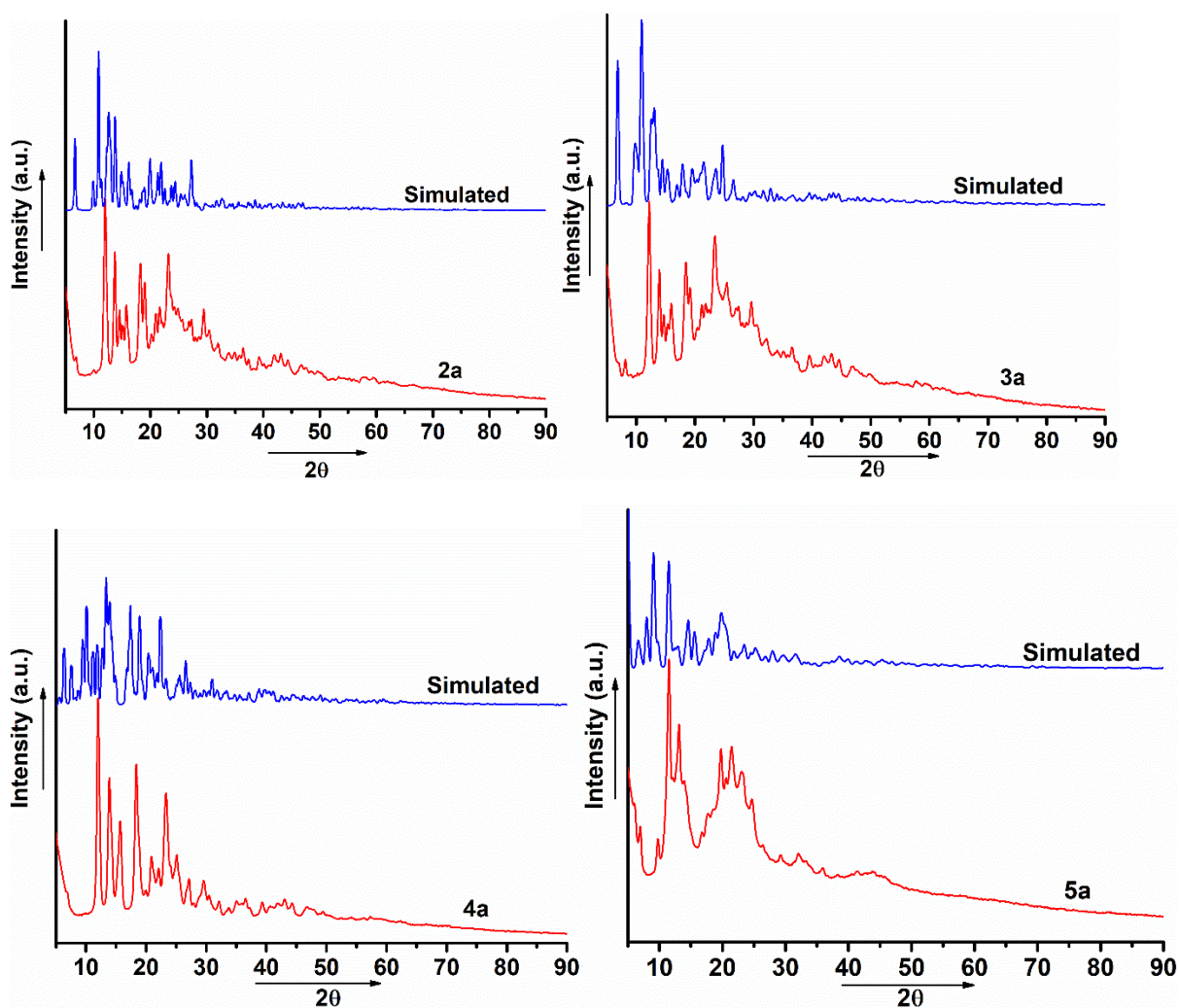


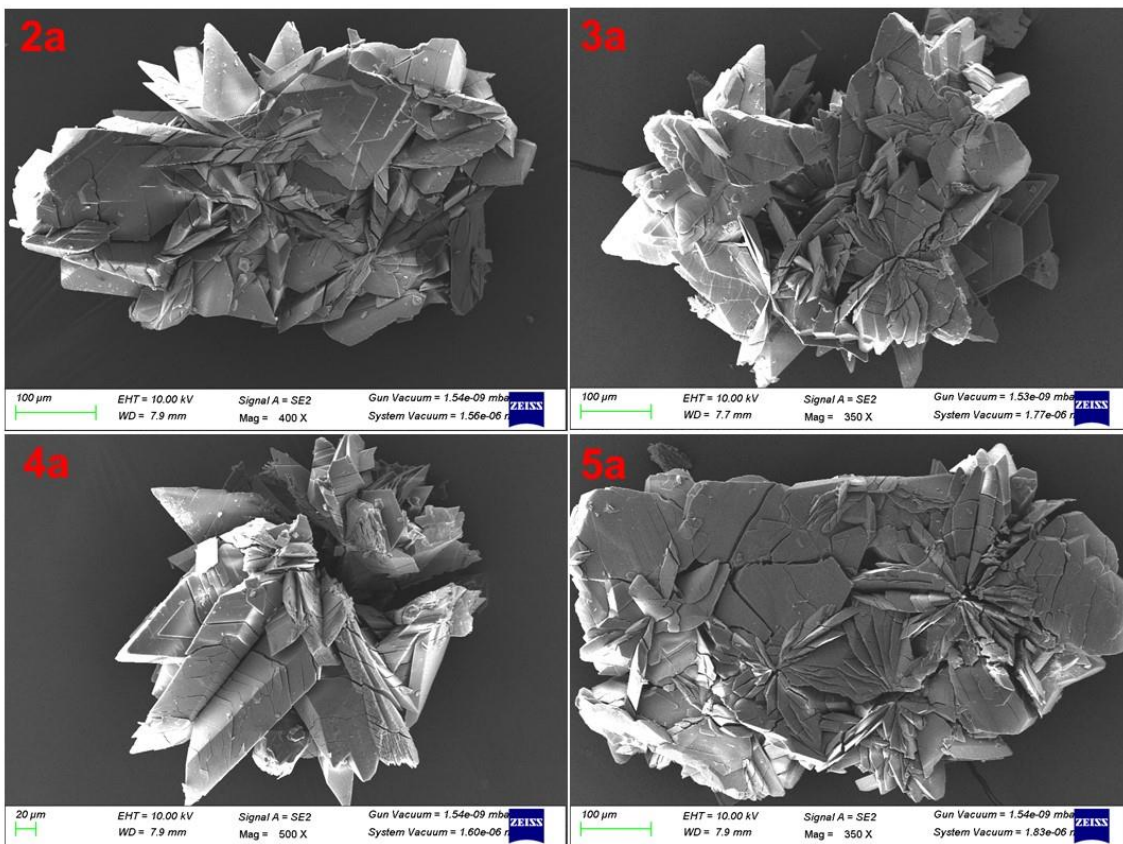
(ESI for New J. Chem) Manuscript ID NJ-ART-12-2022-005936

## Trinuclear dioxidomolybdenum(VI) complexes derived from benzene-1,3,5-tricarbohydrazide and study of catalytic activity

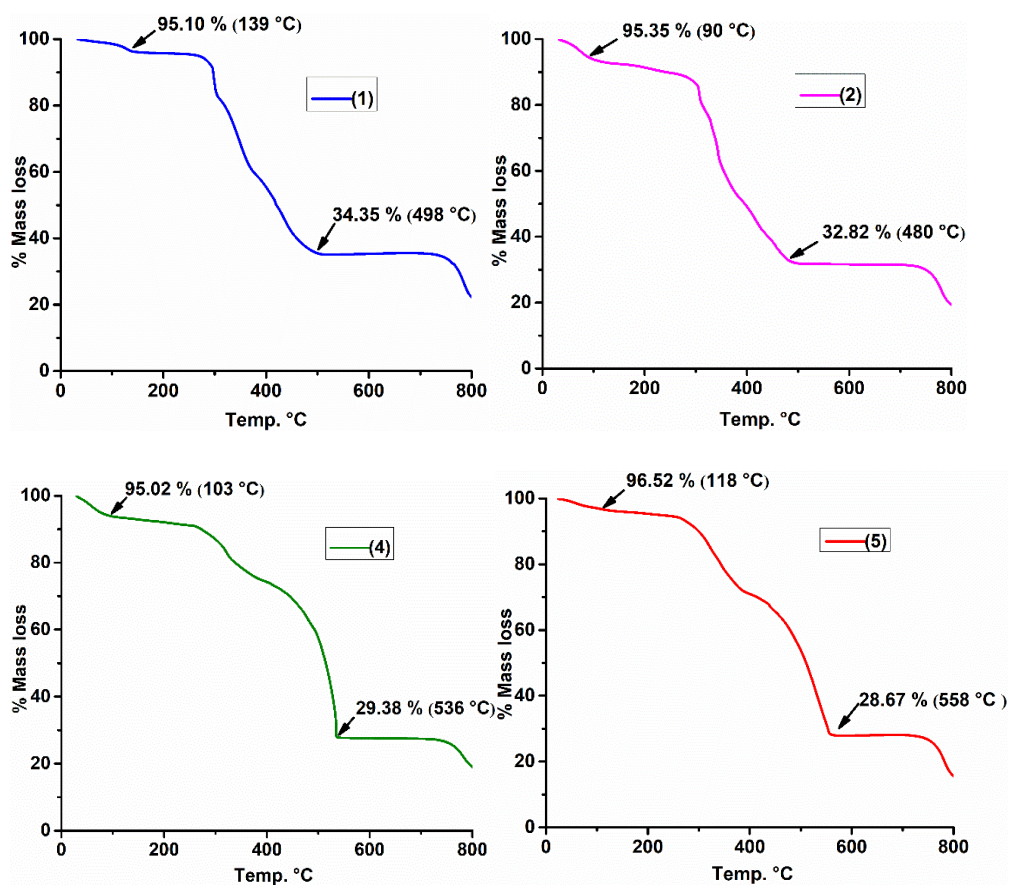
Mannar R. Maurya,\* Devesh Singh, Frnando Avecilla, Akhilesh Sharma and Puneet Gupta



**Fig. S1** P-XRD patterns (red) of complexes **2a**, **3a**, **4a** and **5a** and their comparison with simulated patterns (blue) obtained from SC-XRD.



**Fig. S2** Field emission-scanning electron micrograph of complexes (2a–5a).



**Fig. S3** TGA profiles of complexes **1**, **2**, **4** and **5** showing mass loss vs. temperature. Beyond 750 °C, MoO<sub>3</sub> starts volatilizing. Arrows point the remaining mass percent at particular temperature.



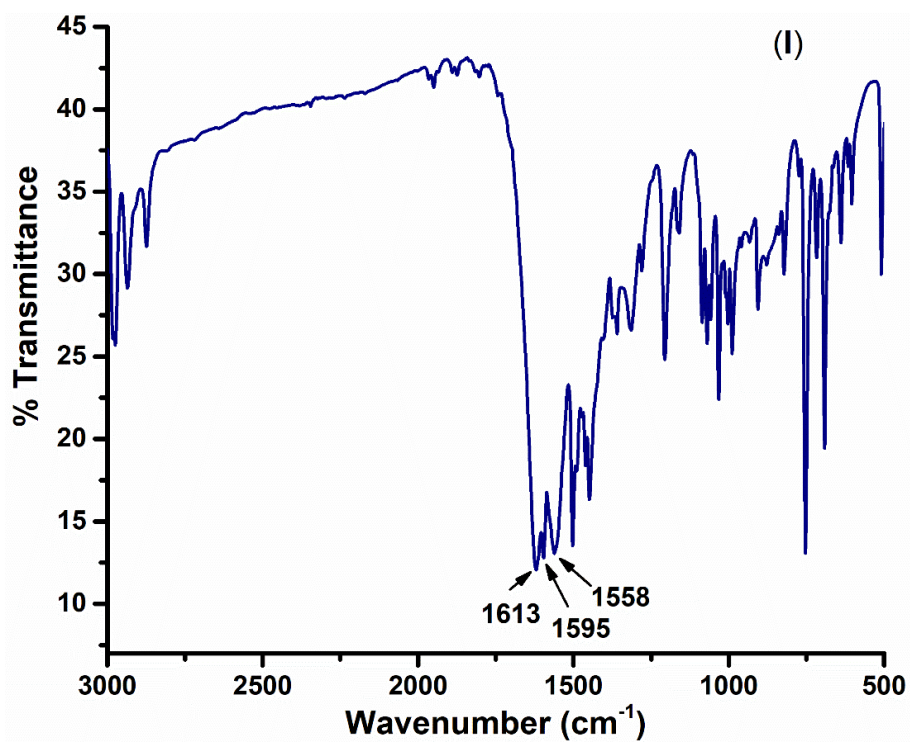


Fig. S4 IR spectrum of  $H_6btzh(fp)_3$  (I)

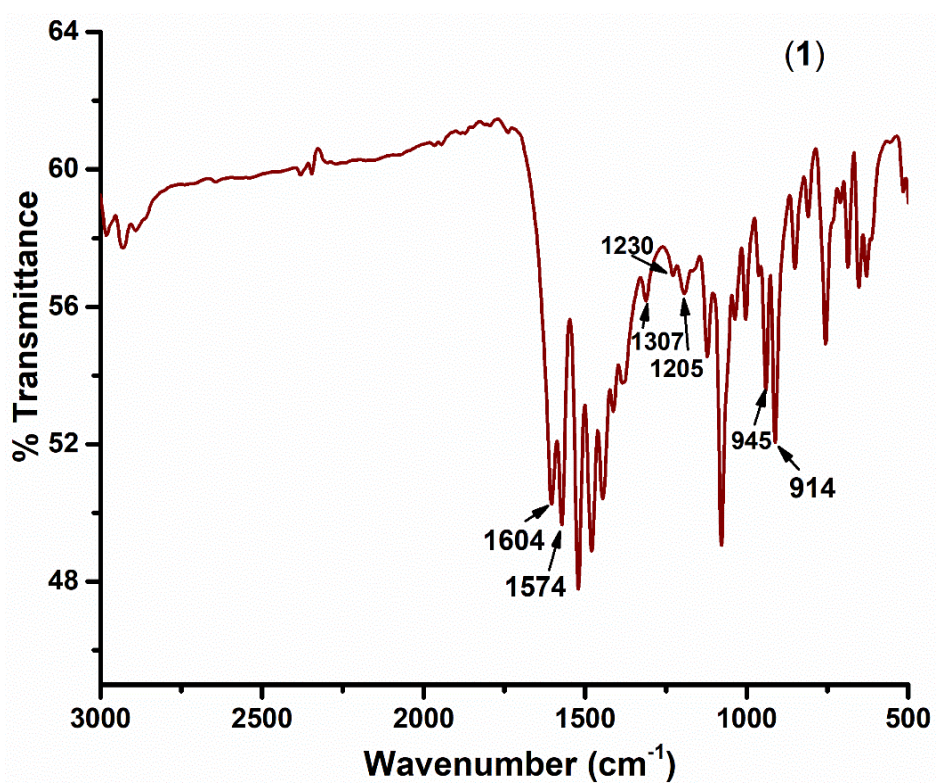


Fig. S5 IR spectrum of  $[Mo^{VI}O_2(H_2O)_3]btzh(fp)_3$  (1).

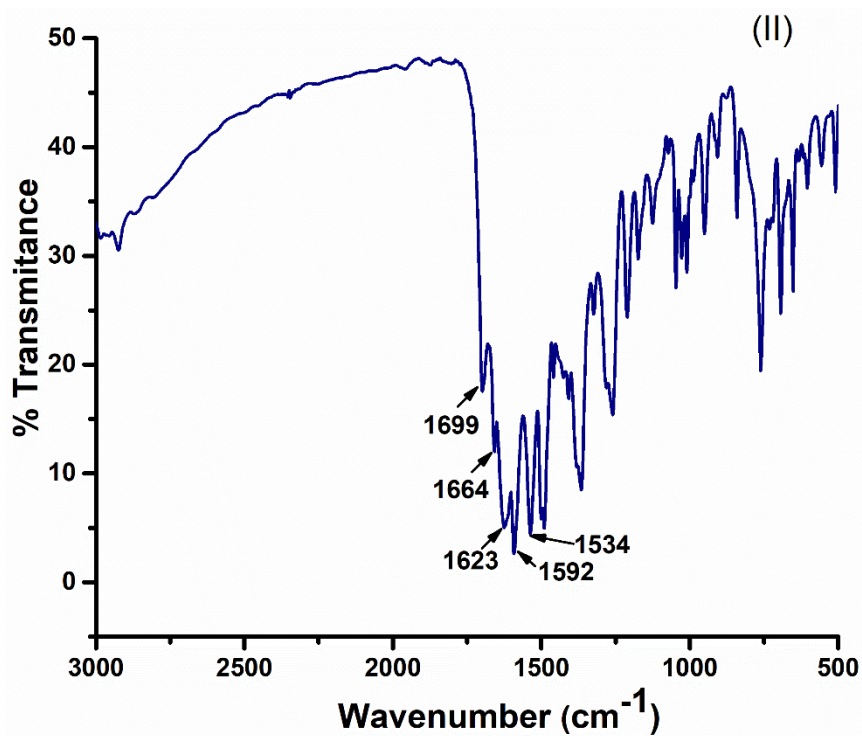


Fig. S6 IR spectrum of  $H_6btzh(mp)_3$  (II).

