Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information

Elucidating the role of the *o*-methoxy group at the lower rim appended salicylideneamine substituents of calix[4]arene ligand on the molecular and electronic structure of dinuclear Fe(III) based "diamond core" complexes

Iuliia V. Strelnikova[a,b], Ilya D. Shutilov,[a] Alexander S. Ovsyannikov[a,*], Daut R. Islamov[c], Andrew V. Pyataev[b], Tatiana P. Gerasimova[a], Ayrat R. Khamatgalimov[a], Mikhail N. Khrizanforov[a,b], Aidar T. Gubaidullin[a], Vladimir A. Burilov[b], Svetlana E. Solovieva[a], Igor S. Antipin[b]

[a]*Kazan Federal University, Kremlevskaya 18 str, Kazan 420008, Russian Federation*
[b]*Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, Arbuzova 8 str, Kazan 420088, Russian Federation*
[c]*Laboratory for structural analysis of biomacromolecules, Kazan Scientific Center of Russian Academy of Sciences, Lobachevskogo 2 str, Kazan 420008, Russian Federation*
[d]*National Research Centre "Kurchatov Institute", Acad. Kurchatov 1 Sq., 123182 Moscow, Russian Federation*

** Corresponding author:*
E-mail address: osaalex2007@ramble.ru

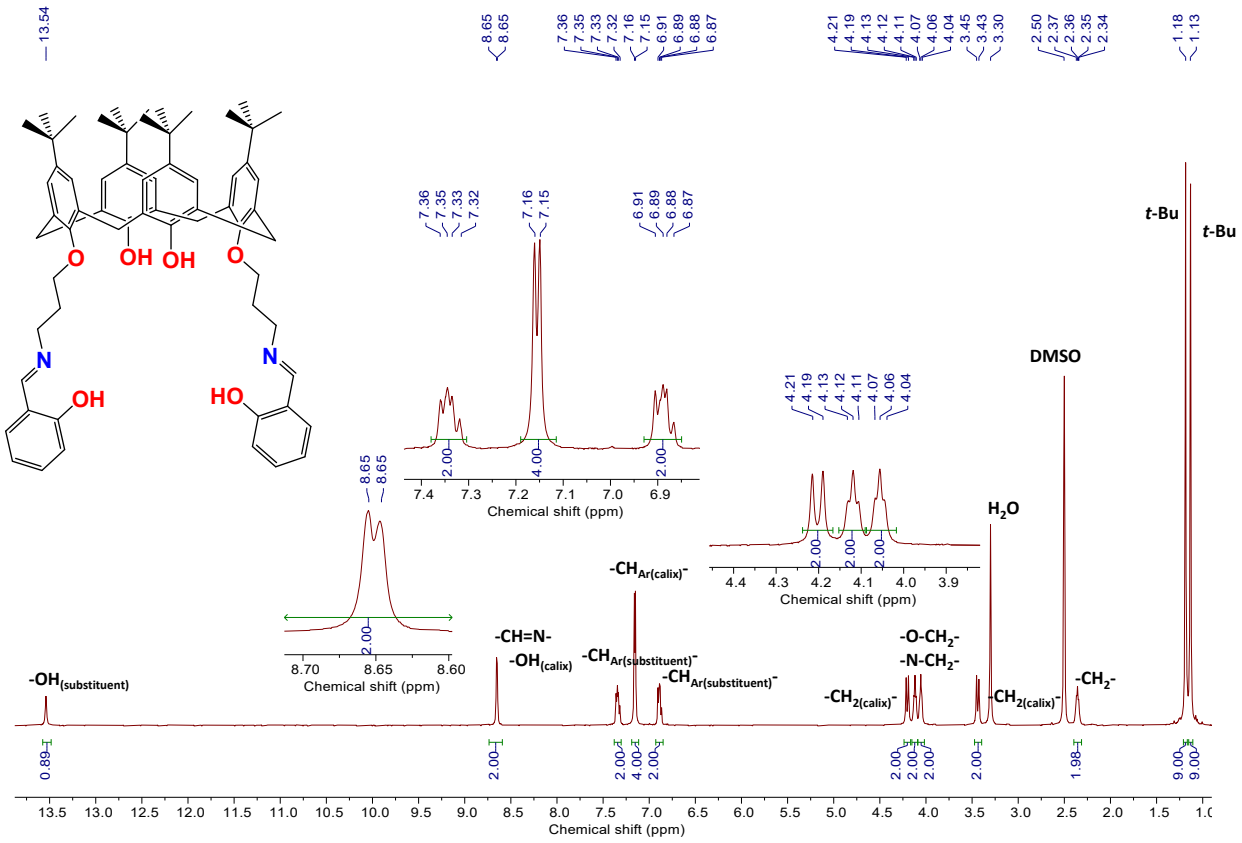


Figure S1. ^{1}H NMR spectrum for **4** (DMSO-d_6, 400 MHz, 25 °C).

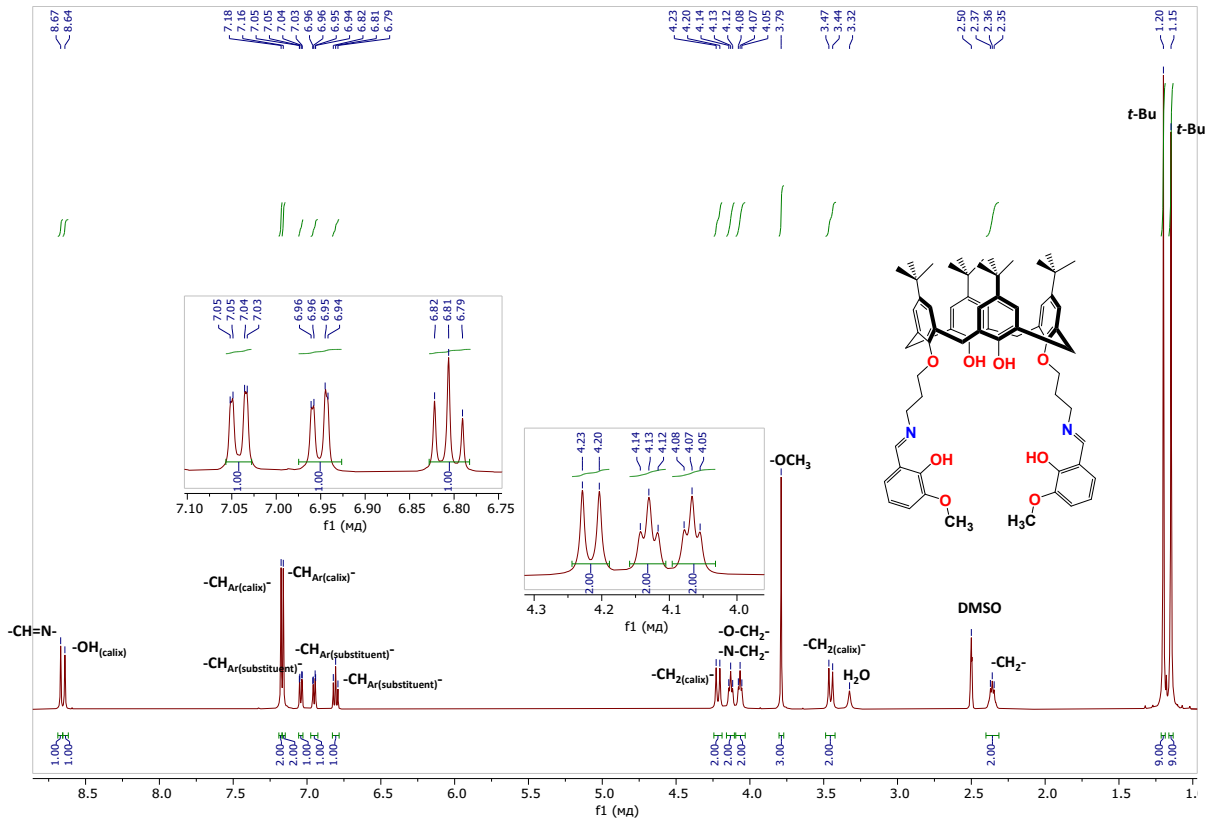


Figure S2. ^{1}H NMR spectrum for **5** (DMSO-d_6, 400 MHz, 25 °C).

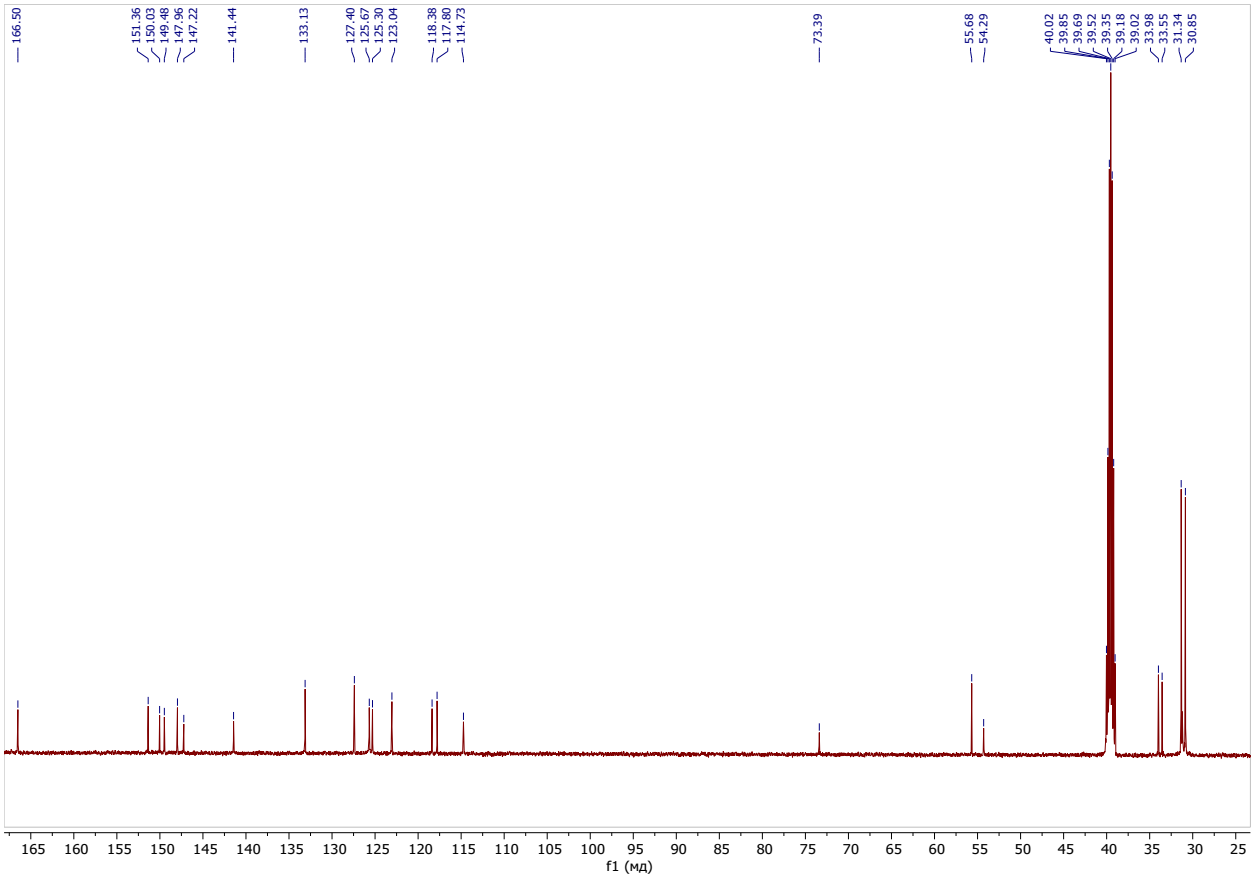


Figure S3. ^{13}C NMR spectrum for **5** (DMSO-d_6, 125 MHz, 25 °C).

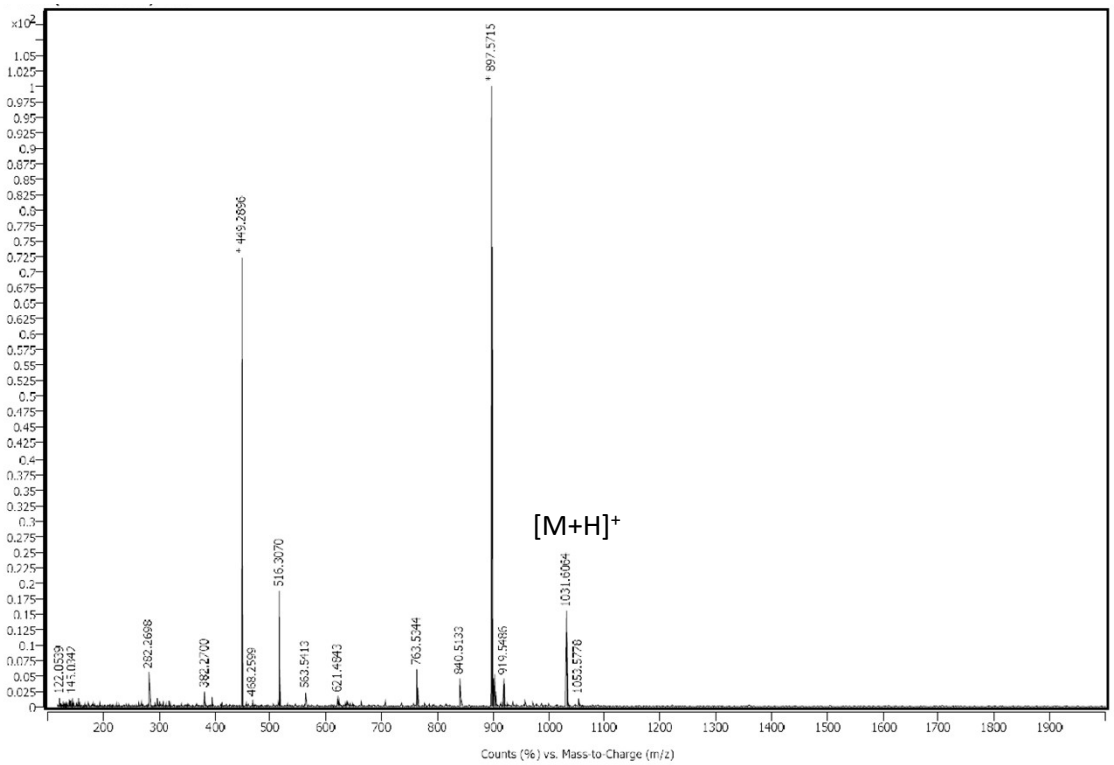


Figure S4. HRESI-MS spectrum for **5**.

