SUPPLEMENTARY INFORMATION

1–COOH–7–SH–*m*–carborane

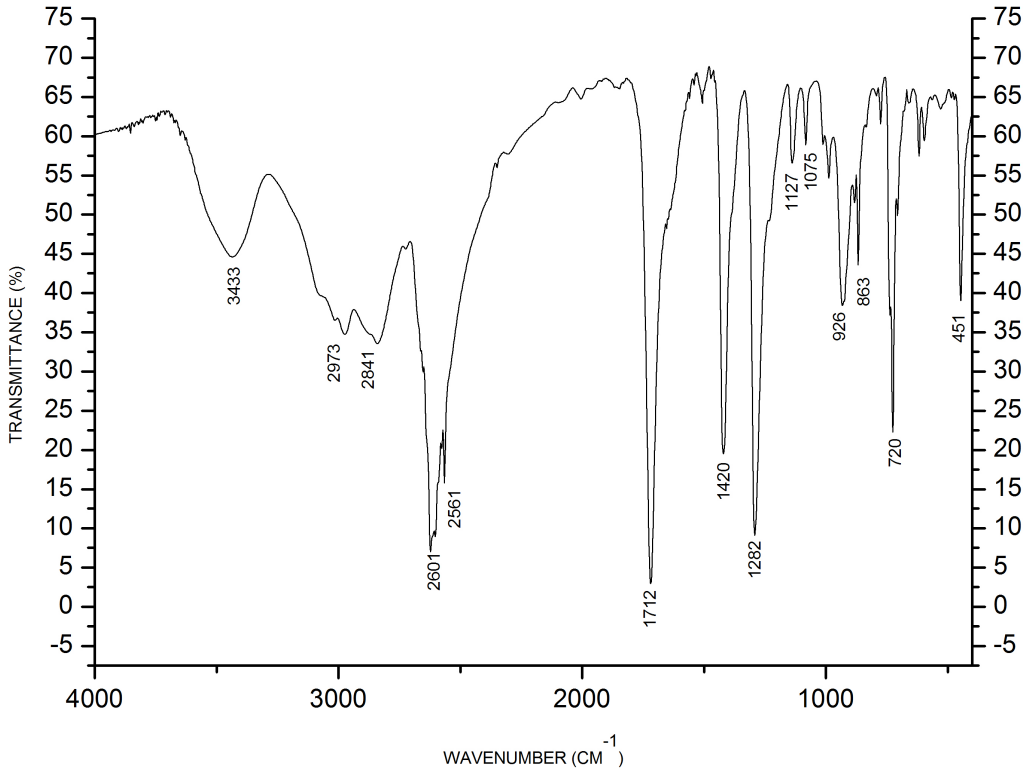
m.p. 92 – 93 °C

Dissociation Constants

pK_{A1} = 3.01

pK_{A2} = 4.25

IR Spectral Analysis



SUPPLEMENTARY INFORMATION

NMR Spectral Analysis

	$\delta(^{13}C)$ / ppm		$\delta(^{11}B)$ / ppm		$\delta(^{1}H)$ / ppm	
	real	comp	real	comp	real	comp
–COOH	167.55[a,c]	174.95	–	–	10.41[a,b,c]	5.97
–SH	–	–	–	–	3.46[a,b,c]	3.69
1	72.64[a,b]	79.26	–	–	–	–
7	64.91[a,b]	77.78	–	–	–	–
2	–	–	–13.59[a]	–17.93	3.22 – 2.02	3.54
3	–	–	–13.59[a]	–17.93		3.54
4	–	–	–12.21[a]	–14.95		2.80
6	–	–	–12.21[a]	–14.95		2.80
8	–	–	–9.64[a]	–11.47		2.96
11	–	–	–9.64[a]	–11.47		2.96
9	–	–	–11.04[a]	–14.17		2.64
10	–	–	–11.04[a]	–14.17		2.64
5	–	–	–9.64[a]	–14.18		2.93
12	–	–	–2.62[a]	–6.03		2.86

