

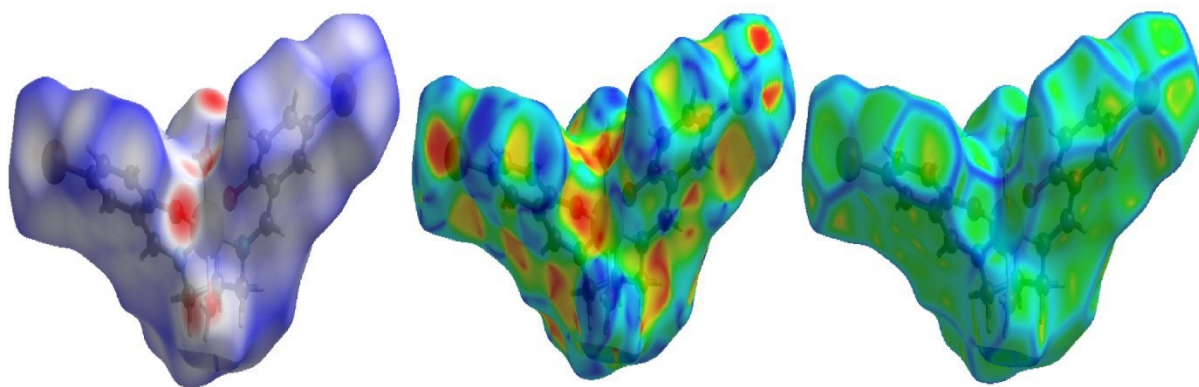
# **An insight to the hydrogen bonding, halogen bonding and chalcogen bonding interactions in the manganese(III) complexes with N<sub>2</sub>O<sub>2</sub> donor salicylidine Schiff base ligands**

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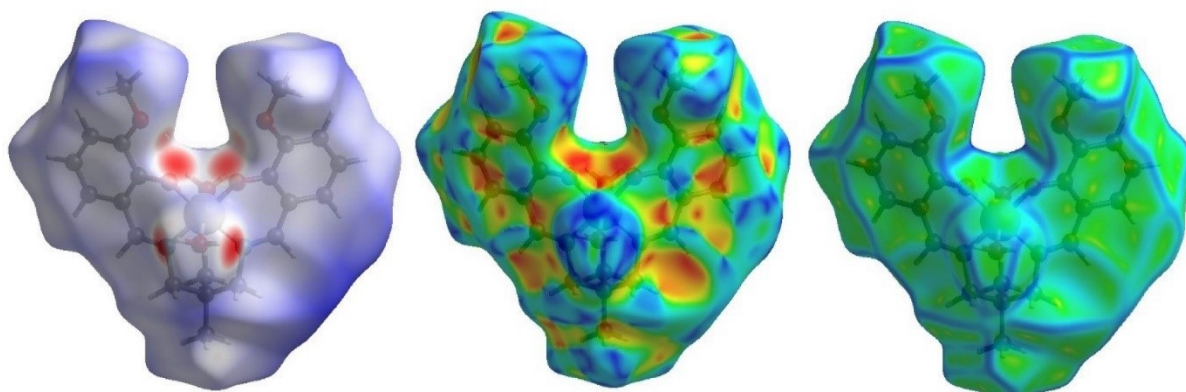
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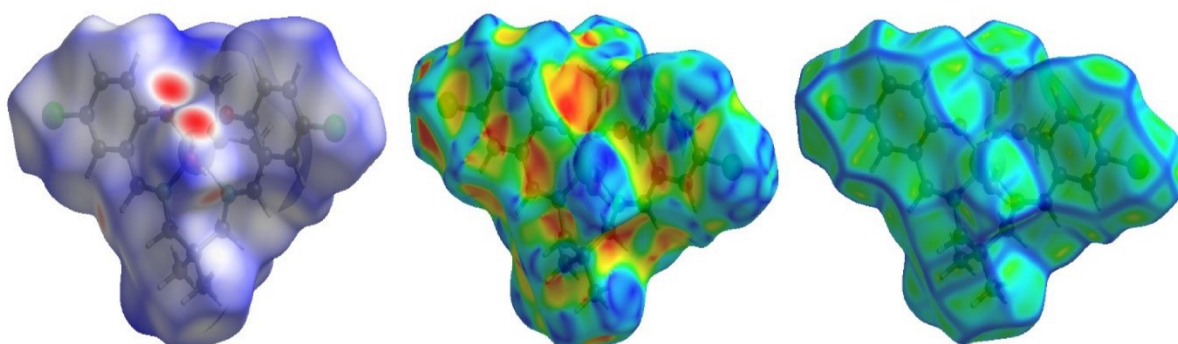
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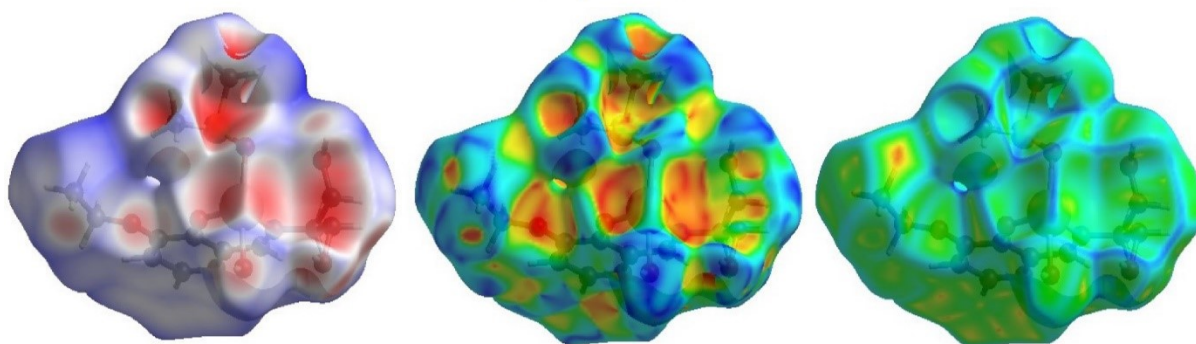
**Complex 1**



