

Supporting Information

Structure of M1-COOH-7-SH-*meta*-carborane obtained by X-ray crystallography, in atomic coordinates as used in the .xyz format.

S	5.238179	0.698012	1.325699
O	1.353825	0.523509	5.607878
O	-0.278153	0.795430	4.101452
C	0.868142	0.970332	4.497733
C	1.868440	1.758719	3.678492
C	4.008308	1.703696	2.160569
B	2.435292	1.048613	2.247081
B	2.787056	2.405695	1.168750
B	2.323184	3.905517	2.002614
B	3.477399	1.215407	3.701488
B	4.023219	3.420152	1.952382
B	3.351170	4.072046	3.456017
B	4.460505	2.675225	3.507366
B	1.346117	2.433738	2.188029
B	1.693138	3.464409	3.606715
B	3.021196	2.707919	4.538813
H	0.355009	2.270000	1.835172
H	0.877213	3.891429	4.138066
H	2.214271	0.050504	1.953498
H	5.454665	2.660738	3.888019
H	3.765155	0.316312	4.194997
H	2.797714	2.244749	0.116094
H	3.621775	5.029087	3.828856
H	2.987019	2.674028	5.602632
H	6.156445	0.818689	2.165592
H	1.963345	4.715434	1.410984
H	0.804723	0.123601	5.994448
H	4.796333	3.814345	1.333960

Structure of M1-COOH-7-SH-*meta*-carborane obtained by quantum chemistry computations, in atomic coordinates as used in the .xyz format.

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B 1.454232 -1.639054 -0.001114
B -0.314003 -1.617818 0.013401
B 0.610507 -1.070480 1.449837
B 0.583693 -1.064928 -1.430984
B 2.056431 -0.228861 0.885072
C 1.908684 -0.214167 -0.810220
B 1.547055 1.204475 0.009300
B 0.629041 0.687425 -1.418597
B 0.666013 0.697505 1.443723
B -0.819949 -0.161677 -0.868856
B -0.797561 -0.161443 0.906114
C -0.154906 1.140538 0.010785
S -1.398450 -3.121048 -0.020335
H 0.603784 -1.687105 2.460384
H 0.668913 -1.633491 -2.463019
H 3.130756 -0.233399 1.377940
H 2.821071 -0.220791 -1.387819
H 2.169771 2.197601 -0.092935
H 0.691013 1.377506 -2.372784
H 0.631409 1.425022 2.374602
H -1.828791 0.000747 -1.459396
H -1.810117 0.000119 1.489806
C -0.954558 2.422857 0.013670
H 2.138868 -2.599820 -0.090845
O -2.144472 2.464382 0.098378
O -0.172375 3.500978 -0.087364
H -0.754702 4.271196 -0.071340
H -0.424612 -4.004769 0.247750
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Structure of M9-COOH-7-SH-*meta*-carborane obtained by X-ray crystallography, in atomic coordinates as used in the .xyz format.

S	6.796870	0.912046	2.860427
C	7.536637	4.808345	4.971013
C	9.796080	3.453561	5.020870
B	9.080279	3.039465	3.509805
B	7.466627	2.135355	5.723719
B	6.571244	3.396968	4.844653
B	7.560183	3.958068	3.481748
B	7.427886	3.790359	6.336946
B	7.554820	2.226456	3.931474
B	9.021206	1.922096	4.901576
B	9.014259	4.699299	4.145438
B	8.931672	2.887629	6.395282
B	8.928533	4.608198	5.929407
H	5.521549	3.506013	4.757655
H	6.890688	4.092649	7.196029
H	7.107029	4.389418	2.628115
H	9.718086	2.857262	2.686652
H	9.481268	2.608805	7.256585
H	7.014649	1.330628	6.239250
H	9.602037	1.038691	4.882803
H	9.547627	5.484702	3.679765
H	9.421985	5.383248	6.457250
H	7.083826	5.762836	4.977674
H	7.465466	1.035240	1.966040
O	11.923791	4.538492	5.026118
O	11.839826	2.333431	5.351100
C	11.308208	3.484618	5.163378
H	12.722903	2.401757	5.334952
O	11.954628	2.474914	4.739488
O	11.813341	4.668242	5.116952
C	11.311717	3.501182	4.939322
H	12.696134	4.624072	5.110896

S	31.169891	0.946900	1.307800
C	27.297913	2.972519	0.447506
C	29.198909	4.779358	-0.128782
B	29.853546	3.218216	-0.556910
B	29.319135	3.316909	2.287792
B	28.881928	4.821458	1.532663
B	27.629683	3.715821	1.949690
B	28.157282	3.617819	-0.890975
B	29.927143	2.275458	0.957990
B	27.568163	4.659270	0.439028
B	28.261929	2.093255	1.564758
B	28.587441	2.033211	-0.192365
B	30.308041	4.011210	0.972927
H	26.794539	5.369445	0.306815
H	29.681570	3.257555	3.280097
H	28.987113	5.736610	2.052836
H	27.677153	3.637143	-1.832818
H	30.561245	3.140228	-1.338280
H	26.847040	3.878699	2.642245
H	27.894953	1.233316	2.058892
H	28.368933	1.149116	-0.730705
H	31.245617	4.437729	1.205057
H	29.497347	5.680017	-0.591427
H	32.081670	1.476942	0.908335
H	31.400870	0.669455	0.244241
O	25.707313	1.231176	0.160271
O	24.980571	3.339684	0.142911
C	25.892084	2.442476	0.229910
H	24.195619	2.960786	-0.010093

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B	1.346117	2.433738	2.188029
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H	2.987019	2.674028	5.602632
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