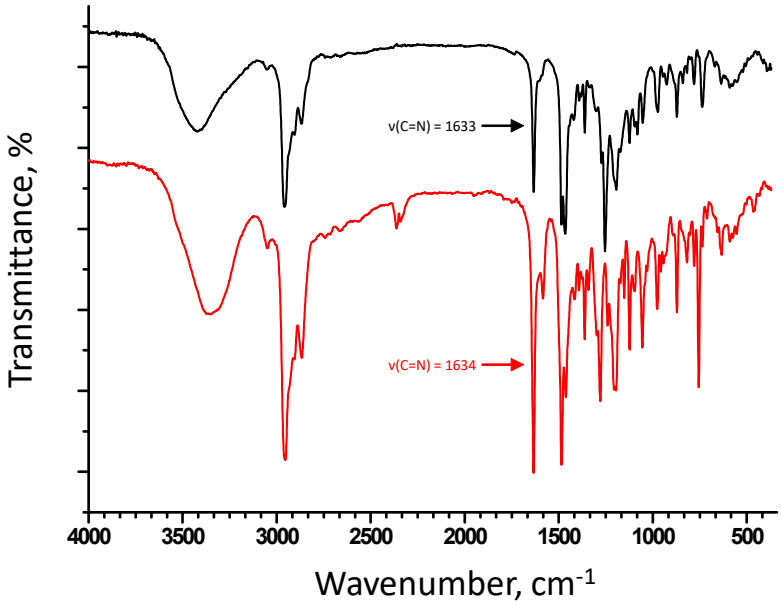


Figure S5. Comparison of IR spectra for **4** (red line) and **5** (black line).

	HOMO	LUMO

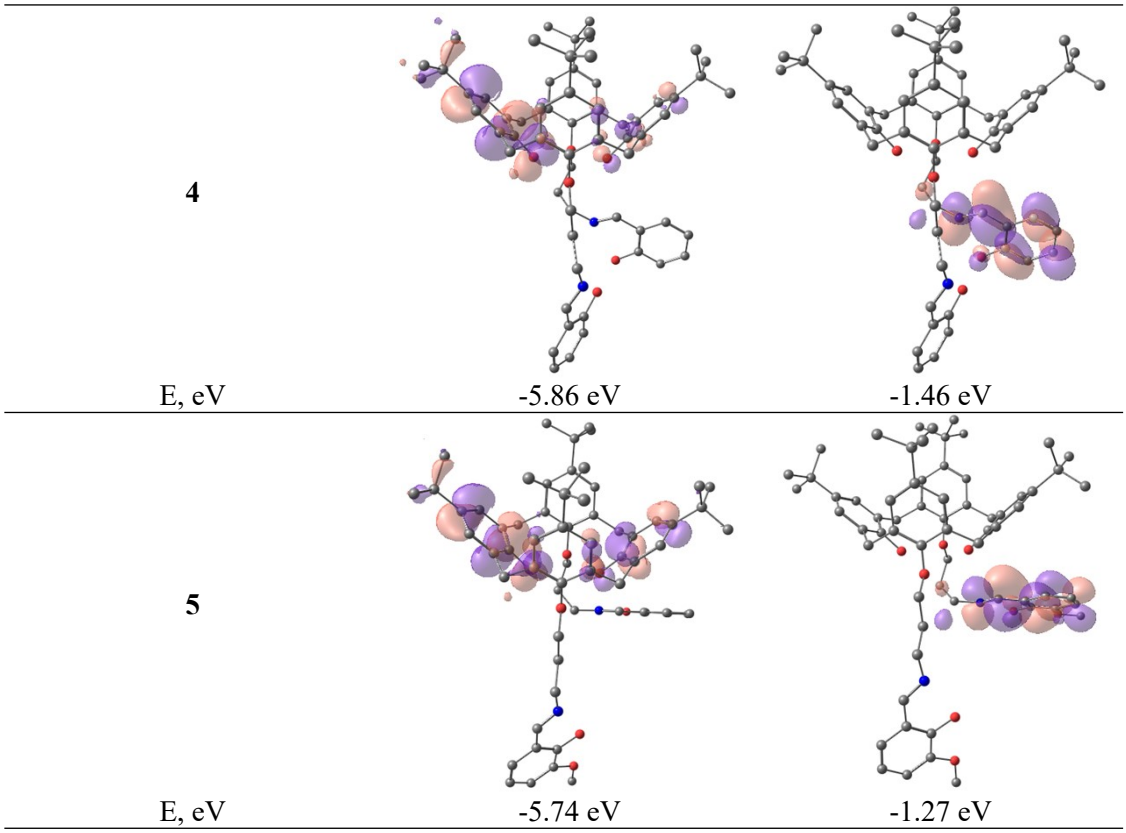


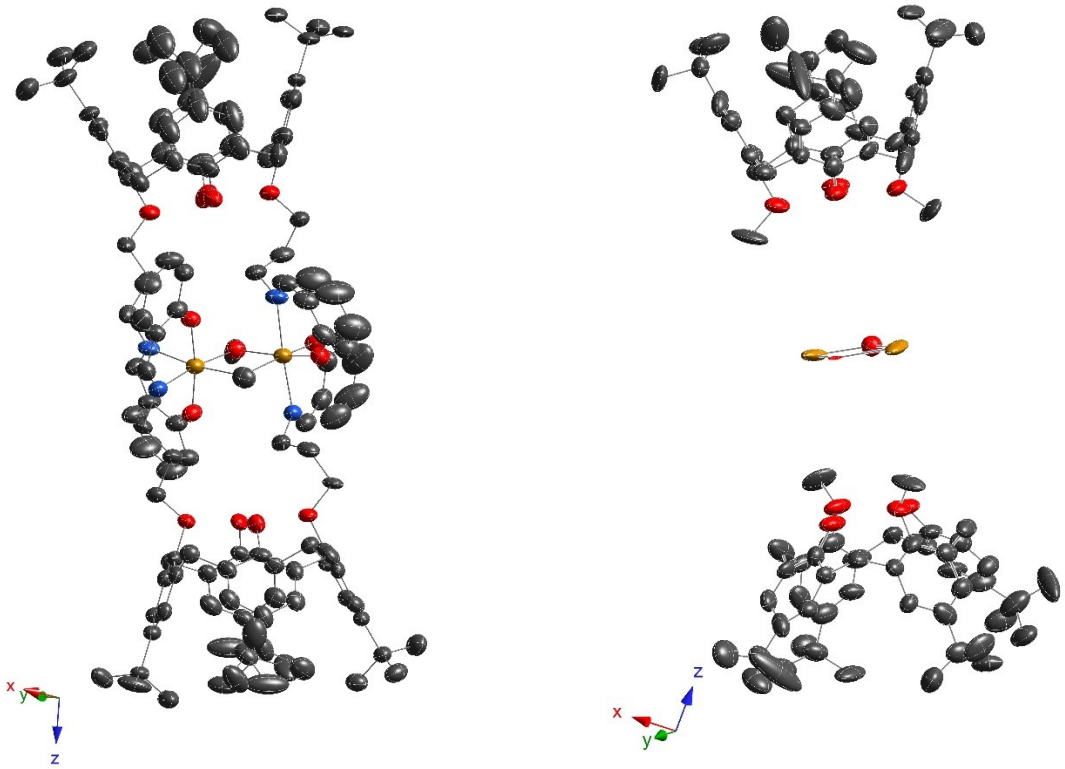
Figure S6. Calculated HOMO and LUMO orbitals for ground singlet states of **4** (top) and **5** (bottom).

Table S1. The calculated bond lengths of salicylideneamine moieties for **4** and **5**, according to DFT-calculations.

	4	**5**
d(N1…C1), Å	1.275	1.275
d(N2…C4), Å	1.287	1.288
d(C1…C2), Å	1.473	1.472
d(C4…C5), Å	1.461	1.459
d(C3…C4), Å	1.420	1.408
d(C5…C6), Å	1.418	1.415
d(C4…O1), Å	1.353	1.355
d(C6…O2), Å	1.361	1.345

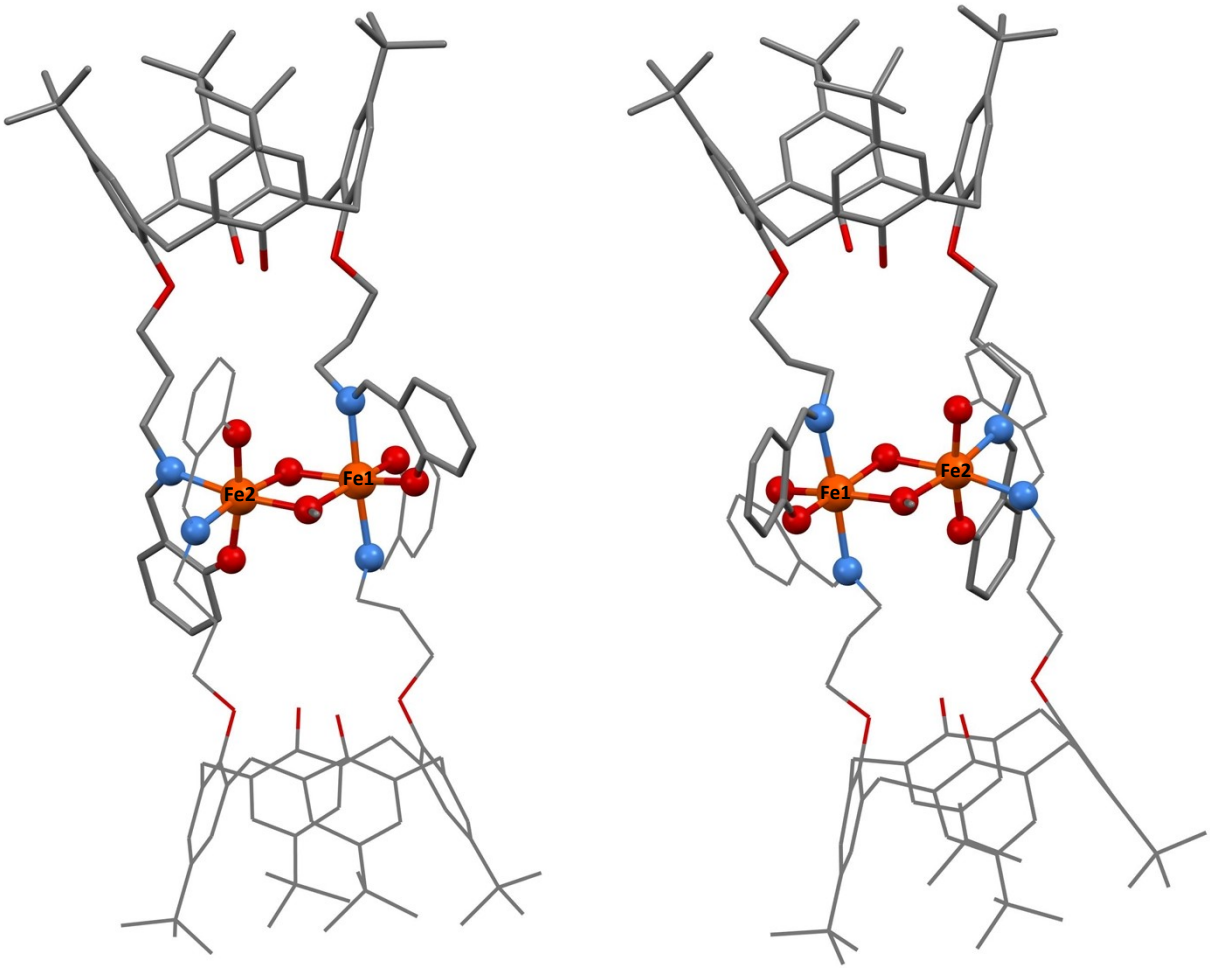
Checkcifs reports responses for 4_2-Fe_2 (CCDC 2256649)

The following Alerts of B level appeared upon checkcif procedure:
RINTA01_ALERT_3_B The value of R_{int} is greater than 0.18……R_{int} given 0.206
PLAT020_ALERT_3_B The Value of R_{int} is Greater Than 0.12 .....0.206 Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.40 Report
Response: *These Alerts B are caused by a poor quality and the partial decomposition of the crystal upon the XRD experiment which was observed even under liquid nitrogen cooling conditions. Unfortunately, all attempts to obtain the crystallographic data of better quality were failed.*



a **b**

Figure S7. ORTEP view for molecular structure of **4_2-$Fe_{2\ exp}$** (a) and **5_2-$Fe_{2\ exp}$** (b) (partially solved structure) with 30% probability. Dark grey, red, goldish and blue ellipsoids represent C-, O-, Fe- and N-atoms, The disordered atoms, H-atoms and solvent molecules are omitted for clarity.



a **b**

Figure S8. For **4_2-$Fe_{2\ exp}$**, two enantiomer complexes (a,b) in crystal unit, showing the macrocycle ligand coordination mode, resulting in *trans*/*cis* orientation of N-atoms of salicylideneamine coordinating sites around coordinated Fe1 and Fe2 metallic centres.