**Complex 2**

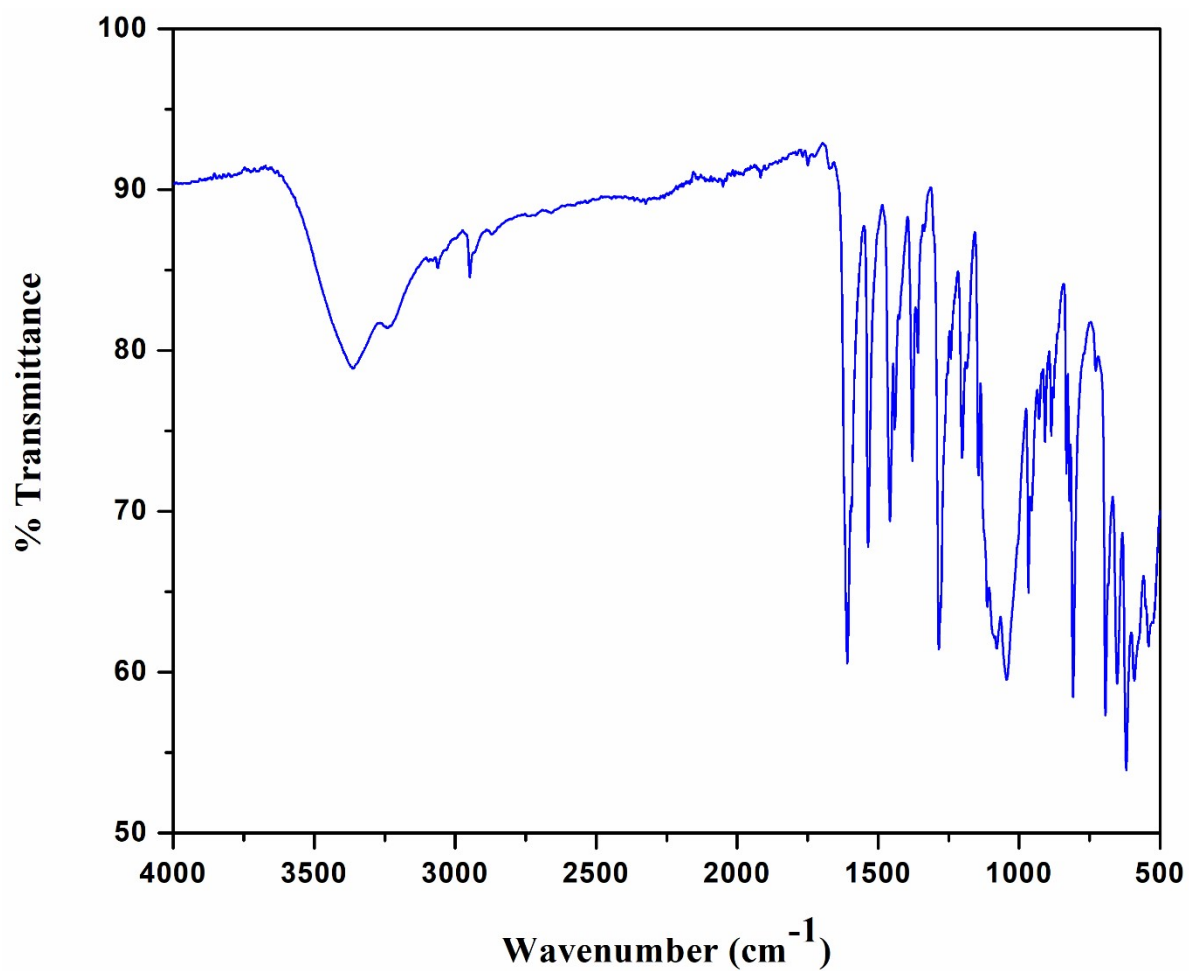


**Complex 3**

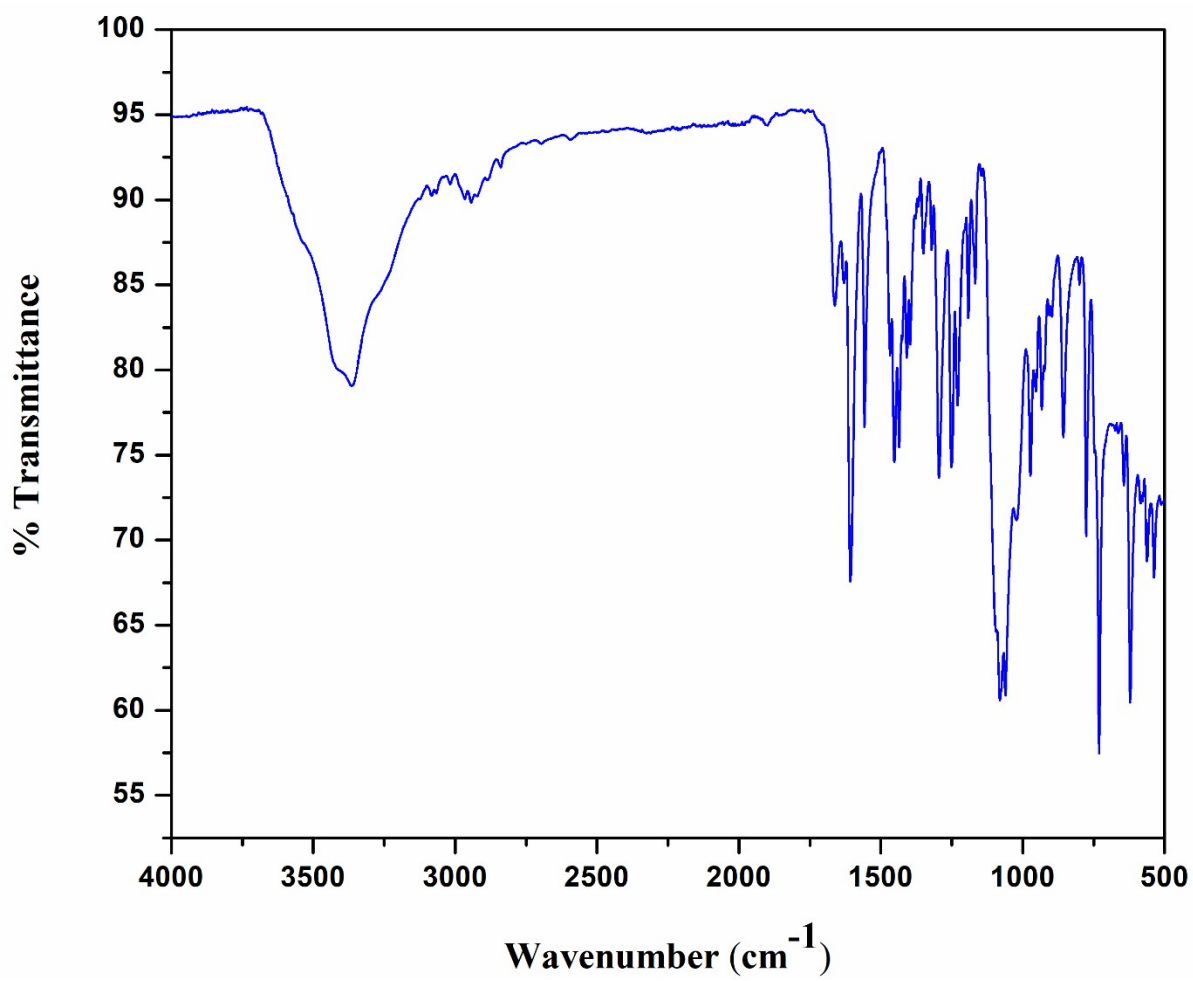


