Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Carboxonium Derivatives Based on *Closo*-Dodecaborate Anion [1,2-$B_{12}H_{10}O_2CR]^-$, R=CH_3, C_2H_5, C_3H_7, C_6H_5: Synthesis and Molecular Orbital Analysis

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1. Experimental data

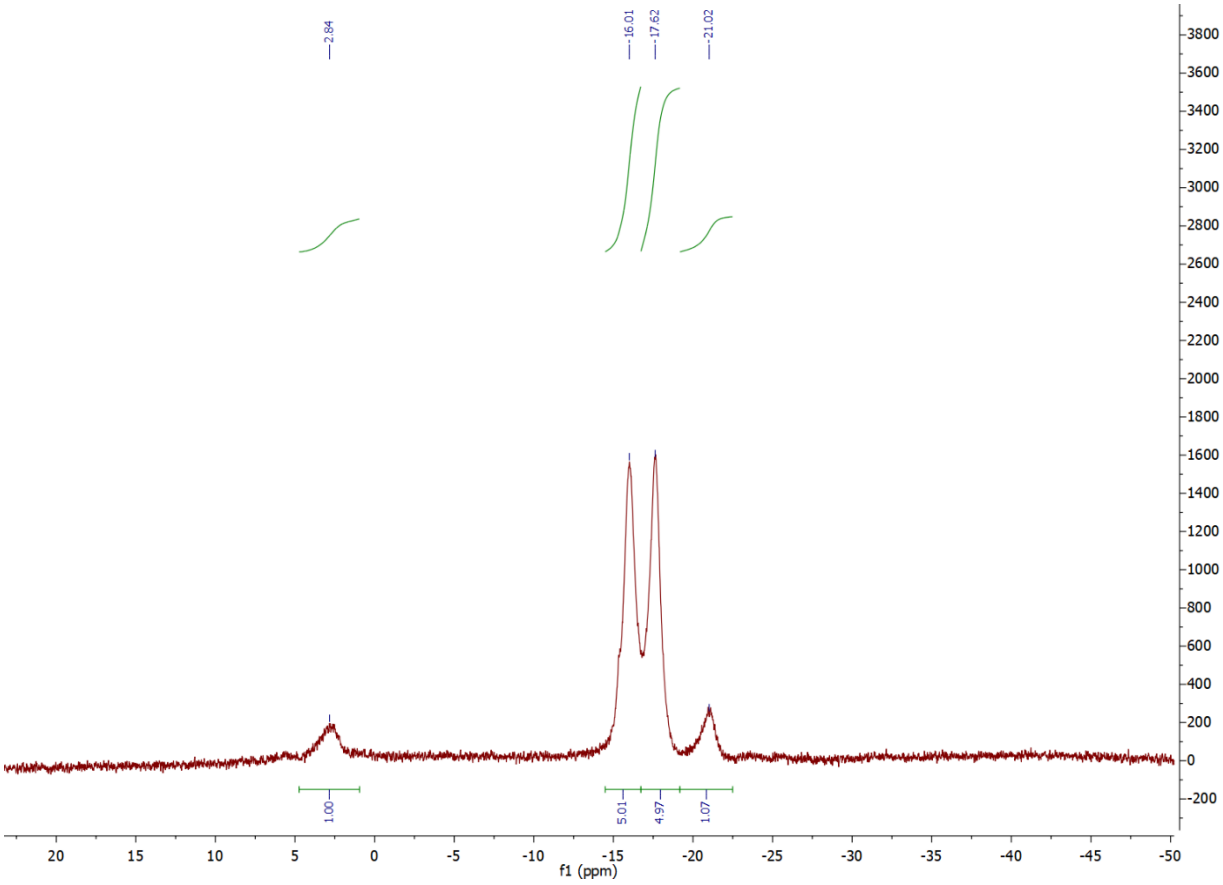


Figure S1. $^{11}B\{^{1}H\}$ NMR spectrum of $((n\text{-}C_4H_9)_4N)_2[B_{12}H_{11}OC(O)CH_3]$