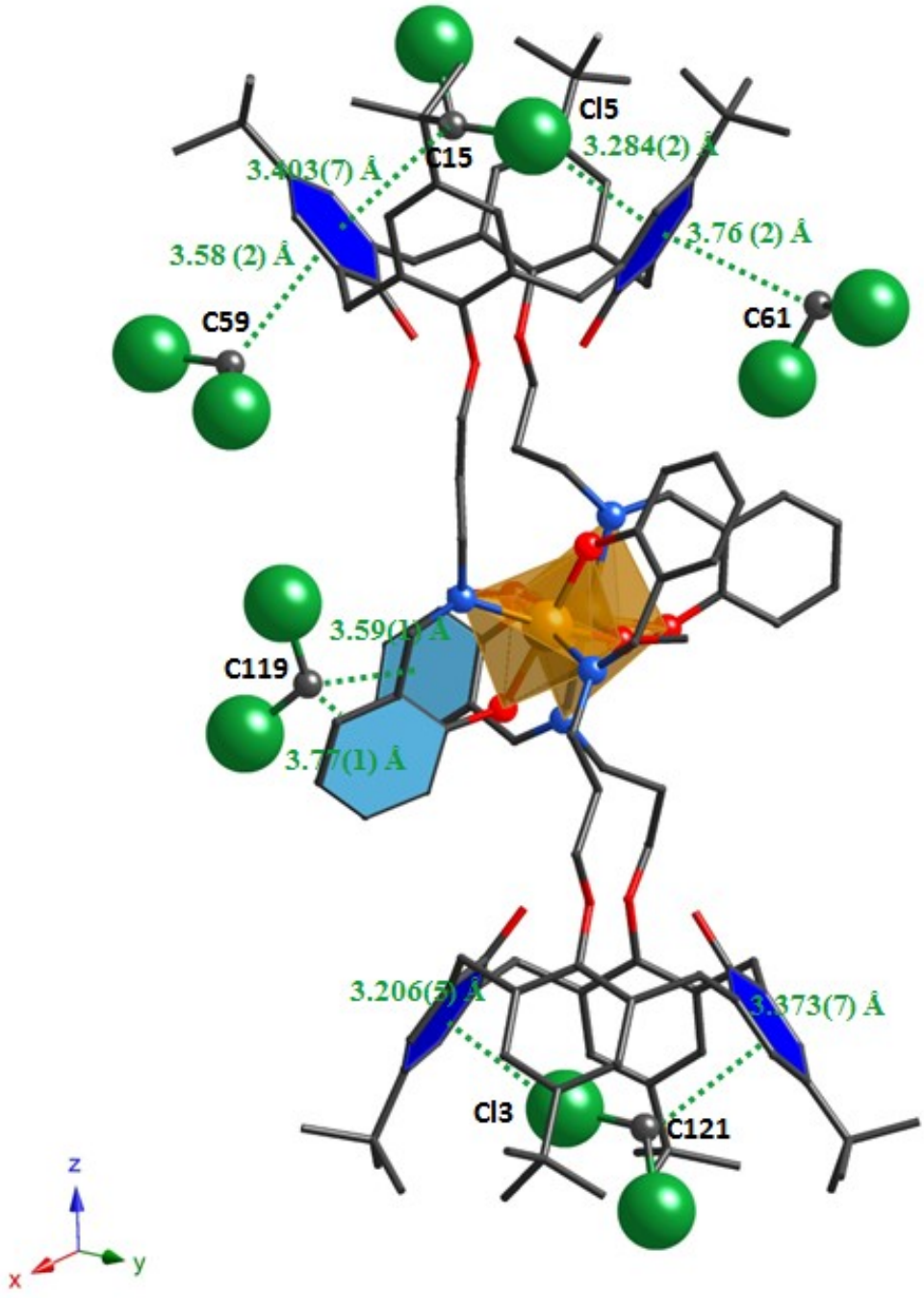


Figure S9. For **4_2-$Fe_{2\ exp}$**, non-covalent interactions within the crystal packing: CH/π bonding involving solvent CH_2Cl_2 molecules and aromatic units of calix[4]arene ligand.

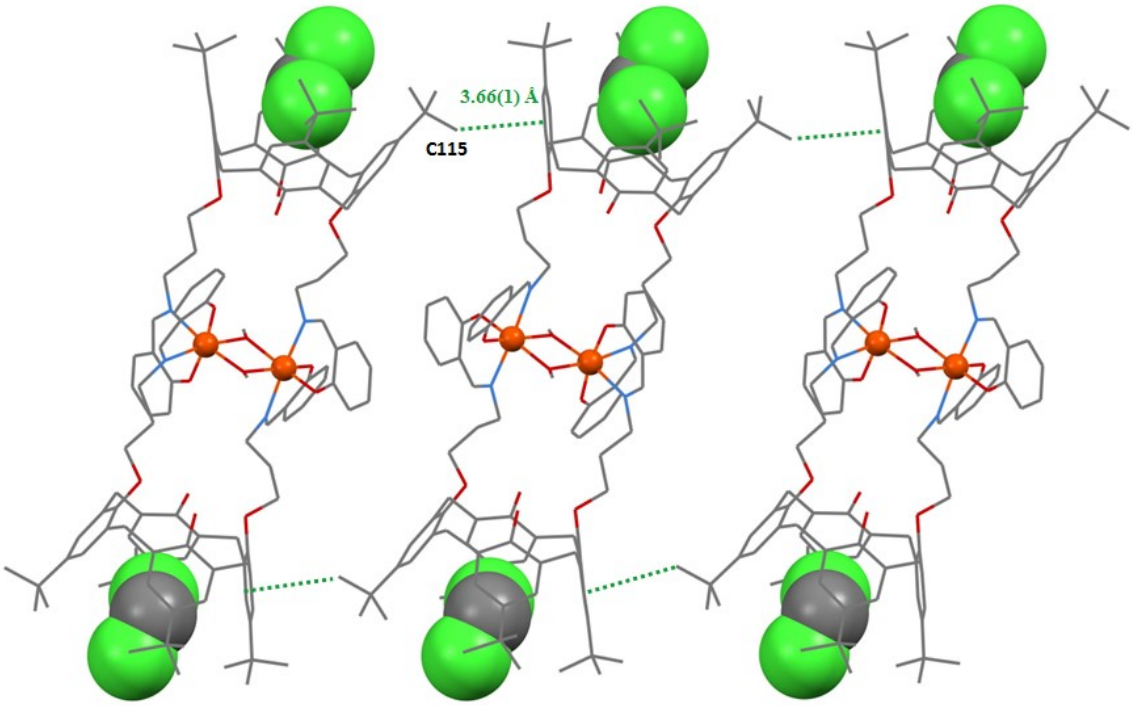


Figure S10. For **4_2-Fe_2 exp**, a portion of crystal packing, showing a formation of 1D chains supported by weak noncovalent CH/π interactions between the C115 atom of tert-butyl group with aromatic system of aryl moiety belonging to calix[4]arene backbone of adjacent complex molecule.Brawn, green and dark grey spheres represent Fe-, Cl- and C-atoms. H-atoms and solvent molecules located in between the complex species are omitted for clarity.

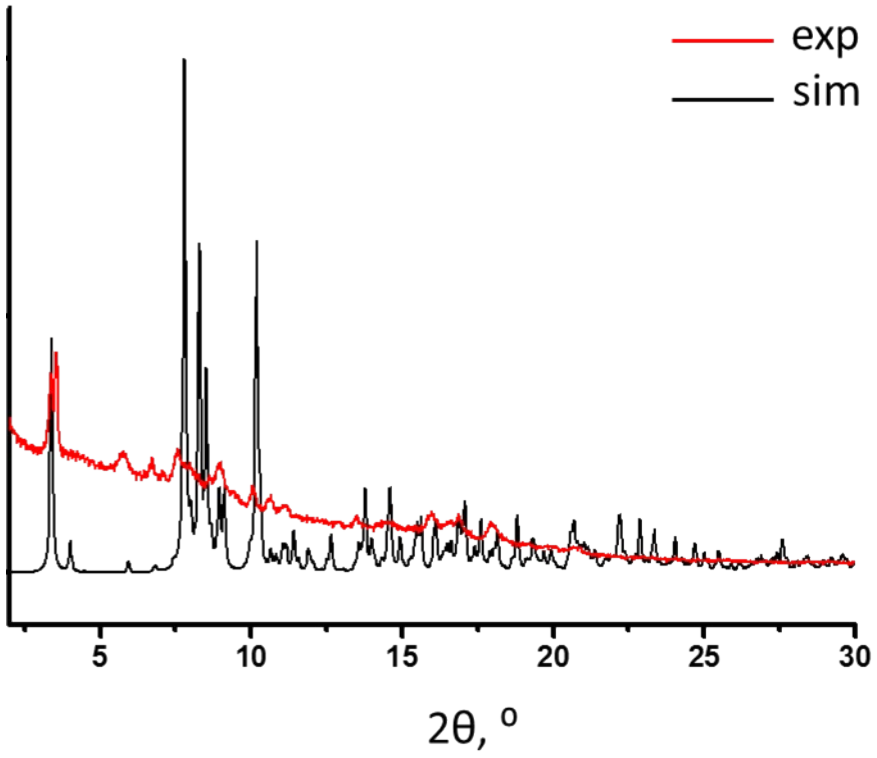
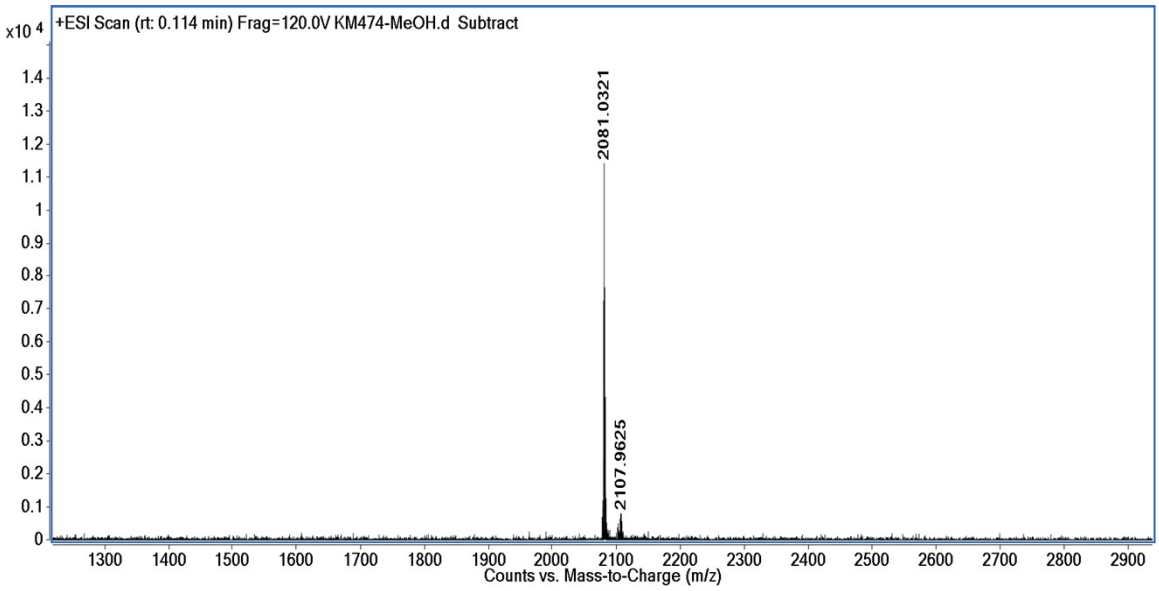
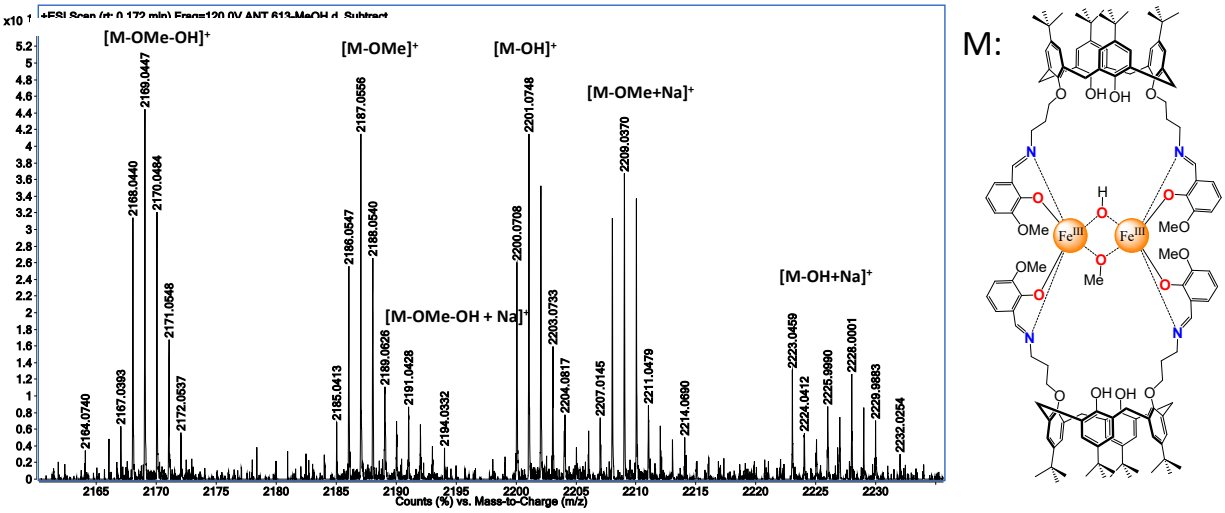


Figure S11. Comparison of experimental PXRD pattern (exp) for $\mathbf{4_2\text{-}Fe_{2\ exp}}$ with the simulated one (sim).