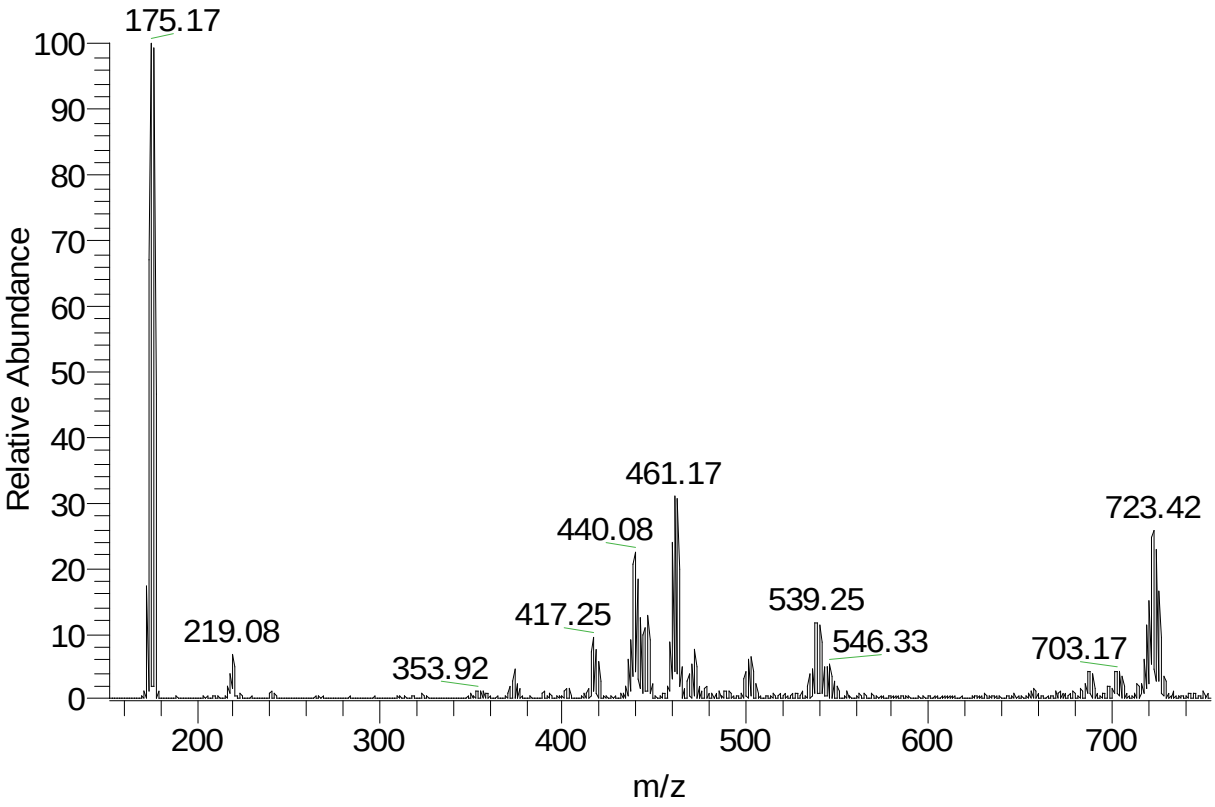
[a)] Signals are assigned *via* comparison to the computational data.

[b)] Signals are assigned *via* comparison to *m*–carborane derivatives, *i.e. m*–carborane, 1–COOH–*m*–CB, 1–SH–*m*–CB.

[c)] Signals are assigned due to spin-spin coupling.

SUPPLEMENTARY INFORMATION

ESI-MS analysis



Main peak in the ESI–MS spectrum (175.36) represents mass of the product without carboxyl moiety, probably decarboxylation in the spectrometer. Carboxyl group is not as stable as thiol group.

