Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Molecular engineering of functionalized crown ether resins for isotopic enrichment of gadolinium: From computer to column chromatography

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Table S1. Calculated values of energies, enthalpy, entropy and Gibbs free energy of the chemical species

System	E(kcal/mol) Zero point energy corrected	H (kcal/mol) Thermal corrected	S (kj/mol/K)	G(kcal/mol)
H_2O	-47951.78	-47951.19	0.195	-47965.10
B15C5	-577974.83	-577974.24	0.578	-578015.52
DB15C5	-673580.68	-673580.09	0.622	-673624.51
B18C6	-674443.35	-674442.75	0.658	-674489.73
DB18C6	-770064.34	-770063.75	0.717	-770114.90
DCH18C6	-774486.25	-774485.66	0.784	-774541.60
CMPS-DB18C6	-1277133.72	-1277133.13	1.185	-1277217.72
Gd^{3+}-$(H_2O)_9$	-911886.53	-911885.94	0.744	-911939.02
B15C5-Gd^{3+}	-1058247.73	-1058247.14	0.598	-1058289.82
DB15C5-Gd^{3+}	-1153847.21	-1153846.62	0.654	-1153893.30
B18C6-Gd^{3+}	-1154729.67	-1154729.08	0.670	-1154776.91
DB18C6-Gd^{3+}	-1250339.26	-1250338.66	0.710	-1250389.35
DCH18C6-Gd^{3+}	-1254779.38	-1254778.79	0.776	-1254834.14
CMPS-DB18C6-Gd^{3+}	-1757428.69	-1757428.10	1.209	-1757514.35

Table S2. Calculated values of IR frequency of different isotopes of Gd with crown ethers

$^{155}Gd^{3+}$-$(H_2O)_9$	$^{157}Gd^{3+}$-$(H_2O)_9$	$^{160}Gd^{3+}$-$(H_2O)_9$	$\Delta_{155\text{-}157}$ (%)	$\Delta_{157\text{-}160}$ (%)
34.35	34.34	34.32	0.03	0.06
43.73	43.71	43.69	0.05	0.05
46.57	46.55	46.53	0.04	0.04
57.55	57.52	57.48	0.05	0.07
63.05	63.03	63.01	0.03	0.03
70.77	70.74	70.7	0.04	0.06
74.82	74.8	74.77	0.03	0.04
82.57	82.53	82.46	0.05	0.08

84.19	84.12	84.02	0.08	0.12
90.37	90.32	90.24	0.06	0.09
104.11	104.07	104.02	0.04	0.05
112.88	112.85	112.82	0.03	0.03
127.37	127.33	127.28	0.03	0.04
143.1	143.09	143.08	0.01	0.01
183.75	183.73	183.7	0.01	0.02
199.62	199.62	199.62	0.00	0.00
223.77	223.71	223.62	0.03	0.04
242.04	242.03	242.03	0.00	0.00
260.12	260.03	259.9	0.03	0.05
275.01	274.99	274.96	0.01	0.01
282.91	282.89	282.85	0.01	0.01
295.98	295.97	295.95	0.00	0.01
305.78	305.5	305.11	0.09	0.13
317.17	317.17	317.16	0.00	0.00
326.91	326.9	326.88	0.00	0.01
340.86	340.72	340.52	0.04	0.06
343.74	343.73	343.72	0.00	0.00
367.84	367.83	367.83	0.00	0.00
369.85	369.76	369.63	0.02	0.04
380.09	379.88	379.58	0.06	0.08
408.43	408.42	408.41	0.00	0.00
416.47	416.45	416.43	0.00	0.00
444.86	444.86	444.85	0.00	0.00
458.7	458.69	458.69	0.00	0.00
465.82	465.82	465.81	0.00	0.00
469.71	469.69	469.67	0.00	0.00
480.68	480.65	480.59	0.01	0.01
489.5	489.48	489.44	0.00	0.01
497.23	497.18	497.12	0.01	0.01
514.7	514.68	514.65	0.00	0.01
522.17	522.16	522.14	0.00	0.00
606.22	606.22	606.22	0.00	0.00
643.48	643.47	643.46	0.00	0.00
690.62	690.62	690.62	0.00	0.00
703.87	703.86	703.85	0.00	0.00
729.09	729.09	729.09	0.00	0.00
793.36	793.36	793.35	0.00	0.00
876.15	876.15	876.15	0.00	0.00
930.5	930.5	930.5	0.00	0.00

949.96	949.96	949.96	0.00	0.00
1194.8	1194.8	1194.8	0.00	0.00
1457.6	1457.6	1457.6	0.00	0.00
1535.1	1535.1	1535.1	0.00	0.00
1548.1	1548.1	1548.1	0.00	0.00
1567.7	1567.7	1567.7	0.00	0.00
1592.9	1592.9	1592.9	0.00	0.00
1596	1596	1596	0.00	0.00
1609	1609	1609	0.00	0.00
1622.7	1622.7	1622.7	0.00	0.00
1638.7	1638.7	1638.7	0.00	0.00
1849.4	1849.4	1849.4	0.00	0.00
2875.4	2875.4	2875.4	0.00	0.00
3014	3014	3014	0.00	0.00
3145.6	3145.6	3145.6	0.00	0.00
3353.7	3353.7	3353.7	0.00	0.00
3589.7	3589.7	3589.7	0.00	0.00
3602.7	3602.7	3602.7	0.00	0.00
3618.8	3618.8	3618.8	0.00	0.00
3626.5	3626.5	3626.5	0.00	0.00
3629	3629	3629	0.00	0.00
3642.6	3642.6	3642.6	0.00	0.00
3647.4	3647.4	3647.4	0.00	0.00
3653.8	3653.8	3653.8	0.00	0.00
3670.1	3670.1	3670.1	0.00	0.00
3676	3676	3676	0.00	0.00
3682.8	3682.8	3682.8	0.00	0.00
3687.7	3687.7	3687.7	0.00	0.00
3692.8	3692.8	3692.8	0.00	0.00

$^{155}Gd^{3+}$-B15C5	$^{157}Gd^{3+}$- B15C5	$^{160}Gd^{3+}$- B15C5	$\Delta_{155\text{-}157}$ (%)	$\Delta_{157\text{-}160}$ (%)
42.96	43.19	43.17	-0.54	0.05
48.54	48.97	48.97	-0.89	0.00
55.55	55.54	55.41	0.02	0.23
91.83	92.34	92.34	-0.56	0.00
105.12	105.09	105.03	0.03	0.06
118.51	118.43	118.12	0.07	0.26

145.35	144.88	144.4	0.32	0.33
155.6	155.68	155.65	-0.05	0.02
174.67	174.35	173.84	0.18	0.29
182.73	182.74	182.72	-0.01	0.01
189.84	189.72	189.49	0.06	0.12
195	194.97	194.89	0.02	0.04
199.3	199.3	199.24	0.00	0.03
228.95	228.85	228.69	0.04	0.07
254.32	254.37	254.36	-0.02	0.00
255.67	255.62	255.52	0.02	0.04
272.13	272.17	272.16	-0.01	0.00
279.17	278.87	278.87	0.11	0.00
295.33	295.44	295.43	-0.04	0.00
314.91	314.89	314.83	0.01	0.02
357.66	357.56	357.48	0.03	0.02
370.57	370.57	370.57	0.00	0.00
384.22	384.11	383.91	0.03	0.05
436.76	435.28	435.26	0.34	0.00
443.69	443.8	443.8	-0.02	0.00
489.13	488.48	488.48	0.13	0.00
497.12	497.16	497.15	-0.01	0.00
517.85	517.87	517.87	0.00	0.00
518.31	518.26	518.25	0.01	0.00
551.52	551.52	551.52	0.00	0.00
586.71	586.04	586.04	0.11	0.00
587.93	586.66	586.66	0.22	0.00
688.83	689.46	689.46	-0.09	0.00
746.13	745.96	745.96	0.02	0.00
749.16	748.92	748.92	0.03	0.00
759.05	758.89	758.89	0.02	0.00
770.77	770.78	770.78	0.00	0.00
794.74	794.72	794.72	0.00	0.00
827.05	827.02	827.02	0.00	0.00
832.79	832.25	832.25	0.06	0.00
884.64	884.56	884.56	0.01	0.00
885.97	885.92	885.91	0.01	0.00
906.65	906.6	906.6	0.01	0.00
916.63	916.61	916.61	0.00	0.00
919.59	919.44	919.44	0.02	0.00
936.85	936.54	936.54	0.03	0.00
946.69	946.62	946.62	0.01	0.00

955.89	955.84	955.84	0.01	0.00
983.63	983.1	983.1	0.05	0.00
987.31	987.21	987.21	0.01	0.00
1009.1	1009.1	1009.1	0.00	0.00
1016.1	1015.9	1015.9	0.01	0.00
1020	1020	1020	0.01	0.00
1026.9	1026.9	1026.9	0.00	0.00
1037.7	1037.7	1037.7	0.00	0.00
1043	1043	1043	0.00	0.00
1059.5	1059.5	1059.5	0.00	0.00
1062.6	1062.6	1062.6	0.00	0.00
1082.5	1082.5	1082.5	0.00	0.00
1087.2	1087.2	1087.2	0.01	0.00
1096.4	1095.5	1095.5	0.08	0.00
1149.6	1148.9	1148.9	0.06	0.00
1158.7	1158.5	1158.5	0.02	0.00
1197.5	1197.5	1197.5	0.00	0.00
1200.9	1200.9	1200.9	0.00	0.00
1209.6	1209.6	1209.6	0.00	0.00
1211.3	1211.2	1211.2	0.00	0.00
1219.3	1219.3	1219.3	0.00	0.00
1222.2	1222.1	1222.1	0.00	0.00
1237.5	1237.5	1237.5	0.00	0.00
1244	1243.8	1243.8	0.02	0.00
1252.9	1252.9	1252.9	0.00	0.00
1261.8	1261.1	1261.1	0.06	0.00
1304.1	1304	1304	0.00	0.00
1318.5	1318.4	1318.4	0.00	0.00
1328.4	1328.3	1328.3	0.01	0.00
1342.3	1342.2	1342.2	0.00	0.00
1357.8	1357.8	1357.8	0.00	0.00
1369.6	1369.8	1369.8	-0.02	0.00
1379	1379.5	1379.5	-0.04	0.00
1399.9	1399.9	1399.9	0.00	0.00
1407.5	1407.5	1407.5	0.00	0.00
1417.6	1417.5	1417.5	0.01	0.00
1418.2	1418.1	1418.1	0.01	0.00
1422.4	1422.3	1422.3	0.01	0.00
1423	1422.9	1422.9	0.01	0.00
1426.2	1426.2	1426.2	0.00	0.00
1436.5	1436.5	1436.5	0.00	0.00