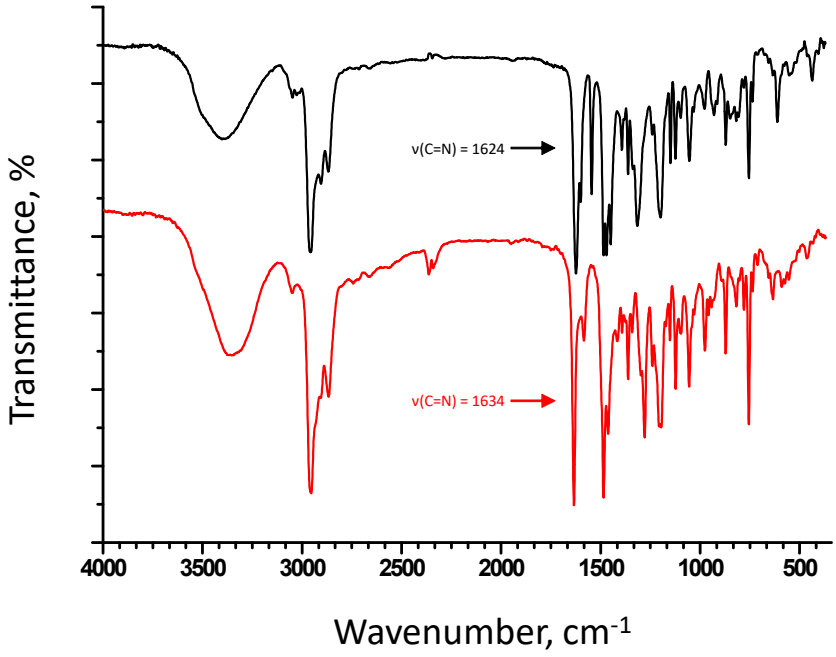


a

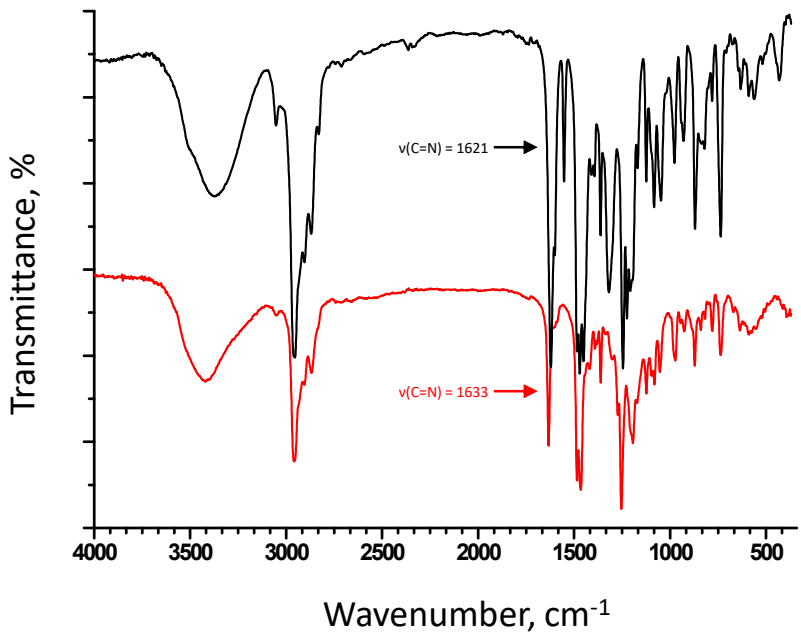


b

Figure S12. The HRESI-MS spectra for $\mathbf{4_2}$-$\mathbf{Fe_{2\ exp}}$ (a) and $\mathbf{5_2}$-$\mathbf{Fe_{2\ exp}}$ (b).

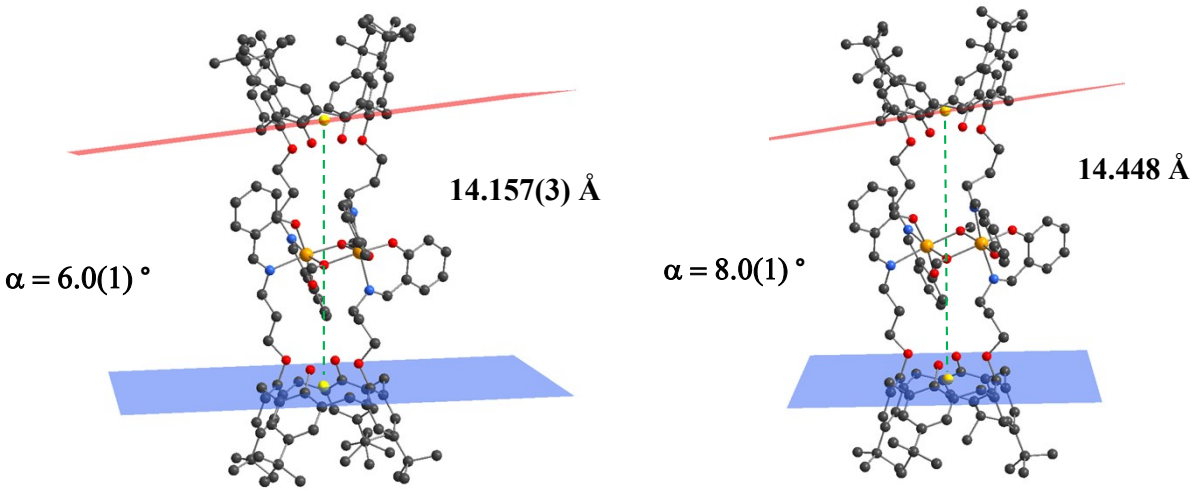


a



b

Figure S13. IR spectra for $\mathbf{4_2}$-$\mathbf{Fe_{2\ exp}}$ (a, black line) and $\mathbf{5_2}$-$\mathbf{Fe_{2\ exp}}$ (b, black line) in comparison with those for free ligands **4** and **5** (red lines), respectively.



a **b**

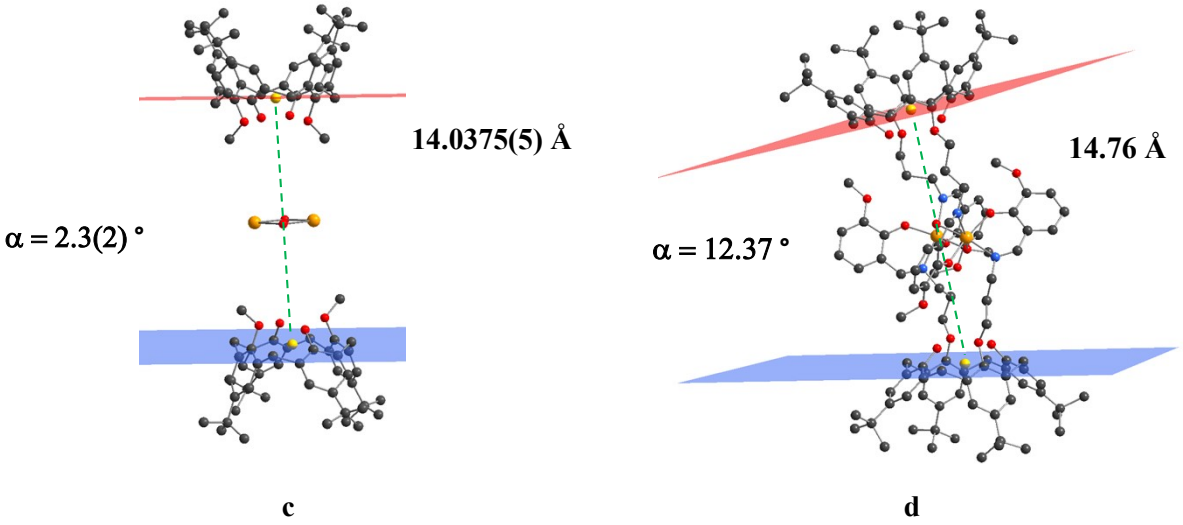


Figure S14. The dihedral angle (α,°) between the planes, passing through four CH_2-bridges of macrocyclic platform, belonging to adjacent calix[4]arene ligands, and the distance (denoted as green dashed line, Å) between the C4-centroids (yellow spheres), built on four C-atoms belonging to CH_2-bridges of adjacent calix[4]arene ligands, observed for **4_2-$Fe_{2\ exp}$** (a), **5_2-$Fe_{2\ exp}$** (b), **4_2-$Fe_{2\ sim}$** (c), **5_2-$Fe_{2\ sim}$** (d). Dark grey, red, goldish, and blue spheres represent C-, O-, Fe- and N-atoms, The disordered atoms, H-atoms and solvent molecules are omitted for clarity.

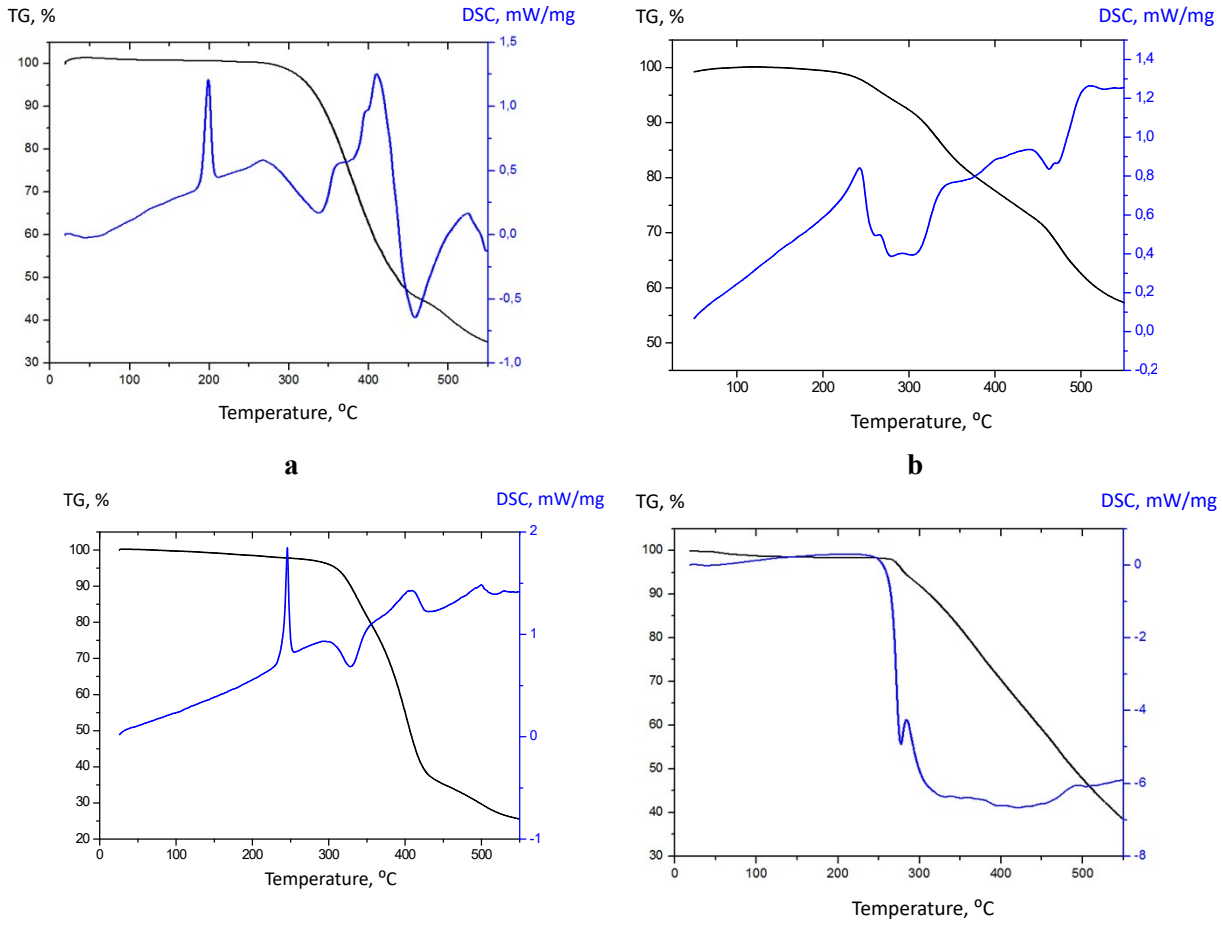
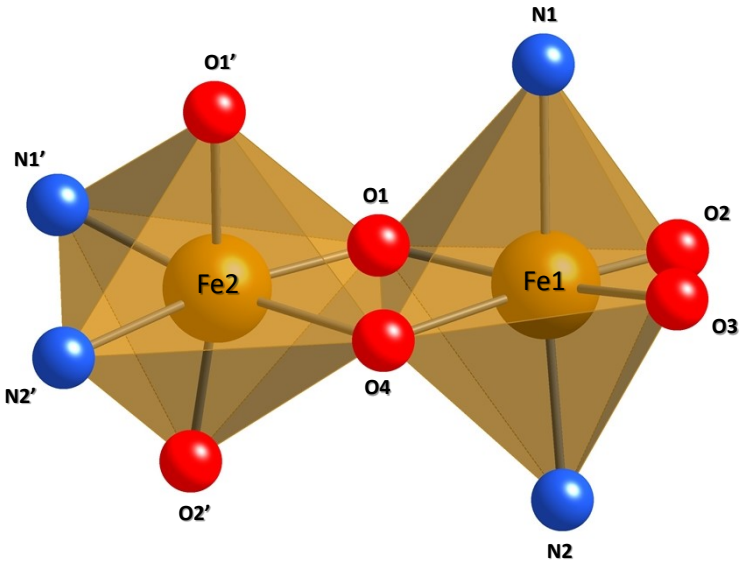


Figure S15. The TGA/DSC traces for samples of **4** (a), **4_2-$Fe_{2\ exp}$** (b), **5** (c) and **5_2-$Fe_{2\ exp}$** (d). Whereas for air-dried sample of **4_2-$Fe_{2\ exp}$** the TGA/DSC analysis revealed the absence of any

solvate molecules, the total mass loss of 1.50% in the temperature range of 25-260°C, observed for **5_2-Fe$_{2\ exp}$**, may be consistent with the presence of *ca* 1 molecule of MeOH per one complex molecule.

Table S2. The coordination bond lengths and angles for **4_2-Fe$_{2\ exp}$** (established by SCXRD), **4_2-Fe$_{2\ sim}$**, **5_2-Fe$_{2\ sim}$** (obtained based on DFT/B3LYP – calculations).