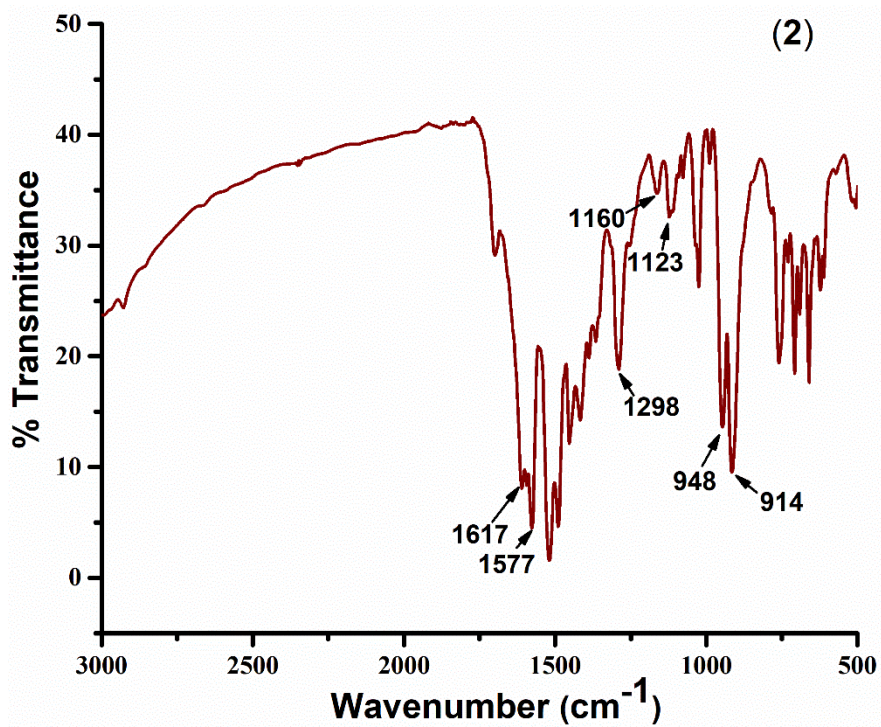


Fig. S7 IR spectrum of  $[Mo^{VI}O_2(H_2O)_3]btzh(mp)_3$  (2).

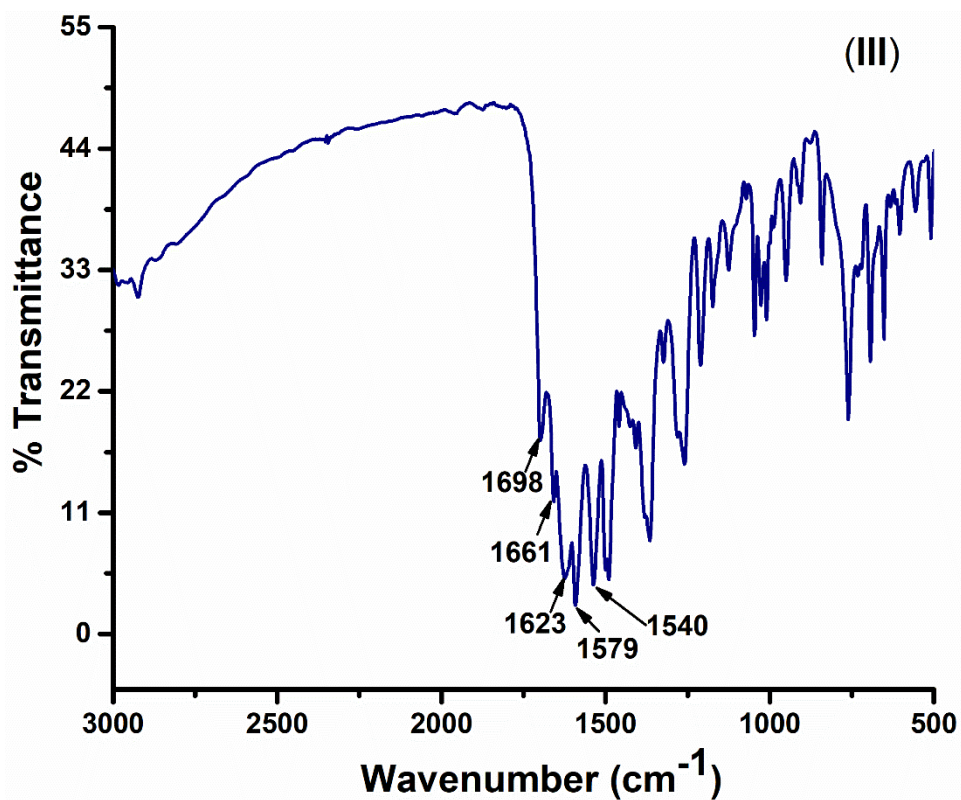


Fig. S8 IR spectrum of  $H_6btzh(ep)_3$  (III).

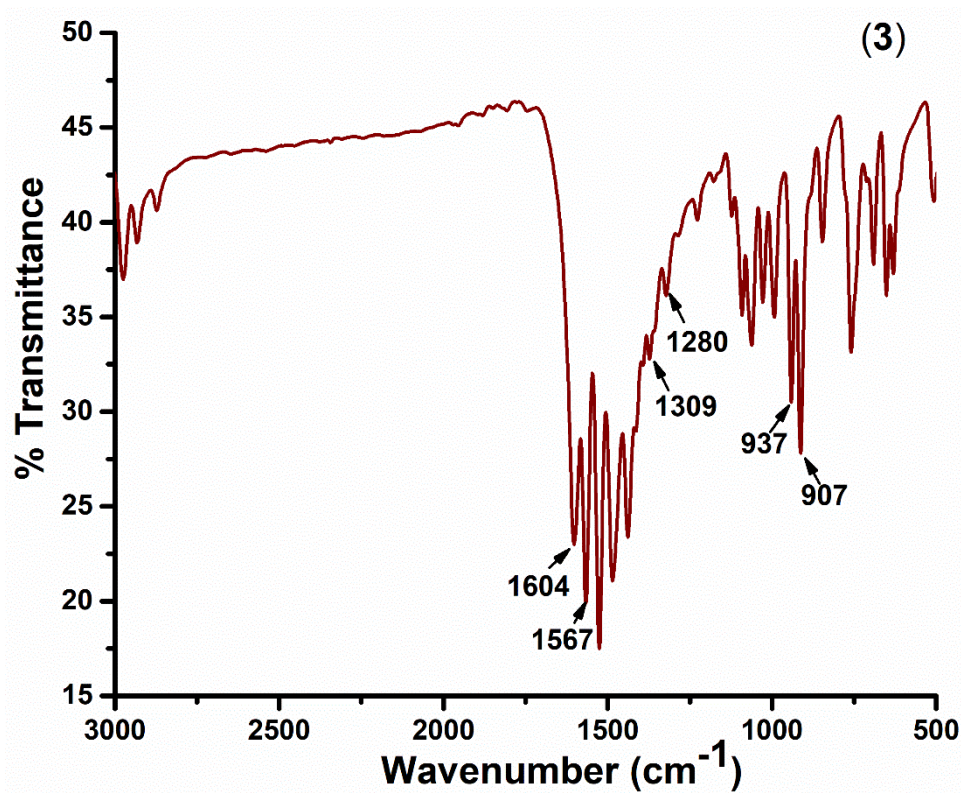


Fig. S9 IR spectrum of  $[Mo^{VI}O_2(H_2O)_3]btzh(ep)_3$  (3).



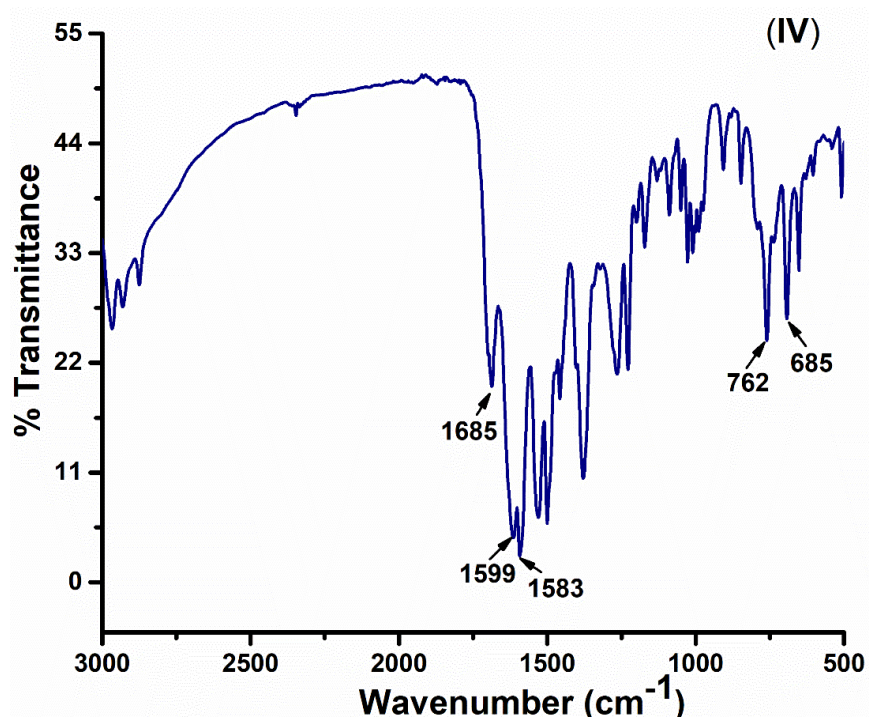


Fig. S10 IR spectrum of  $H_6btzh(pp)_3$  (IV).

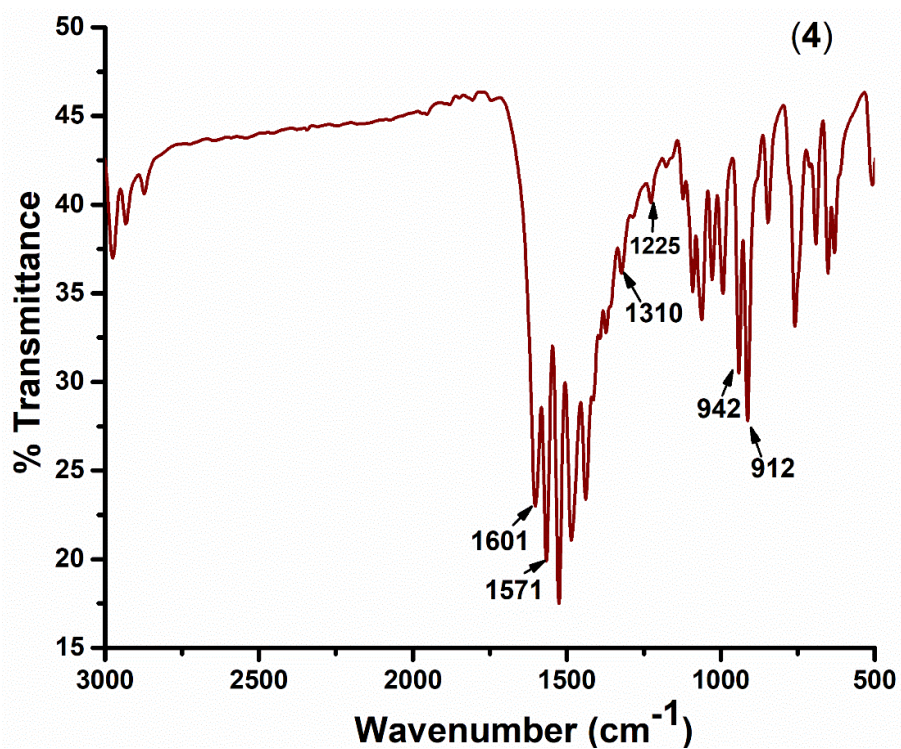


Fig. S11 IR spectrum of  $[Mo^{VI}O_2(H_2O)_3btzh(pp)_3]$  (4).

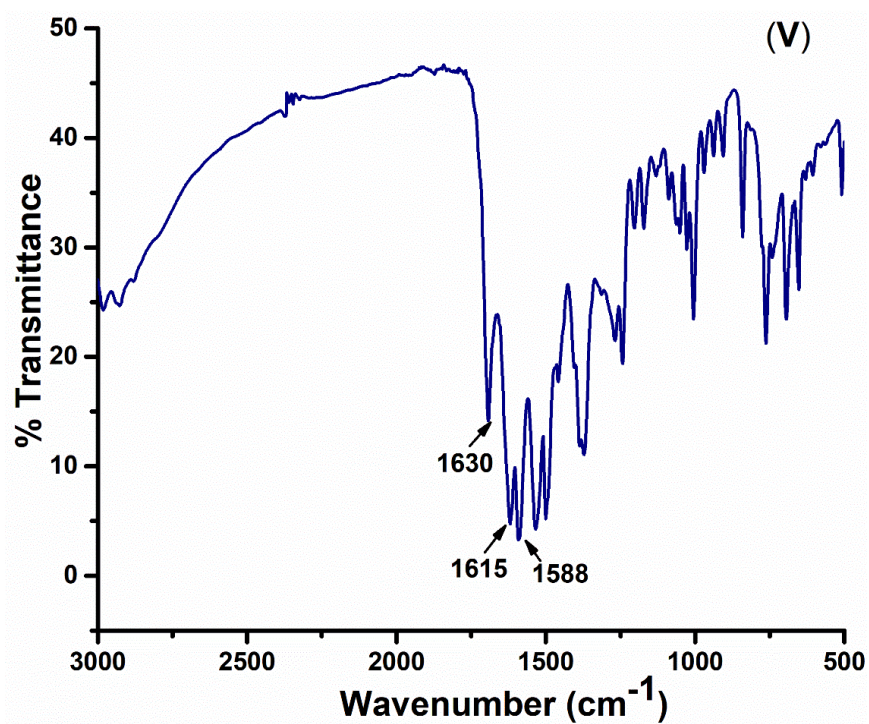


Fig. S12 IR spectrum of  $H_6btzh(php)_3$  (V).