**Complex 4**

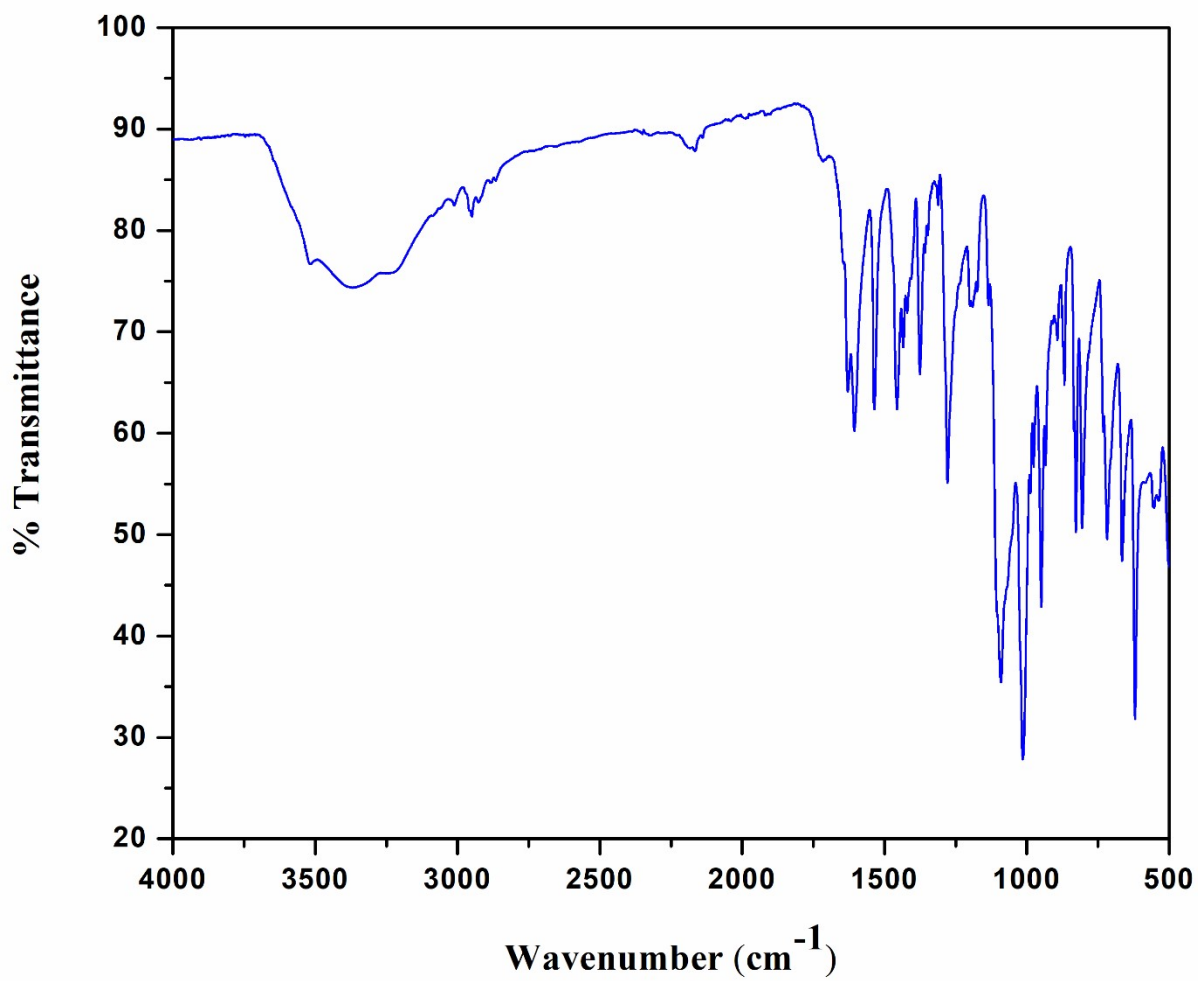
**Figure S1.** Hirshfeld surfaces mapped with  $d_{norm}$  (left-side), shape index (middle), and curvedness (right-side).