SUPPLEMENTARY INFORMATION

XYZ Coordinates

B	1.3768800000	–1.7266830000	0.0051590000
B	0.5450980000	–1.1089430000	1.4434740000
B	0.5598240000	–1.1045340000	–1.4397720000
B	2.0483990000	–0.3567370000	0.9012130000
B	2.0576530000	–0.3543580000	–0.8799770000
B	1.6296550000	1.1085000000	0.0104730000
B	0.7109600000	0.6506310000	–1.4306350000
B	0.6957880000	0.6464320000	1.4410350000
B	–0.7850380000	–0.1248310000	–0.8935210000
B	–0.7941800000	–0.1278040000	0.8866260000
C	–0.3063480000	–1.4801470000	–0.0029930000
C	–0.0859760000	1.1288440000	0.0017680000
S	–1.4509560000	–2.8569000000	–0.0107820000
H	0.3771410000	–1.7957920000	2.3898100000
H	0.4014520000	–1.7885860000	–2.3897950000
H	3.0408170000	–0.4458580000	1.5414310000
H	3.0566050000	–0.4420470000	–1.5101360000
H	2.2180200000	2.1306910000	0.0153560000
H	0.6647110000	1.3565440000	–2.3776460000
H	0.6399690000	1.3497920000	2.3895080000
H	–1.8317000000	–0.0324060000	–1.4250710000
H	–1.8460670000	–0.0374700000	1.4077420000
C	–0.8592260000	2.4276270000	0.0006620000
H	1.7822930000	–2.8391730000	0.0055760000
O	–2.0532560000	2.4877890000	0.0252160000
O	–0.0566200000	3.4899220000	–0.0315490000
H	–0.6249380000	4.2705860000	–0.0305730000
H	–0.4998930000	–3.8038610000	–0.0100130000