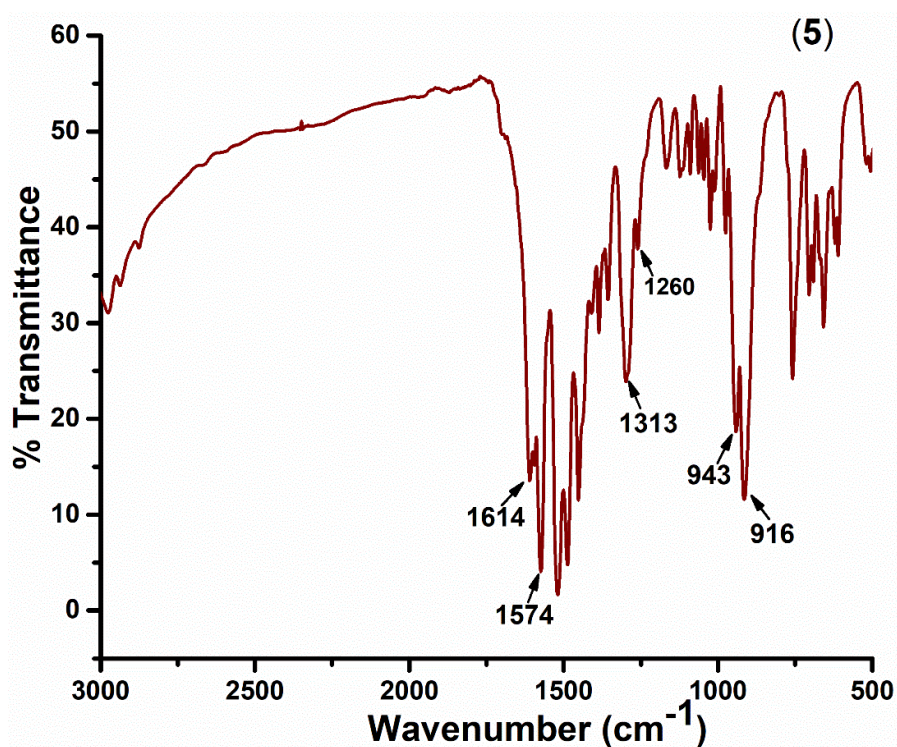
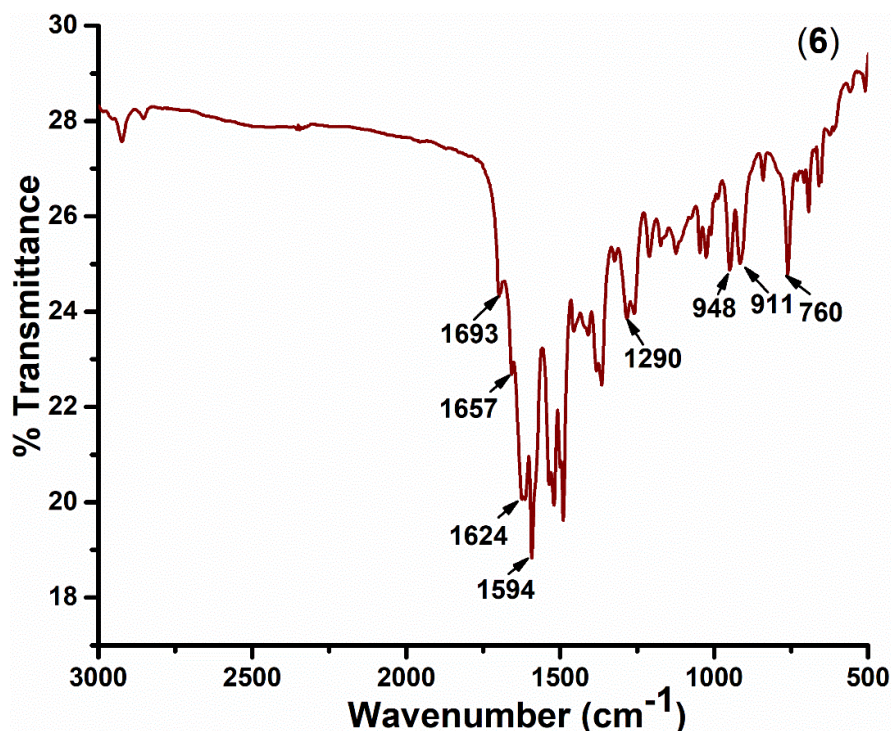


Fig. S13 IR spectrum of  $[Mo^{VI}O_2(H_2O)_3]btzh(php)_3$  (5).

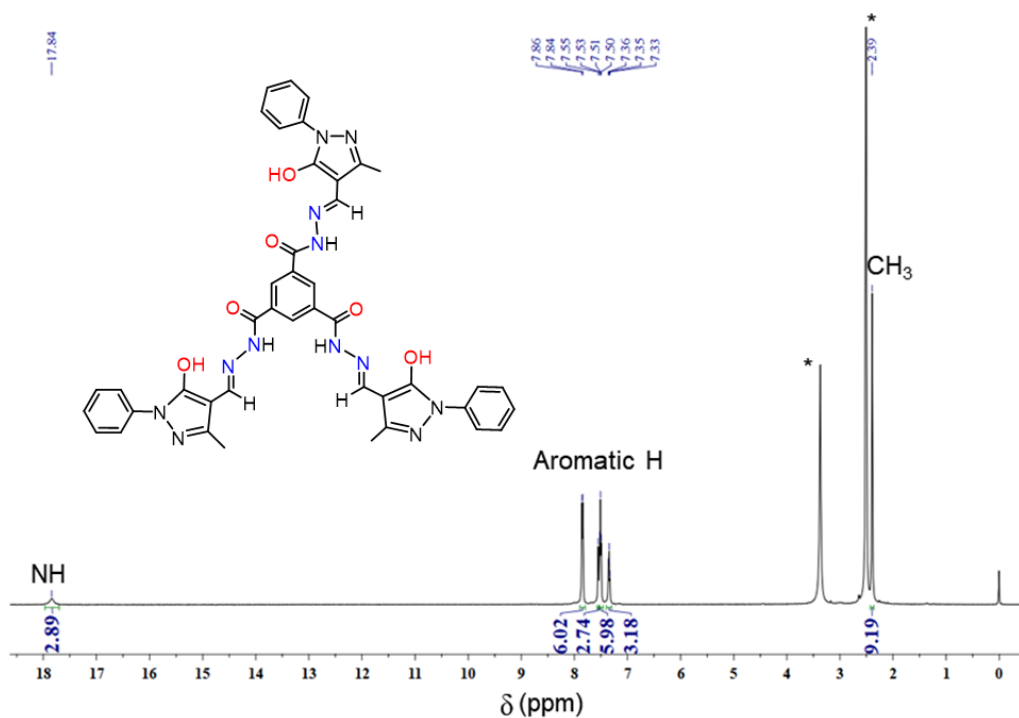




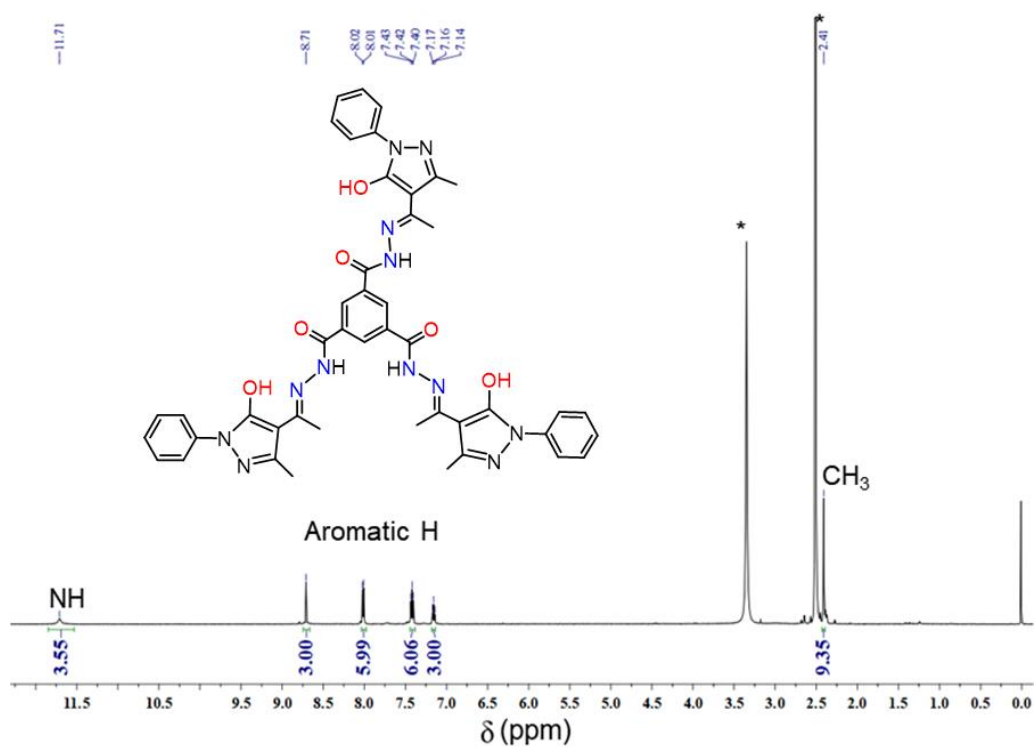
**Fig. S14** IR spectrum of mononuclear complex  $[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}\text{bthz}(\text{pp})_3]$  (**6**).

**Table S1** UV-visible spectral data of ligands and complexes.

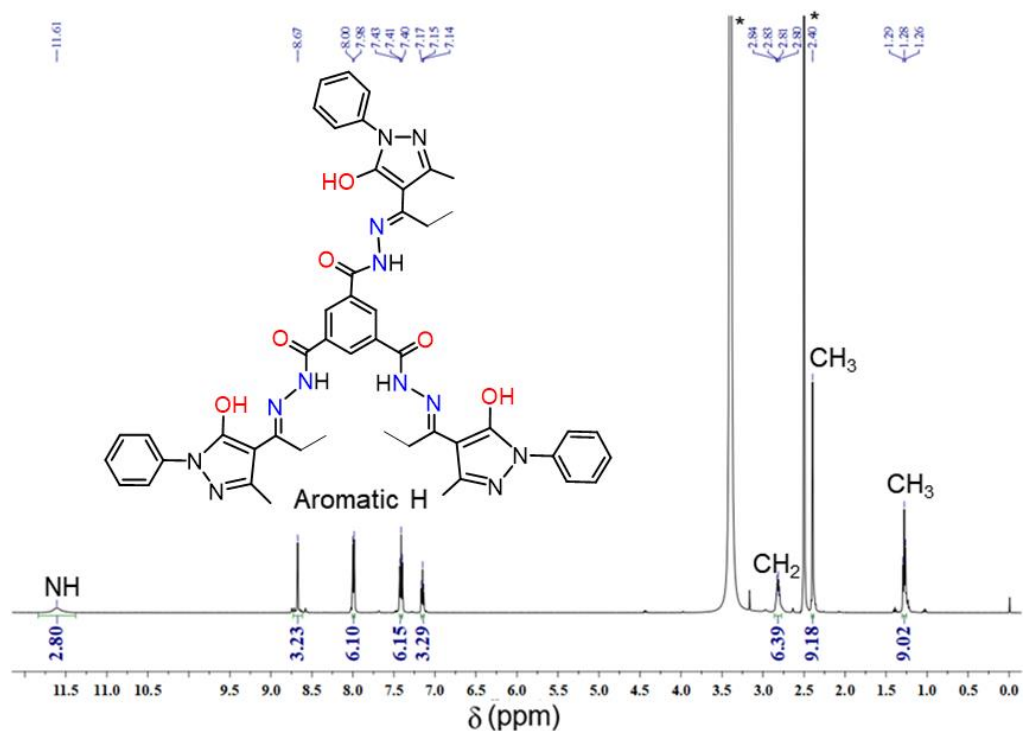
Compounds	$\lambda_{\text{max}}/\text{nm}$ ( $\epsilon/\text{M}^{-1}\text{cm}^{-1}$ )
$\text{H}_6\text{btzh}(\text{fp})_3$ ( <b>I</b> )	262 ( $4.73 \times 10^2$ ), 297 ( $2.73 \times 10^2$ ), 410 ( $0.64 \times 10^2$ )
$[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{bthz}(\text{fp})_3]$ ( <b>1</b> )	262 ( $4.28 \times 10^3$ ), 328 ( $2.22 \times 10^3$ ), 417 ( $1.07 \times 10^3$ )
$\text{H}_6\text{btzh}(\text{mp})_3$ ( <b>II</b> )	258 ( $4.26 \times 10^2$ ), 304 ( $2.87 \times 10^2$ ), 373 ( $2.98 \times 10^2$ )
$[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{bthz}(\text{mp})_3]$ ( <b>2</b> )	258 ( $2.76 \times 10^3$ ), 334 ( $1.92 \times 10^3$ ), 420 ( $7.48 \times 10^2$ )
$\text{H}_6\text{btzh}(\text{ep})_3$ ( <b>III</b> )	259 ( $3.87 \times 10^2$ ), 286 ( $3.73 \times 10^2$ ), 370 ( $3.84 \times 10^2$ ),
$[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{bthz}(\text{ep})_3]$ ( <b>3</b> )	259 ( $4.10 \times 10^3$ ), 328 ( $3.59 \times 10^3$ ), 418 ( $1.06 \times 10^3$ )
$\text{H}_6\text{tzh}(\text{pp})_3$ ( <b>IV</b> )	258 ( $4.32 \times 10^2$ ), 310 ( $2.75 \times 10^2$ ), 372 ( $0.59 \times 10^2$ )
$[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{bthz}(\text{pp})_3]$ ( <b>4</b> )	258 ( $3.56 \times 10^3$ ), 331 ( $3.19 \times 10^3$ ), 418 ( $1.10 \times 10^3$ )
$\text{H}_6\text{tzh}(\text{php})_3$ ( <b>V</b> )	258 ( $4.66 \times 10^2$ ), 297 ( $2.64 \times 10^2$ ), 411 ( $0.66 \times 10^2$ )
$[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{bthz}(\text{php})_3]$ ( <b>5</b> )	259 ( $3.12 \times 10^3$ ), 339 ( $2.64 \times 10^3$ ), 431 ( $1.25 \times 10^3$ )



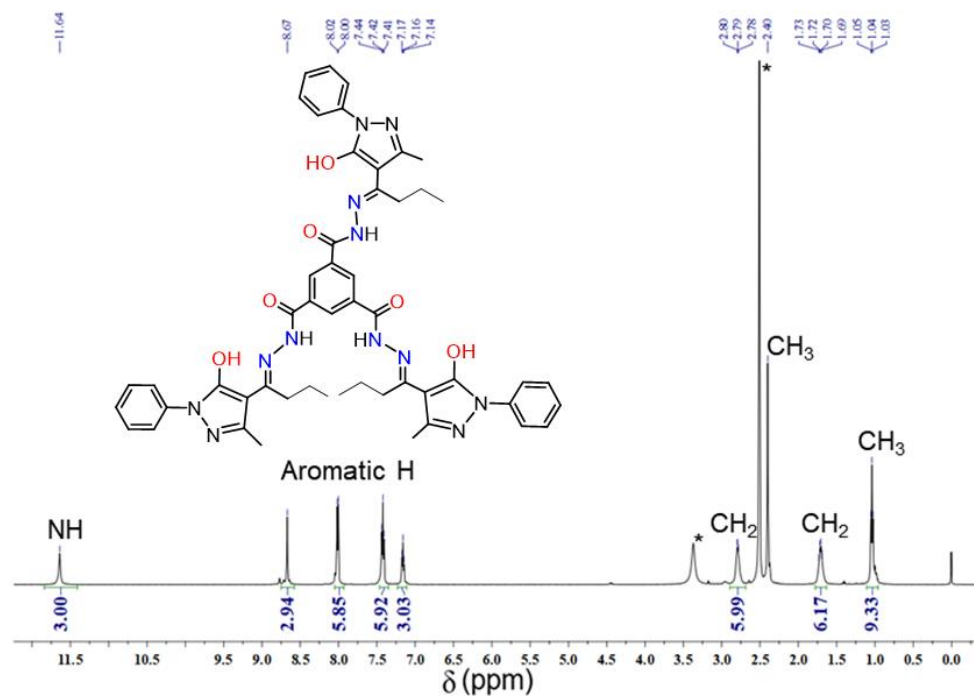
**Fig. S15**  $^1\text{H}$  NMR spectrum of ligand  $\text{H}_6\text{tzh}(\text{fp})_3$  (**I**) recorded in  $\text{DMSO-d}_6$ . \* indicates the proton impurity signal present in  $\text{DMSO-d}_6$  at  $\delta = 2.5$  ppm and that of moisture at  $\delta = 3.33$  ppm.



**Fig. S16**  $^1\text{H}$  NMR spectrum of ligand  $\text{H}_6\text{tzh}(\text{mp})_3$  (**II**) recorded in  $\text{DMSO-d}_6$ . \* indicates the proton impurity signal present in  $\text{DMSO-d}_6$  at  $\delta = 2.5$  ppm and that of moisture at  $\delta = 3.33$  ppm.

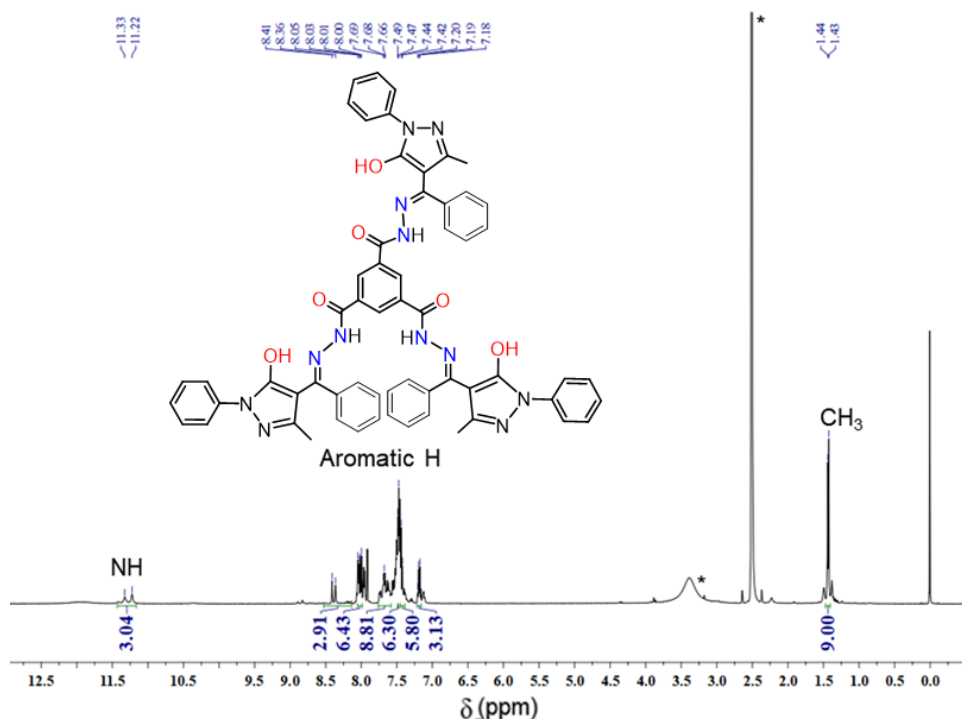


**Fig. S17**  $^1H$  NMR spectrum of ligand  $H_6tzh(ep)_3$  (**III**) recorded in  $DMSO-d_6$ . \* indicates the proton impurity signal present in  $DMSO-d_6$  at  $\delta = 2.5$  ppm and that of moisture at  $\delta = 3.33$  ppm.