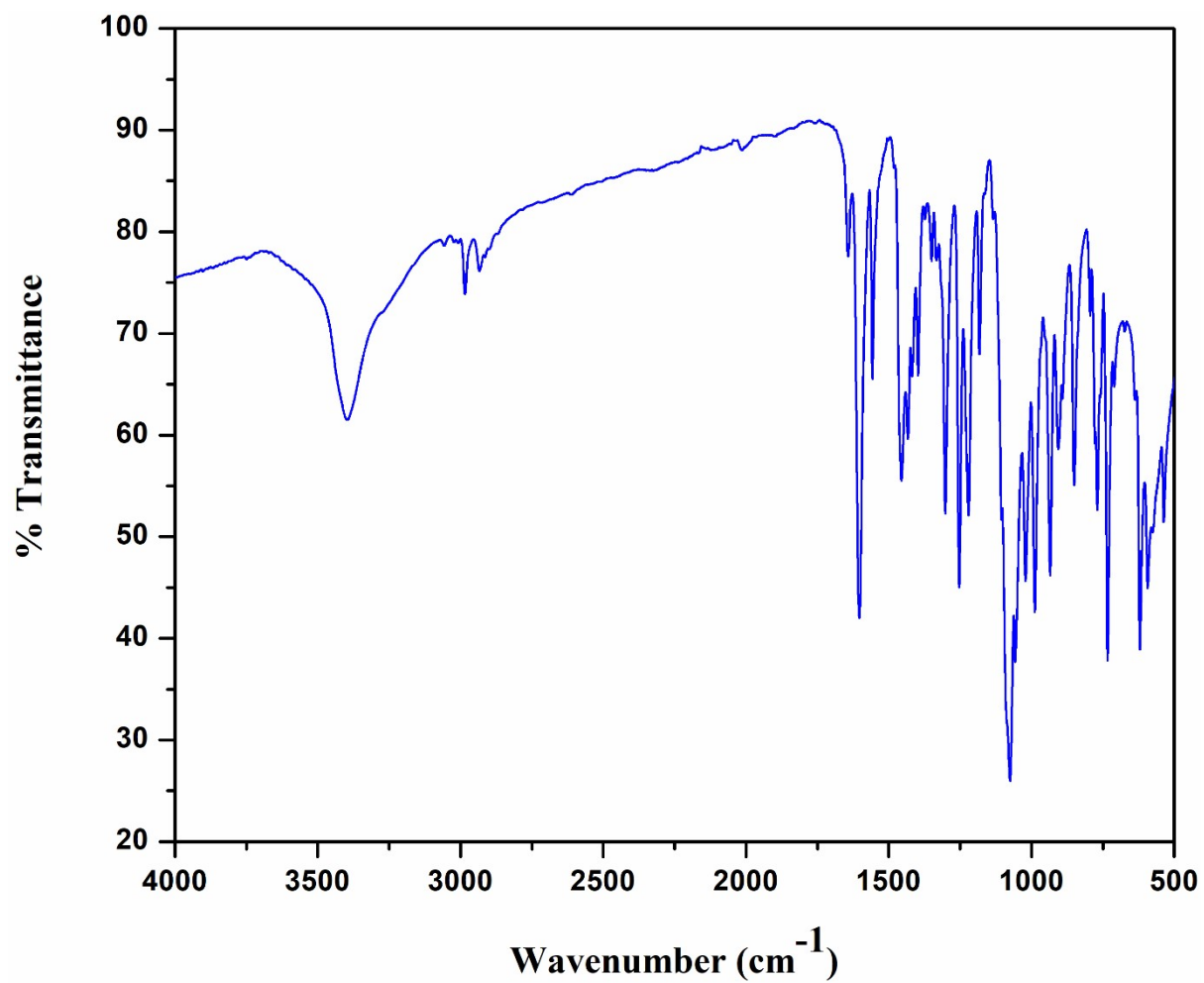
**Figure S2.** The IR spectrum of complex 1.