1437.9	1437.9	1437.9	0.00	0.00
1441.9	1441.9	1441.9	0.00	0.00
1446.5	1446.3	1446.3	0.02	0.00
1453.3	1452.9	1452.9	0.03	0.00
1511.5	1503.3	1503.3	0.55	0.00
1575.3	1575.2	1575.2	0.00	0.00
2982.4	2982.4	2982.4	0.00	0.00
2982.5	2982.5	2982.5	0.00	0.00
2984.3	2984.3	2984.3	0.00	0.00
2985.7	2985.7	2985.7	0.00	0.00
2989.4	2989.4	2989.4	0.00	0.00
2989.7	2989.7	2989.7	0.00	0.00
2999.9	2999.9	2999.9	0.00	0.00
3001.9	3001.9	3001.9	0.00	0.00
3049.8	3049.8	3049.8	0.00	0.00
3050	3050	3050	0.00	0.00
3054.2	3054.2	3054.2	0.00	0.00
3057.3	3057.2	3057.2	0.00	0.00
3063.8	3063.8	3063.8	0.00	0.00
3065	3065	3065	0.00	0.00
3077.1	3077.1	3077.1	0.00	0.00
3079	3079	3079	0.00	0.00
3135.5	3135.6	3135.6	0.00	0.00
3141.6	3141.7	3141.7	0.00	0.00
3146.4	3146.4	3146.4	0.00	0.00
3149.8	3149.9	3149.9	0.00	0.00

$^{155}Gd^{3+}$-B18C6	$^{157}Gd^{3+}$- B18C6	$^{160}Gd^{3+}$- B18C6	$\Delta_{155-157}$ (%)	$\Delta_{157-160}$ (%)
17.32	17.3	17.27	0.12	0.17
32.29	32.24	32.17	0.15	0.22
51.77	51.75	51.71	0.04	0.08
57.89	57.87	57.86	0.03	0.02
61.26	61.25	61.22	0.02	0.05
93.83	93.82	93.8	0.01	0.02
118	117.97	117.93	0.03	0.03
131.36	131.24	131.06	0.09	0.14
149.59	149.32	148.91	0.18	0.27
153.45	153.39	153.3	0.04	0.06

159.3	159.09	158.79	0.13	0.19
174.92	174.63	174.18	0.17	0.26
177.32	177.19	177.05	0.07	0.08
188.23	188.11	187.95	0.06	0.09
192.62	192.57	192.51	0.03	0.03
199.32	199.31	199.28	0.01	0.02
222.31	222.23	222.12	0.04	0.05
257.7	257.69	257.67	0.00	0.01
263.84	263.83	263.83	0.00	0.00
278	277.97	277.93	0.01	0.01
287.79	287.76	287.73	0.01	0.01
297.34	297.33	297.32	0.00	0.00
313.94	313.92	313.89	0.01	0.01
348.65	348.65	348.65	0.00	0.00
352.92	352.88	352.81	0.01	0.02
362.7	362.68	362.64	0.01	0.01
381.79	381.74	381.66	0.01	0.02
392.88	392.87	392.85	0.00	0.01
438.36	438.36	438.36	0.00	0.00
454.44	454.44	454.44	0.00	0.00
483.77	483.77	483.77	0.00	0.00
490	490	490	0.00	0.00
506.59	506.59	506.59	0.00	0.00
534.08	534.08	534.08	0.00	0.00
548.67	548.67	548.67	0.00	0.00
567.59	567.59	567.59	0.00	0.00
573.04	573.04	573.04	0.00	0.00
591.3	591.3	591.29	0.00	0.00
693.22	693.22	693.22	0.00	0.00
727.21	727.21	727.21	0.00	0.00
748.37	748.37	748.37	0.00	0.00
750.37	750.37	750.37	0.00	0.00
760.59	760.59	760.59	0.00	0.00
780.71	780.71	780.71	0.00	0.00
790.14	790.14	790.14	0.00	0.00
824.51	824.51	824.51	0.00	0.00
832.06	832.06	832.06	0.00	0.00
876.79	876.79	876.79	0.00	0.00
887.99	887.99	887.99	0.00	0.00
908.09	908.09	908.09	0.00	0.00
916.15	916.15	916.15	0.00	0.00

922.04	922.04	922.04	0.00	0.00
925	924.99	924.99	0.00	0.00
937.7	937.7	937.7	0.00	0.00
952.05	952.05	952.05	0.00	0.00
959.44	959.44	959.44	0.00	0.00
975.57	975.57	975.57	0.00	0.00
982.34	982.34	982.34	0.00	0.00
992.66	992.66	992.66	0.00	0.00
1009.7	1009.7	1009.7	0.00	0.00
1013.3	1013.3	1013.3	0.00	0.00
1016.7	1016.7	1016.7	0.00	0.00
1019.1	1019.1	1019.1	0.00	0.00
1026.4	1026.4	1026.4	0.00	0.00
1036.4	1036.4	1036.4	0.00	0.00
1051.8	1051.8	1051.8	0.00	0.00
1069.6	1069.6	1069.6	0.00	0.00
1076.2	1076.2	1076.2	0.00	0.00
1078.4	1078.4	1078.4	0.00	0.00
1085.3	1085.3	1085.3	0.00	0.00
1091.8	1091.8	1091.8	0.00	0.00
1101.7	1101.7	1101.7	0.00	0.00
1153.2	1153.2	1153.2	0.00	0.00
1156.5	1156.5	1156.5	0.00	0.00
1201.5	1201.5	1201.5	0.00	0.00
1202.5	1202.5	1202.5	0.00	0.00
1206.6	1206.6	1206.6	0.00	0.00
1212.6	1212.6	1212.5	0.00	0.00
1214.7	1214.7	1214.7	0.00	0.00
1228	1228	1228	0.00	0.00
1236.6	1236.6	1236.6	0.00	0.00
1239.3	1239.3	1239.3	0.00	0.00
1251.1	1251.1	1251.1	0.00	0.00
1254.1	1254.1	1254.1	0.00	0.00
1260.9	1260.9	1260.9	0.00	0.00
1264.1	1264.1	1264.1	0.00	0.00
1307.3	1307.3	1307.3	0.00	0.00
1319.5	1319.5	1319.5	0.00	0.00
1321.6	1321.6	1321.6	0.00	0.00
1335.6	1335.6	1335.6	0.00	0.00
1344.3	1344.3	1344.3	0.00	0.00
1361.7	1361.7	1361.7	0.00	0.00

1364.6	1364.6	1364.6	0.00	0.00
1371.6	1371.6	1371.6	0.00	0.00
1378.4	1378.4	1378.4	0.00	0.00
1392	1392	1392	0.00	0.00
1401.5	1401.5	1401.5	0.00	0.00
1412.6	1412.6	1412.6	0.00	0.00
1414.6	1414.6	1414.6	0.00	0.00
1415.9	1415.9	1415.9	0.00	0.00
1417.7	1417.7	1417.7	0.00	0.00
1423.3	1423.3	1423.3	0.00	0.00
1425.3	1425.3	1425.3	0.00	0.00
1428.2	1428.2	1428.2	0.00	0.00
1433.3	1433.3	1433.3	0.00	0.00
1436.2	1436.2	1436.2	0.00	0.00
1442.8	1442.8	1442.8	0.00	0.00
1448.2	1448.2	1448.2	0.00	0.00
1452.5	1452.5	1452.5	0.00	0.00
1499	1499	1499	0.00	0.00
1575.2	1575.2	1575.2	0.00	0.00
2978.3	2978.3	2978.3	0.00	0.00
2981.6	2981.6	2981.6	0.00	0.00
2982.1	2982.1	2982.1	0.00	0.00
2985.6	2985.6	2985.6	0.00	0.00
2986.2	2986.2	2986.2	0.00	0.00
2992.2	2992.2	2992.2	0.00	0.00
3002.3	3002.3	3002.3	0.00	0.00
3003.9	3003.9	3003.9	0.00	0.00
3006.3	3006.3	3006.3	0.00	0.00
3007.2	3007.2	3007.2	0.00	0.00
3045.1	3045.1	3045.1	0.00	0.00
3050.1	3050.1	3050.1	0.00	0.00
3050.5	3050.5	3050.5	0.00	0.00
3059.7	3059.7	3059.7	0.00	0.00
3060.1	3060.1	3060.1	0.00	0.00
3060.4	3060.4	3060.4	0.00	0.00
3067.7	3067.7	3067.7	0.00	0.00
3069.4	3069.4	3069.4	0.00	0.00
3071.5	3071.5	3071.5	0.00	0.00
3083.1	3083.1	3083.1	0.00	0.00
3135.3	3135.3	3135.3	0.00	0.00
3141	3141	3141	0.00	0.00

3146.3	3146.3	3146.3	0.00	0.00
3151.5	3151.5	3151.5	0.00	0.00

$^{155}Gd^{3+}$-DB18C6	$^{157}Gd^{3+}$-DB18C6	$^{160}Gd^{3+}$-DB18C6	$\Delta_{155-157}$ (%)	$\Delta_{157-160}$ (%)
22.7	22.64	22.56	0.26	0.35
27.12	27.11	27.08	0.04	0.11
45.83	45.82	45.82	0.02	0.00
55.17	55.17	55.17	0.00	0.00
68.66	68.66	68.66	0.00	0.00
82.03	82.01	81.99	0.02	0.02
99.34	99.31	99.27	0.03	0.04
125.75	125.63	125.44	0.10	0.15
138.68	138.58	138.4	0.07	0.13
140.63	140.25	139.71	0.27	0.39
154.15	153.96	153.68	0.12	0.18
157.76	157.57	157.31	0.12	0.17
179.44	179.36	179.24	0.04	0.07
184.24	184.02	183.71	0.12	0.17
197.91	197.91	197.89	0.00	0.01
204.23	204.22	204.21	0.00	0.00
225.61	225.57	225.51	0.02	0.03
233.15	233.14	233.12	0.00	0.01
252.56	252.54	252.5	0.01	0.02
271.2	271.2	271.2	0.00	0.00
290.51	290.49	290.45	0.01	0.01
297.95	297.93	297.9	0.01	0.01
306.56	306.53	306.49	0.01	0.01
333.18	333.17	333.15	0.00	0.01
345.14	345.12	345.1	0.01	0.01
357.71	357.69	357.66	0.01	0.01
385.87	385.86	385.84	0.00	0.01
397	396.99	396.98	0.00	0.00
436.79	436.78	436.76	0.00	0.00
439.83	439.82	439.82	0.00	0.00
450.72	450.72	450.71	0.00	0.00
466.07	466.07	466.06	0.00	0.00
496.39	496.39	496.39	0.00	0.00
508.44	508.44	508.44	0.00	0.00