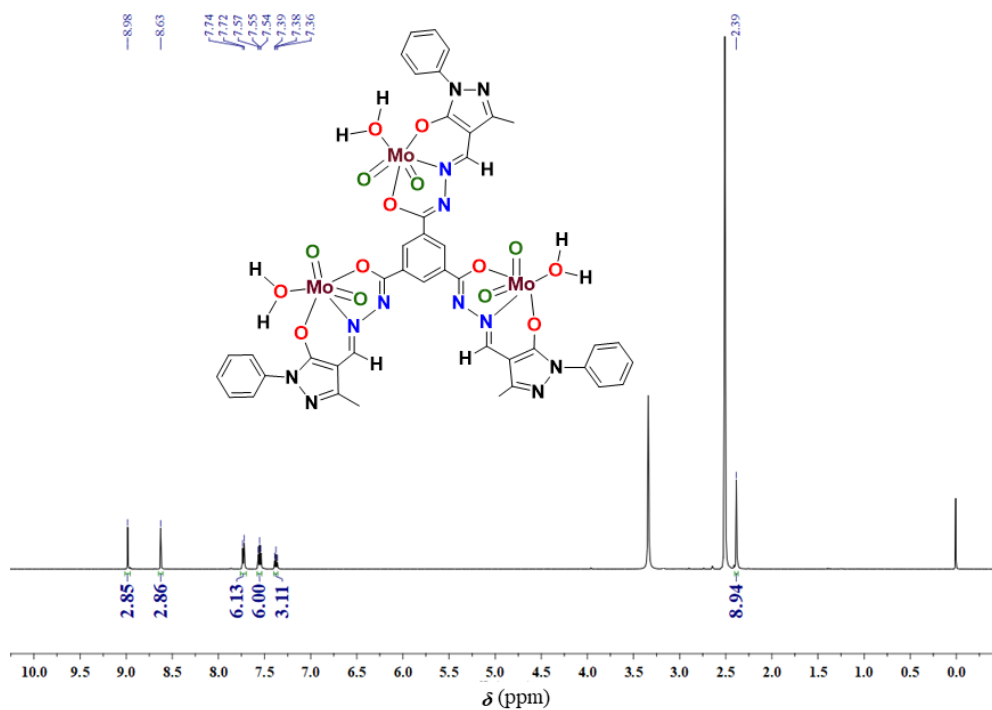


**Fig. S18**  $^1H$  NMR spectrum of ligand  $H_6tzh(pp)_3$  (**IV**) recorded in  $DMSO-d_6$ . \* indicates the proton impurity signal present in  $DMSO-d_6$  at  $\delta = 2.5$  ppm and that of moisture at  $\delta = 3.33$  ppm.

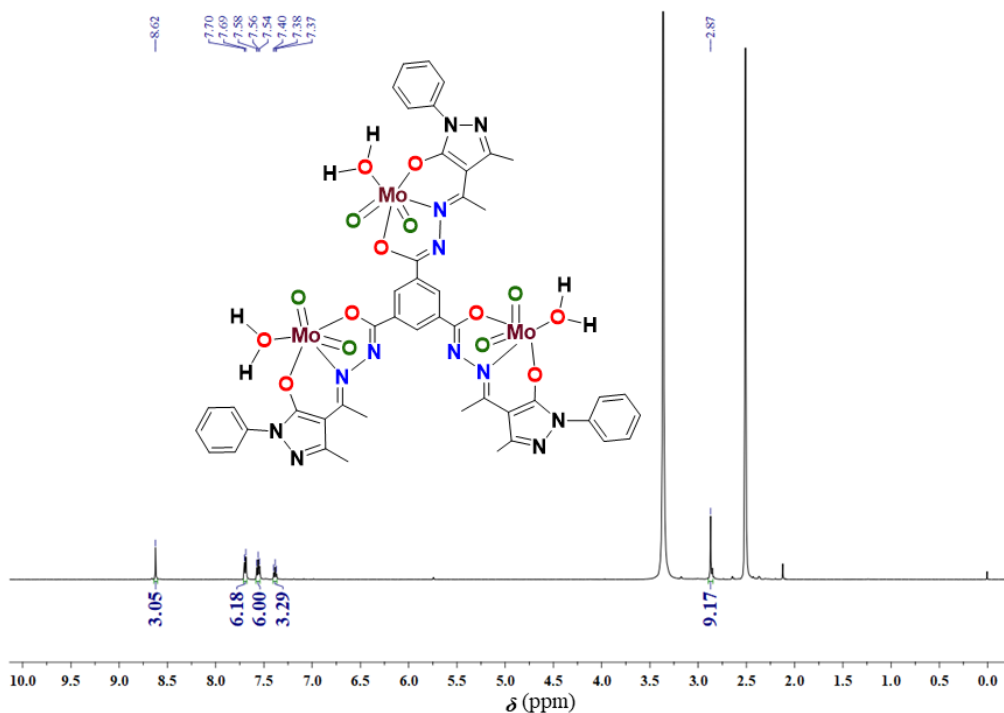




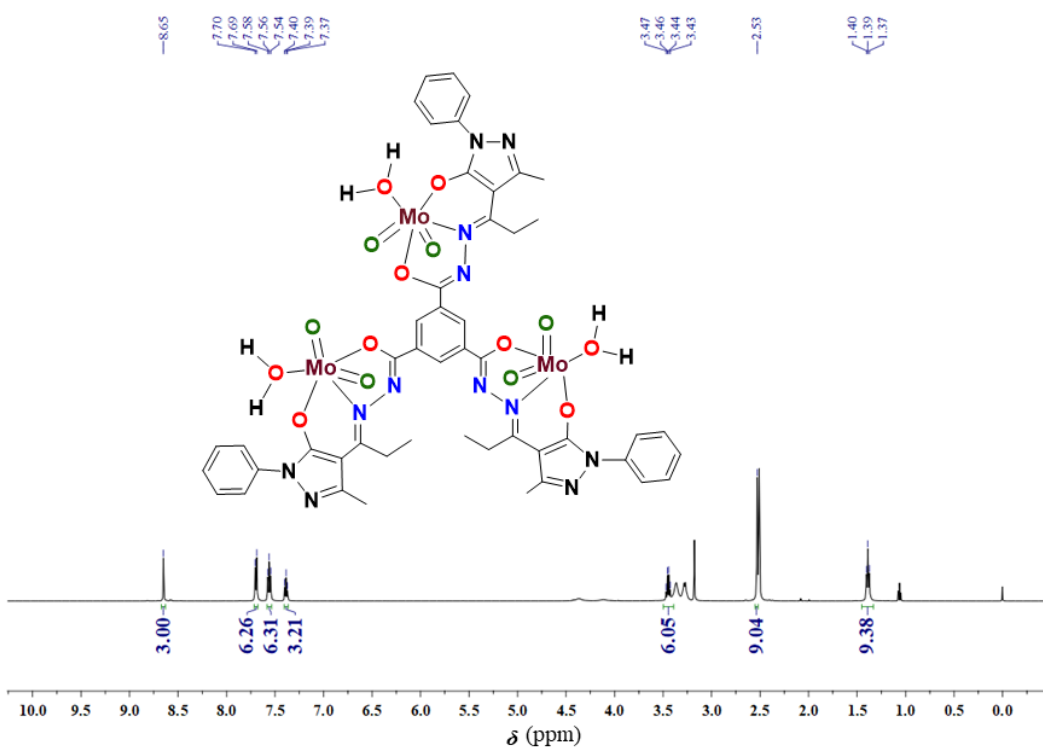
**Fig. S19**  $^1H$  NMR spectrum of ligand  $H_6tzh(php)_3$  (**V**) recorded in  $DMSO-d_6$ . \* indicates the proton impurity signal present in  $DMSO-d_6$  at  $\delta = 2.5$  ppm and that of moisture at  $\delta = 3.33$  ppm.



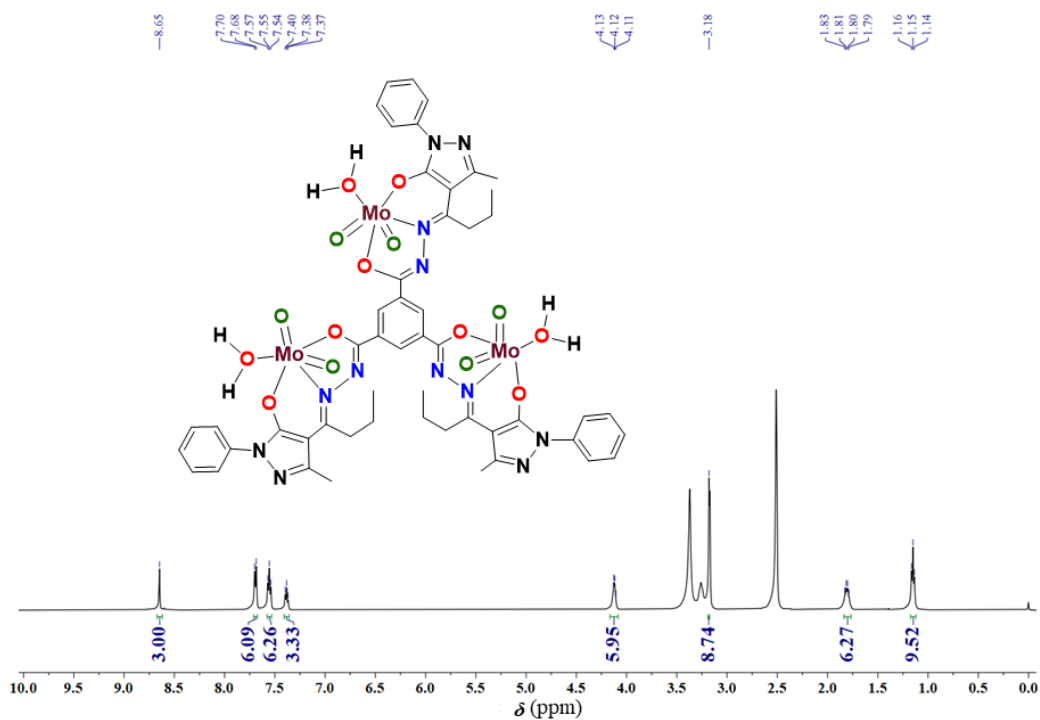
**Fig. S20.**  $^1H$  NMR spectrum of  $[Mo^{VI}O_2(H_2O)_3tzh(fp)_3]$  (**1**) recorded in  $DMSO-d_6$ .



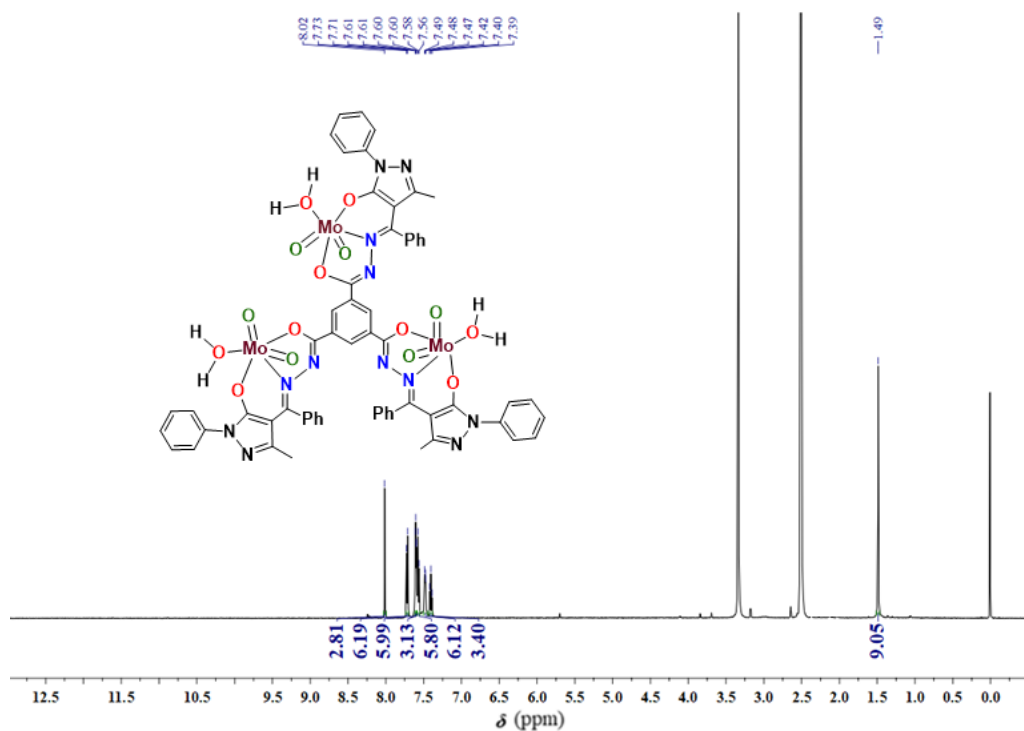
**Fig. 21** <sup>1</sup>H NMR spectrum of [Mo<sup>VI</sup>O<sub>2</sub>(H<sub>2</sub>O)]<sub>3</sub>thz(mp)<sub>3</sub> (**2**) recorded in DMSO-d<sub>6</sub>.



**Fig. 22** <sup>1</sup>H NMR spectrum of {Mo<sup>VI</sup>O<sub>2</sub>(H<sub>2</sub>O)}<sub>3</sub>thz(ep)<sub>3</sub> (**3**) recorded in DMSO-d<sub>6</sub>.

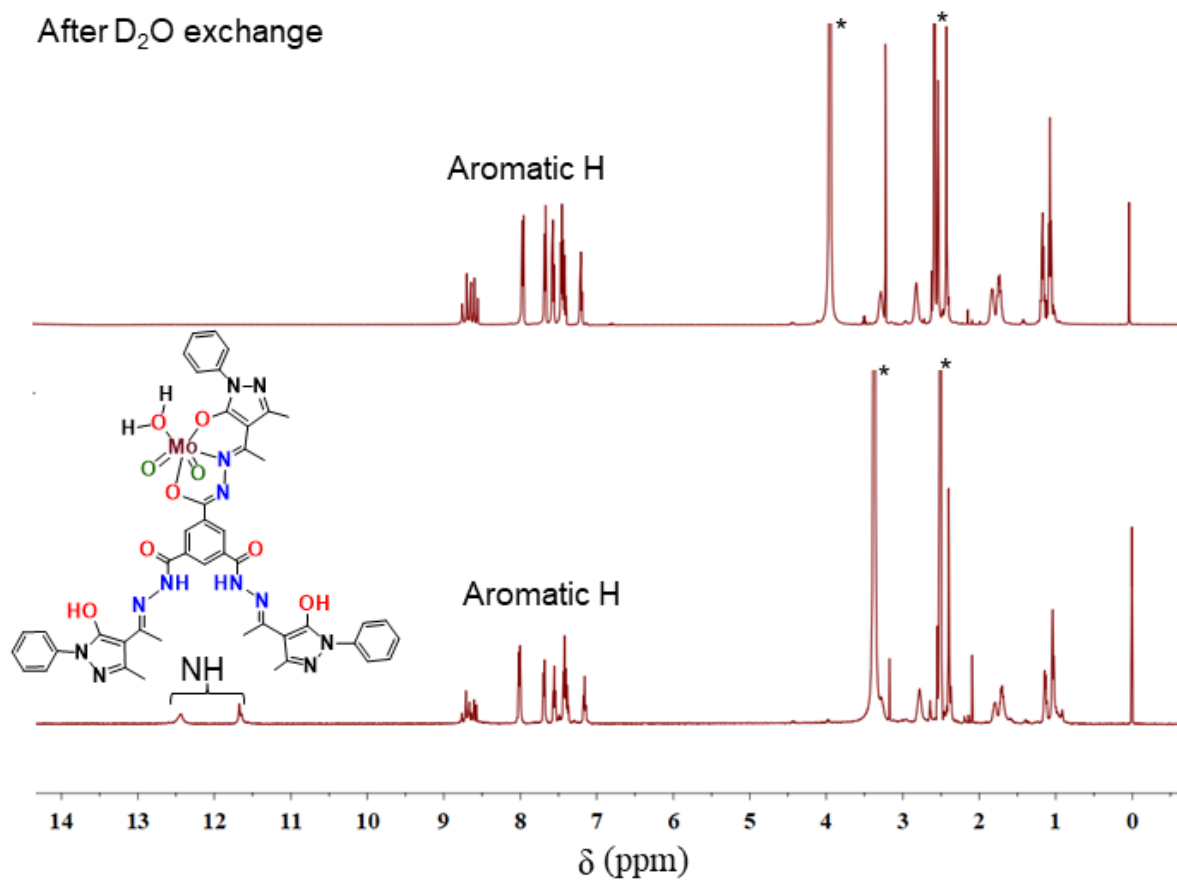


**Fig. 23**  $^1\text{H}$  NMR spectrum of  $[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{thz}(\text{pp})_3]$  (**4**) recorded in  $\text{DMSO-d}_6$ .