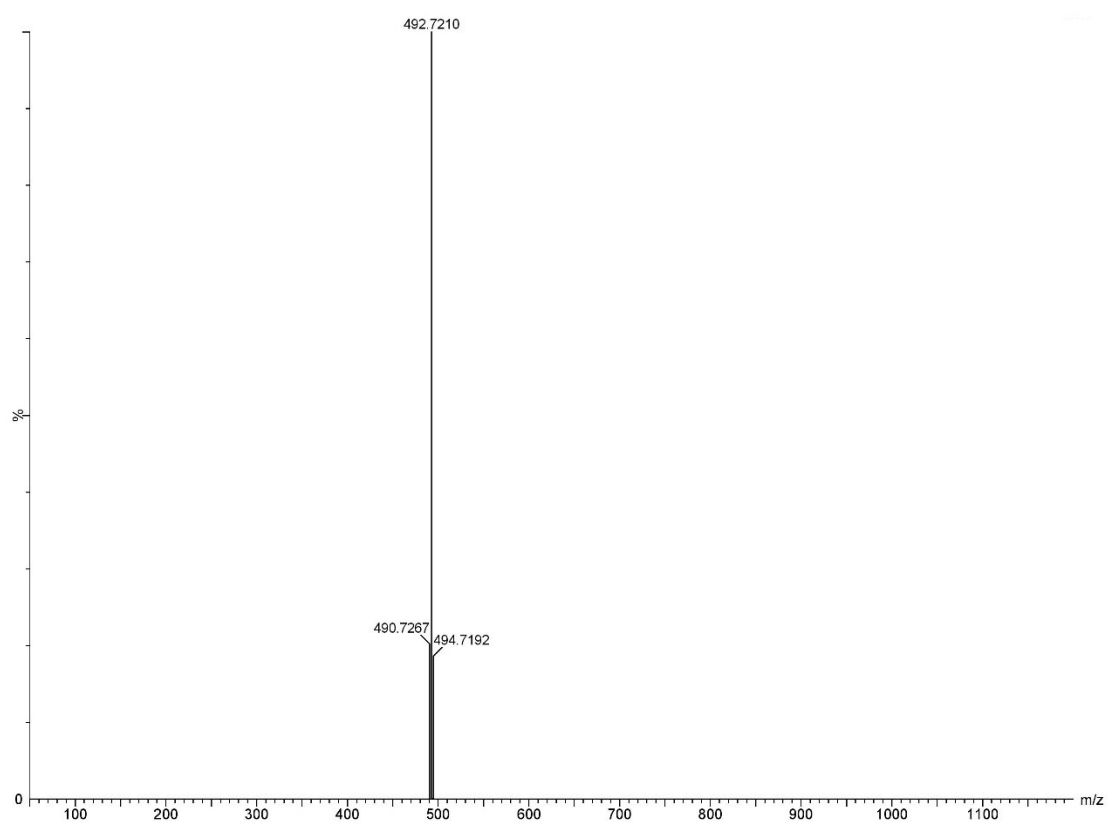
**Figure S3.** The IR spectrum of complex 2.