512.06	512.06	512.06	0.00	0.00
526.64	526.63	526.63	0.00	0.00
530.49	530.49	530.49	0.00	0.00
536.46	536.46	536.46	0.00	0.00
566.75	566.75	566.75	0.00	0.00
578.49	578.49	578.49	0.00	0.00
585.85	585.85	585.85	0.00	0.00
590.01	590.01	590.01	0.00	0.00
685.83	685.83	685.83	0.00	0.00
691.07	691.07	691.07	0.00	0.00
720.84	720.84	720.83	0.00	0.00
725.96	725.96	725.96	0.00	0.00
741.57	741.57	741.57	0.00	0.00
744.99	744.99	744.99	0.00	0.00
750.41	750.41	750.41	0.00	0.00
765.45	765.45	765.45	0.00	0.00
789.55	789.55	789.55	0.00	0.00
796.53	796.53	796.53	0.00	0.00
827.18	827.18	827.18	0.00	0.00
841.41	841.41	841.41	0.00	0.00
856.96	856.96	856.96	0.00	0.00
876.67	876.67	876.67	0.00	0.00
886.49	886.49	886.49	0.00	0.00
903.08	903.08	903.08	0.00	0.00
907.51	907.51	907.51	0.00	0.00
927.18	927.18	927.18	0.00	0.00
936.13	936.13	936.13	0.00	0.00
944.54	944.54	944.54	0.00	0.00
948.99	948.99	948.99	0.00	0.00
957.24	957.24	957.24	0.00	0.00
986.48	986.48	986.48	0.00	0.00
994.9	994.9	994.9	0.00	0.00
997.94	997.94	997.94	0.00	0.00
999.88	999.88	999.88	0.00	0.00
1009.7	1009.7	1009.7	0.00	0.00
1016.8	1016.8	1016.8	0.00	0.00
1020	1020	1020	0.00	0.00
1028.7	1028.7	1028.7	0.00	0.00
1037	1037	1037	0.00	0.00
1044.3	1044.3	1044.3	0.00	0.00
1067.1	1067.1	1067.1	0.00	0.00

1070	1070	1070	0.00	0.00
1073.5	1073.5	1073.5	0.00	0.00
1080.8	1080.8	1080.8	0.00	0.00
1083.4	1083.4	1083.4	0.00	0.00
1091.6	1091.6	1091.6	0.00	0.00
1135.5	1135.4	1135.4	0.00	0.00
1138.6	1138.6	1138.6	0.00	0.00
1144.3	1144.3	1144.3	0.00	0.00
1155.3	1155.3	1155.3	0.00	0.00
1178.4	1178.4	1178.4	0.00	0.00
1197.7	1197.7	1197.7	0.00	0.00
1200.9	1200.9	1200.9	0.00	0.00
1211	1211	1211	0.00	0.00
1217.1	1217.1	1217.1	0.00	0.00
1222.8	1222.8	1222.8	0.00	0.00
1234.7	1234.7	1234.7	0.00	0.00
1237.4	1237.4	1237.4	0.00	0.00
1245.1	1245.1	1245.1	0.00	0.00
1249.3	1249.3	1249.3	0.00	0.00
1252.2	1252.2	1252.2	0.00	0.00
1256.3	1256.3	1256.3	0.00	0.00
1309.7	1309.7	1309.7	0.00	0.00
1315.2	1315.2	1315.2	0.00	0.00
1330.5	1330.5	1330.5	0.00	0.00
1335.3	1335.3	1335.3	0.00	0.00
1352.8	1352.8	1352.8	0.00	0.00
1365.5	1365.5	1365.5	0.00	0.00
1371.6	1371.6	1371.6	0.00	0.00
1377	1377	1377	0.00	0.00
1388.9	1388.9	1388.9	0.00	0.00
1389.7	1389.7	1389.7	0.00	0.00
1416.8	1416.8	1416.8	0.00	0.00
1419.3	1419.3	1419.3	0.00	0.00
1422.2	1422.2	1422.2	0.00	0.00
1422.5	1422.5	1422.5	0.00	0.00
1422.9	1422.9	1422.9	0.00	0.00
1423.7	1423.7	1423.7	0.00	0.00
1430.1	1430.1	1430.1	0.00	0.00
1437.9	1437.9	1437.9	0.00	0.00
1442	1442	1442	0.00	0.00
1448.3	1448.3	1448.3	0.00	0.00

1449.9	1449.9	1449.9	0.00	0.00
1454.7	1454.7	1454.7	0.00	0.00
1530.6	1530.6	1530.6	0.00	0.00
1550.1	1550.1	1550.1	0.00	0.00
1575.3	1575.3	1575.3	0.00	0.00
1592.1	1592.1	1592.1	0.00	0.00
2983.3	2983.3	2983.3	0.00	0.00
2983.8	2983.8	2983.8	0.00	0.00
2986.5	2986.5	2986.5	0.00	0.00
3000.4	3000.4	3000.4	0.00	0.00
3001	3001	3001	0.00	0.00
3004.7	3004.7	3004.7	0.00	0.00
3012.9	3012.9	3012.9	0.00	0.00
3014.6	3014.6	3014.6	0.00	0.00
3049.1	3049.1	3049.1	0.00	0.00
3053.8	3053.8	3053.8	0.00	0.00
3057.4	3057.4	3057.4	0.00	0.00
3070.1	3070.1	3070.1	0.00	0.00
3077.8	3077.8	3077.8	0.00	0.00
3081.1	3081.1	3081.1	0.00	0.00
3086.3	3086.3	3086.3	0.00	0.00
3092.1	3092.1	3092.1	0.00	0.00
3130	3130	3130	0.00	0.00
3135.9	3135.9	3135.9	0.00	0.00
3137	3137	3137	0.00	0.00
3142.4	3142.4	3142.4	0.00	0.00
3143.1	3143.1	3143.1	0.00	0.00
3147.6	3147.6	3147.6	0.00	0.00
3149.4	3149.4	3149.4	0.00	0.00
3152.1	3152.1	3152.1	0.00	0.00

$^{155}Gd^{3+}$-DB15C5	$^{157}Gd^{3+}$-DB15C5	$^{160}Gd^{3+}$-DB15C5	$\Delta_{155\text{-}157}$ (%)	$\Delta_{157\text{-}160}$ (%)
25.35	25.35	25.34	0.00	0.04
35.73	35.72	35.71	0.03	0.03
47.82	47.76	47.67	0.13	0.19
76.74	76.73	76.7	0.01	0.04
83.13	83.07	82.98	0.07	0.11
100.14	100.08	100.01	0.06	0.07

118.11	117.86	117.5	0.21	0.31
130.91	130.72	130.44	0.15	0.21
154.87	154.83	154.76	0.03	0.05
165.22	164.91	164.43	0.19	0.29
171.57	171.4	171.17	0.10	0.13
181.35	181.31	181.27	0.02	0.02
188.45	188.41	188.37	0.02	0.02
198.16	198.03	197.84	0.07	0.10
219.81	219.64	219.38	0.08	0.12
236.54	236.51	236.46	0.01	0.02
247.81	247.8	247.79	0.00	0.00
266.68	266.65	266.6	0.01	0.02
280.11	280.11	280.11	0.00	0.00
296.62	296.62	296.62	0.00	0.00
306.85	306.83	306.81	0.01	0.01
313.13	313.08	313.01	0.02	0.02
365.32	365.28	365.22	0.01	0.02
373.1	373.08	373.05	0.01	0.01
402.65	402.65	402.65	0.00	0.00
439.59	439.59	439.59	0.00	0.00
442.62	442.62	442.62	0.00	0.00
459.41	459.4	459.39	0.00	0.00
499.14	499.14	499.14	0.00	0.00
504.55	504.55	504.55	0.00	0.00
506.51	506.51	506.51	0.00	0.00
513.77	513.76	513.76	0.00	0.00
542.18	542.18	542.17	0.00	0.00
571.46	571.46	571.45	0.00	0.00
578.5	578.49	578.49	0.00	0.00
589.84	589.84	589.84	0.00	0.00
596.43	596.43	596.43	0.00	0.00
685.61	685.61	685.61	0.00	0.00
687.51	687.51	687.51	0.00	0.00
732.84	732.84	732.84	0.00	0.00
746.09	746.09	746.09	0.00	0.00
746.98	746.98	746.98	0.00	0.00
748.74	748.74	748.74	0.00	0.00
756.49	756.49	756.49	0.00	0.00
773.43	773.43	773.43	0.00	0.00
813.06	813.06	813.06	0.00	0.00
831.51	831.51	831.51	0.00	0.00

832.81	832.81	832.81	0.00	0.00
869.31	869.31	869.31	0.00	0.00
887.23	887.23	887.23	0.00	0.00
895.55	895.55	895.55	0.00	0.00
910.19	910.19	910.19	0.00	0.00
914.43	914.43	914.43	0.00	0.00
935.1	935.1	935.1	0.00	0.00
936.95	936.95	936.95	0.00	0.00
946.2	946.19	946.19	0.00	0.00
971.73	971.73	971.73	0.00	0.00
986.46	986.46	986.46	0.00	0.00
989.19	989.19	989.19	0.00	0.00
998.23	998.23	998.23	0.00	0.00
1016.9	1016.9	1016.9	0.00	0.00
1018.4	1018.4	1018.4	0.00	0.00
1024.1	1024.1	1024.1	0.00	0.00
1028.8	1028.8	1028.8	0.00	0.00
1030.8	1030.8	1030.8	0.00	0.00
1060.5	1060.5	1060.5	0.00	0.00
1067.4	1067.4	1067.4	0.00	0.00
1073	1073	1073	0.00	0.00
1083	1083	1083	0.00	0.00
1092.3	1092.3	1092.3	0.00	0.00
1129.8	1129.8	1129.8	0.00	0.00
1136.2	1136.2	1136.2	0.00	0.00
1142	1142	1142	0.00	0.00
1156	1156	1156	0.00	0.00
1175	1175	1175	0.00	0.00
1202.3	1202.3	1202.3	0.00	0.00
1203.7	1203.7	1203.7	0.00	0.00
1205	1205	1205	0.00	0.00
1219.2	1219.2	1219.2	0.00	0.00
1230.7	1230.7	1230.7	0.00	0.00
1236	1236	1236	0.00	0.00
1247.8	1247.8	1247.8	0.00	0.00
1253.6	1253.6	1253.6	0.00	0.00
1258.8	1258.8	1258.8	0.00	0.00
1313	1313	1313	0.00	0.00
1324.8	1324.8	1324.8	0.00	0.00
1335.2	1335.2	1335.2	0.00	0.00
1360.8	1360.8	1360.8	0.00	0.00