	$N_{x,y}/O_{x,y}$	4_2-Fe$_{2\ exp}$	4_2-Fe$_{2\ sim}$	5_2-Fe$_{2\ sim}$
d (Fe1…N_x), Å	N1	2.181(7)	2.2321	2.0570
	N2	2.150(6)	2.2190	2.3150
d (Fe1…O_x), Å	O1	2.001(5)	2.0745	2.0810
	O2	1.929(5)	1.9616	1.9719
	O3	1.957(6)	1.9596	1.9620
	O4	2.021(5)	2.0710	2.0914
d (Fe2…N_x), Å	N1'	2.175(7)	2.2840	2.1556
	N2'	2.183(7)	2.2784	2.2200
d (Fe2…O_x), Å	O1'	1.952(5)	1.9572	1.9595
	O1	1.995(5)	2.0229	2.0398
	O4	2.010(5)	2.0281	2.0359
	O2'	1.946(6)	1.9586	1.9698
∠ N_x – Fe1 – N_y, °	N1/N2	176.1(3)	171.61	163.32
∠ N_x – Fe1 – O_y, °	N1/O1	85.9(2)	89.12	86.20
	N1/O2	90.0(2)	90.36	93.04
	N1/O3	84.7(2)	83.94	86.78
	N1/O4	97.2(2)	96.94	98.58
	O1/N2	96.2(2)	97.92	110.09
	O2/N2	86.5(2)	84.78	81.89
	O3/N2	93.9(2)	90.03	78.13
	O4/N2	86.5(2)	89.26	89.71
∠ O_x – Fe1 – O_y, °	O1/O2	95.3(2)	92.72	96.38
	O1/O3	163.8(2)	166.59	165.31
	O1/O4	75.1(2)	75.62	73.95
	O2/O3	97.9(2)	98.77	96.86
	O2/O4	167.4(2)	166.07	164.24
	O3/O4	92.9(2)	93.80	94.40

∠ N_x – Fe2 – N_y, °	N1′/N2′	92.2(3)	89.41	99.40
∠ N_x – Fe2 – O_y, °	O1′/N1′	88.1(2)	88.22	79.96
	O1′/N2′	86.1(2)	83.92	89.39
	N1′/O1	96.8(2)	96.99	102.73
	N1′/O4	170.8(2)	174.65	171.19
	N1′/O2′	85.9(3)	83.80	85.91
	O1/N2′	170.7(2)	173.59	156.63
	O4/N2′	95.8(2)	95.90	83.24
	N2′/O2′	88.6(3)	88.73	83.39
∠ O_x – Fe2 – O_y, °	O1′/O1	96.8(2)	96.63	101.73
	O1′/O4	87.8(2)	91.69	91.71
	O1′/O2′	171.8(2)	169.21	162.87
	O1/O4	75.5(2)	77.71	76.01
	O1/O2′	89.4(2)	91.56	90.73
	O4/O2′	99.0(2)	96.93	102.78

Table S3. SHAPE[1] analysis of coordination polyhedrons for **4_2-$Fe_{2\ exp}$** (established by SCXRD), **4_2-$Fe_{2\ sim}$**, **5_2-$Fe_{2\ sim}$** (obtained based on DFT/B3LYP – calculations).

Complex name	Fe	HP-6	PPY-6	OC-6	TPR-6	JPPY-6
4_2-$Fe_{2\ exp}$	Fe1	31.639	23.065	1.229	11.535	26.615
	Fe2	29.428	24.358	1.091	12.650	28.564
4_2-$Fe_{2\ sim}$	Fe1	32.303	23.829	1.344	11.021	27.117
	Fe2	29.605	26.008	1.044	14.025	30.125
5_2-$Fe_{2\ sim}$	Fe1	29.704	20.994	2.591	9.179	24.301
	Fe2	33.219	20.867	2.427	9.471	25.235

Label	Symmetry	Shape
HP-6	D_{6h}	Hexagon
PPY-6	C_{5v}	Pentagonal pyramid
OC-6	O_h	Octahedron
TPR-6	D_{3h}	Trigonal prism
JPPY-6	C_{5v}	Johnson pentagonal pyramid (J2)

Table S4. The dihedral angles between the opposite aryl moieties (A-C and B-D) of macrocycle platform for **4_2-$Fe_{2\ exp}$**, **5_2-$Fe_{2\ exp}$** (both established by SCXRD), **4_2-$Fe_{2\ sim}$**, **5_2-$Fe_{2\ sim}$** (both obtained based on DFT/B3LYP – calculations).

	4_2-$Fe_{2\ exp}$	**4_2-$Fe_{2\ sim}$**	**5_2-$Fe_{2\ exp}$**	**5_2-$Fe_{2\ sim}$**
∠A-C, °	45.7(3) 46.2(6)	37.24 38.04	42.2(6)	38.95 39.33
∠B-D, °	70.7(3) 72.6(7)	86.23 89.07	81.3(3)	86.22 88.21
Δ, °	25.0(3) 26.4(6)	48.99 51.03	39.1(6)	47.27 48.88

Table S5. The Fe…Fe distances observed for $\mathbf{4_2\text{-}Fe_{2\ exp}}$, $\mathbf{5_2\text{-}Fe_{2\ exp}}$ (both established by SCXRD), $\mathbf{4_2\text{-}Fe_{2\ sim}}$, $\mathbf{5_2\text{-}Fe_{2\ sim}}$ (both obtained based on DFT/B3LYP – calculations).

	$\mathbf{4_2\text{-}Fe_{2\ exp}}$	$\mathbf{4_2\text{-}Fe_{2\ sim}}$	$\mathbf{5_2\text{-}Fe_{2\ exp}}$	$\mathbf{5_2\text{-}Fe_{2\ sim}}$
d (Fe…Fe), Å	3.175(2)	3.215	3.354(6)	3.272

Table S6. Optimized geometries in Cartesian coordinates for **4**, obtained by DFT-B3LYP calculations.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.749977	4.459356	3.872938
2	8	0	-8.234138	-0.512470	-0.495057
3	8	0	-1.420741	-1.494410	-1.466058
4	8	0	0.358785	0.617133	2.472172
5	8	0	-0.377205	1.155881	-0.187521
6	1	0	-0.122951	1.091005	0.752762
7	7	0	-6.226983	-2.067443	-1.691256
8	8	0	0.093538	-1.887718	1.265157
9	1	0	0.191492	-1.086079	1.813250
10	7	0	-2.976219	2.224936	2.682796
11	6	0	2.237788	2.019073	1.851262
12	6	0	-7.002977	-3.024043	-1.362439
13	1	0	-6.723500	-4.072264	-1.577509
14	6	0	0.319580	-0.501011	-2.811850
15	6	0	1.899973	-2.768444	-2.419855
16	1	0	2.511861	-3.640954	-2.215286
17	6	0	-8.900431	-1.679254	-0.279453
18	6	0	0.657533	-2.684688	-1.774367
19	6	0	0.386721	2.049660	-0.882009
20	6	0	1.748577	0.835504	2.426875
21	6	0	1.565959	-0.631724	-3.429834
22	1	0	1.920951	0.201039	-4.032532
23	6	0	2.370279	-1.771889	-3.281092
24	6	0	-3.642884	5.044116	2.662872
25	6	0	-0.157082	-1.569511	-2.027454
26	6	0	-0.313649	1.064130	3.684341
27	1	0	-0.385614	2.157610	3.659697
28	1	0	0.305803	0.777487	4.541801
29	6	0	3.624494	2.184564	1.795792
30	1	0	4.003842	3.102407	1.354207
31	6	0	2.599951	-0.178643	2.883930
32	6	0	4.525172	1.218205	2.270885
33	6	0	-3.784805	-1.843196	-1.556230
34	1	0	-3.945555	-0.772532	-1.385632
35	1	0	-3.734875	-2.321562	-0.570086
36	6	0	-4.974713	-2.407971	-2.345112
37	1	0	-4.992056	-1.949220	-3.344541
38	1	0	-4.860247	-3.499862	-2.484720
39	6	0	2.103992	-2.651622	2.414352
40	6	0	-1.688972	0.417890	3.775912
41	1	0	-2.116369	0.712037	4.743802
42	1	0	-1.579915	-0.674052	3.790571
43	6	0	-3.236042	4.314995	1.512236
44	6	0	-2.460681	-2.047173	-2.280751
45	1	0	-2.264494	-3.116502	-2.458349
46	1	0	-2.471085	-1.546203	-3.261796
47	6	0	3.982067	0.041508	2.799581
48	1	0	4.636026	-0.747549	3.155268
49	6	0	-8.308842	-2.896821	-0.695363
50	6	0	-2.922387	2.893076	1.582771
51	1	0	-2.628926	2.406268	0.642562

52	6	0	1.187307	3.020793	-0.262036
53	6	0	0.310672	1.964884	-2.286296
54	6	0	-0.447372	0.814776	-2.934246
55	1	0	-1.428588	0.701354	-2.466911
56	1	0	-0.607250	1.054002	-3.993259
57	6	0	2.227480	-4.734474	0.553778
58	1	0	2.255577	-5.526567	-0.188381
59	6	0	1.145860	-2.745881	1.387431
60	6	0	-10.154392	-1.688435	0.346854
61	1	0	-10.595795	-0.743597	0.661287
62	6	0	3.095793	-3.636555	2.488773
63	1	0	3.818398	-3.561753	3.298948
64	6	0	1.322864	3.088335	1.255977
65	1	0	1.730092	4.071275	1.517179
66	1	0	0.332731	3.041703	1.722242
67	6	0	-2.676111	0.798980	2.661126
68	1	0	-2.306579	0.475312	1.677512
69	1	0	-3.613013	0.256766	2.847048
70	6	0	3.179202	-4.705389	1.583961
71	6	0	0.270285	-3.759941	-0.760239
72	1	0	-0.751713	-3.580317	-0.418055
73	1	0	0.296359	-4.747605	-1.237951
74	6	0	-3.943500	6.409638	2.549215
75	1	0	-4.253734	6.946506	3.440811
76	6	0	1.223617	-3.768351	0.426339
77	6	0	0.996278	2.912833	-3.045664
78	1	0	0.913032	2.846277	-4.128527
79	6	0	-9.023425	-4.085093	-0.453432
80	1	0	-8.573971	-5.024110	-0.769766
81	6	0	4.207973	-6.855854	0.648577
82	1	0	3.252362	-7.393363	0.663030
83	1	0	5.003392	-7.593959	0.807319
84	1	0	4.347396	-6.432103	-0.353134
85	6	0	6.042063	1.475780	2.189387
86	6	0	1.869628	3.941417	-1.073772
87	1	0	2.469910	4.696402	-0.575267
88	6	0	3.716621	-1.870546	-4.024212
89	6	0	-10.836209	-2.884107	0.569284
90	1	0	-11.807661	-2.863668	1.056382
91	6	0	2.080263	-1.509552	3.425901
92	1	0	2.705856	-1.798284	4.277962
93	1	0	1.067444	-1.384843	3.825810
94	6	0	4.276457	-5.775276	1.745764
95	6	0	1.783243	3.927396	-2.469830
96	6	0	6.392177	2.751582	2.993872
97	1	0	5.875782	3.635633	2.604168
98	1	0	7.470773	2.947456	2.945087
99	1	0	6.114415	2.639385	4.048806
100	6	0	-3.142585	4.988801	0.278235
101	1	0	-2.826689	4.426379	-0.598096
102	6	0	-10.269956	-4.096798	0.167597
103	1	0	-10.791200	-5.034588	0.335761
104	6	0	-3.842059	7.046675	1.315838
105	1	0	-4.078701	8.105519	1.243554
106	6	0	4.645065	-0.714360	-3.579420
107	1	0	4.205682	0.266074	-3.791719
108	1	0	5.606724	-0.771818	-4.106220

109	1	0	4.841828	-0.764671	-2.501962
110	6	0	-3.440580	6.341759	0.169995
111	1	0	-3.363354	6.846364	-0.788534
112	6	0	4.445729	-3.200161	-3.748051
113	1	0	4.693531	-3.318247	-2.686657
114	1	0	5.386224	-3.227851	-4.311530
115	1	0	3.848170	-4.065625	-4.058853
116	6	0	3.473049	-1.768689	-5.549676
117	1	0	2.827886	-2.584138	-5.898356
118	1	0	4.424489	-1.829757	-6.094048
119	1	0	2.992454	-0.822958	-5.822835
120	6	0	2.497174	4.956793	-3.367364
121	6	0	3.337531	5.962329	-2.556187
122	1	0	2.721580	6.544757	-1.860696
123	1	0	3.822619	6.670731	-3.238315
124	1	0	4.127691	5.464351	-1.981324
125	6	0	5.672689	-5.110166	1.673064
126	1	0	5.815511	-4.604447	0.710623
127	1	0	6.463546	-5.863568	1.783548
128	1	0	5.810615	-4.365552	2.464868
129	6	0	6.453666	1.674829	0.710245
130	1	0	6.221381	0.784055	0.115163
131	1	0	7.532799	1.860917	0.638662
132	1	0	5.937467	2.525402	0.252311
133	6	0	4.120302	-6.477375	3.117036
134	1	0	4.205156	-5.768662	3.948422
135	1	0	4.897599	-7.241525	3.248709
136	1	0	3.142853	-6.968113	3.195843
137	6	0	6.868774	0.308173	2.763017
138	1	0	6.647997	0.131280	3.822615
139	1	0	7.936853	0.542445	2.684456
140	1	0	6.696171	-0.625311	2.214693
141	6	0	1.445429	5.755239	-4.176100
142	1	0	0.834038	5.098841	-4.804928
143	1	0	0.769541	6.300676	-3.506591
144	1	0	1.938300	6.484582	-4.832205
145	6	0	3.446060	4.228472	-4.350140
146	1	0	4.203817	3.650795	-3.807481
147	1	0	3.963795	4.953638	-4.991546
148	1	0	2.903780	3.536713	-5.003900
149	1	0	-3.508410	3.495499	3.762607
150	1	0	-8.765121	0.224944	-0.153289