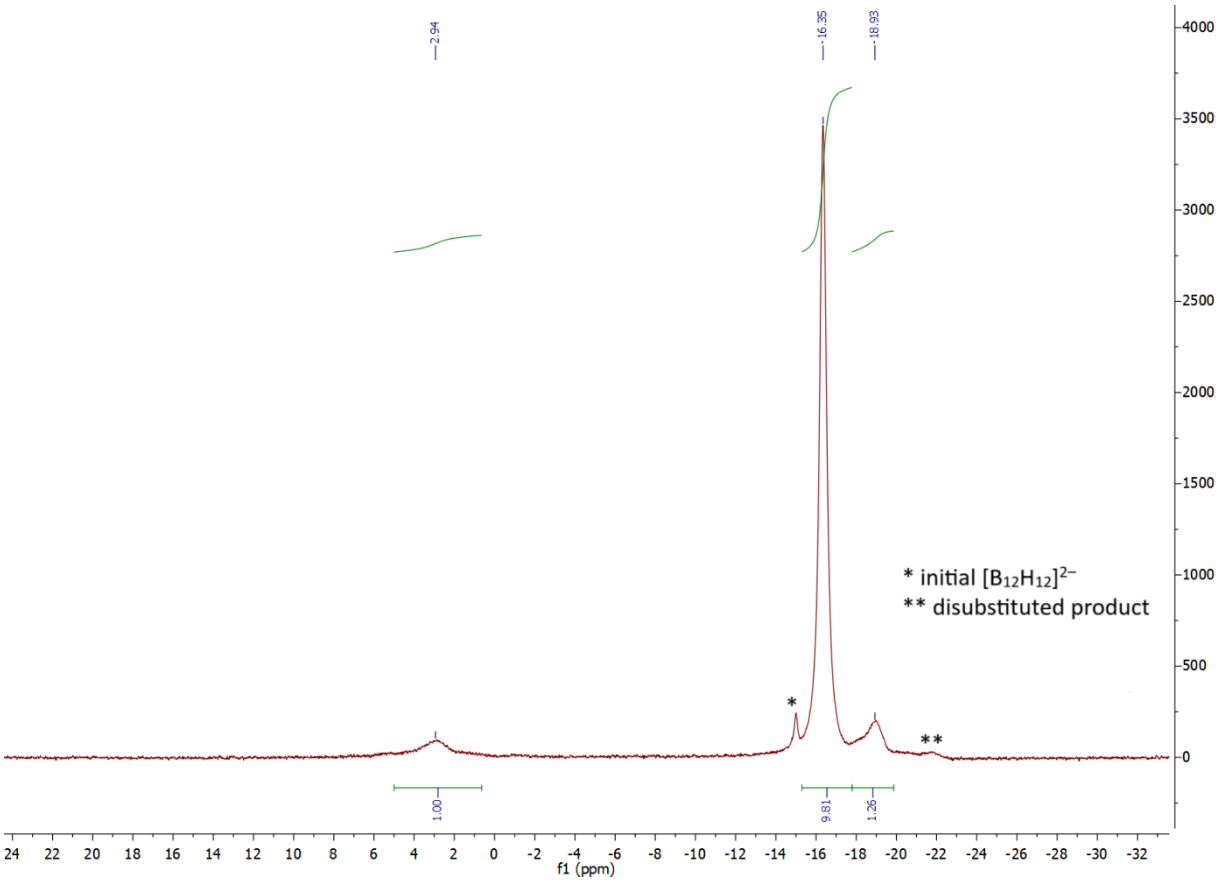


Figure S2. $^{11}B\{^{1}H\}$ NMR spectrum of $((n\text{-}C_4H_9)_4N)[B_{12}H_{11}OC(OH)CH_3]$

