Supporting Information for Manuscript:

Iron(III) Bis(pyrazol-1-yl)acetate Based Decanuclear Metallacycle: Synthesis, Structure, Magnetic Properties and DFT Calculations

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Figure S1 - The IR spectra of $[Fe_{10}(bdtbpza)_{10}(MeO)_{20}]$ (bottom) and bis(3,5-di-t-butylpyrazol-1-yl)acetate ligand (top).

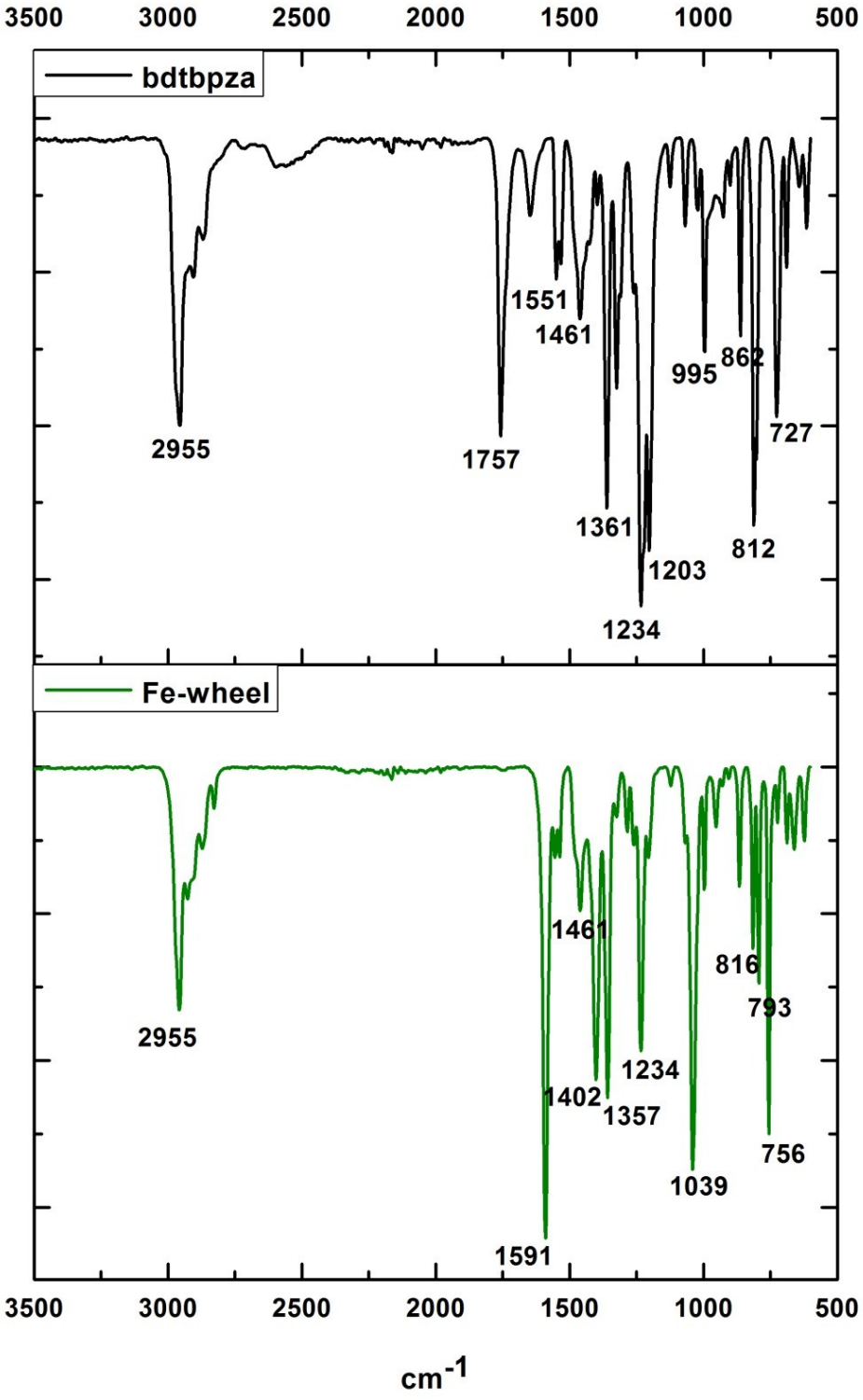


Figure S2 – UV-vis spectra of $[Fe_{10}(bdtbpza)_{10}(MeO)_{20}]$ (**1**) at room temperature in DCM solvent with concentration 6.35 x 10^{-5} M

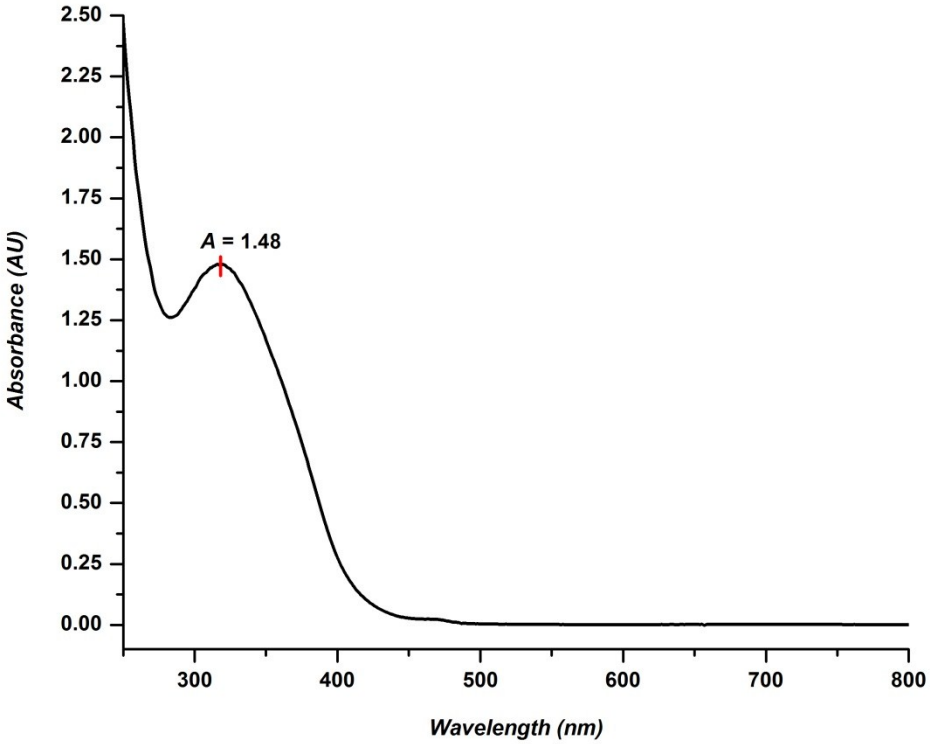


Figure S3 - The Nanospray-ESI spectra of $[Fe_{10}(bdtbpza)_{10}(MeO)_{20}]$ (**1**)