Table S7. Optimized geometries in Cartesian coordinates for **5**, obtained by DFT-B3LYP calculations.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.693036	4.461535	-3.068730
2	8	0	7.695082	-1.456400	0.868574
3	8	0	0.770867	-1.899667	1.515335
4	8	0	-0.606411	0.704122	-2.295860
5	8	0	-0.029902	0.923610	0.449815
6	1	0	-0.210772	0.979876	-0.507756
7	7	0	5.491487	-2.922473	1.871061
8	8	0	-0.576672	-1.918796	-1.327545
9	1	0	-0.587793	-1.064168	-1.798898
10	7	0	2.795429	2.148749	-2.153898
11	6	0	-2.437857	2.153105	-1.641843
12	6	0	6.184839	-3.919061	1.481783
13	1	0	5.801200	-4.949884	1.596295
14	6	0	-0.995363	-0.924503	2.841260
15	6	0	-2.680041	-3.031613	2.121240
16	1	0	-3.327810	-3.836462	1.789186
17	6	0	8.218303	-2.671989	0.579668
18	6	0	-1.391279	-2.971409	1.571318
19	6	0	-0.776550	1.800681	1.182478
20	6	0	-1.981472	1.003743	-2.306833
21	6	0	-2.289251	-1.028180	3.358586
22	1	0	-2.635476	-0.234850	4.016900
23	6	0	-3.149814	-2.090810	3.043378
24	6	0	3.555927	4.912788	-1.809189
25	6	0	-0.529749	-1.943385	1.987275
26	6	0	0.161473	1.224412	-3.419004
27	1	0	0.284706	2.305329	-3.286155
28	1	0	-0.416000	1.052316	-4.334373
29	6	0	-3.814018	2.397725	-1.645869
30	1	0	-4.167249	3.288888	-1.133299
31	6	0	-2.859220	0.096137	-2.913975
32	6	0	-4.736884	1.541411	-2.266774
33	6	0	3.088594	-2.461133	1.672534
34	1	0	3.348276	-1.398802	1.600259
35	1	0	3.043329	-2.850620	0.647843
36	6	0	4.188601	-3.193093	2.454439
37	1	0	4.206420	-2.815720	3.487311
38	1	0	3.969710	-4.277037	2.502105
39	6	0	-2.541624	-2.438009	-2.674658
40	6	0	1.507225	0.517424	-3.493001
41	1	0	2.006252	0.877090	-4.402772
42	1	0	1.348454	-0.561376	-3.617729
43	6	0	3.080677	4.095403	-0.756960
44	6	0	1.719086	-2.605936	2.323305
45	1	0	1.425582	-3.664791	2.400823
46	1	0	1.723566	-2.188993	3.343031
47	6	0	-4.229230	0.392871	-2.885295
48	1	0	-4.903490	-0.313470	-3.358195
49	6	0	7.518365	-3.859698	0.862080
50	6	0	2.720444	2.702034	-0.993173
51	1	0	2.371640	2.133278	-0.120423

52	6	0	-1.468528	2.881755	0.616274
53	6	0	-0.800630	1.575443	2.573185
54	6	0	-0.160394	0.318434	3.144932
55	1	0	0.841147	0.186056	2.728542
56	1	0	-0.057814	0.440755	4.230713
57	6	0	-2.911343	-4.681820	-1.047810
58	1	0	-3.035962	-5.538986	-0.393122
59	6	0	-1.663860	-2.693007	-1.604253
60	6	0	9.496521	-2.738407	-0.022427
61	6	0	-3.579351	-3.346785	-2.912284
62	1	0	-4.238384	-3.149060	-3.755127
63	6	0	-1.502724	3.101553	-0.892821
64	1	0	-1.835988	4.128452	-1.078980
65	1	0	-0.489392	3.037901	-1.303723
66	6	0	2.441412	0.742130	-2.293248
67	1	0	2.002505	0.338802	-1.369284
68	1	0	3.365901	0.179920	-2.482089
69	6	0	-3.785591	-4.491672	-2.128356
70	6	0	-0.998301	-3.966379	0.480072
71	1	0	0.053400	-3.820513	0.222341
72	1	0	-1.113631	-4.992160	0.853124
73	6	0	3.904620	6.260942	-1.540083
74	6	0	-1.865766	-3.798226	-0.759355
75	6	0	-1.472330	2.491958	3.381647
76	1	0	-1.468507	2.314616	4.455141
77	6	0	8.130418	-5.087738	0.527561
78	1	0	7.592229	-6.007467	0.743732
79	6	0	-5.005101	-6.650982	-1.485897
80	1	0	-4.084856	-7.247199	-1.488348
81	1	0	-5.829268	-7.315302	-1.772300
82	1	0	-5.193725	-6.315989	-0.458966
83	6	0	-6.240144	1.877899	-2.233292
84	6	0	-2.137373	3.769152	1.474902
85	1	0	-2.647963	4.612665	1.020419
86	6	0	-4.553545	-2.160236	3.675110
87	6	0	10.080433	-3.959338	-0.342071
88	1	0	11.061443	-4.001364	-0.803112
89	6	0	-2.383201	-1.204959	-3.559137
90	1	0	-2.966881	-1.366378	-4.472249
91	1	0	-1.340187	-1.107248	-3.881622
92	6	0	-4.927533	-5.468591	-2.471497
93	6	0	-2.146586	3.613731	2.864944
94	6	0	-6.476625	3.262062	-2.884982
95	1	0	-5.938934	4.059172	-2.360218
96	1	0	-7.544589	3.513223	-2.865843
97	1	0	-6.145069	3.265787	-3.930300
98	6	0	2.957523	4.629889	0.545123
99	1	0	2.586869	3.990875	1.342830
100	6	0	9.385146	-5.145391	-0.061896
101	1	0	9.834031	-6.102986	-0.308807
102	6	0	3.774018	6.762307	-0.246253
103	1	0	4.038839	7.792311	-0.033604
104	6	0	-5.371684	-0.912883	3.260857
105	1	0	-4.888343	0.016129	3.581626
106	1	0	-6.372654	-0.944098	3.711262
107	1	0	-5.487983	-0.868016	2.171504
108	6	0	3.299900	5.946775	0.797756

109	1	0	3.205620	6.359350	1.797973
110	6	0	-5.336654	-3.412375	3.234004
111	1	0	-5.507986	-3.427547	2.151333
112	1	0	-6.318333	-3.423379	3.723032
113	1	0	-4.817491	-4.337403	3.512384
114	6	0	-4.425809	-2.196704	5.217450
115	1	0	-3.854167	-3.074687	5.541834
116	1	0	-5.418700	-2.244927	5.683593
117	1	0	-3.918390	-1.306672	5.605227
118	6	0	-2.851586	4.598106	3.818194
119	6	0	-3.521917	5.765860	3.067997
120	1	0	-2.794332	6.358335	2.500453
121	1	0	-4.005119	6.437385	3.787849
122	1	0	-4.296461	5.417074	2.374262
123	6	0	-6.285285	-4.725741	-2.429904
124	1	0	-6.472233	-4.308215	-1.433364
125	1	0	-7.106414	-5.413259	-2.671500
126	1	0	-6.321152	-3.900536	-3.149851
127	6	0	-6.724897	1.914700	-0.763211
128	1	0	-6.573164	0.944779	-0.275410
129	1	0	-7.795257	2.153612	-0.721888
130	1	0	-6.191329	2.669530	-0.175659
131	6	0	-4.709071	-6.045329	-3.891763
132	1	0	-4.692921	-5.256770	-4.652358
133	1	0	-5.515522	-6.743720	-4.151455
134	1	0	-3.757103	-6.586172	-3.951912
135	6	0	-7.091856	0.841593	-2.992189
136	1	0	-6.814281	0.780270	-4.051396
137	1	0	-8.148435	1.130255	-2.945145
138	1	0	-7.005605	-0.159692	-2.554417
139	6	0	-1.819059	5.196102	4.804959
140	1	0	-1.332504	4.419209	5.404850
141	1	0	-1.035063	5.742451	4.267135
142	1	0	-2.309074	5.893878	5.496526
143	6	0	-3.947002	3.854473	4.620757
144	1	0	-4.704109	3.430505	3.950281
145	1	0	-4.450236	4.542687	5.312409
146	1	0	-3.529227	3.033311	5.213339
147	1	0	3.413967	3.501789	-3.067393
148	1	0	8.342865	-0.785968	0.584608
149	8	0	10.057996	-1.500565	-0.240868
150	6	0	11.339667	-1.431767	-0.854166
151	1	0	12.097317	-1.932700	-0.238414
152	1	0	11.320415	-1.880143	-1.855476
153	1	0	11.576470	-0.369572	-0.933308
154	8	0	4.352906	6.970609	-2.615630
155	6	0	4.724618	8.325618	-2.418204
156	1	0	3.875124	8.928048	-2.068223
157	1	0	5.554111	8.414151	-1.703314
158	1	0	5.048023	8.688328	-3.395563

Table S8. Optimized geometries in Cartesian coordinates for **4_2-$Fe_{2\ sim}$**, obtained by DFT-B3LYP calculations.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.045899	-0.145384	-1.942346
2	26	0	0.047530	0.036899	1.265982
3	8	0	-0.736811	-1.082344	-0.225392
4	8	0	6.001011	0.064046	-2.222169
5	8	0	5.857866	0.556592	2.269629
6	8	0	-0.729314	-1.568660	-3.106481
7	8	0	0.741728	0.977970	-0.390966
8	8	0	0.527509	1.120806	-3.323648
9	8	0	-1.449248	1.288409	1.420218
10	8	0	1.548386	-1.203180	1.479685
11	8	0	6.388488	1.944057	-0.269026
12	1	0	6.234634	1.337390	-1.026124
13	8	0	6.089438	-1.388420	0.328767
14	1	0	5.979317	-0.760077	1.075566
15	8	0	-5.649325	-0.559241	2.425660
16	8	0	-6.165512	-0.190515	-2.023122
17	8	0	-6.031297	1.418458	0.230661
18	1	0	-6.071582	0.924589	-0.611533
19	7	0	-0.852886	-1.143138	3.001910
20	8	0	-6.408743	-2.075116	0.012260
21	1	0	-6.324847	-1.492135	-0.766593
22	7	0	1.891829	-1.212927	-2.114648
23	7	0	1.051003	1.429819	2.763981
24	7	0	-1.993438	0.934394	-2.095350
25	6	0	9.181539	1.856646	3.180426
26	1	0	9.712608	2.801751	3.142258
27	6	0	9.101482	-0.489132	3.640001
28	1	0	9.574514	-1.410092	3.972574
29	6	0	7.303966	-0.226395	-2.620245
30	6	0	7.791312	-1.541546	-2.535035
31	6	0	9.449417	0.551367	-3.390272
32	1	0	10.077750	1.384042	-3.689121
33	6	0	8.133857	0.837978	-3.002136
34	6	0	7.864686	1.838298	2.696336
35	6	0	7.786102	-0.562444	3.175998
36	6	0	7.409508	-3.111843	-0.571564
37	6	0	-1.671330	2.470893	1.927856
38	6	0	9.822714	0.714831	3.673725
39	6	0	9.110504	-1.772597	-2.937114
40	1	0	9.484103	-2.791529	-2.873537
41	6	0	6.961382	-2.690479	-1.966371
42	1	0	5.908819	-2.402091	-1.939400
43	1	0	7.050164	-3.555256	-2.635566
44	6	0	9.961846	-0.751124	-3.386877
45	6	0	7.661751	2.288162	-2.935727
46	1	0	6.573160	2.336309	-3.047949
47	1	0	8.081921	2.830497	-3.790178
48	6	0	8.080840	3.018431	-1.662932
49	6	0	11.266267	0.731702	4.212665
50	6	0	7.167170	0.624190	2.745405
51	6	0	7.888740	3.446102	0.734906

52	6	0	11.401430	-1.084602	-3.824176
53	6	0	8.263167	-4.206773	-0.392897
54	1	0	8.550868	-4.766868	-1.277557
55	6	0	-7.972442	1.288071	-2.663117
56	6	0	12.178266	-1.686884	-2.628077
57	1	0	12.226639	-0.975533	-1.795280
58	1	0	13.205303	-1.934577	-2.926162
59	1	0	11.707524	-2.603244	-2.255980
60	6	0	9.120041	3.961186	-1.712514
61	1	0	9.581111	4.140216	-2.679105
62	6	0	4.980943	0.050686	-3.244060
63	1	0	4.921841	-0.960035	-3.672198
64	1	0	5.264606	0.741768	-4.049956
65	6	0	6.991561	-2.383486	0.557132
66	6	0	-0.284465	-2.174101	3.539400
67	1	0	-0.786125	-2.646054	4.396443
68	6	0	9.554671	4.675111	-0.590757
69	6	0	7.270537	3.105886	2.085684
70	1	0	6.190412	2.990415	1.974217
71	1	0	7.447509	3.944852	2.770259
72	6	0	8.915078	4.384186	0.626620
73	1	0	9.221882	4.904626	1.531726
74	6	0	7.473924	-2.717176	1.839343
75	6	0	-7.496571	0.866786	3.083836
76	6	0	7.449531	2.780776	-0.428996
77	6	0	8.335475	-3.812746	1.959069
78	1	0	8.685127	-4.067037	2.957578
79	6	0	3.671303	0.473735	-2.595954
80	1	0	2.927438	0.658563	-3.376772
81	1	0	3.835650	1.433733	-2.091827
82	6	0	-0.726763	3.137876	2.771242
83	6	0	-9.093394	-1.405331	3.389469
84	1	0	-9.702328	-2.300895	3.462829
85	6	0	0.528360	2.545082	3.164611
86	1	0	1.082372	3.129430	3.913182
87	6	0	-2.904046	3.124665	1.662386
88	1	0	-3.629517	2.605531	1.042994
89	6	0	4.811220	0.790988	3.229929
90	1	0	5.103035	1.631779	3.872956
91	1	0	4.697441	-0.097523	3.869138
92	6	0	1.825378	-2.287413	2.153953
93	6	0	10.666425	5.740418	-0.646473
94	6	0	-7.774585	-1.555825	2.936879
95	6	0	7.085067	-1.914861	3.077136
96	1	0	5.998617	-1.781794	3.107051
97	1	0	7.344478	-2.508458	3.960888
98	6	0	-6.934750	2.437376	0.292437
99	6	0	3.522623	1.089960	2.469158
100	1	0	3.387954	0.350749	1.675908
101	1	0	3.598950	2.075848	1.994917
102	6	0	-7.461957	-0.014751	-2.538995
103	6	0	-8.816858	0.959997	3.532711
104	1	0	-9.215996	1.954633	3.718428
105	6	0	-9.638413	-0.161327	3.723010
106	6	0	0.080167	2.232477	-3.844164
107	6	0	8.742148	-4.593205	0.865984
108	6	0	-3.175176	4.380174	2.183415