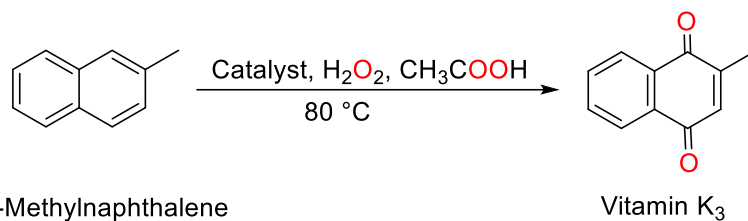
**Fig. 24**  $^1\text{H}$  NMR spectrum of  $[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{thz}(\text{bp})_3]$  (**5**) recorded in  $\text{DMSO-d}_6$ .





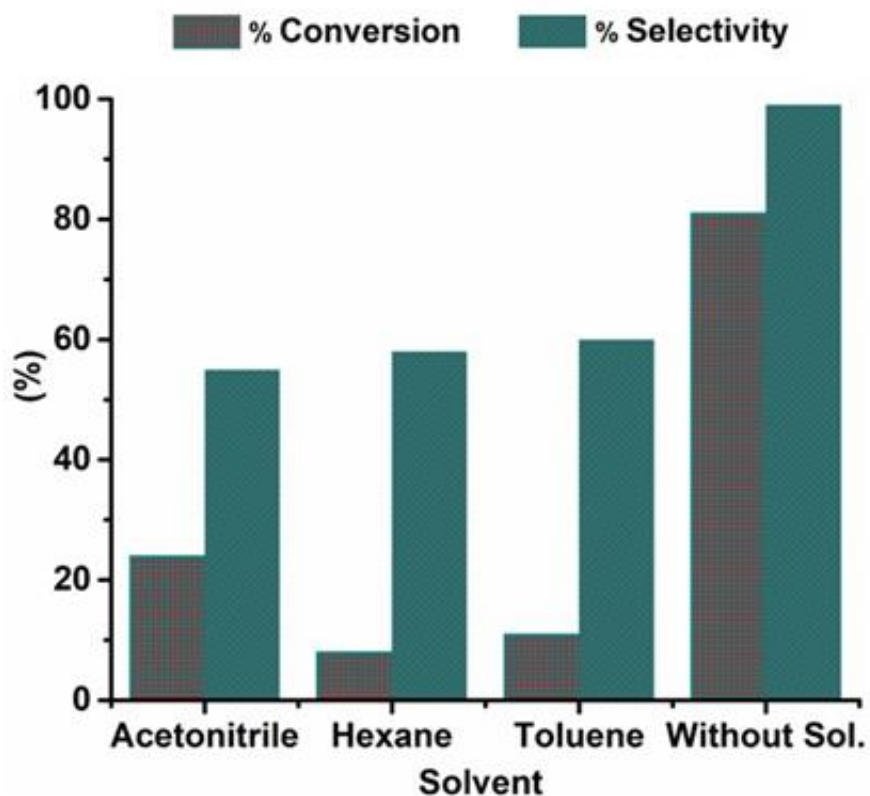
**Fig. 25** <sup>1</sup>H NMR spectrum of mononuclear complex **6** recorded in DMSO-d<sub>6</sub> before and after exchange with D<sub>2</sub>O.

**Table S2** Oxidation of 2-methylnaphthalene (0.71 g, 5 mmol) using  $[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{bthz}(\text{fp})_3]$  (**1**) as a catalyst under different reaction conditions.



S. No.	Catalyst [mg (mmol)]	CH <sub>3</sub> COOH (mL)	H <sub>2</sub> O <sub>2</sub> (mmol)	Solvent	Temp.	Time (h)	Conv. (%)	Selectivity (%)
1	3.0 (2.4×10 <sup>-3</sup> )	2	15	-	80	2	14	>99
2	3.0 (2.4×10 <sup>-3</sup> )	2	15	-	80	3	23	>99
2	3.0 (2.4×10 <sup>-3</sup> )	2	15	-	80	4	30	>99
3	3.0 (2.4×10 <sup>-3</sup> )	2	15	-	80	5	49	>99
4	4.0 (3.2×10 <sup>-3</sup> )	2	15	-	80	5	61	>99
5	5.0 (4.0×10 <sup>-3</sup> )	2	15	-	80	5	70	>99
6	5.0 (4.0×10 <sup>-3</sup> )	1	20	-	80	5	62	87
<b>7<sup>a</sup></b>	<b>5.0 (4.0×10<sup>-3</sup>)</b>	<b>2</b>	<b>20</b>	<b>-</b>	<b>80</b>	<b>5</b>	<b>81</b>	<b>&gt;99</b>
8	5.0 (4.0×10 <sup>-3</sup> )	3	20	-	80	5	85	>99
9	5.0 (4.0×10 <sup>-3</sup> )	2	25	-	80	5	86	>99
10	5.0 (4.0×10 <sup>-3</sup> )	2	20	-	70	5	69	>99
11	5.0 (4.0×10 <sup>-3</sup> )	2	20	-	90	5	84	>99
12	-	2	20	-	80	5	51	71
13	-	2	-	-	80	5	12	63

<sup>a</sup>Optimized reaction conditions among the different sets of reactions carried out.



**Fig. S26** Effect of different solvents on the oxidation of 2-methylnaphthalene and selectivity of the formation of 2-methyl-1,4-naphthoquinone [Reaction conditions: catalyst (5.0 mg,  $4.0 \times 10^{-3}$  mmol), 2-methylnaphthalene (0.71 g, 5 mmol), 30% aqueous  $\text{H}_2\text{O}_2$  (2.31 g, 20 mmol) and  $\text{CH}_3\text{COOH}$  (2 mL) at 80 °C.



**Table S3** Oxidation of styrene (0.52 g, 5 mmol) using [ $\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{bthz}(\text{fp})_3$ ] (**1**) as a catalyst in 1.5 h reaction time under different reaction conditions.

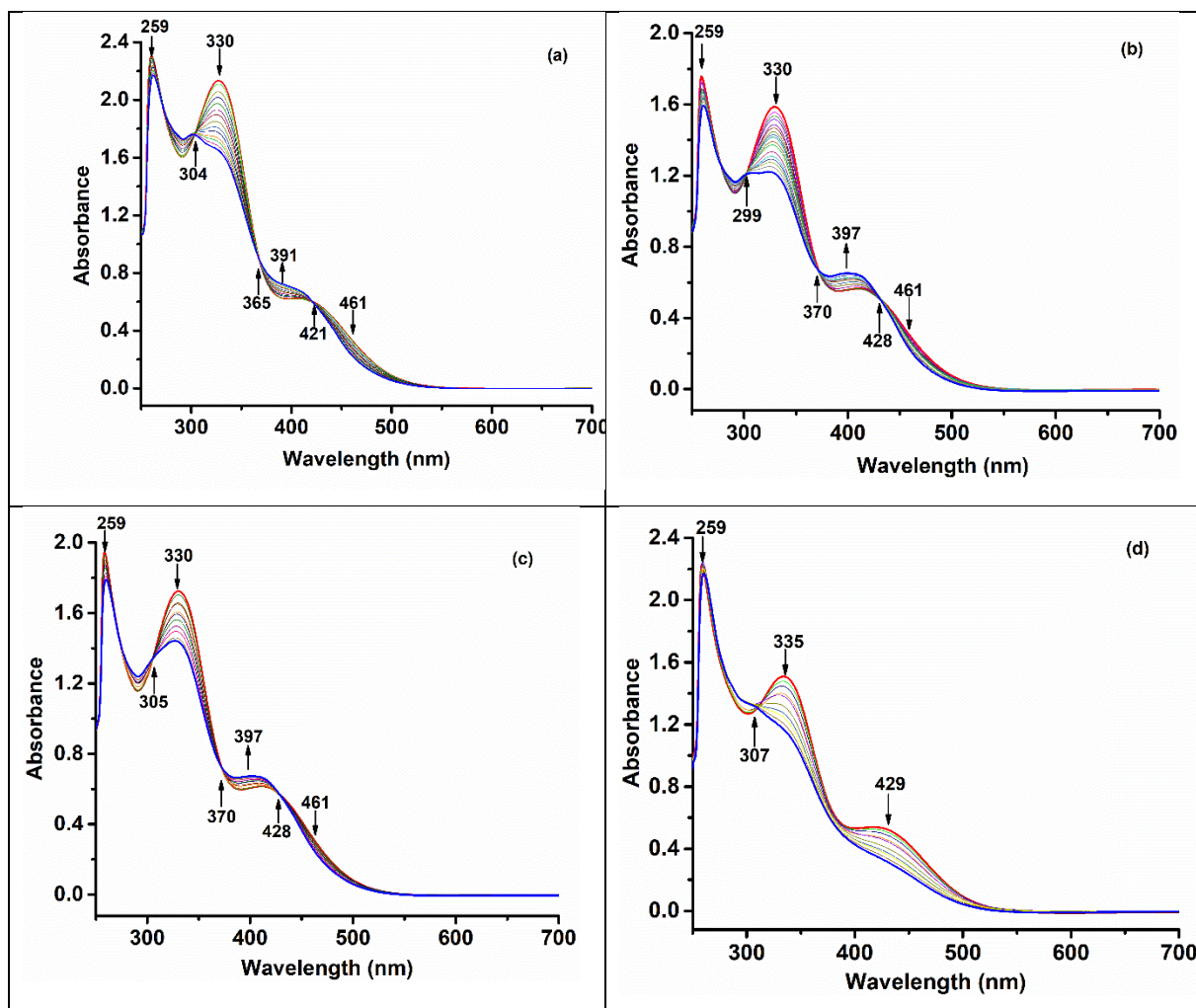
Entry	Catalyst (mg, mmol)	H <sub>2</sub> O <sub>2</sub> (g, mmol)	NaHCO <sub>3</sub> (g, mmol)	MeCN/H <sub>2</sub> O (V/V)	Temp. (°C)	% Conv.
1	0.5, 4.0×10 <sup>-4</sup>	1.13, 10	0.168, 2	2:2	60	59
2	1.0, 8.0×10 <sup>-4</sup>	1.13, 10	0.168, 2	2:1	60	79
3	1.0, 8.0×10 <sup>-4</sup>	1.13, 10	0.168, 2	4:3	60	81
4	1.0, 8.0×10 <sup>-4</sup>	1.13, 10	0.168, 2	3:1	60	77
5	1.0, 8.0×10 <sup>-4</sup>	1.13, 10	0.168, 2	5:0	60	69
6	1.0, 8.0×10 <sup>-4</sup>	1.13, 10	0.168, 2	3:2	50	71
7	1.0, 8.0×10 <sup>-4</sup>	1.13, 10	0.126, 1.5	3:2	70	93
<b>8<sup>a</sup></b>	<b>1.0, 8.0×10<sup>-4</sup></b>	<b>1.13, 10</b>	<b>0.168, 2</b>	<b>2:2</b>	<b>60</b>	<b>88</b>
9	1.5, 1.2×10 <sup>-3</sup>	1.13, 10	0.168, 2	2:2	60	89
10	1.0, 8.0×10 <sup>-4</sup>	0.565, 5	0.168, 2	2:2	60	62
11	1.0, 8.0×10 <sup>-4</sup>	1.69, 15	0.168, 2	2:2	60	91
12	1.0, 8.0×10 <sup>-4</sup>	1.13, 10	0.126, 1.5	2:2	60	76
13	1.0, 8.0×10 <sup>-4</sup>	1.13, 10	0.126, 2.5	2:2	70	92
14	-	1.13, 10	0.168, 2	3:2	60	44
15	-	1.13, 10	-	3:2	60	21
16	1.0, 8.0×10 <sup>-4</sup>	1.13, 10	-	3:2	60	31

<sup>a</sup> Optimized reaction conditions among the different sets of reactions carried out.

**Table S4** Oxidative bromination of thymol (1.50 g, 10 mmol) at room temperature using  $[\{\text{Mo}^{\text{VI}}\text{O}_2(\text{H}_2\text{O})\}_3\text{bthz}(\text{fp})_3]$  (**1**) as a catalyst under different reaction conditions.

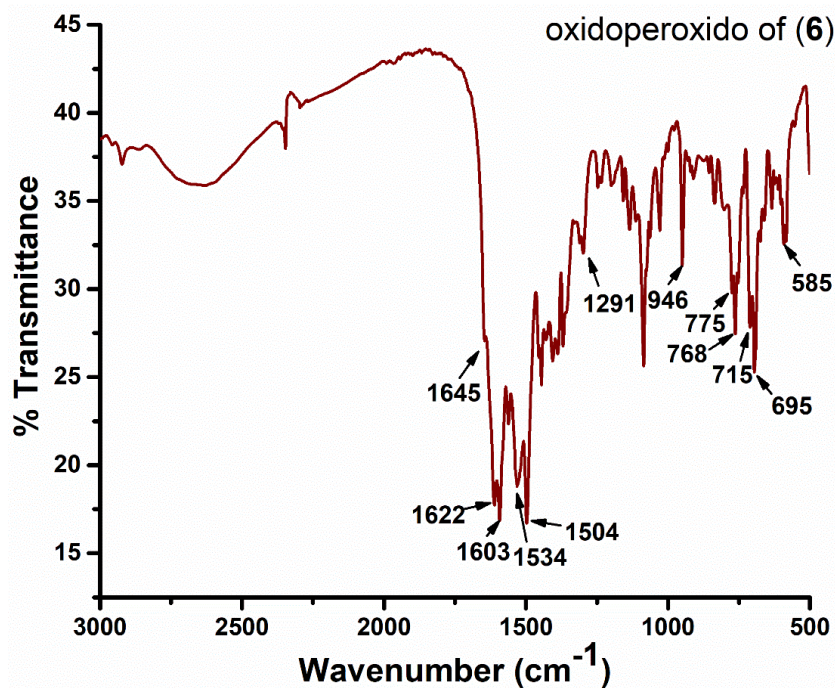
Sr. No.	Catalyst mg (mmol)	KBr (mmol)	H <sub>2</sub> O <sub>2</sub> (mmol)	HClO <sub>4</sub> (mmol)	Time (min)	Conv. (%)	TOF (h <sup>-1</sup> )	2-Brth	4-Brth	2,4-Brth
1.	1.0 (8.00×10 <sup>-4</sup> )	10	10	10	30	31	7948	13	71	16
2.	1.0 (8.00×10 <sup>-4</sup> )	10	10	10	60	41	5256	14	78	8
3.	1.0 (8.00×10 <sup>-4</sup> )	10	15	10	30	52	13332	17	79	4
4.	1.0 (8.00×10 <sup>-4</sup> )	10	15	10	60	61	7820	18	70	12
5.	1.0 (8.00×10 <sup>-4</sup> )	15	10	15	60	57	7307	12	84	4
6.	2.0 (1.60×10 <sup>-3</sup> )	10	10	10	30	39	9999	17	74	9
7.	2.0 (1.60×10 <sup>-3</sup> )	10	10	10	60	51	6538	12	82	6
8.	2.0 (1.60×10 <sup>-3</sup> )	10	10	20	90	61	5215	13	79	8
9	2.0 (1.60×10 <sup>-3</sup> )	15	15	15	30	63	16153	12	85	3
10	2.0 (1.60×10 <sup>-3</sup> )	15	15	15	60	77	9871	13	84	3
11	2.0 (1.60×10 <sup>-3</sup> )	15	20	20	30	81	20768	12	80	8
<b>12<sup>a</sup></b>	<b>2.0</b> (1.60×10 <sup>-3</sup> )	<b>15</b>	<b>20</b>	<b>20</b>	<b>60</b>	<b>98</b>	<b>12563</b>	<b>13</b>	<b>81</b>	<b>6</b>
13	2.0 (1.60×10 <sup>-3</sup> )	20	20	20	60	99	12691	11	60	29
14	3.0 (2.4×10 <sup>-3</sup> )	10	10	10	60	57	2435	17	75	8

<sup>a</sup>Optimized reaction conditions among the different sets of reactions carried out.