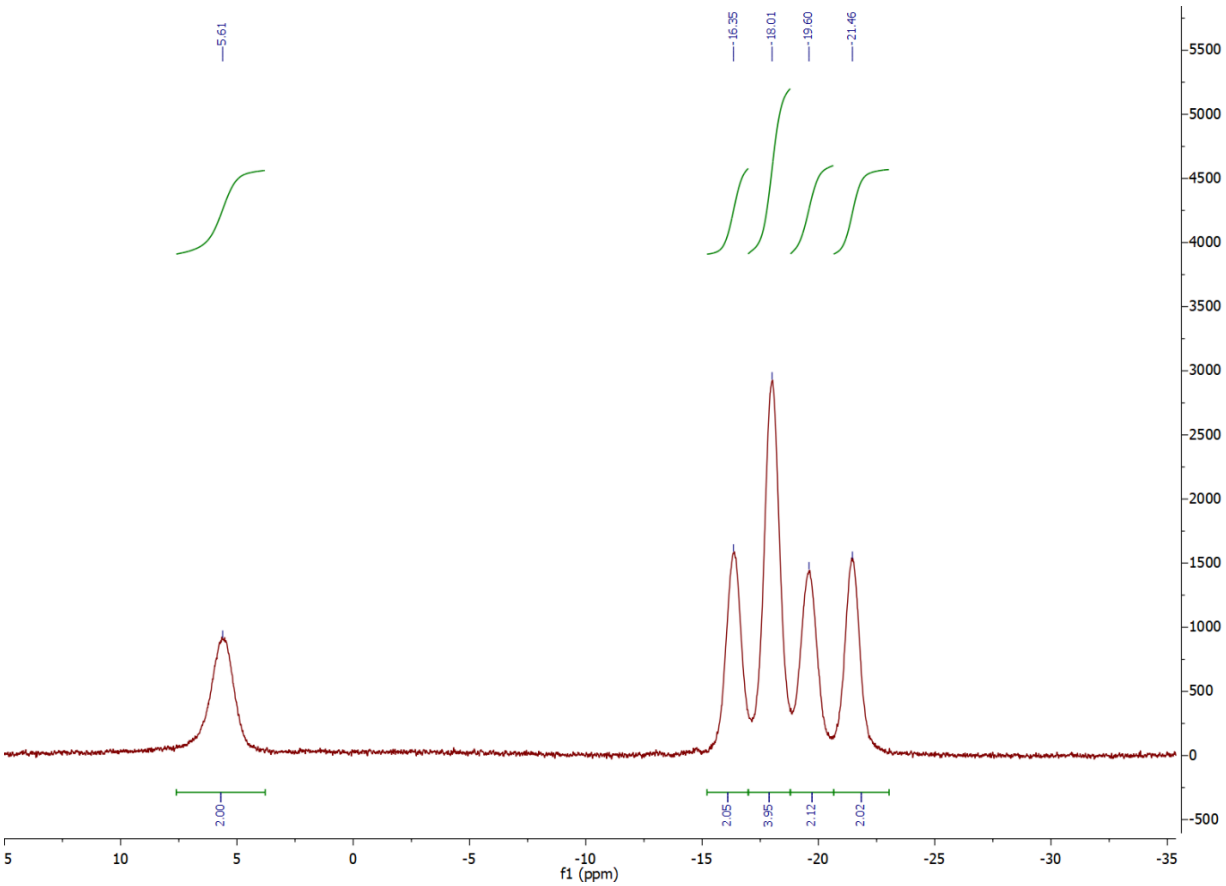


Figure S3. $^{11}B\{^{1}H\}$ NMR spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CCH_3]$

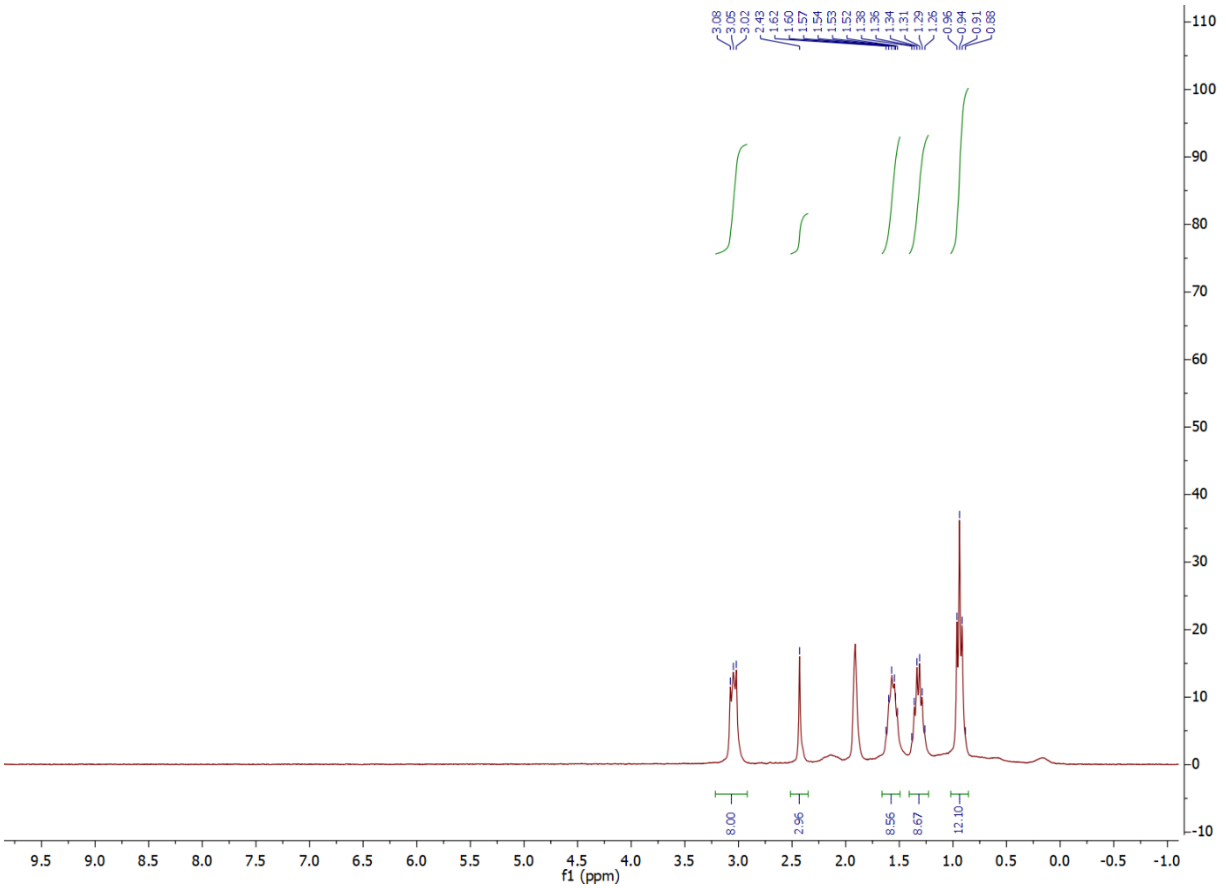


Figure S4. ^{1}H NMR spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CCH_3]$