1368.9	1368.9	1368.9	0.00	0.00
1375.1	1375.1	1375.1	0.00	0.00
1381.7	1381.7	1381.7	0.00	0.00
1401	1401	1401	0.00	0.00
1416.6	1416.6	1416.6	0.00	0.00
1419.6	1419.6	1419.6	0.00	0.00
1421.9	1421.9	1421.9	0.00	0.00
1425.7	1425.7	1425.7	0.00	0.00
1427.9	1427.9	1427.9	0.00	0.00
1439.6	1439.6	1439.6	0.00	0.00
1443.5	1443.5	1443.5	0.00	0.00
1447	1447	1447	0.00	0.00
1450.5	1450.5	1450.5	0.00	0.00
1451.8	1451.8	1451.8	0.00	0.00
1523.2	1523.2	1523.2	0.00	0.00
1525.2	1525.2	1525.2	0.00	0.00
1574.2	1574.2	1574.2	0.00	0.00
1591.5	1591.5	1591.5	0.00	0.00
2982.3	2982.3	2982.3	0.00	0.00
2983	2983	2983	0.00	0.00
2998.3	2998.3	2998.3	0.00	0.00
3005.1	3005.1	3005.1	0.00	0.00
3006.4	3006.4	3006.4	0.00	0.00
3010.3	3010.3	3010.3	0.00	0.00
3050.2	3050.2	3050.2	0.00	0.00
3054.4	3054.4	3054.4	0.00	0.00
3072	3072	3072	0.00	0.00
3081.1	3081.1	3081.1	0.00	0.00
3083.3	3083.3	3083.3	0.00	0.00
3089.2	3089.2	3089.2	0.00	0.00
3134.4	3134.4	3134.4	0.00	0.00
3136	3136	3136	0.00	0.00
3138.4	3138.4	3138.4	0.00	0.00
3141.1	3141.1	3141.1	0.00	0.00
3143.8	3143.8	3143.8	0.00	0.00
3146.1	3146.1	3146.1	0.00	0.00
3150	3150	3150	0.00	0.00
3151	3151	3151	0.00	0.00

$^{155}Gd^{3+}$-DCH18C6	$^{157}Gd^{3+}$-DCH18C6	$^{160}Gd^{3+}$-DCH18C6	$\Delta_{155-157}$ (%)	$\Delta_{157-160}$ (%)
9.84	9.84	9.84	0.00	0.00
25.18	25.15	25.1	0.12	0.20
37.61	37.58	37.54	0.08	0.11
49.73	49.7	49.67	0.06	0.06
60.15	60.11	60.04	0.07	0.12
79.52	79.51	79.48	0.01	0.04
92.95	92.92	92.88	0.03	0.04
98.2	98.16	98.1	0.04	0.06
103.73	103.62	103.45	0.11	0.16
125.52	125.5	125.47	0.02	0.02
139.66	139.6	139.51	0.04	0.06
149.19	149.05	148.83	0.09	0.15
157.72	157.52	157.21	0.13	0.20
161.95	161.76	161.49	0.12	0.17
165.1	165	164.87	0.06	0.08
173.02	172.75	172.36	0.16	0.23
182.65	182.49	182.27	0.09	0.12
203.8	203.76	203.69	0.02	0.03
217.56	217.55	217.55	0.00	0.00
226.22	226.18	226.13	0.02	0.02
244.16	244.14	244.12	0.01	0.01
246.61	246.6	246.59	0.00	0.00
259.37	259.35	259.31	0.01	0.02
287.31	287.3	287.28	0.00	0.01
293.76	293.76	293.76	0.00	0.00
302.59	302.54	302.47	0.02	0.02
313.28	313.27	313.25	0.00	0.01
323.56	323.56	323.55	0.00	0.00
330	329.96	329.91	0.01	0.02
364.49	364.48	364.45	0.00	0.01
371.88	371.87	371.85	0.00	0.01
383.96	383.96	383.95	0.00	0.00
403.79	403.79	403.78	0.00	0.00
419.68	419.67	419.65	0.00	0.00
424.42	424.42	424.41	0.00	0.00
444.75	444.74	444.73	0.00	0.00
462.53	462.53	462.52	0.00	0.00
473.3	473.29	473.29	0.00	0.00

478.65	478.65	478.65	0.00	0.00
492.81	492.81	492.81	0.00	0.00
509.88	509.88	509.88	0.00	0.00
530.8	530.8	530.79	0.00	0.00
551.28	551.28	551.27	0.00	0.00
567.39	567.39	567.39	0.00	0.00
588.43	588.43	588.43	0.00	0.00
599.03	599.03	599.03	0.00	0.00
627.91	627.91	627.91	0.00	0.00
718.17	718.17	718.17	0.00	0.00
725.53	725.53	725.53	0.00	0.00
743.16	743.16	743.16	0.00	0.00
756.73	756.73	756.73	0.00	0.00
765.62	765.62	765.62	0.00	0.00
782.85	782.85	782.85	0.00	0.00
815.35	815.35	815.35	0.00	0.00
824.98	824.98	824.98	0.00	0.00
828.7	828.7	828.7	0.00	0.00
843.29	843.29	843.29	0.00	0.00
851.59	851.59	851.58	0.00	0.00
864.11	864.11	864.11	0.00	0.00
877.52	877.52	877.52	0.00	0.00
886.01	886.01	886.01	0.00	0.00
889.11	889.11	889.11	0.00	0.00
893.64	893.64	893.64	0.00	0.00
909.18	909.18	909.18	0.00	0.00
913.64	913.64	913.64	0.00	0.00
923.78	923.78	923.78	0.00	0.00
930.25	930.25	930.25	0.00	0.00
939.9	939.9	939.9	0.00	0.00
950.05	950.05	950.05	0.00	0.00
960.26	960.26	960.26	0.00	0.00
968.25	968.25	968.25	0.00	0.00
968.89	968.89	968.89	0.00	0.00
979.2	979.2	979.2	0.00	0.00
986.87	986.87	986.87	0.00	0.00
1002.6	1002.6	1002.6	0.00	0.00
1005.5	1005.5	1005.5	0.00	0.00
1016.1	1016.1	1016.1	0.00	0.00
1018.7	1018.7	1018.7	0.00	0.00
1019.8	1019.8	1019.8	0.00	0.00

1024.3	1024.3	1024.3	0.00	0.00
1030.8	1030.8	1030.8	0.00	0.00
1040.9	1040.9	1040.9	0.00	0.00
1050.6	1050.6	1050.6	0.00	0.00
1058.1	1058.1	1058.1	0.00	0.00
1062.1	1062.1	1062.1	0.00	0.00
1067.7	1067.7	1067.7	0.00	0.00
1069.7	1069.7	1069.7	0.00	0.00
1073.2	1073.2	1073.2	0.00	0.00
1076.8	1076.8	1076.8	0.00	0.00
1082.4	1082.4	1082.4	0.00	0.00
1086.2	1086.2	1086.2	0.00	0.00
1099.1	1099.1	1099.1	0.00	0.00
1116.7	1116.7	1116.7	0.00	0.00
1127.2	1127.2	1127.2	0.00	0.00
1148	1148	1148	0.00	0.00
1166.3	1166.3	1166.3	0.00	0.00
1186.9	1186.9	1186.9	0.00	0.00
1203.2	1203.2	1203.2	0.00	0.00
1206.2	1206.2	1206.2	0.00	0.00
1208.6	1208.6	1208.6	0.00	0.00
1216.1	1216.1	1216.1	0.00	0.00
1217.6	1217.6	1217.6	0.00	0.00
1228	1228	1228	0.00	0.00
1229.5	1229.5	1229.5	0.00	0.00
1239	1239	1239	0.00	0.00
1245.2	1245.2	1245.2	0.00	0.00
1254.1	1254.1	1254.1	0.00	0.00
1257.4	1257.4	1257.4	0.00	0.00
1258.2	1258.2	1258.2	0.00	0.00
1263.9	1263.9	1263.9	0.00	0.00
1272.1	1272.1	1272.1	0.00	0.00
1278.6	1278.6	1278.6	0.00	0.00
1282.6	1282.6	1282.6	0.00	0.00
1294.3	1294.3	1294.3	0.00	0.00
1295.5	1295.5	1295.5	0.00	0.00
1299.5	1299.5	1299.5	0.00	0.00
1303.5	1303.5	1303.5	0.00	0.00
1306.3	1306.3	1306.3	0.00	0.00
1310.1	1310.1	1310.1	0.00	0.00
1315.6	1315.6	1315.5	0.00	0.00

1319.5	1319.5	1319.5	0.00	0.00
1320.9	1320.9	1320.9	0.00	0.00
1324.7	1324.7	1324.7	0.00	0.00
1333.6	1333.6	1333.6	0.00	0.00
1334.8	1334.8	1334.8	0.00	0.00
1341.7	1341.7	1341.7	0.00	0.00
1345.7	1345.7	1345.7	0.00	0.00
1349	1349	1349	0.00	0.00
1353.2	1353.2	1353.2	0.00	0.00
1357.6	1357.6	1357.6	0.00	0.00
1359.3	1359.3	1359.3	0.00	0.00
1371.5	1371.5	1371.5	0.00	0.00
1379.8	1379.8	1379.8	0.00	0.00
1385.2	1385.2	1385.2	0.00	0.00
1391.7	1391.7	1391.7	0.00	0.00
1394.6	1394.6	1394.6	0.00	0.00
1397.2	1397.2	1397.2	0.00	0.00
1402.6	1402.6	1402.6	0.00	0.00
1406.1	1406.1	1406.1	0.00	0.00
1410.8	1410.8	1410.8	0.00	0.00
1413.3	1413.3	1413.3	0.00	0.00
1416.9	1416.9	1416.9	0.00	0.00
1419.3	1419.3	1419.3	0.00	0.00
1424.4	1424.4	1424.4	0.00	0.00
1426	1426	1426	0.00	0.00
1429	1429	1429	0.00	0.00
1436.2	1436.2	1436.2	0.00	0.00
2722.7	2722.7	2722.7	0.00	0.00
2919.5	2919.5	2919.5	0.00	0.00
2945.5	2945.5	2945.5	0.00	0.00
2948.7	2948.7	2948.7	0.00	0.00
2954.1	2954.1	2954.1	0.00	0.00
2960.4	2960.4	2960.4	0.00	0.00
2965.7	2965.7	2965.7	0.00	0.00
2967	2967	2967	0.00	0.00
2971	2971	2971	0.00	0.00
2975.6	2975.6	2975.6	0.00	0.00
2976.1	2976.1	2976.1	0.00	0.00
2978.9	2978.9	2978.9	0.00	0.00
2983.1	2983.1	2983.1	0.00	0.00
2990.2	2990.2	2990.2	0.00	0.00