**Fig. S27** UV-Vis spectral changes obtained during the titration of complexes **2–5** with H<sub>2</sub>O<sub>2</sub>. (a) Spectra were recorded at every 2 min after the addition of one drop of 30% H<sub>2</sub>O<sub>2</sub> (0.830 g, 7.3 mmol) dissolved in 10 mL DMSO to a solution of **2** (0.001 g,  $7.81 \times 10^{-5}$  M) in 10 mL DMSO. (b) Spectra were recorded at every 2 min after the addition of one drop of 30% H<sub>2</sub>O<sub>2</sub> (0.830 g, 7.3 mmol) dissolved in 10 mL DMSO to a solution of **3** (0.001 g,  $7.57 \times 10^{-5}$  M) in 10 mL DMSO. (c) Spectra were recorded at every 2 min after the addition of one drop of 30% H<sub>2</sub>O<sub>2</sub> (0.830 g, 7.3 mmol) dissolved in 10 mL DMSO to a solution of **4** (0.001 g,  $7.33 \times 10^{-5}$  M) in 10 mL DMSO. (d) Spectra were recorded at every 2 min after the addition of one drop of 30% H<sub>2</sub>O<sub>2</sub> (0.830 g, 7.3 mmol) dissolved in 10 mL DMSO to a solution of **5** (0.001 g,  $6.82 \times 10^{-5}$  M) in 10 mL DMSO.





**Fig. S28** IR spectrum of oxidoperoxido complex of **6** isolated after stirring **6** with H<sub>2</sub>O<sub>2</sub> in MeOH.

### Energy table for the molecules in the catalytic cycle

All DFT computations were performed using the ORCA 4.2.1<sup>[1]</sup> quantum chemical program package. Geometries were optimized along the reaction profile diagram with the GGA (generalized gradient approximation) density functional BP86<sup>[2,3]</sup> in conjunction with the split valence basis sets def2-SVP<sup>[4]</sup>. The RI<sup>[5-7]</sup> (resolution-of-identity) approximation was applied to accelerate the overall calculations. Becke-Johnson (D3BJ) damping<sup>[8]</sup> was used to account for the noncovalent interactions by using atom-pairwise dispersion corrections. single point calculations were carried out with BP86/def2-TZVP<sup>[3]</sup> method to calculate Gibbs free energies on the BP86/def2-SVP geometries.

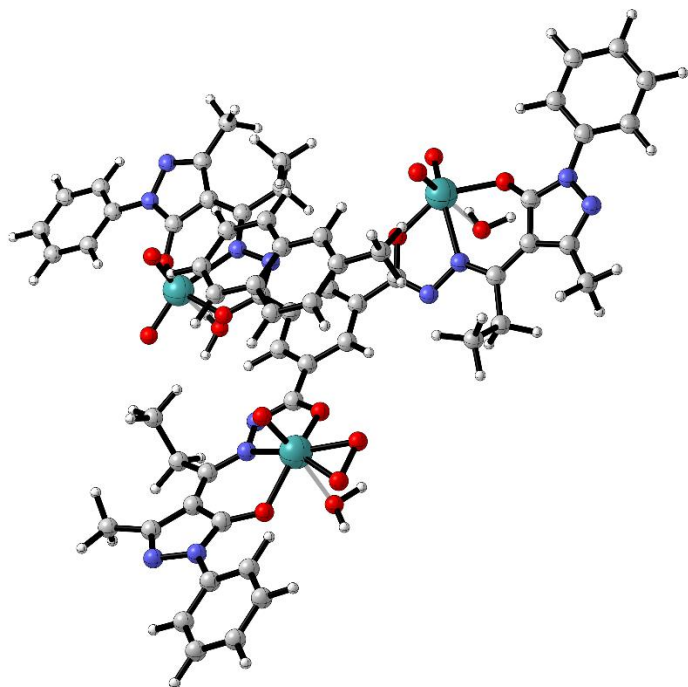
Molecule	E <sub>tot</sub> [a.u]	G <sub>298</sub> [a.u]
<b>1'</b>	-3850.788928	-3849.979133
<b>1'a</b>	-4114.1507270	-4113.33700
<b>1'b</b>	-4114.1487847	-4113.331751
<b>1'c</b>	-3925.972891	-3925.159704
<b>2'a</b>	-4078.68768	-4077.84274
<b>2'b</b>	-4078.679905	-4077.831577
<b>2'c</b>	-4351.402763	-4350.425618
<b>3'a</b>	-6424.515701	-6423.716332
<b>HCO<sub>3</sub><sup>-</sup></b>	-264.5917988	-264.592210
<b>HCO<sub>4</sub><sup>-</sup></b>	-339.7866902	-339.785643

<b>Styrene peroxide</b>	-385.016789	-384.913900
<b>Styrene</b>	-309.7767579	-309.677908
<b>CH<sub>3</sub>COOOH</b>	-304.3631954	-304.330059
<b>CH<sub>3</sub>COOH</b>	-229.1996011	-229.166645
<b>Naphthalene</b>	-425.3896532	-425.253043
<b>Phenol</b>	-307.608288	-307.535466
<b>o-Bromophenol</b>	-2881.448991	2881.388836
<b>HBr</b>	-2574.816593	-2574.829980
<b>H<sub>2</sub>O<sub>2</sub></b>	-151.629918	-151.626874
<b>H<sub>2</sub>O</b>	-76.46495919	-76.462013
<b>HOBr</b>	-2650.2472	-2650.259187

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### XYZ coordinates of the molecules present in the catalytic cycle

1'



O	-8.696218494	9.014075113	12.959080343
H	-8.104825702	9.249313284	13.704353067
H	-8.195237337	8.323351402	12.477594733
Mo	-10.232718150	7.533055994	14.247434679
O	-11.346821939	6.418711343	14.887886666
N	-12.181384986	9.225184692	12.507218238
O	-8.963340329	7.736372063	15.388294879
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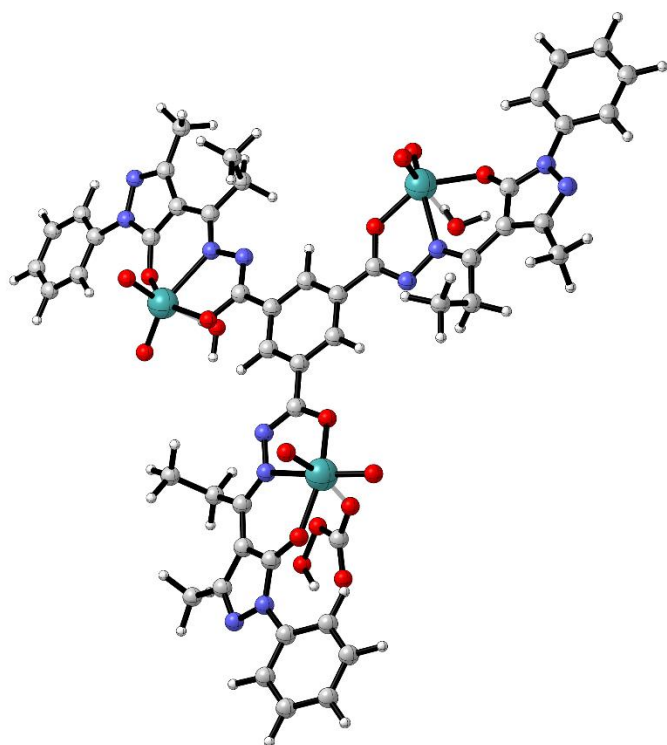
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C	-11.949544419	9.803725774	13.658302490
C	-11.733479830	7.307056311	11.317435660
C	-9.899277844	5.695179482	11.943056034
C	-11.006206507	6.080663076	11.141257693
C	-11.127019620	5.003112112	10.180840660
C	-8.336450769	3.711664434	11.890457970
C	-7.765582552	3.884584110	13.168513097
H	-8.178165558	4.621368267	13.866928765
C	-6.665801983	3.096384333	13.538695583
H	-6.223090239	3.233926507	14.536674977
C	-6.138531696	2.137196607	12.658964961
H	-5.274570958	1.525194388	12.958455982
C	-6.726100948	1.962920200	11.394133726
H	-6.326250637	1.210314332	10.697346298
C	-7.820411427	2.744786615	11.003121665
H	-8.298447140	2.623795845	10.022742132
C	-12.115451672	4.794620242	9.075116409
H	-11.985708141	5.534042134	8.257716754
H	-11.964271951	3.784325570	8.651391297
H	-13.160414787	4.876035035	9.434680549
C	-12.793219524	7.745947213	10.337437571
H	-12.716738011	8.845472174	10.232369060
H	-12.595533432	7.292367748	9.349788805
C	-14.209619844	7.388239904	10.827418054
H	-14.326185512	6.295746853	10.975857803
H	-14.419469447	7.887620501	11.792868121
C	-12.624862878	11.059803107	14.026982636
C	-12.323913844	11.678498573	15.252226677
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O	-15.090873688	14.741335779	9.444406497
H	-14.756964493	14.083705195	8.798704195
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C	-12.968036844	12.883418713	15.610911681
C	-13.909331556	13.463012292	14.743551675
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C	-14.217149610	12.836136852	13.515441857
C	-13.576472014	11.637993723	13.157081212
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H	-16.210486334	16.737162834	13.755707332
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C	-11.324755206	15.281881803	21.278659615
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C	-11.402528226	10.706733530	19.923760363
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1'a



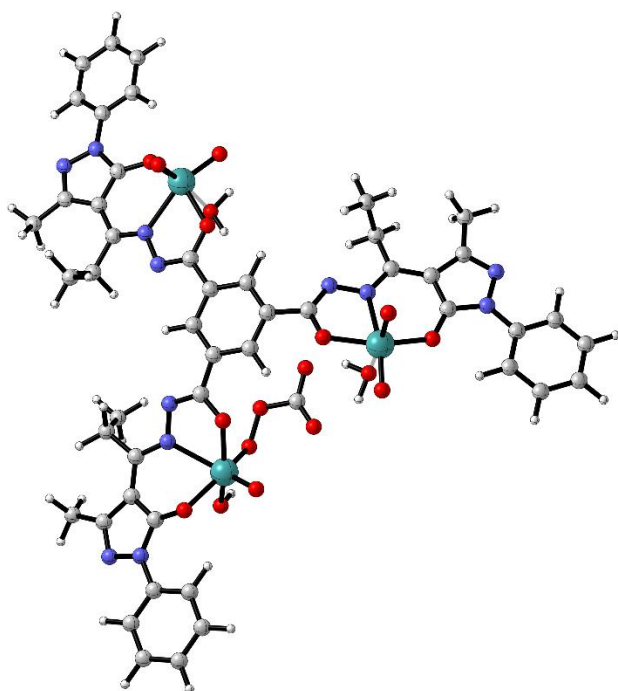
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H	-39.782013139	23.742564015	-26.356127827
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1'b



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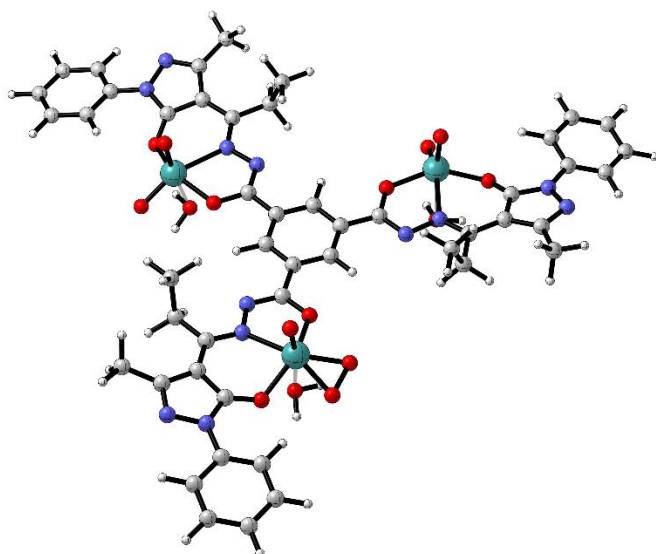


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C	4.202730638	-12.737680649	-17.903225494
H	4.001005143	-11.792318242	-18.450153728
H	4.856887120	-13.366910713	-18.537086668
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C	2.070615549	-11.081398673	-16.083927492
H	1.578834579	-10.108788984	-15.886217152
H	2.509649573	-11.046022861	-17.096999244
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H	1.475476574	-13.201726152	-16.130052116
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1'c



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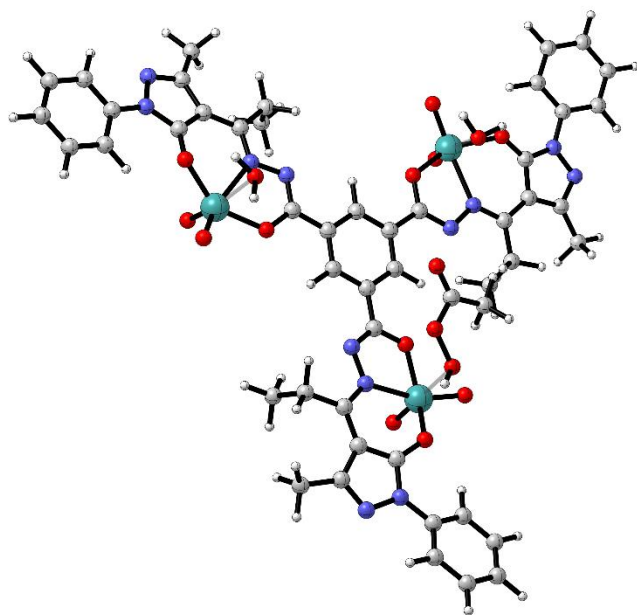
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2'a



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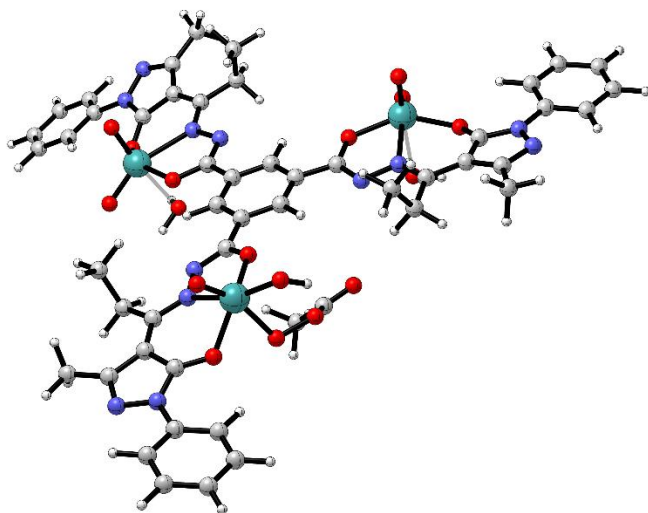
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C	-58.334449341	9.761379597	-51.068952150
C	-58.220996960	8.968297054	-52.229732046
H	-57.762185935	7.974692119	-52.184074806
C	-58.710795368	9.464711402	-53.447116470
H	-58.621849972	8.842680250	-54.350597195
C	-59.316333204	10.729775549	-53.518034822
H	-59.699133880	11.107719161	-54.477610801
C	-59.435073030	11.505612873	-52.351950707
H	-59.911237248	12.496723938	-52.392962192
C	-58.946867446	11.030164638	-51.128036668
H	-59.034342028	11.615281290	-50.203745049
C	-57.921371082	9.801912214	-46.249731808
H	-57.040694070	10.296291166	-45.788519611
H	-58.749814224	10.534582889	-46.282605630
H	-58.215910786	8.962044169	-45.589017748
C	-55.568763018	7.527228390	-45.974853604
H	-54.491845684	7.323281431	-45.817983203
H	-55.777784689	8.558186742	-45.639469507
C	-56.393533492	6.512602030	-45.161224049
H	-57.483182953	6.651046650	-45.317558254
H	-56.133460188	5.478555480	-45.460657800
H	-56.180645220	6.622124202	-44.078989376
O	-53.611149174	7.255137903	-50.698352835
H	-53.902113689	8.140468973	-50.384194823
O	-50.690443084	5.830921314	-49.463498104
C	-51.590936205	6.079540900	-50.232004706
O	-52.478497041	7.040802064	-49.760356718
C	-51.838148983	5.493288974	-51.590214525
H	-51.045865314	4.749922860	-51.785297515
H	-52.836509239	5.017112395	-51.638770760
H	-51.831525476	6.288645563	-52.361637207