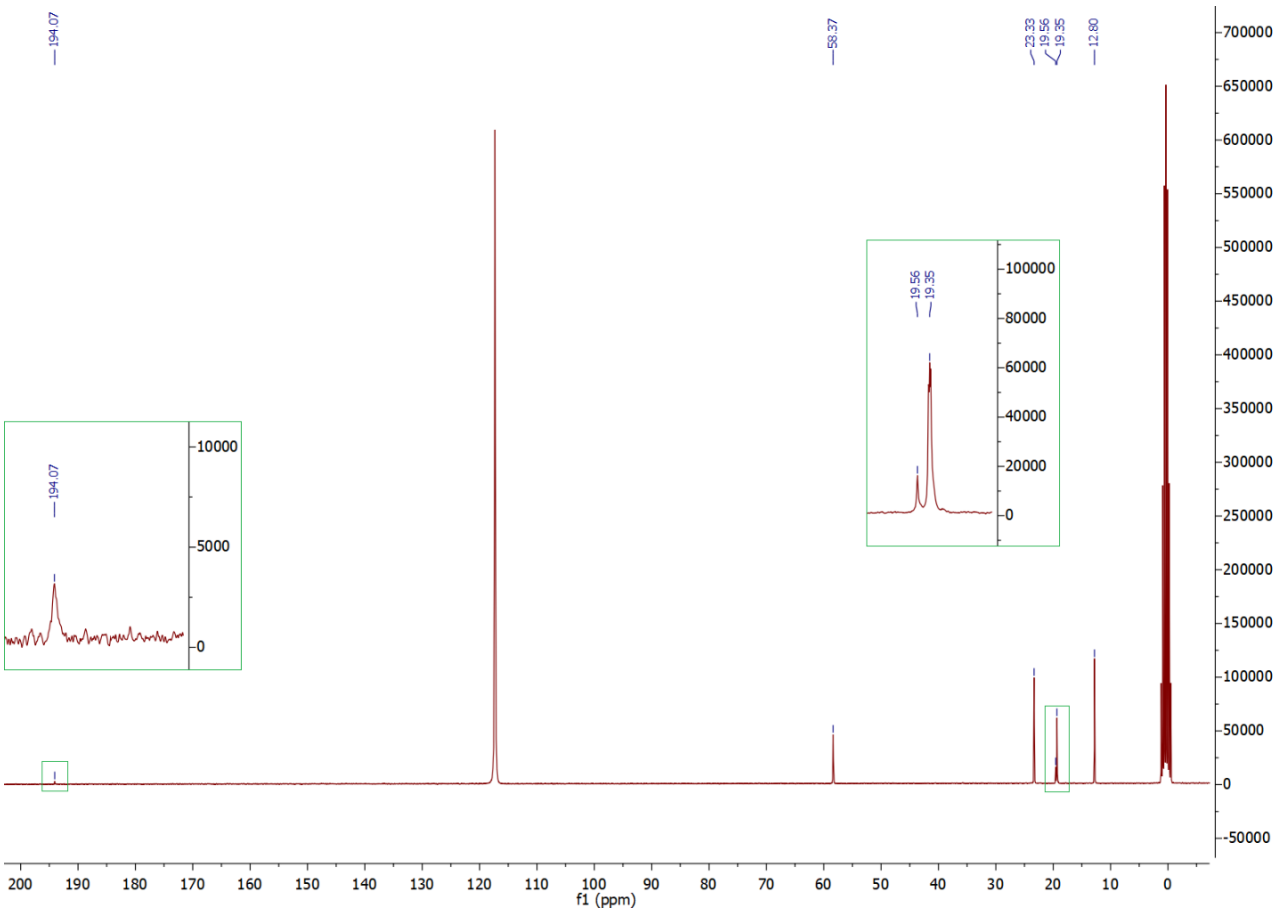


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CCH_3]$

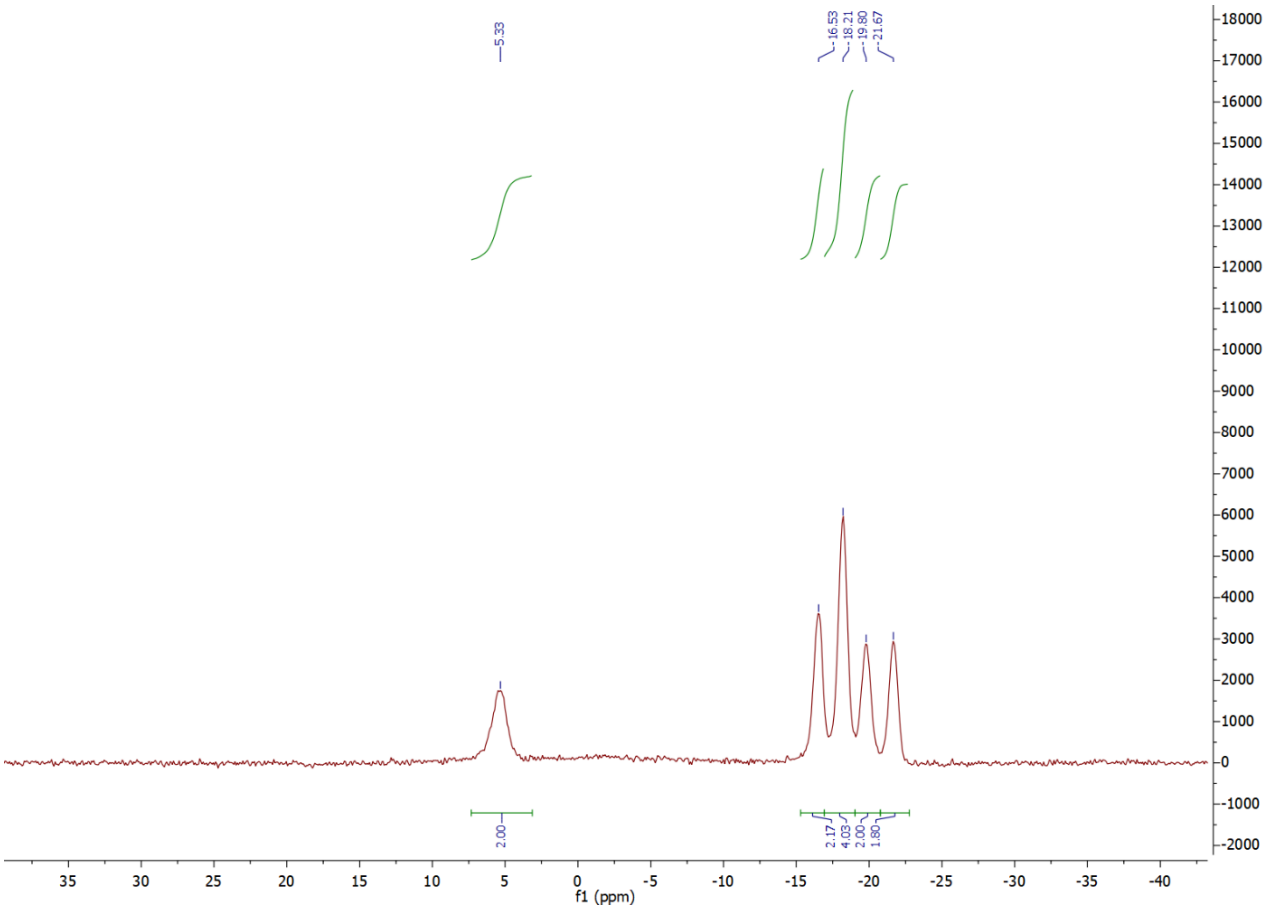


Figure S6. $^{11}B\{^{1}H\}$ NMR spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CC_2H_5]$

