SUPPLEMENTARY INFORMATION

Fluorescent probe: Complexation of Fe^{3+} with the *myo*-inositol 1,2,3-trisphosphate motif

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Coordinates and absolute energies for structures 7A and 7B.

Structure 7A:

Absolute energy = -3888.877237 au

1	P	-2.3479	-1.0884	-0.9558
2	P	-0.3012	2.7253	-0.0415
3	P	2.5732	-0.7391	-0.7573
4	H	1.7075	-0.9632	4.7426
5	H	-1.9042	-1.1219	4.5774
6	C	-1.2975	-0.5211	1.4960
7	C	-0.0367	0.3633	1.5093
8	C	1.3000	-0.3905	1.6287
9	C	1.2949	-1.3482	2.8397
10	C	0.0235	-2.3386	2.8782
11	C	-1.3143	-1.4686	2.7135
12	O	-1.3704	-1.3157	0.2944
13	O	-3.5451	-0.2723	-0.3718
14	O	-1.5572	-0.3529	-2.0603
15	O	-2.8642	-2.4739	-1.4257
16	O	0.0183	1.1416	0.2854
17	O	0.6918	3.6971	0.6563
18	O	-1.7020	2.9457	0.6031
19	O	-0.1827	2.6233	-1.5642
20	O	1.5882	-1.1528	0.4404
21	O	1.7432	-0.1280	-1.9036
22	O	3.3430	-2.0136	-1.1952
23	O	3.5891	0.2584	-0.1039
24	O	1.2864	-0.5403	3.9704
25	O	0.1162	-3.2721	1.8694
26	O	-1.4834	-0.6559	3.8307
27	H	-2.1823	0.1168	1.5643
28	H	2.1032	0.3322	1.7954
29	H	2.1693	-2.0107	2.7967
30	H	0.0014	-2.7944	3.8753
31	H	-2.1213	-2.2048	2.5996

32	H	-0.1157	1.0361	2.3693
33	Fe	0.0216	0.6891	-1.992
34	H	0.1738	-4.1840	2.2110
35	C	-2.4402	-3.3003	-2.5730
36	C	-4.8523	-0.0715	-1.0468
37	C	3.1286	-2.8901	-2.3631
38	C	4.9447	0.5577	-0.6313
39	C	-2.3334	4.2712	0.8658
40	C	1.8916	4.3492	0.0749
41	H	-2.1985	-2.6561	-3.4185
42	H	-3.3003	-3.9298	-2.7938
43	H	-1.5882	-3.9034	-2.2593
44	H	-5.4528	0.4751	-0.3230
45	H	-5.2905	-1.0464	-1.2612
46	H	-4.6975	0.5151	-1.9531
47	H	2.3737	-3.6300	-2.0970
48	H	4.0927	-3.3652	-2.5342
49	H	2.8296	-2.2891	-3.2220
50	H	5.3968	1.2001	0.1214
51	H	4.8490	1.0756	-1.5864
52	H	5.4985	-0.3758	-0.7304
53	H	-3.2222	4.0351	1.4465
54	H	-2.5957	4.7251	-0.0900
55	H	-1.6389	4.8859	1.4378
56	H	2.0434	5.2361	0.6872
57	H	1.6934	4.6130	-0.9638
58	H	2.7302	3.6597	0.1691

Structure 7B:

Absolute energy = -3888.877008 au

1	P	-2.4837	-0.3389	-1.2668
2	P	0.6249	2.7113	-0.0197
3	P	2.3394	-1.4156	-0.5275
4	H	0.8291	-1.4086	4.8489
5	H	-1.5159	-0.2610	4.1031
6	C	-1.2681	0.1307	1.2730
7	C	0.2010	0.4245	1.6107
8	C	1.0888	-0.8090	1.8623
9	C	0.4174	-1.7348	2.9083
10	C	-1.0386	-2.1209	2.5451
11	C	-1.9099	-0.8787	2.2678
12	O	-1.2630	-0.3227	-0.1476
13	O	-3.4346	0.7918	-0.8127
14	O	-1.5361	-0.0521	-2.4665

15	O	-3.2743	-1.6585	-1.3397
16	O	0.8124	1.1606	0.4939
17	O	1.8792	3.5791	0.1977
18	O	-0.5417	3.2757	0.8279
19	O	0.3190	2.3586	-1.5047
20	O	1.2892	-1.5801	0.6457
21	O	1.5627	-0.6898	-1.6872
22	O	2.8597	-2.7965	-0.9860
23	O	3.5432	-0.5882	0.0093
24	O	0.3817	-0.9620	4.1104
25	O	-1.0796	-2.9554	1.3895
26	O	-2.1902	-0.1077	3.4136
27	H	-1.8593	1.0470	1.3015
28	H	2.0630	-0.4841	2.2353
29	H	1.0272	-2.6374	3.0143
30	H	-1.4712	-2.6283	3.4152
31	H	-2.8632	-1.2196	1.8493
32	H	0.2294	1.0463	2.5088
33	Fe	0.1185	0.4599	-1.6334
34	H	-1.2346	-3.8753	1.6588
35	C	-2.9528	-2.9333	-2.0360
36	C	-4.8705	0.9984	-1.2016
37	C	2.2666	-3.8092	-1.8846
38	C	4.9786	-0.7603	-0.3613
39	C	-0.8370	4.7166	1.1313
40	C	3.0325	3.8696	-0.7012
41	H	-2.5530	-2.7065	-3.0241
42	H	-3.9089	-3.4483	-2.1041
43	H	-2.2495	-3.4791	-1.4084
44	H	-5.2279	1.7436	-0.4950
45	H	-5.3995	0.0529	-1.0917
46	H	-4.8874	1.3722	-2.2247
47	H	1.4533	-4.3033	-1.3533
48	H	3.0799	-4.5038	-2.0857
49	H	1.9333	-3.3208	-2.8005
50	H	5.5157	-0.1416	0.3543
51	H	5.1188	-0.4054	-1.3823
52	H	5.2461	-1.8107	-0.2561
53	H	-1.5812	4.6699	1.9229
54	H	-1.2383	5.1738	0.2275
55	H	0.0810	5.1948	1.4699
56	H	3.3922	4.8418	-0.3701
57	H	2.6827	3.9021	-1.7327
58	H	3.7787	3.0940	-0.5352

Full citation for ref. 9:

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