2'b



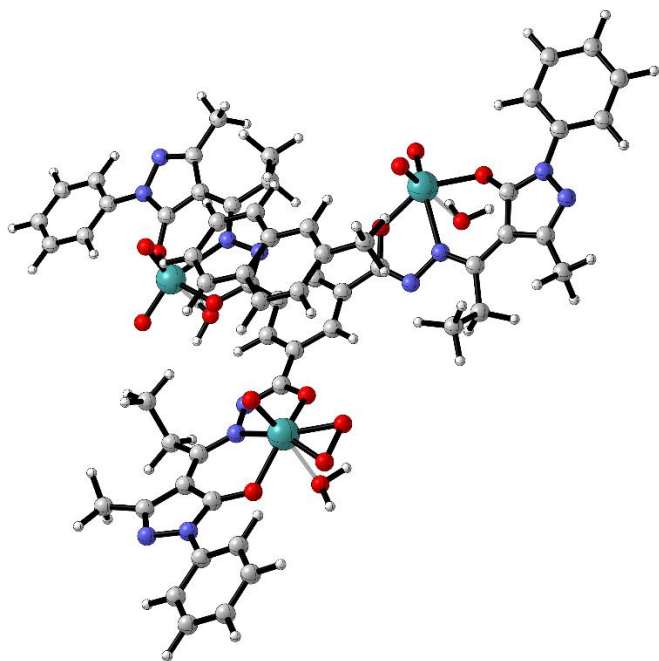
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H	-36.799478000	-16.493596000	-16.887641000
H	-36.866327000	-15.888978000	-18.301516000
Mo	-38.945119000	-17.800389000	-18.058184000
O	-40.068694000	-18.923507000	-18.664990000
N	-40.784834000	-15.325447000	-17.638862000
O	-37.711364000	-18.665084000	-17.229928000
N	-40.105805000	-15.919890000	-18.670182000
O	-39.837083000	-17.065368000	-16.451938000
N	-38.742523000	-16.481480000	-23.065168000
O	-37.973537000	-17.385130000	-19.753482000
N	-38.042440000	-17.179612000	-22.105569000
C	-40.618472000	-15.985453000	-16.521120000
C	-40.304399000	-15.412791000	-19.887995000
C	-38.513527000	-16.899305000	-20.849327000
C	-39.579224000	-15.971779000	-20.994231000
C	-39.655934000	-15.756882000	-22.424752000
C	-36.958433000	-18.015982000	-22.492622000
C	-36.483007000	-19.036729000	-21.643949000
H	-36.950073000	-19.212803000	-20.668527000
C	-35.407287000	-19.831259000	-22.067268000
H	-35.039218000	-20.627921000	-21.403022000
C	-34.811444000	-19.626908000	-23.322320000
H	-33.967722000	-20.255751000	-23.643940000
C	-35.304440000	-18.616377000	-24.165625000

H	-34.850088000	-18.450820000	-25.154107000
C	-36.373366000	-17.808082000	-23.758262000
H	-36.778993000	-17.016531000	-24.401712000
C	-40.590485000	-14.907384000	-23.230075000
H	-40.420701000	-13.824036000	-23.057073000
H	-40.422174000	-15.115818000	-24.303809000
H	-41.651604000	-15.119702000	-22.989105000
C	-41.309222000	-14.304479000	-20.078654000
H	-41.208368000	-13.609276000	-19.222549000
H	-41.075937000	-13.746455000	-21.002943000
C	-42.753122000	-14.840603000	-20.118043000
H	-42.895120000	-15.572896000	-20.938498000
H	-43.002460000	-15.342507000	-19.163242000
C	-41.283359000	-15.554655000	-15.278765000
C	-41.134907000	-16.320534000	-14.109016000
H	-40.527143000	-17.234614000	-14.123960000
O	-42.521152000	-9.423386000	-14.489317000
H	-42.228346000	-9.245712000	-15.408089000
H	-42.820013000	-8.546179000	-14.173282000
Mo	-44.719959000	-10.386690000	-15.203380000
C	-41.778066000	-15.913693000	-12.919113000
C	-42.546534000	-14.737459000	-12.895560000
H	-43.032211000	-14.400950000	-11.971044000
C	-42.674022000	-13.957501000	-14.064939000
C	-42.058084000	-14.372281000	-15.257705000
H	-42.163742000	-13.772010000	-16.170850000
O	-46.284505000	-10.996228000	-15.473043000
N	-43.880197000	-12.249514000	-12.867561000
O	-44.113546000	-9.775471000	-16.691771000
N	-44.566979000	-11.076227000	-13.022733000
O	-43.601654000	-12.019693000	-15.149768000
N	-47.113342000	-7.468713000	-11.622749000
O	-45.180943000	-8.660733000	-14.310743000
N	-46.605595000	-7.404499000	-12.902656000
C	-43.428708000	-12.693604000	-14.010553000
C	-45.112345000	-10.563424000	-11.917839000
C	-45.831206000	-8.503175000	-13.179123000
C	-45.831722000	-9.324815000	-12.021319000
C	-46.661037000	-8.596935000	-11.083746000

C	-46.889812000	-6.268447000	-13.711633000
C	-46.621705000	-6.262037000	-15.096848000
H	-46.191277000	-7.144273000	-15.583317000
C	-46.916859000	-5.113235000	-15.846741000
H	-46.704989000	-5.114284000	-16.926739000
C	-47.479984000	-3.979686000	-15.238359000
H	-47.710337000	-3.084864000	-15.835949000
C	-47.752672000	-4.001416000	-13.859687000
H	-48.198492000	-3.121648000	-13.370698000
C	-47.460757000	-5.136549000	-13.092682000
H	-47.671568000	-5.178320000	-12.016583000
C	-47.075865000	-8.943015000	-9.686714000
H	-46.218899000	-8.910202000	-8.981694000
H	-47.830287000	-8.208625000	-9.346839000
H	-47.517084000	-9.958330000	-9.628891000
C	-44.988877000	-11.304744000	-10.610627000
H	-43.954093000	-11.692671000	-10.528579000
H	-45.151818000	-10.600588000	-9.776307000
C	-45.973527000	-12.484669000	-10.514967000
H	-47.028491000	-12.152253000	-10.598259000
H	-45.778449000	-13.215371000	-11.323568000
H	-43.468212000	-14.007941000	-20.266855000
H	-45.852450000	-13.006208000	-9.544323000
Mo	-42.295564000	-17.243230000	-8.873585000
O	-43.033945000	-18.770797000	-8.775591000
N	-40.671430000	-17.578621000	-11.525428000
O	-43.791179000	-16.228494000	-8.360385000
N	-40.704853000	-18.109791000	-10.264634000
O	-42.434719000	-16.395817000	-10.658652000
N	-39.215716000	-20.870934000	-6.837772000
O	-40.977820000	-17.899870000	-7.484559000
N	-39.927363000	-19.750380000	-6.458290000
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C	-39.878212000	-19.141881000	-10.024432000
C	-40.304342000	-19.015936000	-7.549677000
C	-39.781002000	-19.672439000	-8.704379000
C	-39.105944000	-20.835914000	-8.160141000
C	-40.214979000	-19.527361000	-5.082148000
C	-40.673863000	-18.273330000	-4.628041000

H	-40.803645000	-17.441505000	-5.330646000
C	-40.958287000	-18.105291000	-3.264495000
H	-41.320497000	-17.127840000	-2.911810000
C	-40.781353000	-19.161209000	-2.355732000
H	-41.010370000	-19.018349000	-1.288991000
C	-40.308607000	-20.401110000	-2.819522000
H	-40.160771000	-21.235468000	-2.117025000
C	-40.025179000	-20.592230000	-4.177924000
H	-39.654421000	-21.550530000	-4.562740000
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H	-37.419839000	-21.605811000	-9.290505000
H	-38.161249000	-22.743464000	-8.121597000
H	-38.987350000	-22.377180000	-9.679603000
C	-39.091706000	-19.726519000	-11.171791000
H	-38.721115000	-18.884307000	-11.787457000
H	-38.217155000	-20.272241000	-10.777801000
C	-39.960036000	-20.649816000	-12.047916000
H	-40.370401000	-21.496881000	-11.462533000
H	-40.810239000	-20.088039000	-12.479892000
H	-39.360721000	-21.062785000	-12.882913000
O	-41.180263000	-15.618249000	-8.143594000
O	-41.922476000	-12.670943000	-9.877950000
C	-41.297717000	-13.636662000	-9.490836000
O	-41.898340000	-14.387341000	-8.498208000
C	-39.933876000	-14.074145000	-9.945432000
H	-39.549926000	-13.326955000	-10.661558000
H	-39.256393000	-14.182274000	-9.076226000
H	-39.980693000	-15.068289000	-10.430618000
H	-43.625299000	-15.248779000	-8.372601000

**$1^{\circ}\text{c}$  for mechanism the oxidation of 7-methylnaphthalene in Fig 20.**



Mo	2.685635462	-1.509227046	12.987899302
O	2.154160517	-2.989824657	12.369450620
N	3.296505882	-2.676624133	15.751704319
O	3.992576316	-0.834342076	11.736366957
N	2.224238510	-2.170605742	15.059355459
O	4.426277992	-1.981542579	13.875958765
N	-2.296958379	-1.251913914	14.496882829
O	0.882018398	-0.593702202	13.162188925
N	-1.436724420	-0.728612092	13.553438424
C	4.400247211	-2.597711450	15.055833640
C	1.040590138	-2.267610757	15.685998878
C	-0.130642082	-1.022777941	13.857486062
C	-0.143500868	-1.786844031	15.056471722
C	-1.549923091	-1.879425295	15.398254311
C	-1.958490786	0.025751387	12.466324400
C	-1.196044913	0.251553728	11.301147643
H	-0.182850066	-0.155793183	11.213600851
C	-1.754177244	1.000510301	10.254258751
H	-1.156204340	1.174536348	9.346771416
C	-3.057529370	1.514754878	10.350630956
H	-3.485839015	2.097786636	9.521374783
C	-3.811843809	1.272363998	11.511693541

H	-4.836163597	1.665159135	11.597392853
C	-3.270097031	0.532492332	12.571215657
H	-3.843430654	0.324948372	13.483858988
C	-2.229717052	-2.573177781	16.538449960
H	-2.006230840	-2.087735397	17.511672161
H	-3.323638319	-2.533226918	16.376959269
H	-1.920653060	-3.634815953	16.617573557
C	0.987238333	-2.938226510	17.037708242
H	1.860996367	-2.590100546	17.621559334
H	0.073323219	-2.613882520	17.565474967
C	1.035680952	-4.472803245	16.930167657
H	0.186077746	-4.868378090	16.338054596
H	1.975827830	-4.788715931	16.439402200
H	1.005133803	-4.934333769	17.936188526
O	2.696825727	-0.247640638	11.504772215
O	3.274100547	0.554000023	14.133894500
H	2.881931735	1.203760102	13.513070145
H	4.235781438	0.597211105	13.951224415
H	8.204626345	-6.700635998	12.838235837
C	7.190526964	-6.287087804	12.952173596
C	6.689186794	-5.421278581	11.981600061
C	5.370527211	-4.895410376	12.150637205
C	4.580520543	-5.264543061	13.228117537
C	5.069887840	-6.164749438	14.218800395
C	6.413896987	-6.673930188	14.082906716
C	6.917513957	-7.554004568	15.086952598
C	6.125019968	-7.937843447	16.161753934
C	4.797584819	-7.446609967	16.287788250
C	4.287208625	-6.570748319	15.338486305
H	4.973212910	-4.189807450	11.403730714
H	3.560767839	-4.861694766	13.323225128
H	3.260713079	-6.183387364	15.431285961
H	4.187575600	-7.767157447	17.144125554
H	6.517205536	-8.620449950	16.930730007
H	7.947201875	-7.930557340	14.984047385
C	7.484775327	-5.083476830	10.746228143
H	7.118301524	-5.675529009	9.879818873
H	7.372822778	-4.017397848	10.472346927
H	8.560107412	-5.310804735	10.873326910

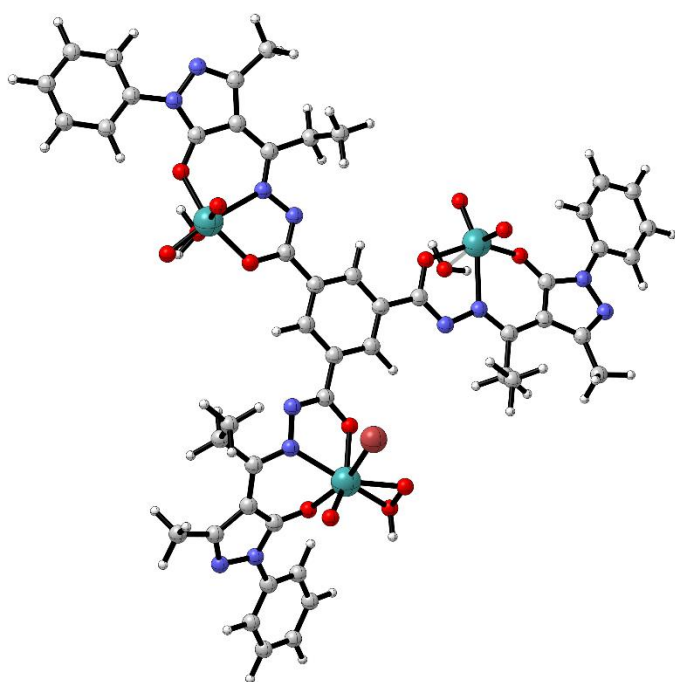
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H	6.642825979	-5.824516273	22.453049600
Mo	5.384907594	-7.109790353	20.283875574
O	4.900520396	-8.479316024	19.393461277
N	7.846806227	-6.290187800	18.574390645
O	3.991953197	-6.417723266	21.015348500
N	7.568185888	-7.164107807	19.590668394
O	5.632978777	-5.724995936	18.901196674
N	8.429060973	-10.666330815	22.502931000
O	6.177955570	-8.035978487	21.869395004
N	7.275928704	-9.947208986	22.728753588
C	6.781865798	-5.611370795	18.227968982
C	8.535627207	-8.019052422	19.923255316
C	7.159326854	-8.911080034	21.836584995
C	8.293268853	-8.957150117	20.983827727
C	9.046856595	-10.092284373	21.474321813
C	6.421490415	-10.314038840	23.806159026
C	5.098993527	-9.831012742	23.894313352
H	4.698772999	-9.163957372	23.122784089
C	4.297561865	-10.223235492	24.977292771
H	3.266131989	-9.845285528	25.040282758
C	4.792881021	-11.092443033	25.962863839
H	4.154711013	-11.396251803	26.806222523
C	6.108410542	-11.575995416	25.858266746
H	6.507035021	-12.262095567	26.621466025
C	6.926424655	-11.191709536	24.788026244
H	7.953755144	-11.561921147	24.682199371
C	10.331175687	-10.686923659	20.983399945
H	11.193683095	-10.009936963	21.156716891
H	10.519059229	-11.629227947	21.530709509
H	10.292548543	-10.908612757	19.898623122
C	9.829702934	-8.012293557	19.147022873
H	10.104012362	-6.954503515	18.967191446
H	10.628433368	-8.475395142	19.752584787
C	9.690786384	-8.728302372	17.789908994
H	9.381120982	-9.785672160	17.914612828
H	8.930656833	-8.216913265	17.168921722
C	6.800829414	-4.727997834	17.054317416



C	5.650710833	-4.002794117	16.701099909
H	4.744517169	-4.077305044	17.314890170
O	12.538653936	-3.625253526	14.351260031
H	12.858785747	-4.253957842	15.031538702
H	13.328772266	-3.474216559	13.792804159
Mo	11.333384048	-5.335269309	12.967242925
C	5.643871186	-3.226013616	15.522423354
C	6.790880081	-3.158525897	14.715367137
H	6.773122986	-2.589189614	13.778649994
C	7.937694281	-3.899829869	15.063945853
C	7.941366135	-4.689545790	16.225981445
H	8.815385834	-5.301520034	16.479352921
O	10.493074555	-6.333554550	11.869505430
N	9.247945367	-3.035891337	13.214657573
O	12.312929956	-6.338311499	13.959579306
N	10.307083413	-3.350647953	12.400332794
O	9.959885776	-4.935993763	14.317291506
N	13.143133052	-2.788530693	8.779449926
O	12.742969424	-4.618042214	11.756116204
N	13.468176318	-3.792103573	9.664858727
C	9.089670312	-3.931433368	14.154913758
C	10.580570375	-2.480662324	11.428640708
C	12.601559076	-3.811884168	10.728520727
C	11.657447833	-2.772733812	10.523711955
C	12.075273704	-2.168784781	9.275976519
C	14.609881230	-4.604957336	9.420096584
C	14.767078208	-5.855954385	10.052153571
H	14.002542582	-6.229289279	10.742982421
C	15.909977138	-6.622374243	9.777883334
H	16.026414058	-7.599504134	10.269846602
C	16.886638389	-6.162259270	8.879498625
H	17.777417801	-6.773040507	8.669041094
C	16.712856359	-4.919405299	8.246520647
H	17.469322202	-4.550849321	7.536709663
C	15.581757807	-4.136541083	8.512245718
H	15.421787723	-3.166589860	8.024706842
C	11.474759526	-1.035836717	8.501440011
H	11.582255425	-0.067594311	9.033877046
H	11.994992170	-0.953548902	7.529303436