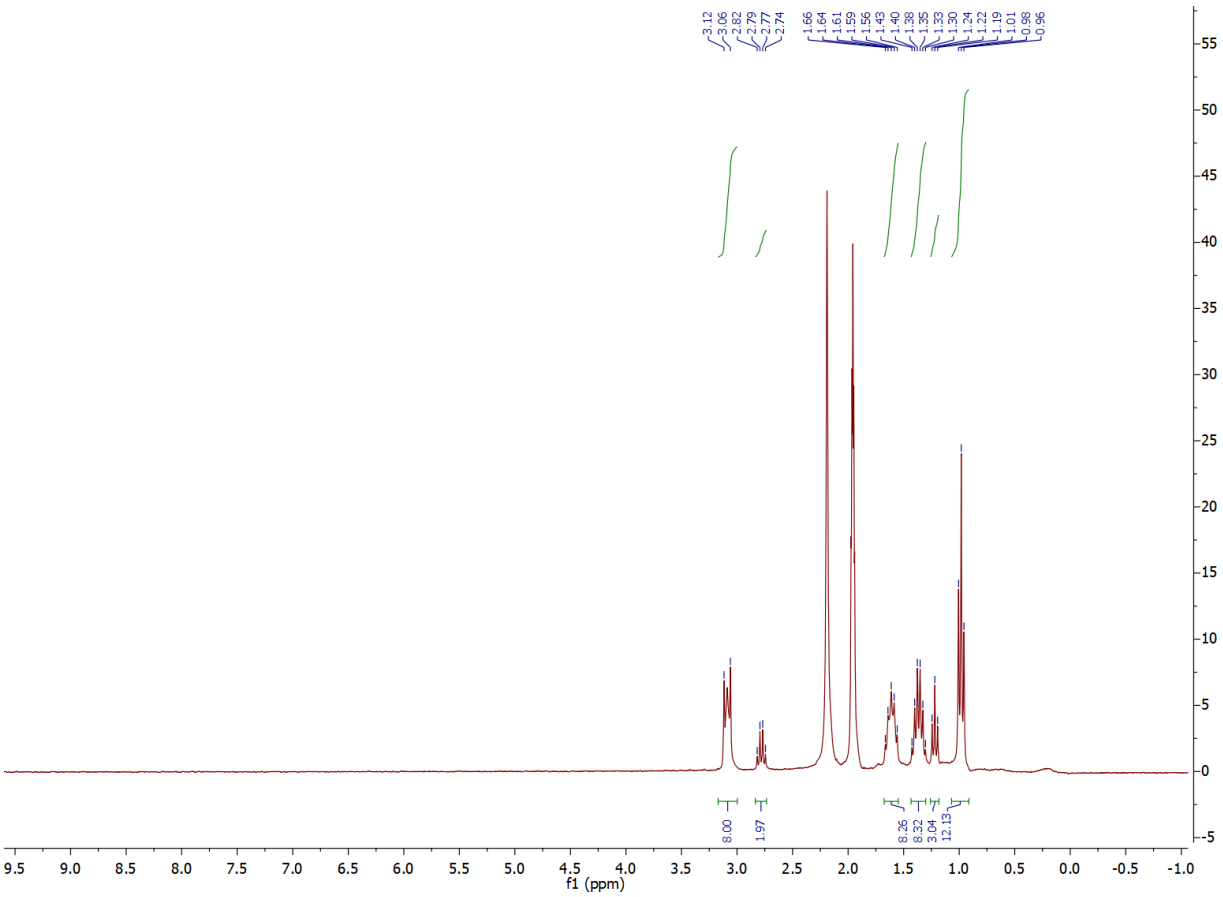


Figure S7. ^{1}H NMR spectrum of ((*n*-C_4H_9)$_4$N)[1,2-$B_{12}H_{10}O_2CC_2H_5$]