SUPPLEMENTARY INFORMATION

1–COOH–9–SH–*m*–carborane

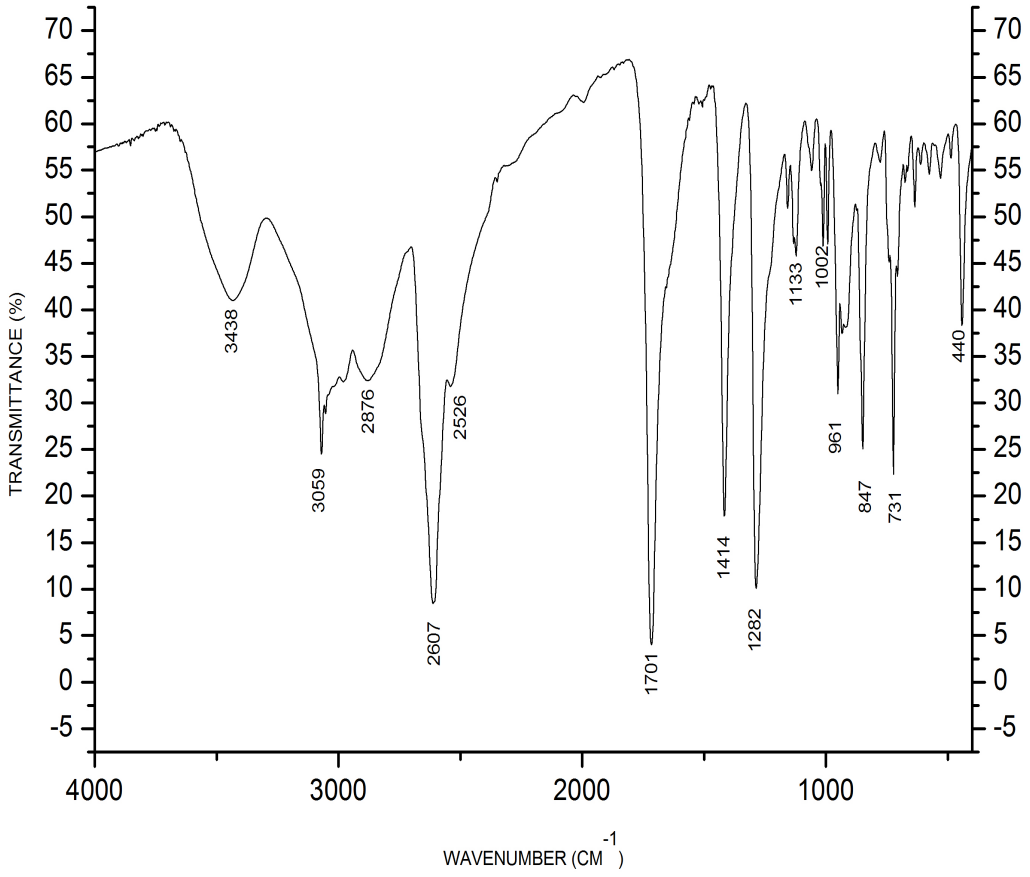
m.p. 115 – 116 °C

Dissociation Constants

pK_{A1} = 3.21

pK_{A2} = 9.23

IR Spectral Analysis



SUPPLEMENTARY INFORMATION

NMR Spectral Analysis

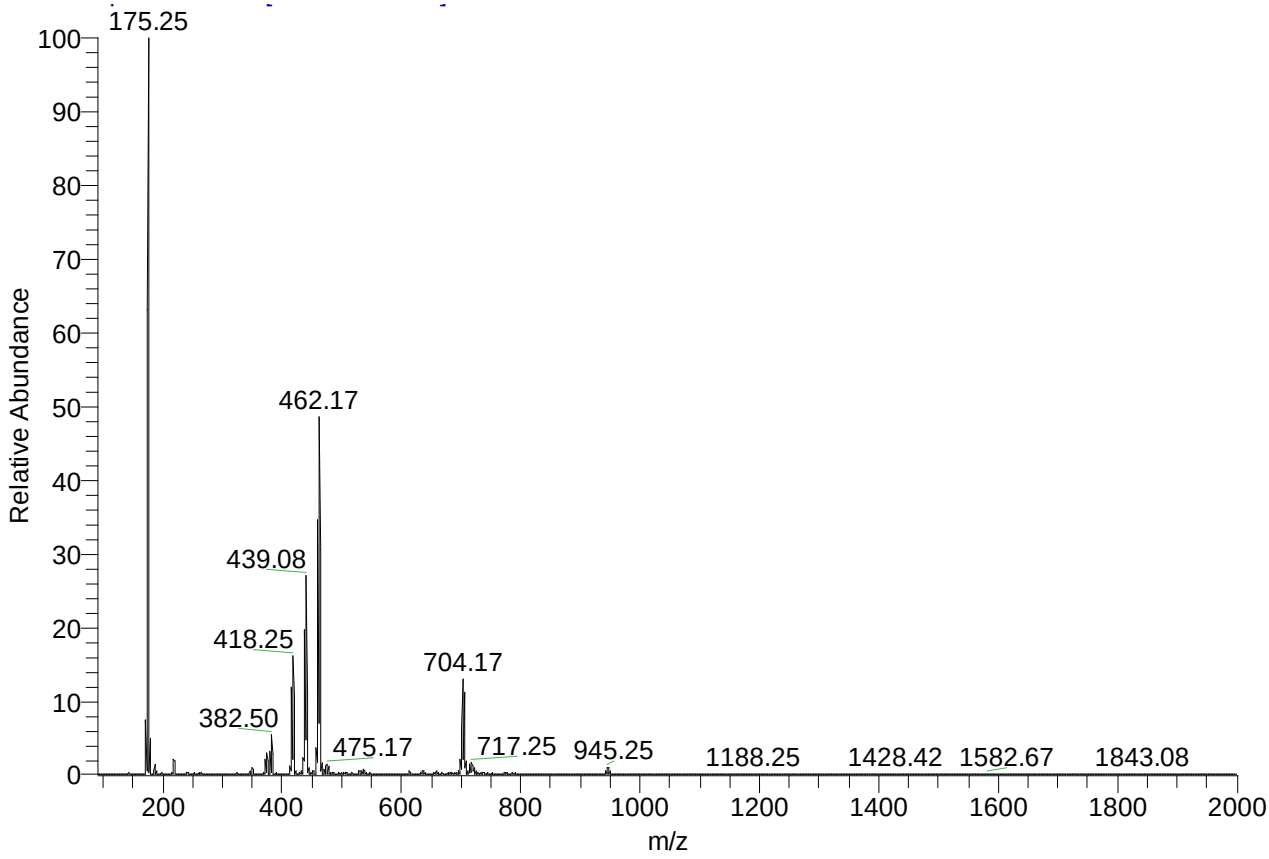
	δ(^{13}C) / ppm		δ(^{11}B) / ppm		δ(^{1}H) / ppm	
	real	comp	real	comp	real	comp
–COOH	167.40[a,b,]	174.01	–	–	9.94[a,b]	6.06
–SH	–	–	–	–	0.52[a,b]	0.99
1	70.90[a,b]	77.23	–	–	–	–
7	54.64[a,b]	61.84	–	–	3.09[a,b]	2.79
9	–	–	–3.00[a]	–2.74	–	–
2	–	–	–20.48[a]	–26.38		3.19
3	–	–	–17.37[a]	–21.37		3.16
4	–	–	–13.42[a]	–15.49		2.92
6	–	–	–11.78[a]	–15.42		2.79
8	–	–	–13.42[a]	–15.95	2.93 – 2.20	2.86
11	–	–	–14.73[a]	–19.47		2.47
10	–	–	–10.00[a]	–11.85		2.82
5	–	–	–5.24[a]	–7.79		3.33
12	–	–	–6.62[a]	–11.70		2.73