H	10.394092858	-1.192518915	8.312932339
C	9.767362772	-1.213699071	11.300310483
H	9.594536589	-0.835621274	12.327436619
H	10.365209203	-0.459228927	10.757670636
C	8.404681398	-1.412240072	10.614370403
H	8.511620749	-1.866692921	9.609359838
H	7.761918161	-2.073463680	11.225264866
H	10.653252264	-8.711079682	17.240760248
H	7.886871680	-0.439902829	10.497811772

**3'a**



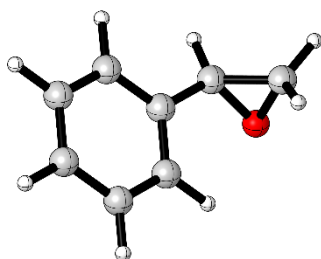
Mo	-32.824735452	-14.495868848	-30.052540993
O	-32.871181481	-15.745026299	-28.897351473
N	-31.127131624	-15.342384769	-32.421544465
O	-34.561589160	-13.571587322	-29.976079099
N	-31.203134916	-15.493559139	-31.075562224
O	-32.464541201	-13.580172098	-31.866784294
N	-28.944704639	-15.672413286	-27.082324993
O	-31.203341481	-13.770186470	-28.994547635
N	-29.697328049	-14.543144366	-27.342023116
C	-31.825648932	-14.273927891	-32.779055850
C	-30.249987397	-16.224600368	-30.464403639
C	-30.382856890	-14.662048610	-28.525447204
C	-29.992199283	-15.923058435	-29.099286744

C	-29.092599884	-16.490192605	-28.116408285
C	-29.765437680	-13.504708061	-26.373765400
C	-30.263365590	-12.228992194	-26.712262591
H	-30.589169173	-12.019986786	-27.737776698
C	-30.327095405	-11.234945872	-25.723841401
H	-30.715715053	-10.240265729	-25.990203248
C	-29.889224423	-11.492771733	-24.414750096
H	-29.939024700	-10.704880258	-23.648172540
C	-29.379091932	-12.762977943	-24.094646875
H	-29.025378414	-12.975182496	-23.074347750
C	-29.316026216	-13.771987250	-25.064333431
H	-28.920370143	-14.769724681	-24.837123616
C	-28.397396653	-17.816021744	-28.117075640
H	-27.529034412	-17.826540889	-28.808930728
H	-28.019441415	-18.027783463	-27.099717071
H	-29.082546270	-18.630466678	-28.424336928
C	-29.437207633	-17.193423583	-31.282277855
H	-29.032583354	-16.639099925	-32.153477126
H	-28.578848784	-17.551841560	-30.687467673
C	-30.299086811	-18.367614474	-31.782349957
H	-30.712825722	-18.950572486	-30.935646548
H	-31.145839556	-17.994896143	-32.390797187
H	-29.691479514	-19.048151627	-32.411078756
O	-33.684083118	-12.659861376	-29.186809492
H	-33.926879090	-12.863555282	-28.249542200
Br	-34.339950082	-15.957941536	-31.539061019
O	-26.969174537	-14.606263870	-38.086199459
H	-26.461176517	-14.956757678	-37.324289399
H	-26.354507062	-14.718076876	-38.840716857
Mo	-28.347507017	-16.666606398	-38.389844174
O	-29.310775284	-17.995071570	-38.834734312
N	-30.398350522	-14.358939456	-38.786194572
O	-27.182572348	-17.213778804	-37.249734166
N	-29.546812687	-15.100571252	-39.561625899
O	-29.477031722	-15.660883174	-37.116093460
N	-27.597631443	-16.541217800	-43.512965819
O	-27.189982257	-16.554584052	-40.017425427
N	-26.973456091	-16.919551792	-42.344163687
C	-30.326874341	-14.717596003	-37.529068489

C	-29.619199061	-14.912271243	-40.879611466
C	-27.616223170	-16.395204777	-41.251764829
C	-28.717814219	-15.638212441	-41.730596577
C	-28.631221882	-15.778026476	-43.169449827
C	-25.796122503	-17.716868311	-42.404885220
C	-25.296671012	-18.381932871	-41.265370401
H	-25.816646048	-18.305594266	-40.304385368
C	-24.127612304	-19.149636629	-41.378266450
H	-23.742142731	-19.665788050	-40.486151604
C	-23.459102965	-19.269154808	-42.607565518
H	-22.541809787	-19.871652597	-42.684333588
C	-23.974451055	-18.614009061	-43.739210070
H	-23.464224419	-18.703389265	-44.710376231
C	-25.136669962	-17.837764073	-43.645868939
H	-25.559729257	-17.321133542	-44.516455240
C	-29.514081836	-15.236027219	-44.251052993
H	-29.435890688	-14.132000426	-44.334761738
H	-29.203909687	-15.677525346	-45.216252037
H	-30.580512051	-15.481026643	-44.074770578
C	-30.668867114	-13.988074102	-41.444485868
H	-30.746423696	-13.115279244	-40.768075087
H	-30.349043724	-13.625317285	-42.437287925
C	-32.045130215	-14.676359894	-41.533336475
H	-32.012573376	-15.573779951	-42.184002558
H	-32.378849384	-14.994996570	-40.527397866
C	-31.178847411	-14.079191217	-36.511025115
C	-31.088149273	-14.481959585	-35.166653262
H	-30.391300493	-15.280196554	-34.877961817
O	-33.470132709	-8.201238813	-37.397633891
H	-32.957797654	-8.152048610	-38.232268688
H	-33.981962346	-7.366212866	-37.394549131
Mo	-35.206175445	-9.760531455	-38.288924139
C	-31.894129128	-13.857645144	-34.190191070
C	-32.791195077	-12.842038028	-34.559112201
H	-33.424612998	-12.367364510	-33.798833446
C	-32.889590598	-12.445214155	-35.910832941
C	-32.082333885	-13.059163136	-36.883417097
H	-32.153734927	-12.749698350	-37.934200373
O	-36.537313237	-10.728267262	-38.717632751

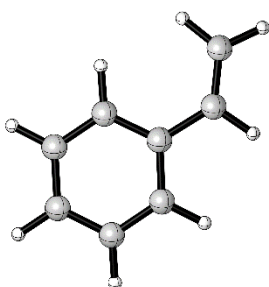
N	-34.633258294	-10.836088917	-35.425203950
O	-34.354138440	-9.349216439	-39.724540674
N	-35.481681383	-9.939678060	-36.019537819
O	-33.881465681	-11.055121900	-37.597114261
N	-38.987646295	-6.911986395	-36.186224777
O	-36.169355453	-8.038709260	-37.966386047
N	-38.157346527	-6.958241973	-37.284621582
C	-33.847317783	-11.398684910	-36.307645852
C	-36.419691518	-9.400240199	-35.240451605
C	-37.137148776	-7.854950813	-37.095665052
C	-37.312393475	-8.429008451	-35.808721294
C	-38.500198825	-7.775512880	-35.299204430
C	-38.406578235	-6.101238209	-38.392128810
C	-37.869709691	-6.377386277	-39.666645598
H	-37.255079846	-7.270238447	-39.829211236
C	-38.142179247	-5.501420304	-40.728208365
H	-37.723473558	-5.721014824	-41.721793238
C	-38.947502810	-4.366811962	-40.536552876
H	-39.158532592	-3.688052243	-41.376608498
C	-39.488143483	-4.109747108	-39.264768105
H	-40.124641332	-3.226357548	-39.102746909
C	-39.221813618	-4.968912632	-38.190667833
H	-39.639588225	-4.793866093	-37.191143885
C	-39.224846651	-7.958382231	-34.001331532
H	-38.633215395	-7.583510488	-33.140307540
H	-40.171468612	-7.388866074	-34.040118943
H	-39.460004510	-9.023766210	-33.807512186
C	-36.546524444	-9.850670315	-33.806242018
H	-35.522663961	-9.967884869	-33.400925472
H	-37.062338042	-9.071221019	-33.218222974
C	-37.286017655	-11.197696811	-33.688139386
H	-38.309523311	-11.139233839	-34.110062685
H	-36.734524849	-11.987322497	-34.233681022
H	-32.800535516	-13.976818149	-41.942930458
H	-37.364162798	-11.504209398	-32.626506128

## Styrene epoxide



C	-0.498291000	0.309113000	0.622157000
C	-1.733912000	0.168144000	1.278039000
C	0.642963000	0.695555000	1.340436000
H	-2.629117000	-0.134278000	0.713573000
H	1.613063000	0.832689000	0.838764000
C	-1.823549000	0.424209000	2.656679000
C	0.560505000	0.942596000	2.725993000
H	-2.790054000	0.323746000	3.174526000
C	-0.682838000	0.814177000	3.376136000
H	-0.758007000	1.024564000	4.455337000
H	-0.424707000	0.120930000	-0.460236000
C	1.779452000	1.320825000	3.503045000
H	1.591324000	1.918540000	4.417279000
C	3.005820000	0.483255000	3.482016000
H	3.005143000	-0.436373000	2.865597000
H	3.678877000	0.469941000	4.361324000
O	2.942275000	1.714204000	2.760181000

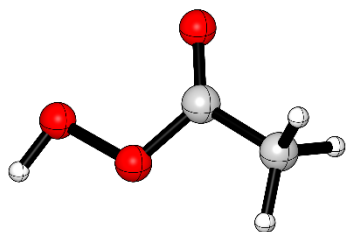
## Styrene



C	-0.689758000	0.821409000	0.590813000
C	-1.733547000	0.223222000	1.314859000
C	0.546908000	1.058996000	1.208971000
H	-2.705507000	0.032699000	0.834588000
H	1.364187000	1.527707000	0.637216000
C	-1.527375000	-0.133770000	2.660726000

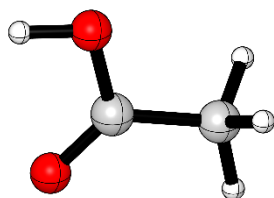
C	0.771515000	0.708221000	2.561603000
H	-2.340905000	-0.603862000	3.234746000
C	-0.293029000	0.104790000	3.275812000
H	-0.149187000	-0.184088000	4.327700000
H	-0.839409000	1.105289000	-0.462089000
C	2.087866000	0.982292000	3.162766000
H	2.822838000	1.432025000	2.471379000
C	2.472967000	0.747918000	4.436138000
H	1.798075000	0.305768000	5.186497000
H	3.489700000	0.997765000	4.773699000

### CH<sub>3</sub>COOOH



O	5.281330000	-5.806897000	6.490189000
O	5.140124000	-6.334588000	7.844207000
O	5.852907000	-4.253759000	8.487791000
C	5.487168000	-5.370214000	8.760690000
C	5.324708000	-5.969716000	10.144805000
H	6.298797000	-5.909772000	10.669144000
H	4.600191000	-5.352027000	10.711267000
H	4.978708000	-7.018896000	10.119383000
H	4.967522000	-6.609779000	6.021865000

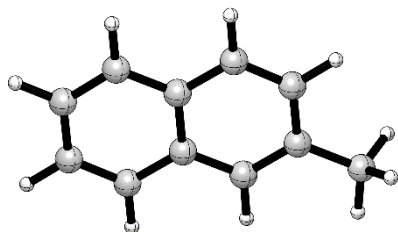
### CH<sub>3</sub>COOH



H	5.052003000	-5.702546000	6.917957000
O	4.826377000	-6.109920000	7.783403000
O	6.325234000	-4.529171000	8.393435000
C	5.571364000	-5.432031000	8.701810000
C	5.328373000	-5.950325000	10.100394000

H	5.938632000	-5.377832000	10.818883000
H	4.253556000	-5.861809000	10.357158000
H	5.586641000	-7.027031000	10.156092000

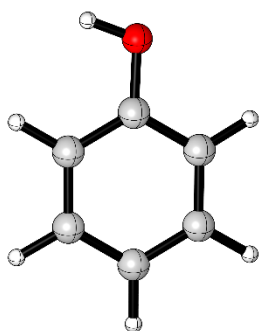
## Naphthalene



H	0.632138000	-2.915241000	12.237376000
C	0.667013000	-2.419448000	13.220566000
C	0.701145000	-1.034387000	13.309157000
C	0.745614000	-0.400371000	14.581613000
C	0.755000000	-1.159936000	15.743586000
C	0.720658000	-2.585336000	15.687323000
C	0.675814000	-3.227599000	14.395476000
C	0.641799000	-4.653610000	14.348449000
C	0.651152000	-5.405846000	15.511260000
C	0.695243000	-4.784422000	16.799241000
C	0.729065000	-3.394745000	16.862261000
H	0.693971000	-0.422592000	12.394158000
H	0.773174000	0.698866000	14.642686000
H	0.789891000	-0.669393000	16.729361000
H	0.763941000	-2.893159000	17.843309000
H	0.623637000	-6.506131000	15.449923000
H	0.606975000	-5.151114000	13.366123000
C	0.704106000	-5.638135000	18.043150000
H	-0.197895000	-6.284865000	18.094169000
H	1.583752000	-6.316873000	18.059609000
H	0.733145000	-5.022365000	18.962780000

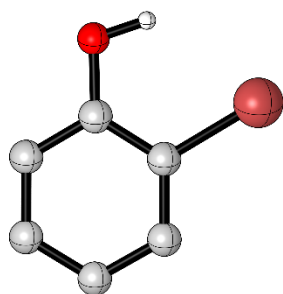


## Phenol



C	4.093923000	4.055395000	9.244492000
C	2.881909000	4.052370000	9.965740000
C	5.320189000	4.046433000	9.941336000
C	2.899509000	4.040351000	11.369519000
C	5.324094000	4.034529000	11.342622000
C	4.118181000	4.031312000	12.067139000
H	1.922237000	4.059576000	9.421322000
H	6.255965000	4.048926000	9.363616000
H	1.946020000	4.037981000	11.920054000
H	6.286703000	4.027458000	11.877274000
H	4.129302000	4.021538000	13.167344000
O	4.137355000	4.066861000	7.880300000
H	3.221335000	4.070942000	7.544573000

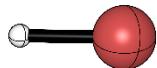
## o-Bromophenol



C	-0.890734000	0.635809000	13.074295000
C	-0.965423000	-0.604610000	12.394362000
Br	-0.486471000	-2.180640000	13.378257000
C	-1.371933000	-0.693201000	11.056688000
H	-1.417566000	-1.676083000	10.566202000
C	-1.716178000	0.478051000	10.363378000
H	-2.038672000	0.415449000	9.314225000
C	-1.647557000	1.719874000	11.020385000
H	-1.916656000	2.641914000	10.483733000

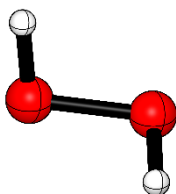
C	-1.240526000	1.800521000	12.357974000
H	-1.182332000	2.763933000	12.885397000
O	-0.503152000	0.749332000	14.364457000
H	-0.301030000	-0.157208000	14.691158000

### HBr



Br	0.541700000	-0.080282000	-3.049753000
H	1.156954000	-0.961308000	-2.097324000

### H<sub>2</sub>O<sub>2</sub>



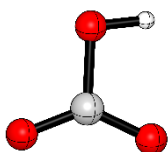
O	0.639307000	-0.220052000	-2.898655000
O	0.606222000	1.007571000	-2.106667000
H	1.059347000	-0.821538000	-2.248421000
H	1.157021000	1.584089000	-2.676878000

### H<sub>2</sub>O



O	0.841883000	0.000000000	-2.822519000
H	0.841883000	0.758979000	-2.210228000
H	0.841883000	-0.758979000	-2.210228000

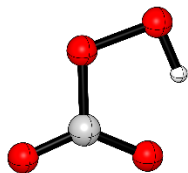
### HCO<sub>3</sub><sup>-</sup>



O	-0.443830000	2.212447000	1.252114000
O	-0.464127000	0.727707000	3.004791000

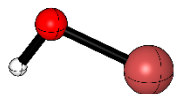
C	-0.456011000	1.846329000	2.458727000
O	-0.461697000	2.971827000	3.396361000
H	-0.453418000	3.708887000	2.753676000

### HCO<sub>4</sub><sup>-</sup>



O	-0.943685000	2.511857000	1.519926000
O	-0.300132000	0.698334000	2.781194000
C	-0.531620000	1.891579000	2.545783000
O	-0.273340000	2.739793000	3.687032000
O	-0.575012000	4.139315000	3.313184000
H	-0.849957000	3.879954000	2.359430000

### HOBr



O	-0.213692000	0.337031000	14.667713000
H	-0.336896000	-0.490002000	15.182571000
Br	1.643593000	0.552610000	14.744590000

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