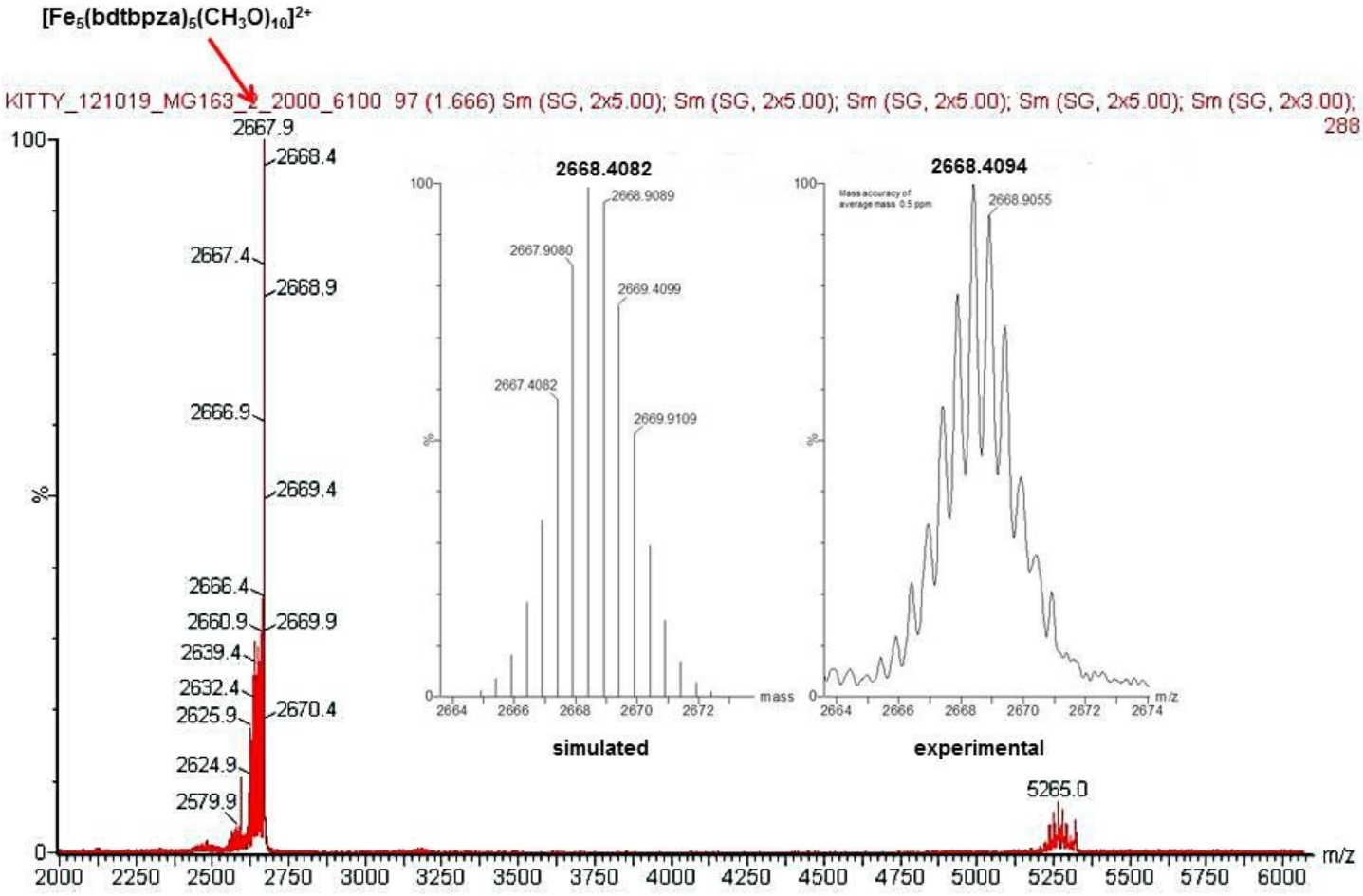
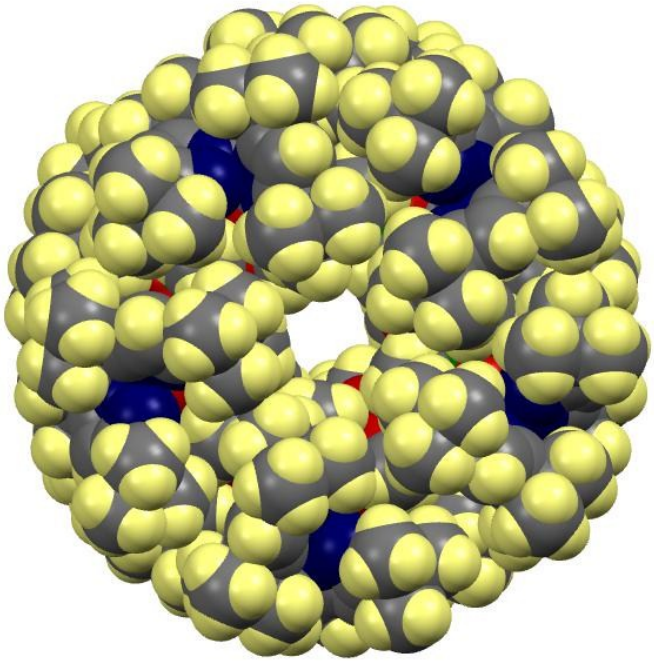
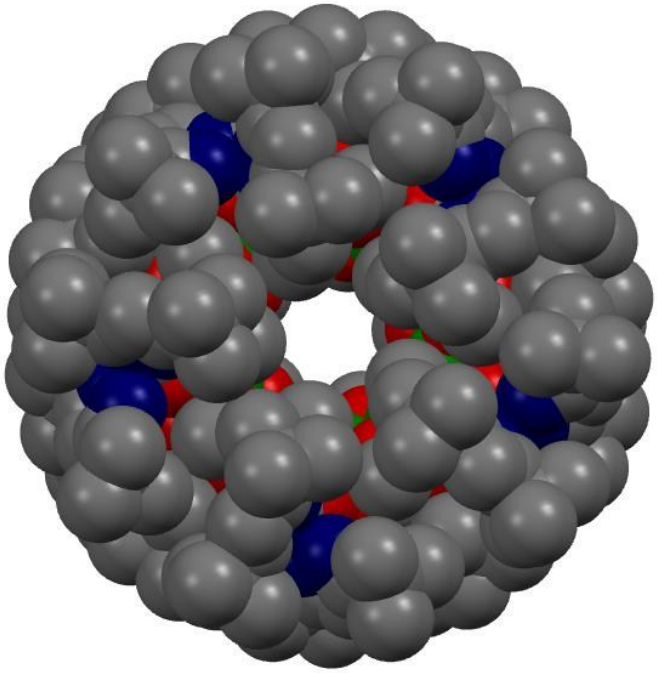