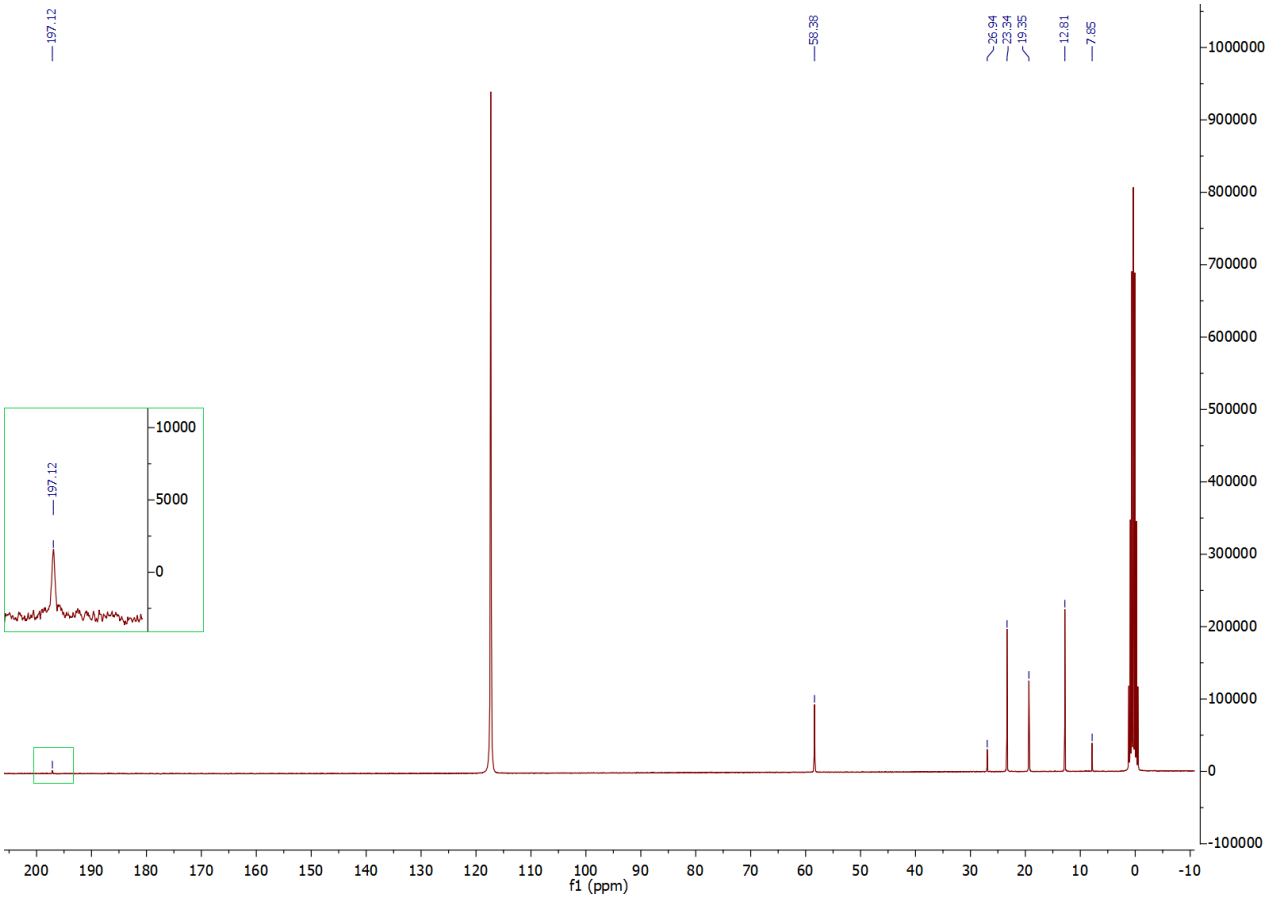


Figure S8. ^{13}C{^{1}H} NMR spectrum of ((*n*-C_4H_9)$_4$N)[1,2-$B_{12}H_{10}O_2CC_2H_5$]

