-1.490598000
C	-0.643644000	-3.047862000	-1.692502000
H	-1.539961000	-2.490488000	-1.958705000
H	-0.518161000	-3.913051000	-2.359309000
C	-0.140536000	4.137481000	-2.218984000
H	-0.368080000	4.239246000	-3.278017000
H	6.869710000	-1.850995000	1.502975000
H	-0.062857000	6.253348000	-1.876005000
H	-1.031280000	2.743257000	4.154305000
H	1.280601000	2.087347000	3.967492000
H	1.611546000	-3.380857000	-0.410681000

H	-0.773336000	-3.387268000	-0.663525000
O	-1.633517000	-0.967198000	-0.069202000
C	-2.897849000	-0.636087000	0.030849000
C	-3.676839000	-1.649848000	0.925826000
C	-3.567758000	-0.310499000	-1.279454000
C	-4.991127000	-2.119811000	0.472226000
C	-4.752097000	-0.828476000	-1.620490000
H	-3.016460000	0.372483000	-1.922736000
C	-5.476836000	-1.733444000	-0.720559000
H	-5.519209000	-2.808576000	1.123222000
H	-5.209884000	-0.590446000	-2.575764000
H	-6.441827000	-2.105219000	-1.053783000
O	-3.142694000	-2.074520000	1.933589000
H	2.787841000	0.815480000	-1.417561000
O	-2.975604000	0.715625000	0.787762000
O	-3.872013000	0.748157000	1.728288000
H	-0.467585000	0.476255000	4.498633000

Intermediate J

Mn	-0.073107000	0.185158000	-0.875968000
O	1.745081000	0.843487000	-1.768511000
C	5.411550000	-0.321733000	-0.176895000
C	5.209538000	0.999821000	-0.564155000
H	6.007086000	1.728384000	-0.467545000
C	3.981332000	1.397301000	-1.087472000
H	3.823985000	2.424926000	-1.405761000
C	2.961799000	0.468061000	-1.204561000
C	3.125898000	-0.860930000	-0.810006000
C	2.079360000	-1.884915000	-0.861706000
H	2.444760000	-2.910610000	-0.798036000
N	0.816857000	-1.686177000	-0.947381000
C	-0.012979000	-2.875236000	-0.761992000
H	0.447025000	-3.732157000	-1.269795000
H	-1.004327000	-2.696502000	-1.179765000
C	-0.143363000	-3.147795000	0.749050000
H	-0.826052000	-4.000068000	0.888211000
H	-0.619939000	-2.278467000	1.204989000
N	1.157800000	-3.370901000	1.351134000

C	1.311720000	-2.681490000	2.623024000
H	1.090283000	-1.620424000	2.475795000
H	2.344499000	-2.784395000	2.971565000
C	1.507609000	-4.778102000	1.434784000
H	1.418610000	-5.245989000	0.447913000
H	0.861498000	-5.334971000	2.134568000
C	4.377488000	-1.239170000	-0.310321000
H	4.519739000	-2.271423000	-0.002640000
O	0.792669000	0.495421000	0.768665000
C	1.072333000	3.944612000	3.062371000