2990.7	2990.7	2990.7	0.00	0.00
2992.9	2992.9	2992.9	0.00	0.00
2995.5	2995.5	2995.5	0.00	0.00
2995.6	2995.6	2995.6	0.00	0.00
3002.1	3002.1	3002.1	0.00	0.00
3002.5	3002.5	3002.5	0.00	0.00
3004.9	3004.9	3004.9	0.00	0.00
3007.2	3007.2	3007.2	0.00	0.00
3020.7	3020.7	3020.7	0.00	0.00
3028.8	3028.8	3028.8	0.00	0.00
3034.7	3034.7	3034.7	0.00	0.00
3041.7	3041.7	3041.7	0.00	0.00
3050.4	3050.4	3050.4	0.00	0.00
3050.6	3050.6	3050.6	0.00	0.00
3054.3	3054.3	3054.3	0.00	0.00
3056.7	3056.7	3056.7	0.00	0.00
3057	3057	3057	0.00	0.00
3064.5	3064.5	3064.5	0.00	0.00
3064.5	3064.5	3064.5	0.00	0.00
3065.7	3065.7	3065.7	0.00	0.00
3069.4	3069.4	3069.4	0.00	0.00
3077.8	3077.8	3077.8	0.00	0.00

$^{155}Gd^{3+}$-CMPS-DB18C6	$^{157}Gd^{3+}$- CMPS-DB18C6	$^{160}Gd^{3+}$- CMPS-DB18C6	$\Delta_{155\text{-}157}$ (%)	$\Delta_{157\text{-}160}$ (%)
2.92	2.92	2.9	0.00	0.68
11.68	11.68	11.67	0.00	0.09
15.55	15.55	15.55	0.00	0.00
17.69	17.69	17.68	0.00	0.06
20.2	20.2	20.2	0.00	0.00
21.68	21.68	21.68	0.00	0.00
28.76	28.73	28.69	0.10	0.14
30.5	30.5	30.49	0.00	0.03
34.63	34.63	34.63	0.00	0.00
36.32	36.32	36.31	0.00	0.03
40.44	40.39	40.31	0.12	0.20
48.24	48.23	48.22	0.02	0.02
59.36	59.35	59.34	0.02	0.02
66.97	66.96	66.95	0.01	0.01

77.55	77.48	77.38	0.09	0.13
80.39	80.36	80.33	0.04	0.04
88.4	88.32	88.2	0.09	0.14
93.61	93.6	93.57	0.01	0.03
98.32	98.21	98.05	0.11	0.16
115.56	115.55	115.52	0.01	0.03
116.86	116.74	116.57	0.10	0.15
120.65	120.62	120.56	0.02	0.05
126.51	126.29	125.99	0.17	0.24
135.14	135.09	135.01	0.04	0.06
141.6	141.49	141.33	0.08	0.11
154.32	154.18	153.98	0.09	0.13
161.88	161.71	161.47	0.11	0.15
169.01	168.99	168.97	0.01	0.01
173.95	173.89	173.82	0.03	0.04
188.18	188.17	188.15	0.01	0.01
197.94	197.89	197.82	0.03	0.04
204.24	204.24	204.23	0.00	0.00
210.11	210.11	210.11	0.00	0.00
214.41	214.41	214.41	0.00	0.00
220.3	220.29	220.28	0.00	0.00
234.84	234.84	234.83	0.00	0.00
235.38	235.38	235.38	0.00	0.00
248.04	248.04	248.04	0.00	0.00
255.33	255.32	255.31	0.00	0.00
257.79	257.78	257.78	0.00	0.00
272.74	272.74	272.73	0.00	0.00
276.9	276.9	276.89	0.00	0.00
280.74	280.74	280.73	0.00	0.00
290.7	290.69	290.68	0.00	0.00
304.01	304	303.98	0.00	0.01
311.86	311.84	311.82	0.01	0.01
329.04	329.03	329.03	0.00	0.00
330.76	330.76	330.76	0.00	0.00
348.41	348.41	348.4	0.00	0.00
365.94	365.94	365.93	0.00	0.00
369.29	369.29	369.29	0.00	0.00
375.02	375.01	375.01	0.00	0.00
378.73	378.73	378.73	0.00	0.00
384.9	384.9	384.9	0.00	0.00
385.87	385.87	385.87	0.00	0.00

403.39	403.39	403.39	0.00	0.00
431.94	431.94	431.93	0.00	0.00
432.93	432.93	432.93	0.00	0.00
444.15	444.15	444.15	0.00	0.00
446.4	446.4	446.4	0.00	0.00
448.67	448.67	448.67	0.00	0.00
450.3	450.3	450.3	0.00	0.00
456.51	456.51	456.51	0.00	0.00
473.91	473.9	473.9	0.00	0.00
484.39	484.39	484.39	0.00	0.00
491.11	491.11	491.11	0.00	0.00
507.63	507.63	507.62	0.00	0.00
519.64	519.64	519.64	0.00	0.00
531.09	531.09	531.09	0.00	0.00
536.49	536.49	536.49	0.00	0.00
546.4	546.4	546.4	0.00	0.00
559.93	559.93	559.93	0.00	0.00
584.35	584.35	584.35	0.00	0.00
591.52	591.52	591.52	0.00	0.00
595.02	595.02	595.02	0.00	0.00
603.72	603.71	603.71	0.00	0.00
604.33	604.33	604.33	0.00	0.00
607.29	607.29	607.29	0.00	0.00
609.49	609.49	609.49	0.00	0.00
615.41	615.41	615.41	0.00	0.00
668.14	668.14	668.14	0.00	0.00
669.34	669.34	669.34	0.00	0.00
695.85	695.85	695.85	0.00	0.00
711.8	711.8	711.8	0.00	0.00
718.52	718.52	718.52	0.00	0.00
721.78	721.78	721.78	0.00	0.00
735.41	735.41	735.41	0.00	0.00
750.04	750.04	750.04	0.00	0.00
753.74	753.74	753.74	0.00	0.00
757.36	757.36	757.36	0.00	0.00
774.06	774.06	774.06	0.00	0.00
776.74	776.74	776.74	0.00	0.00
779.16	779.16	779.16	0.00	0.00
781.91	781.91	781.91	0.00	0.00
799.29	799.29	799.29	0.00	0.00
801.99	801.99	801.99	0.00	0.00

804.34	804.34	804.34	0.00	0.00
809.63	809.63	809.63	0.00	0.00
809.74	809.74	809.74	0.00	0.00
811.27	811.27	811.27	0.00	0.00
814.9	814.9	814.9	0.00	0.00
818.68	818.68	818.68	0.00	0.00
829.27	829.27	829.27	0.00	0.00
831.35	831.35	831.35	0.00	0.00
868.4	868.4	868.39	0.00	0.00
877.34	877.34	877.34	0.00	0.00
891.47	891.47	891.47	0.00	0.00
906.5	906.5	906.5	0.00	0.00
918.15	918.15	918.15	0.00	0.00
923.76	923.76	923.76	0.00	0.00
924.99	924.99	924.99	0.00	0.00
926.99	926.99	926.99	0.00	0.00
931.36	931.36	931.36	0.00	0.00
942.71	942.71	942.71	0.00	0.00
943.52	943.52	943.52	0.00	0.00
943.93	943.93	943.93	0.00	0.00
944.53	944.53	944.53	0.00	0.00
958.34	958.34	958.34	0.00	0.00
961.46	961.46	961.46	0.00	0.00
965.12	965.12	965.12	0.00	0.00
968.86	968.86	968.86	0.00	0.00
977.24	977.24	977.24	0.00	0.00
987.59	987.59	987.59	0.00	0.00
988.32	988.32	988.32	0.00	0.00
989.32	989.32	989.32	0.00	0.00
990.43	990.43	990.43	0.00	0.00
1002.8	1002.8	1002.8	0.00	0.00
1004.9	1004.9	1004.9	0.00	0.00
1019.7	1019.7	1019.7	0.00	0.00
1022.3	1022.3	1022.3	0.00	0.00
1022.5	1022.5	1022.5	0.00	0.00
1027.9	1027.9	1027.9	0.00	0.00
1035.1	1035.1	1035.1	0.00	0.00
1036.2	1036.2	1036.2	0.00	0.00
1059.8	1059.8	1059.8	0.00	0.00
1068.7	1068.7	1068.7	0.00	0.00
1072.4	1072.4	1072.4	0.00	0.00

1077.3	1077.3	1077.3	0.00	0.00
1079.1	1079.1	1079.1	0.00	0.00
1084.4	1084.4	1084.4	0.00	0.00
1088.7	1088.7	1088.7	0.00	0.00
1092.7	1092.7	1092.7	0.00	0.00
1102.2	1102.2	1102.2	0.00	0.00
1107.3	1107.3	1107.3	0.00	0.00
1109.7	1109.7	1109.7	0.00	0.00
1114.1	1114.1	1114.1	0.00	0.00
1145	1145	1145	0.00	0.00
1153.3	1153.3	1153.3	0.00	0.00
1153.9	1153.9	1153.9	0.00	0.00
1156.6	1156.6	1156.6	0.00	0.00
1178.1	1178.1	1178.1	0.00	0.00
1182.1	1182.1	1182.1	0.00	0.00
1185.3	1185.3	1185.3	0.00	0.00
1187.7	1187.7	1187.7	0.00	0.00
1195.5	1195.5	1195.5	0.00	0.00
1196.7	1196.7	1196.7	0.00	0.00
1201	1201	1201	0.00	0.00
1201.2	1201.2	1201.2	0.00	0.00
1204.1	1204.1	1204.1	0.00	0.00
1205.6	1205.6	1205.6	0.00	0.00
1205.9	1205.9	1205.9	0.00	0.00
1207	1207	1207	0.00	0.00
1213.2	1213.2	1213.2	0.00	0.00
1218.1	1218.1	1218.1	0.00	0.00
1230.9	1230.9	1230.9	0.00	0.00
1236.8	1236.8	1236.8	0.00	0.00
1243.9	1243.9	1243.9	0.00	0.00
1245.9	1245.9	1245.9	0.00	0.00
1254.8	1254.8	1254.8	0.00	0.00
1256.5	1256.5	1256.5	0.00	0.00
1258.2	1258.2	1258.2	0.00	0.00
1262.2	1262.2	1262.2	0.00	0.00
1263.5	1263.5	1263.5	0.00	0.00
1263.8	1263.8	1263.8	0.00	0.00
1286.6	1286.6	1286.6	0.00	0.00
1291.4	1291.4	1291.4	0.00	0.00
1311.7	1311.7	1311.7	0.00	0.00
1313.6	1313.6	1313.6	0.00	0.00