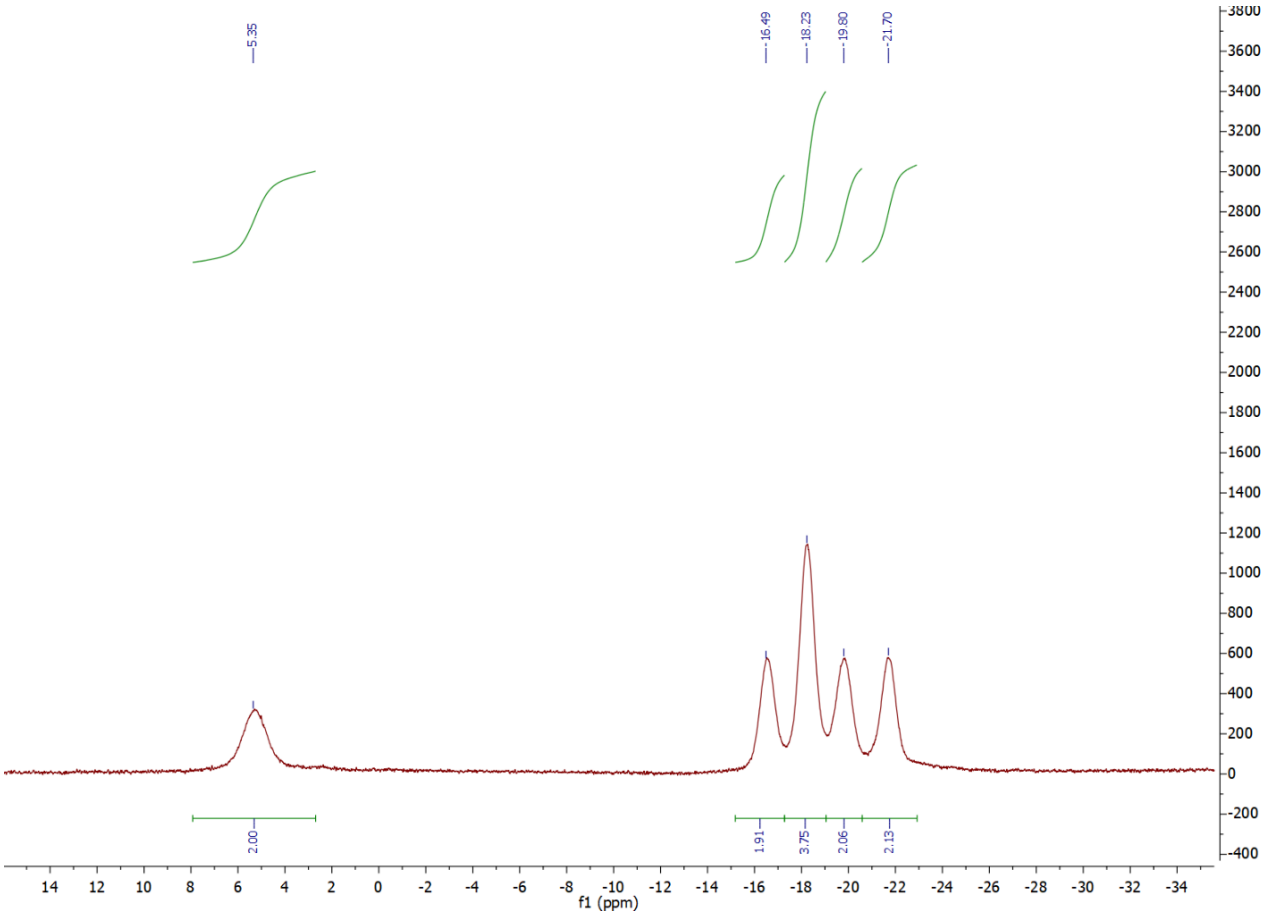


Figure S9. $^{11}B\{^{1}H\}$ NMR spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CC_3H_7]$