109	1	0	-4.128441	4.852761	1.956919
110	6	0	-6.958639	-0.414517	2.842067
111	6	0	-5.076975	-0.340821	-2.986939
112	1	0	-4.954008	0.610463	-3.520609
113	1	0	-5.375285	-1.104139	-3.714125
114	6	0	-9.278349	1.430319	-3.140275
115	1	0	-9.670994	2.438964	-3.240947
116	6	0	1.035252	-3.189814	-3.298787
117	6	0	-8.242133	-1.146418	-2.812502
118	6	0	-10.088254	0.334192	-3.475461
119	6	0	2.032728	-2.392160	-2.622321
120	1	0	3.025561	-2.859488	-2.565882
121	6	0	-3.334686	-0.969859	2.745221
122	1	0	-3.249223	-0.384880	1.826635
123	1	0	-3.369870	-2.029194	2.461584
124	6	0	-0.295625	-2.724071	-3.538370
125	6	0	-0.926758	-2.483565	-0.145812
126	1	0	-1.583524	-2.818264	-0.956545
127	1	0	-1.391409	-2.749239	0.811056
128	1	0	0.030071	-3.016128	-0.229066
129	6	0	3.100473	-0.559221	-1.588543
130	1	0	3.860873	-1.311267	-1.344752
131	1	0	2.816289	-0.067219	-0.660710
132	6	0	-2.241728	5.044303	3.003726
133	1	0	-2.463134	6.027242	3.408887
134	6	0	-2.110543	-0.702510	3.628116
135	1	0	-2.030161	0.372015	3.821541
136	1	0	-2.229684	-1.203790	4.602017
137	6	0	0.960480	2.373516	-0.487861
138	1	0	1.512953	2.603088	-1.405736
139	1	0	1.547204	2.726426	0.368851
140	1	0	0.009393	2.922675	-0.506729
141	6	0	-8.198908	-3.164372	-1.227059
142	6	0	-3.821777	-0.755455	-2.232054
143	1	0	-3.087548	-1.134284	-2.950571
144	1	0	-4.078296	-1.597684	-1.578382
145	6	0	-1.214876	2.759742	-3.542903
146	6	0	-4.642308	-0.587568	3.437950
147	1	0	-4.912066	-1.314687	4.219931
148	1	0	-4.557407	0.400359	3.918007
149	6	0	-9.544928	-0.941900	-3.289782
150	1	0	-10.140735	-1.822648	-3.504669
151	6	0	0.959447	-2.807108	3.167649
152	6	0	-2.159198	2.063339	-2.700981
153	1	0	-3.132329	2.564131	-2.598314
154	6	0	-7.493678	3.037481	-0.846359
155	6	0	11.279929	0.225632	5.675637
156	1	0	10.894010	-0.796282	5.758856
157	1	0	10.666679	0.868244	6.318853
158	1	0	12.304236	0.227897	6.069884
159	6	0	-7.255948	2.896089	1.585264
160	6	0	12.170104	0.158065	-4.315120
161	1	0	11.681757	0.627674	-5.177575
162	1	0	13.179906	-0.134743	-4.626403
163	1	0	12.275462	0.912985	-3.527111
164	6	0	-6.719630	2.153093	2.803189
165	1	0	-5.663842	1.922596	2.652875

166	1	0	-6.791615	2.815833	3.674675
167	6	0	-9.046015	-4.266941	1.198415
168	1	0	-9.355153	-4.677993	2.154596
169	6	0	-7.524211	-2.856901	-0.030650
170	6	0	3.039323	-2.978860	1.897364
171	1	0	3.700697	-2.578249	1.134469
172	6	0	-9.286331	-4.042829	-1.168413
173	1	0	-9.786512	-4.288490	-2.103041
174	6	0	-7.180394	2.527337	-2.250828
175	1	0	-7.408388	3.329028	-2.962125
176	1	0	-6.105792	2.334229	-2.345003
177	6	0	-1.042193	4.415603	3.292853
178	1	0	-0.313544	4.907165	3.935810
179	6	0	-3.155549	0.367758	-1.398419
180	1	0	-3.874840	1.163177	-1.166707
181	1	0	-2.797324	-0.033516	-0.452917
182	6	0	2.312658	1.042478	3.411726
183	1	0	2.192434	0.021948	3.791143
184	1	0	2.492903	1.694226	4.281937
185	6	0	-9.730683	-4.626130	0.027929
186	6	0	12.152015	-0.194227	3.343479
187	1	0	11.795370	-1.229820	3.355562
188	1	0	13.185172	-0.191384	3.714284
189	1	0	12.162585	0.142069	2.300114
190	6	0	-7.295184	-2.937018	2.493529
191	1	0	-6.210722	-2.920148	2.364929
192	1	0	-7.530766	-3.669868	3.275464
193	6	0	11.247398	5.910841	-2.064033
194	1	0	11.701247	4.983774	-2.434501
195	1	0	12.030159	6.678893	-2.051605
196	1	0	10.483985	6.230620	-2.783333
197	6	0	11.367640	-2.112416	-4.981245
198	1	0	10.881353	-3.047543	-4.683051
199	1	0	12.387811	-2.355952	-5.304840
200	1	0	10.822914	-1.712979	-5.845169
201	6	0	-1.166730	-3.565791	-4.278895
202	1	0	-2.172352	-3.204124	-4.473826
203	6	0	0.896499	2.962446	-4.748117
204	1	0	1.873202	2.553129	-4.989660
205	6	0	-7.962623	-3.381367	1.197271
206	6	0	-8.098600	4.000951	1.705412
207	1	0	-8.322724	4.358989	2.708202
208	6	0	11.826026	5.339406	0.297486
209	1	0	11.492862	5.251911	1.337500
210	1	0	12.624458	6.092293	0.266134
211	1	0	12.254852	4.374662	0.001280
212	6	0	1.334325	-3.978501	3.867211
213	1	0	0.664459	-4.358524	4.637152
214	6	0	-11.243644	-6.155621	1.418998
215	1	0	-10.396804	-6.697072	1.857281
216	1	0	-12.085341	-6.855781	1.355176
217	1	0	-11.533415	-5.354978	2.109873
218	6	0	-11.514799	0.567302	-4.008520
219	6	0	-8.349236	4.136516	-0.668219
220	1	0	-8.759738	4.599502	-1.560481
221	6	0	11.886206	2.142839	4.192069
222	1	0	12.904532	2.102542	4.596805

223	1	0	11.314877	2.849025	4.806612
224	1	0	11.952535	2.547328	3.175404
225	6	0	-11.076919	0.014020	4.246207
226	6	0	10.097325	7.108641	-0.197371
227	1	0	9.282853	7.429129	-0.857973
228	1	0	10.880629	7.877638	-0.222781
229	1	0	9.701731	7.069099	0.823611
230	6	0	1.424740	-4.460046	-3.780398
231	1	0	2.441422	-4.797952	-3.585661
232	6	0	3.370234	-4.129729	2.596769
233	1	0	4.306070	-4.636354	2.371115
234	6	0	-7.754898	-2.573247	-2.562391
235	1	0	-8.147285	-3.210143	-3.363008
236	1	0	-6.663589	-2.625474	-2.642926
237	6	0	-10.913999	-5.613834	0.014099
238	6	0	-8.662098	4.653975	0.593416
239	6	0	-11.451118	1.417270	-5.301059
240	1	0	-10.988925	2.394865	-5.125885
241	1	0	-12.462212	1.592016	-5.689949
242	1	0	-10.870885	0.906726	-6.079031
243	6	0	-1.623401	3.980629	-4.125873
244	1	0	-2.611869	4.366588	-3.881120
245	6	0	2.517346	-4.644891	3.592245
246	1	0	2.783934	-5.546225	4.136233
247	6	0	0.464416	4.156817	-5.304221
248	1	0	1.117344	4.692247	-5.990160
249	6	0	-0.752115	-4.806545	-4.738627
250	1	0	-1.447525	-5.427017	-5.299828
251	6	0	0.552339	-5.271889	-4.488459
252	1	0	0.871124	-6.245626	-4.848298
253	6	0	-11.888438	0.883833	3.255348
254	1	0	-11.442775	1.875572	3.124343
255	1	0	-12.914723	1.022750	3.620086
256	1	0	-11.937734	0.408121	2.268669
257	6	0	-0.803243	4.684549	-4.993489
258	1	0	-1.134230	5.622063	-5.430310
259	6	0	-11.811650	-1.330782	4.411026
260	1	0	-11.913719	-1.860897	3.456823
261	1	0	-12.822147	-1.152845	4.798281
262	1	0	-11.298189	-1.993133	5.118364
263	6	0	-11.043936	0.711676	5.627889
264	1	0	-10.482378	0.112731	6.355046
265	1	0	-12.062927	0.848170	6.013008
266	1	0	-10.572665	1.699216	5.574766
267	6	0	-9.569436	5.883317	0.796256
268	6	0	-10.098955	6.449249	-0.535967
269	1	0	-9.285455	6.779380	-1.193133
270	1	0	-10.736585	7.319564	-0.339830
271	1	0	-10.703641	5.713829	-1.080148
272	6	0	-12.178551	-4.907410	-0.533228
273	1	0	-12.451069	-4.050376	0.094256
274	1	0	-13.029120	-5.601420	-0.551479
275	1	0	-12.028079	-4.538619	-1.553957
276	6	0	-12.347258	1.320062	-2.941950
277	1	0	-12.415186	0.739213	-2.014716
278	1	0	-13.366044	1.495591	-3.310181
279	1	0	-11.909739	2.293184	-2.694051

280	6	0	-10.575399	-6.821559	-0.893463
281	1	0	-10.377338	-6.512588	-1.925758
282	1	0	-11.411165	-7.533167	-0.912576
283	1	0	-9.686493	-7.348477	-0.526690
284	6	0	-12.241594	-0.750950	-4.340324
285	1	0	-11.715268	-1.325824	-5.111787
286	1	0	-13.245217	-0.530071	-4.722370
287	1	0	-12.360150	-1.387925	-3.456052
288	6	0	-8.772245	7.004059	1.507806
289	1	0	-8.397340	6.677968	2.484168
290	1	0	-7.909662	7.313747	0.905527
291	1	0	-9.407869	7.884325	1.670677
292	6	0	-10.789545	5.497794	1.667637
293	1	0	-11.381203	4.710151	1.186199
294	1	0	-11.440319	6.368330	1.821515
295	1	0	-10.486338	5.131581	2.654592
296	6	0	8.962918	-6.832423	2.011330
297	1	0	8.724828	-6.396446	2.987920
298	1	0	9.610286	-7.702482	2.182385
299	1	0	8.025471	-7.187455	1.566646
300	6	0	9.662483	-5.810688	1.081524
301	6	0	10.004539	-6.528549	-0.238723
302	1	0	9.107472	-6.909935	-0.740977
303	1	0	10.657139	-7.385781	-0.034054
304	1	0	10.535175	-5.870217	-0.936959
305	6	0	10.990176	-5.357019	1.736008
306	1	0	11.517162	-4.638770	1.096766
307	1	0	11.651346	-6.218144	1.898907
308	1	0	10.822152	-4.878426	2.707054

Table S9. Optimized geometries in Cartesian coordinates for **5_2-$Fe_{2\,sim}$**, obtained by DFT-B3LYP calculations.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.074337	0.062894	1.648066
2	26	0	0.045830	-0.431700	-1.537550
3	8	0	-0.941658	0.625186	-0.134677
4	8	0	5.994778	-0.065070	2.009665
5	8	0	6.088993	-0.107498	-2.462090
6	8	0	-0.777874	1.657641	2.532332
7	8	0	0.813737	-1.138618	0.217014
8	8	0	0.527510	-0.956381	3.205952
9	8	0	-1.073929	-2.048283	-1.692360
10	8	0	1.217631	1.134311	-1.854106
11	8	0	6.351229	-1.803617	-0.072380
12	1	0	6.199927	-1.246167	0.723409
13	8	0	6.342187	1.604582	-0.352693
14	1	0	6.206789	1.069916	-1.166092
15	8	0	-5.922088	-0.350692	-2.546273
16	8	0	-6.197708	0.227382	1.850736
17	8	0	-6.499032	-1.754171	-0.054657
18	1	0	-6.373485	-1.139875	0.695510
19	7	0	-1.182475	0.444106	-3.222590
20	8	0	-6.231965	1.729477	-0.505101
21	1	0	-6.204390	1.284110	0.364341
22	7	0	1.873139	1.195591	1.695505
23	7	0	1.434031	-1.544389	-2.933615
24	7	0	-1.969386	-1.117225	1.966779
25	6	0	9.337030	-1.559228	-3.423596
26	1	0	9.800905	-2.538966	-3.466316
27	6	0	9.433170	0.818537	-3.656378
28	1	0	9.975528	1.731140	-3.891977
29	6	0	7.279140	0.090618	2.523465
30	6	0	7.861083	1.367250	2.601127
31	6	0	9.302321	-0.911084	3.366016
32	1	0	9.847775	-1.812284	3.626907
33	6	0	8.005051	-1.062622	2.857923
34	6	0	8.012381	-1.493651	-2.964998
35	6	0	8.114078	0.940224	-3.214241
36	6	0	7.729251	3.127253	0.767917
37	6	0	-0.832921	-3.300943	-1.970542
38	6	0	10.069366	-0.425297	-3.792711
39	6	0	9.157362	1.462433	3.117168
40	1	0	9.601292	2.452738	3.182282
41	6	0	7.158014	2.621678	2.088225
42	1	0	6.092444	2.415171	1.968855
43	1	0	7.260551	3.415734	2.838194
44	6	0	9.899815	0.344300	3.527365
45	6	0	7.447697	-2.462076	2.609792
46	1	0	6.353271	-2.446167	2.644205
47	1	0	7.770652	-3.116339	3.427228
48	6	0	7.916185	-3.081533	1.295943
49	6	0	11.519451	-0.495704	-4.308971
50	6	0	7.400307	-0.233400	-2.915406
51	6	0	7.858405	-3.256172	-1.140465