1324.3	1324.3	1324.3	0.00	0.00
1329.1	1329.1	1329.1	0.00	0.00
1336	1336	1336	0.00	0.00
1337.2	1337.2	1337.2	0.00	0.00
1337.6	1337.6	1337.6	0.00	0.00
1339.4	1339.4	1339.4	0.00	0.00
1355	1355	1355	0.00	0.00
1359.4	1359.4	1359.4	0.00	0.00
1363.6	1363.6	1363.6	0.00	0.00
1368.7	1368.7	1368.7	0.00	0.00
1369.1	1369.1	1369.1	0.00	0.00
1381.7	1381.7	1381.7	0.00	0.00
1393.7	1393.7	1393.7	0.00	0.00
1396.7	1396.7	1396.7	0.00	0.00
1400.1	1400.1	1400.1	0.00	0.00
1406.6	1406.6	1406.6	0.00	0.00
1408.8	1408.8	1408.8	0.00	0.00
1409.9	1409.9	1409.9	0.00	0.00
1412.2	1412.2	1412.2	0.00	0.00
1414.3	1414.3	1414.3	0.00	0.00
1416.1	1416.1	1416.1	0.00	0.00
1420.2	1420.2	1420.2	0.00	0.00
1420.9	1420.9	1420.9	0.00	0.00
1422	1422	1422	0.00	0.00
1422.1	1422.1	1422.1	0.00	0.00
1424.7	1424.7	1424.7	0.00	0.00
1426	1426	1426	0.00	0.00
1426.6	1426.6	1426.6	0.00	0.00
1430.3	1430.3	1430.3	0.00	0.00
1434.9	1434.9	1434.9	0.00	0.00
1436.1	1436.1	1436.1	0.00	0.00
1439.4	1439.4	1439.4	0.00	0.00
1443	1443	1443	0.00	0.00
1443.5	1443.5	1443.5	0.00	0.00
1463.7	1463.7	1463.7	0.00	0.00
1476.4	1476.4	1476.4	0.00	0.00
1477.6	1477.6	1477.6	0.00	0.00
1480.5	1480.5	1480.5	0.00	0.00
1482.9	1482.9	1482.9	0.00	0.00
1490.3	1490.3	1490.3	0.00	0.00
1510.3	1510.3	1510.3	0.00	0.00

1515.8	1515.8	1515.8	0.00	0.00
1573.4	1573.4	1573.4	0.00	0.00
1574	1574	1574	0.00	0.00
1597.2	1597.2	1597.2	0.00	0.00
1602.6	1602.6	1602.6	0.00	0.00
1615.9	1615.9	1615.9	0.00	0.00
1618.3	1618.3	1618.3	0.00	0.00
2927.1	2927.1	2927.1	0.00	0.00
2927.8	2927.8	2927.8	0.00	0.00
2960.9	2960.9	2960.9	0.00	0.00
2965.5	2965.5	2965.5	0.00	0.00
2966.3	2966.3	2966.3	0.00	0.00
2969.5	2969.5	2969.5	0.00	0.00
2970	2970	2970	0.00	0.00
2970.3	2970.3	2970.3	0.00	0.00
2971.3	2971.3	2971.3	0.00	0.00
2972.1	2972.1	2972.1	0.00	0.00
2975.1	2975.1	2975.1	0.00	0.00
2975.7	2975.7	2975.7	0.00	0.00
2976.5	2976.5	2976.5	0.00	0.00
2988.3	2988.3	2988.3	0.00	0.00
3000.7	3000.7	3000.7	0.00	0.00
3013.3	3013.3	3013.3	0.00	0.00
3026.7	3026.7	3026.7	0.00	0.00
3031.4	3031.4	3031.4	0.00	0.00
3032.3	3032.3	3032.3	0.00	0.00
3032.6	3032.6	3032.6	0.00	0.00
3034.4	3034.4	3034.4	0.00	0.00
3038.7	3038.7	3038.7	0.00	0.00
3048.1	3048.1	3048.1	0.00	0.00
3069.9	3069.9	3069.9	0.00	0.00
3070.1	3070.1	3070.1	0.00	0.00
3071.1	3071.1	3071.1	0.00	0.00
3073.5	3073.5	3073.5	0.00	0.00
3076.2	3076.2	3076.2	0.00	0.00
3076.8	3076.8	3076.8	0.00	0.00
3081.5	3081.5	3081.5	0.00	0.00
3104.8	3104.8	3104.8	0.00	0.00
3105	3105	3105	0.00	0.00
3108.4	3108.4	3108.4	0.00	0.00
3110.5	3110.5	3110.5	0.00	0.00

3122.1	3122.1	3122.1	0.00	0.00
3123.3	3123.3	3123.3	0.00	0.00
3124	3124	3124	0.00	0.00
3124.3	3124.3	3124.3	0.00	0.00
3125.4	3125.4	3125.4	0.00	0.00
3129.5	3129.5	3129.5	0.00	0.00
3132.8	3132.8	3132.8	0.00	0.00
3135.8	3135.8	3135.8	0.00	0.00
3157.5	3157.5	3157.5	0.00	0.00
3165.4	3165.4	3165.4	0.00	0.00
3499.4	3499.4	3499.4	0.00	0.00
3504.9	3504.9	3504.9	0.00	0.00

Table S2: Optimized coordinates of the complexes

Gd_{3+}-$(H_2O)_9$

```
28
Energy = -1452.828964312
O    -1.4823893    2.0523852    0.5009973
Gd   -0.0024713    0.1707938    0.1803233
O     0.9099513   -1.0608141   -1.9360728
O     1.3768302    1.9252791   -0.6867569
O    -0.7742288    1.0603864   -2.1672137
O     2.3493255   -0.5429719    0.6240739
O    -1.5027152   -0.6318507    1.9088822
O     0.7645971    0.9495455    2.3236823
O    -1.9207698   -1.1390019   -0.8069574
O     0.3630624   -2.3987314    0.6646744
H    -1.3004499    2.9916533    0.2831743
H    -2.4031754    2.0478367    0.8393558
H    -0.4324185    0.6653052   -2.9970234
H     3.2202256   -0.2313000    0.3007973
H     2.4343370   -1.4990908    0.8311706
H    -1.3898621    1.7677438   -2.4507440
H    -2.4091834   -0.9646638    1.7395376
H    -1.4348304   -0.4943403    2.8768988
H     0.5053313    1.7052538    2.8935511
H    -2.1351689   -2.0936774   -0.7472681
H     1.6653705    0.6760055    2.6071460
H    -2.4269301   -0.8052132   -1.5765015
H     0.6670642   -3.0895759    0.0377165
H    -0.0133581   -2.8996892    1.4207401
H     1.8292326   -1.2666359   -2.2099209
H     0.3595362   -1.6596459   -2.4814252
```

```
H     1.1759023    2.1636865   -1.6176712
H     2.0071860    2.6013267   -0.3551694
```

Gd^{3+}-B15C5

```
40
Energy = -1686.264966257
C     3.4005316    0.7059864   -0.2648865
C     3.2087277    1.2601338    1.0509875
C     4.2854163    1.3709777    1.9371900
C     5.5508971    0.9162236    1.5274975
C     5.7401042    0.3692221    0.2290301
C     4.6655821    0.2722000   -0.6729424
H     4.1673064    1.7950904    2.9456202
H     6.4044544    0.9893627    2.2215794
H     6.7394534    0.0196746   -0.0787821
H     4.8403457   -0.1503808   -1.6736501
O     1.9085763    1.6946811    1.3254058
O     2.2580739    0.6855051   -1.0708154
C     2.1572348   -0.2364358   -2.2268832
C     0.9774988    0.2063161   -3.0797285
H     2.0302667   -1.2591335   -1.8116057
H     3.0802441   -0.1872451   -2.8397004
H     0.7326061   -0.6029608   -3.8026103
O    -0.1603751    0.4381617   -2.1905645
C    -1.4866423    0.6307421   -2.7993029
C    -2.5016935    0.6173140   -1.6667432
H    -1.6982773   -0.2035595   -3.5032005
H    -1.4890416    1.5881441   -3.3702623
H    -3.4878297    0.9726424   -2.0388061
H    -2.6167900   -0.3977561   -1.2270248
H     1.1938497    1.1364546   -3.6559087
O    -2.0206048    1.5234579   -0.6135178
C    -2.8362036    1.5470159    0.6093930
C    -2.1401877    2.4444403    1.6209296
H    -2.9363640    0.5038147    0.9817080
H    -3.8446801    1.9535153    0.3743639
O    -0.7282278    2.0301623    1.6630137
H    -2.5988635    2.3065010    2.6247384
H    -2.1937971    3.5241520    1.3495433
C     0.1251445    2.6153334    2.6964950
C     1.4332984    1.8384728    2.7222973
H    -0.3676839    2.5223657    3.6899133
H     0.2776885    3.6989165    2.4819048
H     2.1742878    2.4045532    3.3229550
H     1.3180048    0.8112878    3.1294923
Gd    0.2792215    1.9214112   -0.4425350
```

Gd^{3+}-DB15C5

44
Energy = -1838.827271909
C 2.6823254 -0.0141178 -1.3076443
C 3.2156954 -0.2560770 -0.0072152
C 4.5888663 -0.4125673 0.1881694
C 5.4394641 -0.2903473 -0.9271849
C 4.9121646 -0.0479928 -2.2164862
C 3.5243551 0.0761540 -2.4185171
H 5.0134476 -0.6262901 1.1797543
H 6.5264642 -0.3942306 -0.7900032
H 5.5910136 0.0389754 -3.0782313
H 3.1358636 0.2456305 -3.4325150
C 0.5899910 0.4381787 -2.5929033
C -0.8093237 0.8885980 -2.2255763
H 0.5994635 -0.4422766 -3.2679611
H 1.1264369 1.2804807 -3.0745488
H -1.4221813 0.9420353 -3.1457409
H -0.8286661 1.8750863 -1.7191052
C -2.2771340 -0.3243319 2.6702511
C -1.0465047 0.3783545 3.2119939
H -2.4206977 -1.3416516 3.0886390
H -3.1738056 0.2887411 2.8858241
H -1.0116952 0.2661838 4.3161473
H -1.0412754 1.4601181 2.9592301
C 1.4009674 0.3373843 3.1241663
C 2.5643109 -0.3442335 2.4283194
H 1.4710320 0.1699680 4.2197722
H 1.3874581 1.4304117 2.9262722
H 3.4881219 0.2452149 2.5900768
H 2.7337175 -1.3874130 2.7658171
O -2.0936729 -0.4550629 1.2148300
O 0.1476270 -0.2391445 2.6208473
O 2.2347395 -0.3656914 0.9915005
O 1.2782793 0.0781987 -1.3416798
O -1.3780488 -0.1109296 -1.2973628
C -5.0981414 0.0613071 -1.6809468
C -3.7383076 0.0956824 -2.0392604
C -2.7751923 -0.0824083 -1.0426575
C -3.1637645 -0.2889804 0.3087196
C -4.5144190 -0.3324467 0.6657100
C -5.4822388 -0.1526228 -0.3394724
H -5.8652086 0.1843763 -2.4602473
H -3.4565012 0.2383875 -3.0924874
H -4.8332328 -0.5212438 1.7008702
H -6.5491214 -0.1955221 -0.0732764
Gd 0.0370632 -1.0585933 0.3840319