Figure S4 The space-filling representations of {Fe_{10}} wheel showing the interior cavity diameters; (a) whole molecule, (b) without H atoms; (C-grey, H-cream, O-red, N-blue, Fe green)



a)



b)

Table S1 Selected Bond valence sums for Fe atoms in (**1**)

Atom no.	Valence state assumed	Most consistent valence state	BVS	% Deviation from assumed valence state
Fe1	Fe1(2)		2.939	47
Fe1	**Fe1(3)**	*	**3.144**	**5**
Fe1	Fe1(6)		3.039	49
Fe1	Fe1(9)		3.053	66
Fe2	Fe2(2)		3.022	51
Fe2	**Fe2(3)**	*	**3.233**	**8**
Fe2	Fe2(6)		3.13	48
Fe2	Fe2(9)		3.162	65
Fe3	Fe3(2)		3.001	50
Fe3	**Fe3(3)**	*	**3.211**	**7**
Fe3	Fe3(6)		3.108	48
Fe3	Fe3(9)		3.136	65
Fe4	Fe4(2)		2.956	48
Fe4	**Fe4(3)**	*	**3.162**	**5**
Fe4	Fe4(6)		3.058	49
Fe4	Fe4(9)		3.077	66
Fe5	Fe5(2)		3.016	51
Fe5	**Fe5(3)**	*	**3.227**	**8**
Fe5	Fe5(6)		3.123	48
Fe5	Fe5(9)		3.154	65

(Only bonds that have all of the valence states defined in a given model have their bond valence parameters reported)