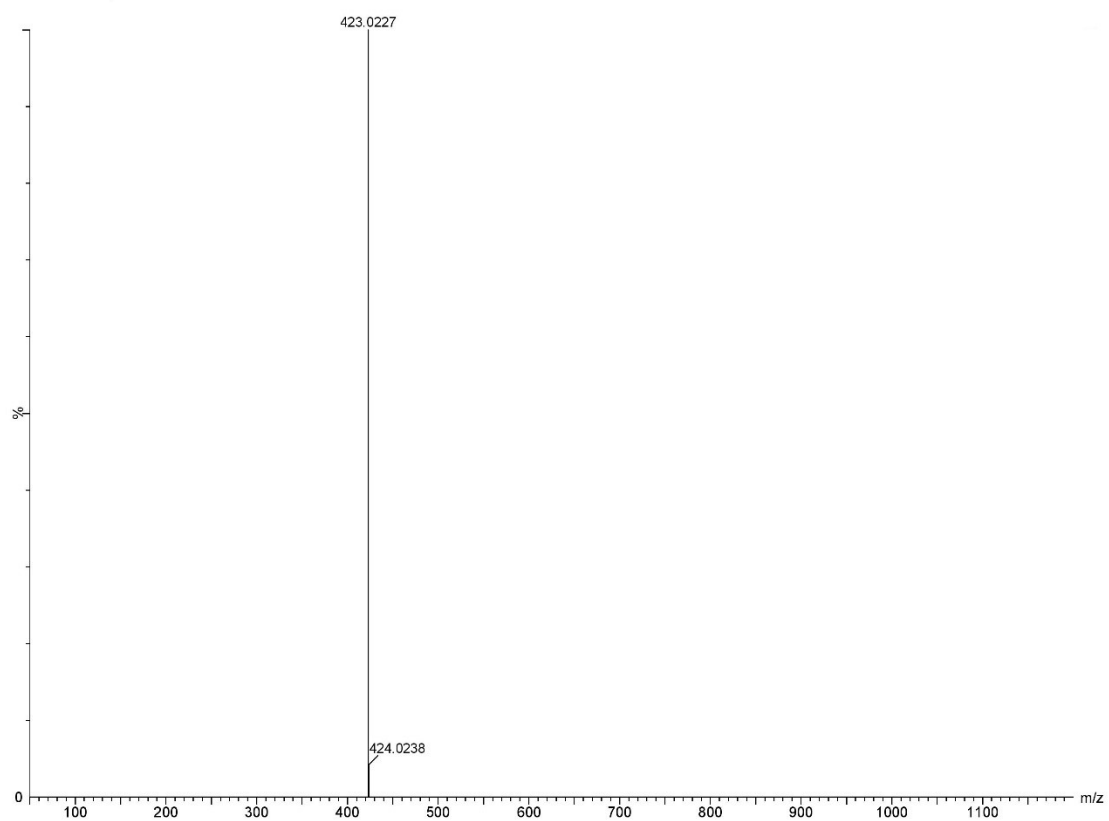
**Figure S4.** The IR spectrum of complex **3**.