Gd^{3+}-B18C6

47

Energy = -1840.267388122

C	-0.4502963	-1.6027137	-3.5396745
C	0.5834228	-0.5931869	-4.0059434
C	-2.4519259	-0.3268418	-2.8426139
C	-3.1095088	0.1877463	-1.5830830
H	-3.1354631	-1.0315466	-3.3610194
H	-2.1952827	0.5026874	-3.5351752
H	-3.9426918	0.8724202	-1.8444415
H	-3.5028192	-0.6430875	-0.9592767
C	-2.5592888	1.6051643	0.3745540
C	-2.5255436	0.6625899	1.5670153
H	-3.5826466	2.0043655	0.2186143
H	-1.8818993	2.4707132	0.5224923
H	-2.6583803	1.2381101	2.5060101
H	-3.2945821	-0.1363549	1.5176892
C	-0.7114514	-0.5747428	2.6908241
C	-1.4733413	-0.8593373	3.8338159
C	-0.8502698	-1.4818576	4.9253392
C	0.5315410	-1.8115556	4.8812231
C	1.3056782	-1.5106966	3.7466259
C	0.6892958	-0.8958064	2.6525717
H	-2.5451410	-0.6227014	3.8836874
H	-1.4423702	-1.7290871	5.8197184
H	0.9999454	-2.3203277	5.7377654
H	2.3702106	-1.7850842	3.7254162
C	2.7911665	-0.2332093	1.5075502
C	2.9948100	1.0240277	0.6808842
H	3.3263750	-1.1155412	1.1016605
H	3.1193834	-0.0535145	2.5500766
H	4.0785630	1.2136473	0.5419472
H	2.5535851	1.9140948	1.1737922
C	3.2324238	0.7732878	-1.7788075
H	3.9364416	1.6312137	-1.7835343
H	3.8071783	-0.1737987	-1.7061977
C	2.3667027	0.8122322	-3.0191341
H	1.9559306	1.8252642	-3.2192719
H	2.9631745	0.4934812	-3.8990268
O	-1.2008443	0.0314313	1.5474000
O	1.3465768	-0.5330630	1.4816924
O	2.3397529	0.8778602	-0.6182656
O	-2.0921584	0.9304076	-0.8293686
O	1.2605783	-0.1181402	-2.8002454
O	-1.2347152	-1.0314126	-2.4434618
H	-1.1173027	-1.9128877	-4.3693071
H	0.0258496	-2.5170538	-3.1307343
H	1.3188593	-1.0821062	-4.6795274
H	0.1380079	0.2738657	-4.5396839
Gd	0.1105249	-0.0559161	-0.6754579

Gd^{3+}-DB18C6

51
Energy = -1992.427831014
C -2.9661919 -0.7117060 -0.5805248
C -2.8962852 0.7064203 -0.6991802
C -3.7250410 1.3897807 -1.5957667
C -4.6466292 0.6494009 -2.3574441
C -4.7189057 -0.7565750 -2.2368009
C -3.8692608 -1.4482000 -1.3537063
O -1.9327076 1.2972907 0.1220911
C -1.9506418 2.7549707 0.3118710
C -1.2460555 3.0285420 1.6293182
O 0.0064938 2.2751347 1.6569441
C 1.2848191 2.9709073 1.8049870
C 2.1301127 2.7043448 0.5716621
O 2.0624778 1.2597433 0.3268176
C 2.9919315 0.6744217 -0.5462490
C 2.9313275 -0.7415739 -0.5974620
C 3.7687787 -1.4643868 -1.4502710
C 4.6978228 -0.7608278 -2.2390684
C 4.7595266 0.6476528 -2.1876840
C 3.8969867 1.3779187 -1.3506759
O 1.9254799 -1.3233551 0.2019868
C 2.2563606 -2.5033778 1.0222626
C 0.9680473 -3.2479687 1.2817274
O -0.0133267 -2.2857048 1.7800338
C -1.3573649 -2.8178777 1.9915380
C -2.1897999 -2.6573673 0.7301448
O -2.0522853 -1.2514839 0.3279175
Gd 0.0294501 -0.0126326 0.9444823
H -3.9344150 -2.5428668 -1.2840009
H -3.6757757 2.4811158 -1.7140098
H -5.3141298 1.1749289 -3.0564553
H -5.4435017 -1.3219421 -2.8415815
H 3.7125235 -2.5610578 -1.5154143
H 5.3723642 -1.3175230 -2.9062511
H 5.4852818 1.1880668 -2.8134254
H 3.9543967 2.4750751 -1.3388769
H -3.0018619 3.1026165 0.3691761
H -1.4531121 3.2323051 -0.5570520
H -1.0464324 4.1135506 1.7376006
H -1.8544757 2.7036783 2.4979133
H 1.1193189 4.0595522 1.9309809
H 1.7673223 2.5899475 2.7281325
H 1.7614543 3.2368514 -0.3293710
H 3.1826953 2.9959185 0.7652129
H 2.7413479 -2.1441182 1.9540808
H 2.9664002 -3.1579462 0.4816564
H 1.1386129 -4.0341738 2.0468411
H 0.5814073 -3.7206945 0.3540005
H -1.7880785 -2.2465248 2.8386096
H -1.3070322 -3.8822255 2.3000146
H -1.8535891 -3.3049964 -0.1058459

```
H    -3.2558327   -2.8730048    0.9491392
```

Gd^{3+}-DCH18C6

```
63
Energy = -1999.661617548
C     2.8201017   -0.4987239   -1.0455992
C     2.6564700    1.0365133   -1.1497659
C     4.0431138    1.7272484   -1.0886205
C     5.1402382    0.8311778   -1.6752147
C     5.3213743   -0.4535039   -0.8507624
C     4.0069664   -0.8937928   -0.1610540
O     1.7695725    1.4478253   -0.0385061
Gd   -0.2660266    0.1557361    0.4817734
O    -2.1581919   -1.4692449    0.3203965
C    -1.9566091   -2.7911642    0.8927313
C    -0.9823027   -2.6646890    2.0549862
O     0.2193651   -1.9538076    1.6245262
C     1.3078480   -2.7655488    1.0731939
C     1.4430467   -2.4884213   -0.4187026
O     1.5181640   -1.0483606   -0.6295488
C     1.6700706    2.8826466    0.2129117
C     1.0277302    3.0610403    1.5731770
O    -0.1913432    2.2577846    1.5722195
C    -1.2859789    2.6245697    2.4746066
C    -2.5696601    2.3508763    1.7111861
O    -2.4198780    1.0164925    1.1490612
C    -3.4394660    0.5522667    0.2004380
C    -3.5520051   -0.9618443    0.4002154
C    -4.4581400   -1.6146991   -0.6496185
C    -4.0800393   -1.2328859   -2.0896713
C    -4.0027203    0.2899478   -2.2671209
C    -3.0640168    0.9406691   -1.2362412
H     5.7157335   -1.2679704   -1.4956105
H     3.8924045   -0.4102103    0.8350558
H     2.9916694   -0.8814547   -2.0771210
H     2.1344453    1.3024922   -2.0960278
H     4.2850452    1.9207371   -0.0204599
H     4.9215094    0.6034539   -2.7453223
H     6.0945601    1.4006915   -1.7277411
H     4.0076785    2.7016271   -1.6129601
H     6.1009563   -0.3191641   -0.0686323
H     4.0445816   -1.9858710    0.0224116
H    -4.4674188   -2.7147067   -0.5038626
H    -5.4961042   -1.2863457   -0.4195648
H    -3.1046135   -1.6936699   -2.3622563
H    -4.8229943   -1.6597945   -2.7915229
H    -3.6837891    0.5643736   -3.2921715
H    -5.0142648    0.7392748   -2.1418077
H    -3.0383615    2.0438143   -1.3521649
```

H	-2.0104858	0.5837719	-1.4575710
H	-4.4136613	1.0069710	0.4801167
H	-3.9095055	-1.1725665	1.4312141
H	1.0776957	3.3615106	-0.5970836
H	2.6782651	3.3416449	0.2263739
H	1.6888509	2.7269961	2.4003475
H	0.7690963	4.1285245	1.7301890
H	-1.2048859	2.0230556	3.4044831
H	-1.2109176	3.6976029	2.7435429
H	-3.4448134	2.3785015	2.3942388
H	-2.7211610	3.0882808	0.8951726
H	-1.5788055	-3.4625172	0.0941184
H	-2.9178088	-3.2106582	1.2540006
H	-0.7044921	-3.6565520	2.4667895
H	-1.4116326	-2.0619714	2.8804095
H	1.1060960	-3.8407576	1.2550404
H	2.2233044	-2.4848558	1.6303002
H	2.3403978	-2.9915596	-0.8309051
H	0.5657352	-2.8508519	-0.9920340

Gd^{3+}-CMPS-DB18C6

93
Energy = -2800.684524878

C	-10.1113393	-0.0676453	2.1348691
C	-9.2237446	0.3426128	1.1110205
C	-9.7044880	0.4159827	-0.2233318
C	-11.0276742	0.0840948	-0.5198123
C	-11.9294542	-0.3207407	0.5015574
C	-11.4356127	-0.3918960	1.8358939
C	-7.8074366	0.7508798	1.4518530
N	-6.8245199	0.1834785	0.5369650
C	-5.5432052	0.6318823	0.3505424
C	-5.0303143	1.7652507	1.0455328
C	-3.7173332	2.1986633	0.8360110
C	-2.8900806	1.5320841	-0.0762238
C	-3.3767684	0.3982603	-0.7655044
C	-4.6780888	-0.0583841	-0.5576483
O	-2.4379189	-0.1795116	-1.6322224
C	-2.7355953	-1.3883200	-2.3706487
C	-2.1965086	-2.5838191	-1.6102237
O	-0.8065219	-2.2987605	-1.3236224
Gd	0.0330256	0.0640616	-0.9635018
O	0.6673024	2.3511759	-1.6573358
C	1.8014921	2.4163075	-2.5544910
C	2.9779050	1.8026675	-1.8204485
O	2.5456571	0.5202002	-1.3019593
C	3.4412239	-0.2021755	-0.5006945
C	2.9198024	-1.3835163	0.0671120
C	3.7169416	-2.1436590	0.9372551
C	5.0274432	-1.7586426	1.2092160
C	5.5810142	-0.5808387	0.6236802