[a)] Signals are assigned *via* comparison to the computational data.

[b)] Signals are assigned *via* comparison to *m*–carborane derivatives, *i.e.* *m*–carborane, 1–COOH–*m*–CB, 9–SH–*m*–CB and due to spin-spin coupling.

SUPPLEMENTARY INFORMATION

ESI-MS Analysis



Main peak in the ESI–MS spectrum (175.36) represents mass of the product without carboxyl group, as for the 1–COOH–7–SH–*m*–carborane.

SUPPLEMENTARY INFORMATION

XYZ Coordinates

B	1.4542320000	–1.6390540000	–0.0011140000
B	–0.3140030000	–1.6178180000	0.0134010000
B	0.6105070000	–1.0704800000	1.4498370000
B	0.5836930000	–1.0649280000	–1.4309840000
B	2.0564310000	–0.2288610000	0.8850720000
C	1.9086840000	–0.2141670000	–0.8102200000
B	1.5470550000	1.2044750000	0.0093000000
B	0.6290410000	0.6874250000	–1.4185970000
B	0.6660130000	0.6975050000	1.4437230000
B	–0.8199490000	–0.1616770000	–0.8688560000
B	–0.7975610000	–0.1614430000	0.9061140000
C	–0.1549060000	1.1405380000	0.0107850000
S	–1.3984500000	–3.1210480000	–0.0203350000
H	0.6037840000	–1.6871050000	2.4603840000
H	0.6689130000	–1.6334910000	–2.4630190000
H	3.1307560000	–0.2333990000	1.3779400000
H	2.8210710000	–0.2207910000	–1.3878190000
H	2.1697710000	2.1976010000	–0.0929350000
H	0.6910130000	1.3775060000	–2.3727840000
H	0.6314090000	1.4250220000	2.3746020000
H	–1.8287910000	0.0007470000	–1.4593960000
H	–1.8101170000	0.0001190000	1.4898060000
C	–0.9545580000	2.4228570000	0.0136700000
H	2.1388680000	–2.5998200000	–0.0908450000
O	–2.1444720000	2.4643820000	0.0983780000
O	–0.1723750000	3.5009780000	–0.0873640000
H	–0.7547020000	4.2711960000	–0.0713400000
H	–0.4246120000	–4.0047690000	0.2477500000