52	6	0	11.315726	0.530177	4.105931
53	6	0	8.675776	4.157894	0.739408
54	1	0	8.956016	4.606593	1.687601
55	6	0	-8.187065	-0.767043	2.812079
56	6	0	12.224910	1.202404	3.048393
57	1	0	12.295185	0.586427	2.144238
58	1	0	13.238009	1.339028	3.448417
59	1	0	11.847421	2.186834	2.751720
60	6	0	8.917104	-4.065415	1.307798
61	1	0	9.310260	-4.360593	2.275846
62	6	0	4.900268	-0.083520	2.956790
63	1	0	4.804039	0.917354	3.401802
64	1	0	5.131040	-0.793564	3.761549
65	6	0	7.323689	2.541756	-0.445542
66	6	0	-0.951810	1.604577	-3.745510
67	1	0	-1.623963	1.943801	-4.546211
68	6	0	9.398890	-4.676192	0.144810
69	6	0	7.323533	-2.768897	-2.482335
70	1	0	6.247891	-2.602408	-2.401441
71	1	0	7.482552	-3.558322	-3.227519
72	6	0	8.845813	-4.239025	-1.070981
73	1	0	9.190520	-4.676860	-2.005651
74	6	0	7.892651	2.960376	-1.666179
75	6	0	-8.020301	-1.471372	-2.943793
76	6	0	7.372677	-2.693444	0.058272
77	6	0	8.844101	3.985989	-1.635036
78	1	0	9.265553	4.305757	-2.585826
79	6	0	3.642925	-0.507100	2.213331
80	1	0	2.869876	-0.750377	2.946503
81	1	0	3.870763	-1.440524	1.685251
82	6	0	0.281120	-3.716614	-2.764766
83	6	0	-9.163513	0.960945	-3.698205
84	1	0	-9.592434	1.925653	-3.949705
85	6	0	1.274932	-2.789945	-3.248873
86	1	0	1.987071	-3.232483	-3.959281
87	6	0	-1.702802	-4.329656	-1.489185
88	6	0	5.029668	-0.309833	-3.417480
89	1	0	5.332636	-1.099009	-4.117639
90	1	0	4.879767	0.615126	-3.994756
91	6	0	1.110178	2.276141	-2.473289
92	6	0	10.476839	-5.777298	0.154922
93	6	0	-7.828280	0.941448	-3.269638
94	6	0	7.503858	2.321497	-2.996863
95	1	0	6.412850	2.263557	-3.081015
96	1	0	7.840681	2.984574	-3.801634
97	6	0	-7.568780	-2.583652	0.100988
98	6	0	3.771965	-0.704052	-2.649459
99	1	0	3.547288	0.055007	-1.895780
100	1	0	3.966007	-1.646576	-2.123992
101	6	0	-7.473121	0.377979	2.421932
102	6	0	-9.349168	-1.394527	-3.369225
103	1	0	-9.934233	-2.311331	-3.362010
104	6	0	-9.947392	-0.194523	-3.781370
105	6	0	0.194445	-2.075515	3.794402
106	6	0	9.254753	4.617892	-0.451099
107	6	0	-1.480278	-5.662906	-1.800215
108	1	0	-2.162929	-6.402560	-1.388806

109	6	0	-7.241028	-0.296348	-2.950314
110	6	0	-5.049335	0.378930	2.748687
111	1	0	-4.997256	-0.511013	3.389544
112	1	0	-5.245033	1.247627	3.386230
113	6	0	-9.467592	-0.586323	3.342468
114	1	0	-10.015338	-1.474793	3.645871
115	6	0	0.977405	3.287374	2.640384
116	6	0	-8.036724	1.659777	2.493200
117	6	0	-10.062374	0.677230	3.479057
118	6	0	1.990932	2.422858	2.074636
119	1	0	2.977632	2.895094	1.980795
120	6	0	-3.605981	0.012865	-2.889475
121	1	0	-3.501604	-0.505769	-1.932652
122	1	0	-3.673342	1.083742	-2.662529
123	6	0	-0.357075	2.847433	2.860447
124	6	0	3.097299	0.537157	1.207639
125	1	0	3.862662	1.289355	0.982456
126	1	0	2.834788	0.050704	0.270854
127	6	0	-0.401496	-6.054475	-2.613176
128	1	0	-0.245711	-7.102302	-2.851699
129	6	0	-2.366469	-0.253791	-3.755060
130	1	0	-2.147972	-1.323670	-3.781234
131	1	0	-2.549409	0.080125	-4.788415
132	6	0	1.230620	-2.471179	0.457482
133	1	0	1.731456	-2.540046	1.428693
134	1	0	1.934410	-2.798357	-0.318578
135	1	0	0.374647	-3.157495	0.462495
136	6	0	-7.752078	3.311056	0.549130
137	6	0	-3.788184	0.582585	1.923085
138	1	0	-3.032187	1.039087	2.568200
139	1	0	-3.999857	1.329015	1.148552
140	6	0	-1.005933	-2.783954	3.491606
141	6	0	-4.910942	-0.427948	-3.551300
142	1	0	-5.163536	0.222860	-4.402080
143	1	0	-4.840857	-1.459755	-3.934984
144	6	0	-9.324579	1.780430	3.035240
145	1	0	-9.751178	2.776489	3.090337
146	6	0	0.079943	2.557997	-3.416722
147	6	0	-2.019914	-2.228764	2.620679
148	1	0	-2.940131	-2.824160	2.557769
149	6	0	-8.143421	-2.865882	1.349720
150	6	0	11.596622	0.133034	-5.721662
151	1	0	11.283923	1.182940	-5.719013
152	1	0	10.952462	-0.406044	-6.426765
153	1	0	12.625762	0.092519	-6.101033
154	6	0	-8.055002	-3.191837	-1.073664
155	6	0	11.965946	-0.806913	4.512706
156	1	0	11.382599	-1.328982	5.280652
157	1	0	12.963468	-0.618702	4.927468
158	1	0	12.087615	-1.480466	3.656285
159	6	0	-7.477930	-2.803156	-2.430493
160	1	0	-6.390098	-2.744875	-2.365549
161	1	0	-7.726112	-3.593088	-3.150316
162	6	0	-8.542475	4.083133	-2.018853
163	1	0	-8.833118	4.360804	-3.027466
164	6	0	-7.202859	2.681570	-0.583709
165	6	0	2.078647	3.311237	-2.229567

166	6	0	-8.685691	4.334238	0.352753
167	1	0	-9.087924	4.825598	1.236351
168	6	0	-7.646639	-2.182404	2.620504
169	1	0	-7.959161	-2.787619	3.478730
170	1	0	-6.550863	-2.174228	2.637132
171	6	0	0.461017	-5.082721	-3.088337
172	1	0	1.311377	-5.363535	-3.706938
173	6	0	-3.192658	-0.691015	1.272371
174	1	0	-3.921921	-1.513145	1.265856
175	1	0	-2.916827	-0.477806	0.241523
176	6	0	2.565833	-0.866128	-3.587847
177	1	0	2.224329	0.114748	-3.928343
178	1	0	2.863038	-1.441897	-4.478781
179	6	0	-9.096808	4.756870	-0.920560
180	6	0	12.449327	0.287602	-3.350313
181	1	0	12.164263	1.342554	-3.276113
182	1	0	13.486564	0.246048	-3.707114
183	1	0	12.418421	-0.137650	-2.340355
184	6	0	-7.096629	2.270651	-3.084305
185	1	0	-6.025528	2.092436	-2.970017
186	1	0	-7.238458	2.888004	-3.980268
187	6	0	10.950112	-6.123116	1.580259
188	1	0	11.393996	-5.256867	2.085155
189	1	0	11.716281	-6.906457	1.534529
190	1	0	10.129665	-6.499847	2.202676
191	6	0	11.246037	1.429758	5.364134
192	1	0	10.836257	2.419631	5.135541
193	1	0	12.249131	1.572965	5.786189
194	1	0	10.613012	0.975933	6.136127
195	6	0	-1.265447	3.770945	3.480157
196	6	0	1.049761	-2.628793	4.796443
197	6	0	-7.616499	3.043567	-1.877189
198	6	0	-9.089326	-4.120331	-0.958047
199	1	0	-9.442504	-4.598185	-1.869560
200	6	0	11.709389	-5.308133	-0.656376
201	1	0	11.450220	-5.088963	-1.698174
202	1	0	12.485042	-6.085209	-0.662301
203	1	0	12.140867	-4.398593	-0.221521
204	6	0	0.033374	3.809180	-4.084348
205	1	0	-0.764703	3.990440	-4.801110
206	6	0	-10.433000	6.229585	-2.535633
207	1	0	-9.541582	6.538094	-3.094819
208	1	0	-11.154105	7.054423	-2.583967
209	1	0	-10.880503	5.370793	-3.049866
210	6	0	-11.475512	0.801915	4.079509
211	6	0	-9.191289	-3.798424	1.408126
212	1	0	-9.611889	-4.017513	2.384981
213	6	0	12.041077	-1.943123	-4.402957
214	1	0	13.069105	-1.938711	-4.784401
215	1	0	11.437789	-2.551399	-5.087639
216	1	0	12.054996	-2.437829	-3.424873
217	6	0	-11.408278	-0.186554	-4.271459
218	6	0	9.910095	-7.068034	-0.485169
219	1	0	9.039386	-7.430681	0.074015
220	1	0	10.669394	-7.861107	-0.487893
221	1	0	9.595652	-6.903762	-1.521697
222	6	0	1.369167	4.597748	3.006501

223	1	0	2.396357	4.907031	2.824577
224	6	0	1.996208	4.531258	-2.889169
225	1	0	2.727252	5.307053	-2.690067
226	6	0	-7.333580	2.907494	1.960100
227	1	0	-7.566030	3.740558	2.633263
228	1	0	-6.246334	2.780159	1.997418
229	6	0	-10.107132	5.912071	-1.062711
230	6	0	-9.681080	-4.454851	0.273786
231	6	0	-11.486694	0.202870	5.506972
232	1	0	-11.209484	-0.856867	5.508421
233	1	0	-12.489238	0.285041	5.945588
234	1	0	-10.784617	0.733399	6.161426
235	6	0	-1.272537	-4.025242	4.110619
236	1	0	-2.189161	-4.550724	3.850059
237	6	0	0.971827	4.785135	-3.824303
238	1	0	0.930859	5.746044	-4.328631
239	6	0	0.764723	-3.855054	5.380145
240	1	0	1.464603	-4.246521	6.114013
241	6	0	-0.851210	5.049616	3.830655
242	1	0	-1.545559	5.741853	4.294646
243	6	0	0.472107	5.470710	3.589914
244	1	0	0.775145	6.475531	3.869192
245	6	0	-12.339109	-0.697410	-3.144704
246	1	0	-12.083550	-1.716218	-2.834661
247	1	0	-13.383099	-0.702676	-3.484597
248	1	0	-12.270883	-0.053442	-2.259953
249	6	0	-0.392787	-4.572431	5.031236
250	1	0	-0.599669	-5.533459	5.492806
251	6	0	-11.884396	1.221173	-4.680051
252	1	0	-11.854411	1.923073	-3.838367
253	1	0	-12.922378	1.171644	-5.030691
254	1	0	-11.279849	1.636671	-5.495238
255	6	0	-11.544159	-1.113636	-5.503897
256	1	0	-10.900463	-0.771695	-6.323373
257	1	0	-12.580855	-1.122026	-5.865210
258	1	0	-11.264127	-2.146274	-5.268556
259	6	0	-10.804654	-5.507983	0.329101
260	6	0	-11.331482	-5.731773	1.760247
261	1	0	-10.545395	-6.092791	2.434232
262	1	0	-12.125690	-6.487838	1.746669
263	1	0	-11.756637	-4.815465	2.187312
264	6	0	-11.431436	5.539195	-0.352422
265	1	0	-11.871128	4.636543	-0.793140
266	1	0	-12.160296	6.354972	-0.445727
267	1	0	-11.280781	5.348770	0.716069
268	6	0	-12.481871	0.029435	3.191854
269	1	0	-12.498109	0.435313	2.173682
270	1	0	-13.494332	0.109385	3.607725
271	1	0	-12.232489	-1.034763	3.122413
272	6	0	-9.528432	7.194404	-0.416379
273	1	0	-9.318285	7.053563	0.649650
274	1	0	-10.239041	8.026170	-0.509391
275	1	0	-8.592065	7.489101	-0.904915
276	6	0	-11.947835	2.266261	4.173253
277	1	0	-11.288355	2.869732	4.808617
278	1	0	-12.950915	2.299875	4.614424
279	1	0	-12.006770	2.741838	3.187310

280	6	0	-10.273015	-6.862280	-0.200571
281	1	0	-9.918681	-6.783805	-1.234269
282	1	0	-9.436870	-7.220494	0.411869
283	1	0	-11.065153	-7.622021	-0.175455
284	6	0	-11.994567	-5.051295	-0.549770
285	1	0	-12.396404	-4.093842	-0.197651
286	1	0	-12.802698	-5.793713	-0.517525
287	1	0	-11.701625	-4.925159	-1.597793
288	6	0	9.727057	6.931860	-1.346494
289	1	0	9.508099	6.620944	-2.374115
290	1	0	10.453525	7.753709	-1.393900
291	1	0	8.799171	7.322157	-0.911207
292	6	0	10.285802	5.762287	-0.499310
293	6	0	10.620193	6.309102	0.902481
294	1	0	9.735411	6.719915	1.403270
295	1	0	11.355801	7.117884	0.817339
296	1	0	11.053000	5.536833	1.549675
297	6	0	11.601330	5.256308	-1.139608
298	1	0	12.023946	4.426449	-0.561020
299	1	0	12.345680	6.062461	-1.175406
300	1	0	11.445184	4.902583	-2.164605
301	8	0	2.215170	-1.980601	5.149288
302	6	0	2.028808	-0.751023	5.863555
303	1	0	1.478482	-0.023553	5.258742
304	1	0	1.495121	-0.935155	6.805777
305	1	0	3.030635	-0.373483	6.083541
306	8	0	3.045108	2.992969	-1.321010
307	6	0	4.001726	3.993327	-0.991991
308	1	0	4.587277	4.292825	-1.871285
309	1	0	3.515361	4.878382	-0.559948
310	1	0	4.669711	3.535689	-0.264263
311	8	0	-2.529465	3.286207	3.684637
312	6	0	-3.468970	4.132014	4.328705
313	1	0	-3.132544	4.411414	5.336462
314	1	0	-3.660942	5.041274	3.742903
315	1	0	-4.390837	3.551875	4.405488
316	8	0	-2.737732	-3.994639	-0.645520
317	6	0	-3.958834	-3.673898	-1.319580
318	1	0	-3.801002	-2.865700	-2.041382
319	1	0	-4.355970	-4.557705	-1.838483
320	1	0	-4.664884	-3.339254	-0.560316
321	1	0	-0.982352	1.583299	-0.272847

References:

1. M. Llunell, D. Casanova, J. Cirera, J. M. Bofill, P. Alemany, S. Alvarez, M. Pinsky, D. Avnir, *SHAPE, version 2.3*, University of Barcelona, Barcelona, Spain, and Hebrew University of Jerusalem, Jerusalem, Israel, 2013.