**Figure S5.** The IR spectrum of complex 4.

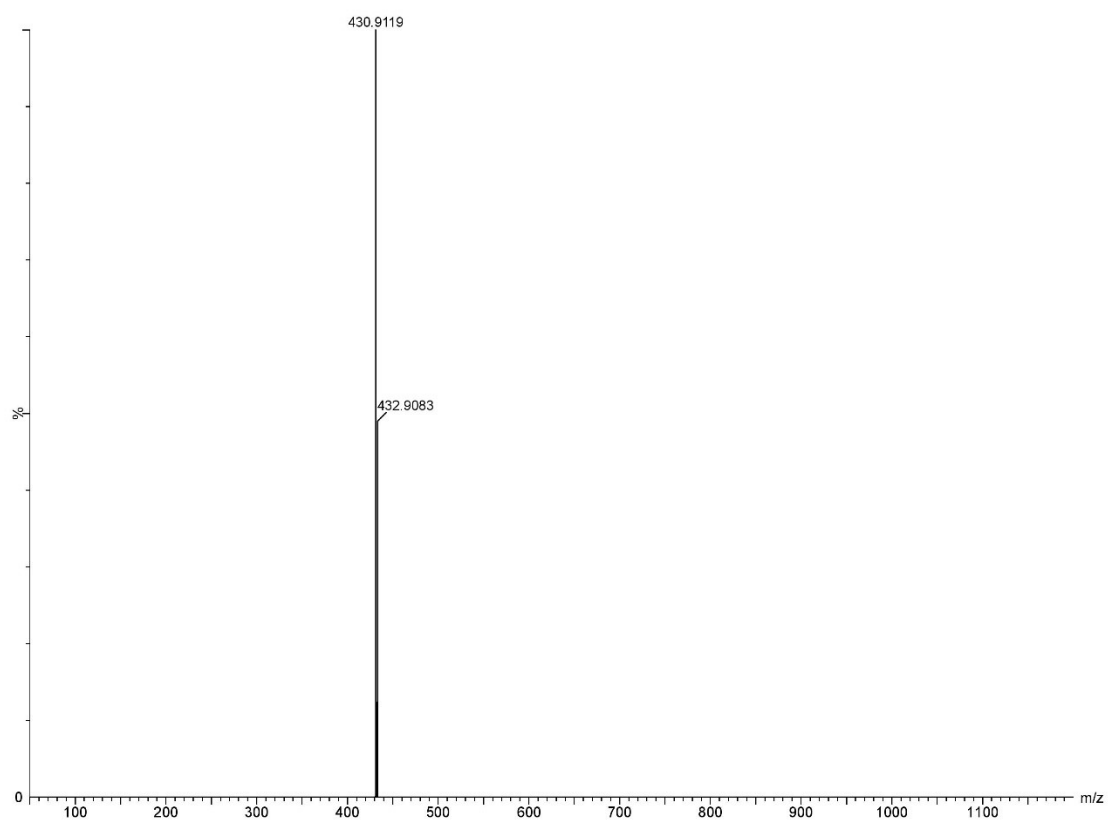


**Figure S6.** HRMS-ESI mass spectrum of complex **1** in acetonitrile medium.



**Figure S7.** HRMS-ESI mass spectrum of complex **2** in acetonitrile medium.





**Figure S8.** HRMS-ESI mass spectrum of complex **3** in acetonitrile medium.



**Figure S9.** HRMS-ESI mass spectrum of complex **4** in acetonitrile medium.

**Table S1.** Crystal data and refinement details of Complexes **1 - 4**.

Complex	1	2	3	4
Formula	C <sub>17</sub> H <sub>20</sub> Br <sub>2</sub> ClMnN <sub>2</sub> O <sub>9</sub>	C <sub>42</sub> H <sub>58</sub> Cl <sub>2</sub> Mn <sub>2</sub> N <sub>4</sub> O <sub>21</sub>	C <sub>21</sub> H <sub>26</sub> Cl <sub>3</sub> MnN <sub>2</sub> O <sub>8</sub> S	C <sub>23</sub> H <sub>30</sub> ClMnN <sub>2</sub> O <sub>11</sub> S
Molecular Weight	646.54	1133.69	627.79	632.94
Temperature (K)	273	273	273	273
Crystal system	Orthorhombic	Monoclinic	Triclinic	Monoclinic
Space group	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	<i>C2/c</i>	<i>P-1</i>	<i>C2/m</i>
a (Å)	7.8022(3)	29.4946(9)	10.626(6)	15.4932(6)
b (Å)	13.8143(6)	7.7686(2)	11.755(7)	17.3487(7)
c (Å)	20.8527(9)	25.9950(8)	11.982(8)	12.3645(5)
α	(90)	(90)	81.815(15)	(90)
β	(90)	120.781(1)	67.238(15)	123.207(1)
γ	(90)	(90)	74.590(12)	(90)
d <sub>calc</sub> (g cm <sup>-3</sup> )	1.911	1.472	1.569	1.512
Z	4	4	2	4
μ	4.314	0.678	0.924	0.706
F(000)	1280	2352	644	1312
Total Reflections	67027	31809	17133	17693
Unique Reflections	3977	4539	4862	2534
Observed data [I>2σ(I)]	3837	4002	3045	2347
No. of	305	334	333	210

parameters				
R(int)	0.048	0.034	0.078	0.034
$\mathcal{R}_1, \mathcal{wR}_2$ (all data)	0.0214, 0.0477	0.0642, 0.1911	0.1406, 0.3176	0.0565, 0.1623
$\mathcal{R}_1, \mathcal{wR}_2$ [I>2σ(I)]	0.0199, 0.0471	0.0586, 0.1847	0.1028, 0.2774	0.0534, 0.1588

$$(\mathcal{R}) \mathcal{R}_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|; (\mathcal{w}) \mathcal{wR}_2 = \Sigma w(|F_o|^2-|F_c|^2)^2/\Sigma w|F_o|^2)^{1/2}$$