C	4.7527930	0.2076318	-0.2324645
N	6.8714748	-0.2327072	0.9137705
C	7.6050259	0.9257694	0.4181626
C	9.1004716	0.7233523	0.5400773
C	9.8964404	1.6289746	1.2766824
C	11.2765868	1.4342525	1.3791523
C	11.9141555	0.3228847	0.7556106
C	11.1038243	-0.5792129	0.0163942
C	9.7257891	-0.3862169	-0.0906979
C	13.4037117	0.1459631	0.8424296
C	14.1680375	1.0135865	-0.1906881
O	1.5874775	-1.7302812	-0.2436058
C	1.3829685	-3.0782775	-0.7759976
C	-0.0926626	-3.3845749	-0.6847773
O	-1.5557054	1.8818850	-0.3369606
C	-1.2149005	3.2848573	-0.5464229
C	-0.3591562	3.3659573	-1.7975542
C	-13.3540021	-0.6852303	0.1909167
C	-13.5800600	-2.2177852	0.1254746
H	-2.2189505	-1.2749703	-3.3446116
H	-3.8185977	-1.4829960	-2.5752195
H	-2.7471117	-2.7561043	-0.6590431
H	-2.2742078	-3.4989846	-2.2363720
H	-0.3005337	-4.3403304	-1.2119979
H	-0.4289345	-3.4821420	0.3709344
H	1.7546042	-3.1099080	-1.8222121
H	1.9519941	-3.8132278	-0.1745410
H	3.2917944	2.4472416	-0.9724004
H	3.8314997	1.6660126	-2.5167330
H	1.5682937	1.8790583	-3.5007833
H	2.0357463	3.4718535	-2.8049946
H	-0.9518700	3.1793654	-2.7194931
H	0.1093128	4.3704420	-1.8710974
H	-2.1396259	3.8815233	-0.6729441
H	-0.6670392	3.6465161	0.3474022
H	3.3108437	-3.0466239	1.4162109
H	5.6400856	-2.3690254	1.8889256
H	5.1499902	1.1319158	-0.6662620
H	-3.3383325	3.0637999	1.4001155
H	-5.6535266	2.3051799	1.7694061
H	-5.0649615	-0.9369472	-1.0920195
H	7.3596550	-0.8061768	1.6068422
H	-7.0986157	-0.6849356	0.0713766
H	-11.3914459	0.1622918	-1.5558710
H	-9.0379151	0.7628191	-1.0286688
H	-9.7580542	-0.1264439	3.1762062
H	-12.1151753	-0.7008160	2.6452034
H	-13.6569137	-0.2260819	-0.7717838
H	-14.0173560	-0.2633450	0.9766232
H	-7.5738754	0.4757789	2.5059331
H	-7.7415046	1.8626083	1.4009741
H	-14.6448571	-2.4268344	-0.0958121

H	-13.3292773	-2.7094932	1.0865708
H	-12.9636409	-2.6807176	-0.6703807
H	11.8837906	2.1454080	1.9605199
H	9.4288402	2.4911170	1.7775805
H	9.1214370	-1.0952811	-0.6784382
H	11.5751964	-1.4401722	-0.4822422
H	13.6625460	-0.9213277	0.6883758
H	13.7455009	0.4239541	1.8624125
H	7.2954941	1.8523249	0.9542416
H	7.3486275	1.0759003	-0.6557086
H	15.2580528	0.8541009	-0.0769771
H	13.9632295	2.0931934	-0.0465662
H	13.8844376	0.7443367	-1.2272962

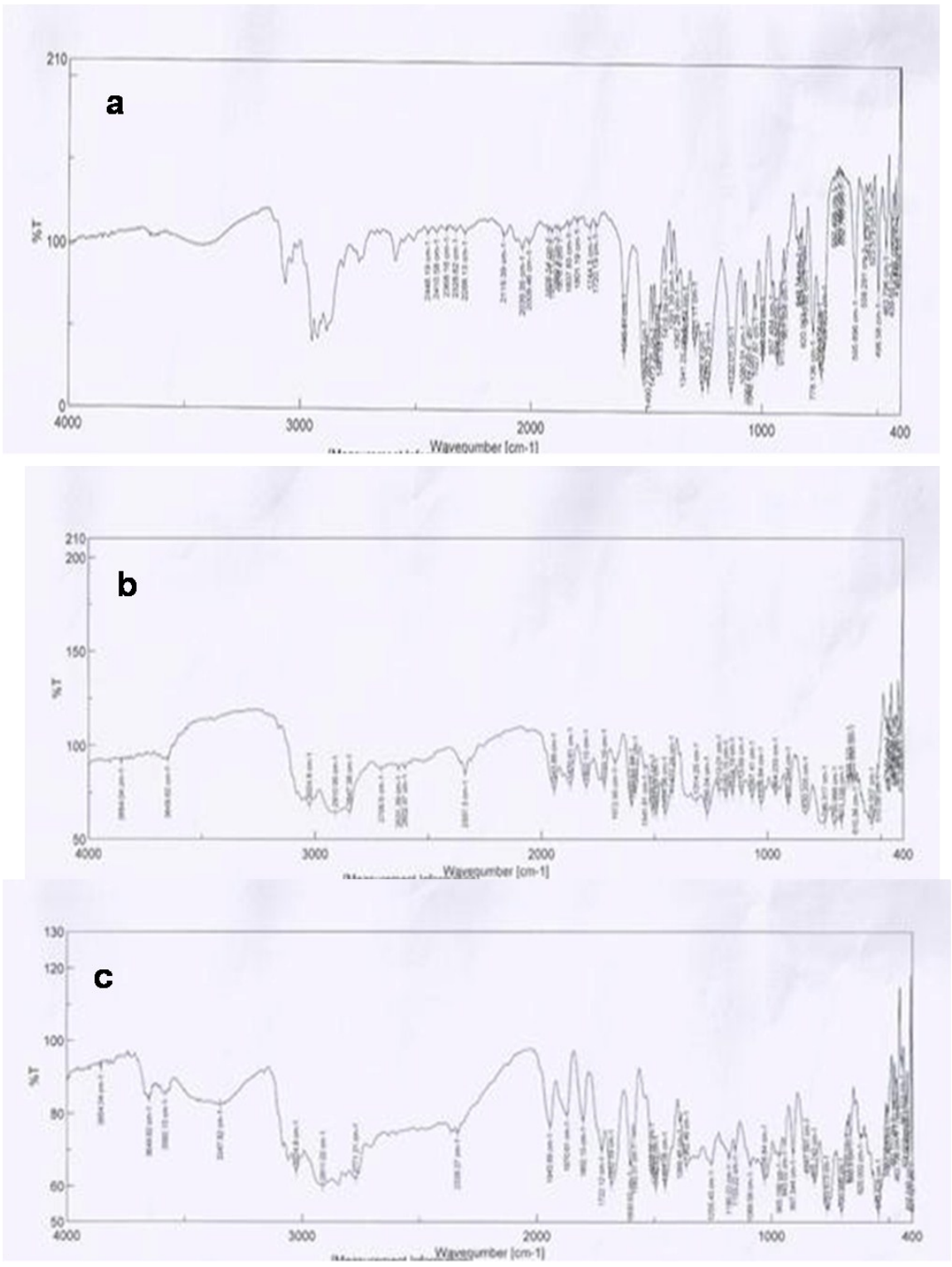

Fig S1. IR spectrum of (a)DADB18C6, (b)CMPS resin and (c) DB18C6 functionalized CMPS resin

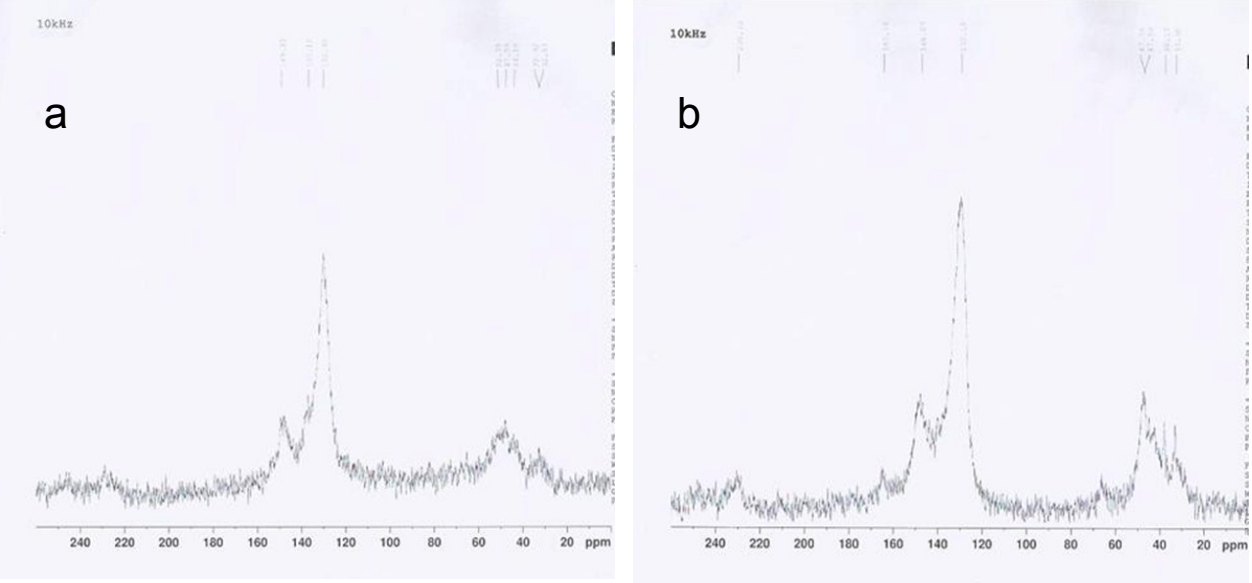

Fig. S2. ^{13}C NMR of (a) CMPS and (b) DB18C6 modified CMPS resin