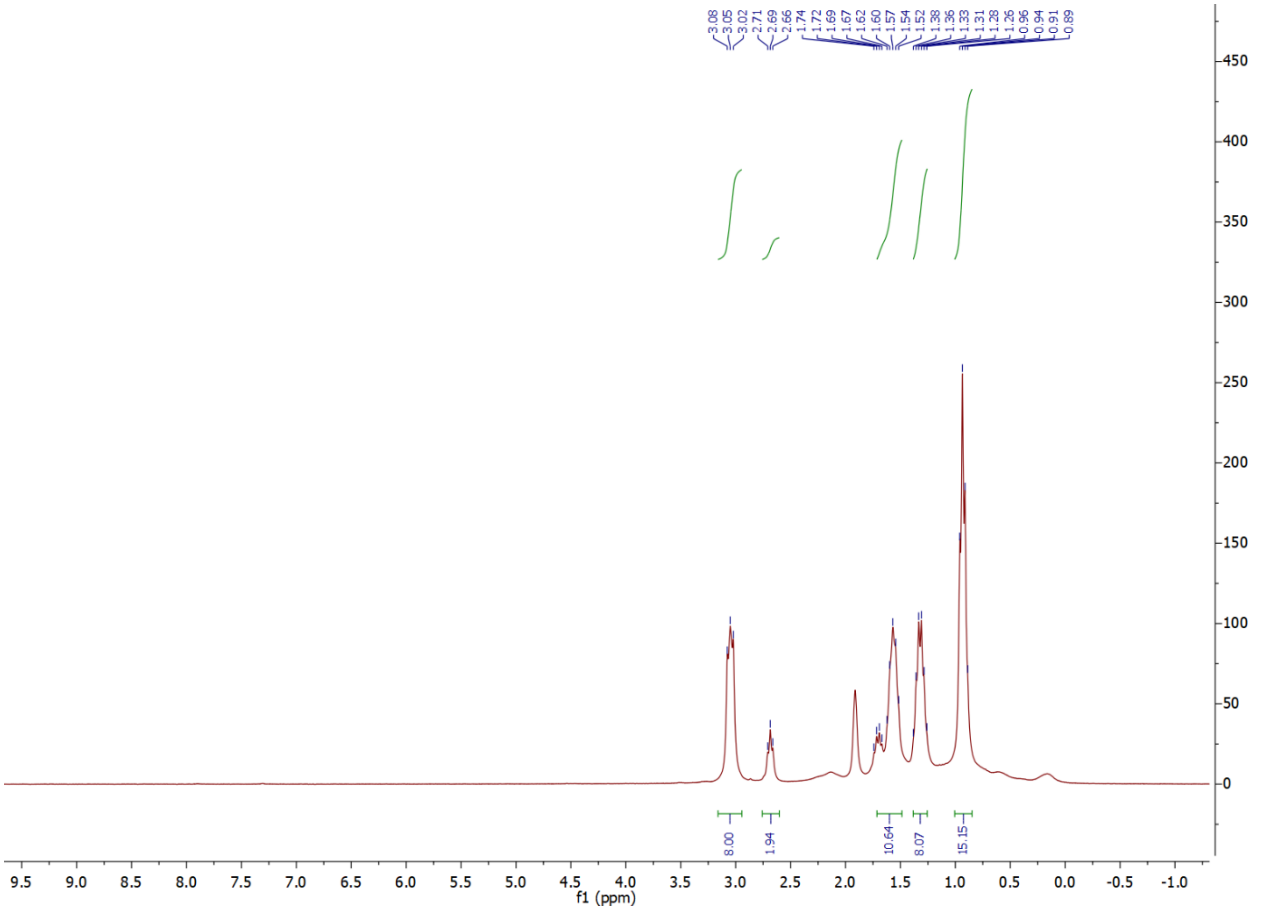


Figure S10. ^{1}H NMR spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CC_3H_7]$

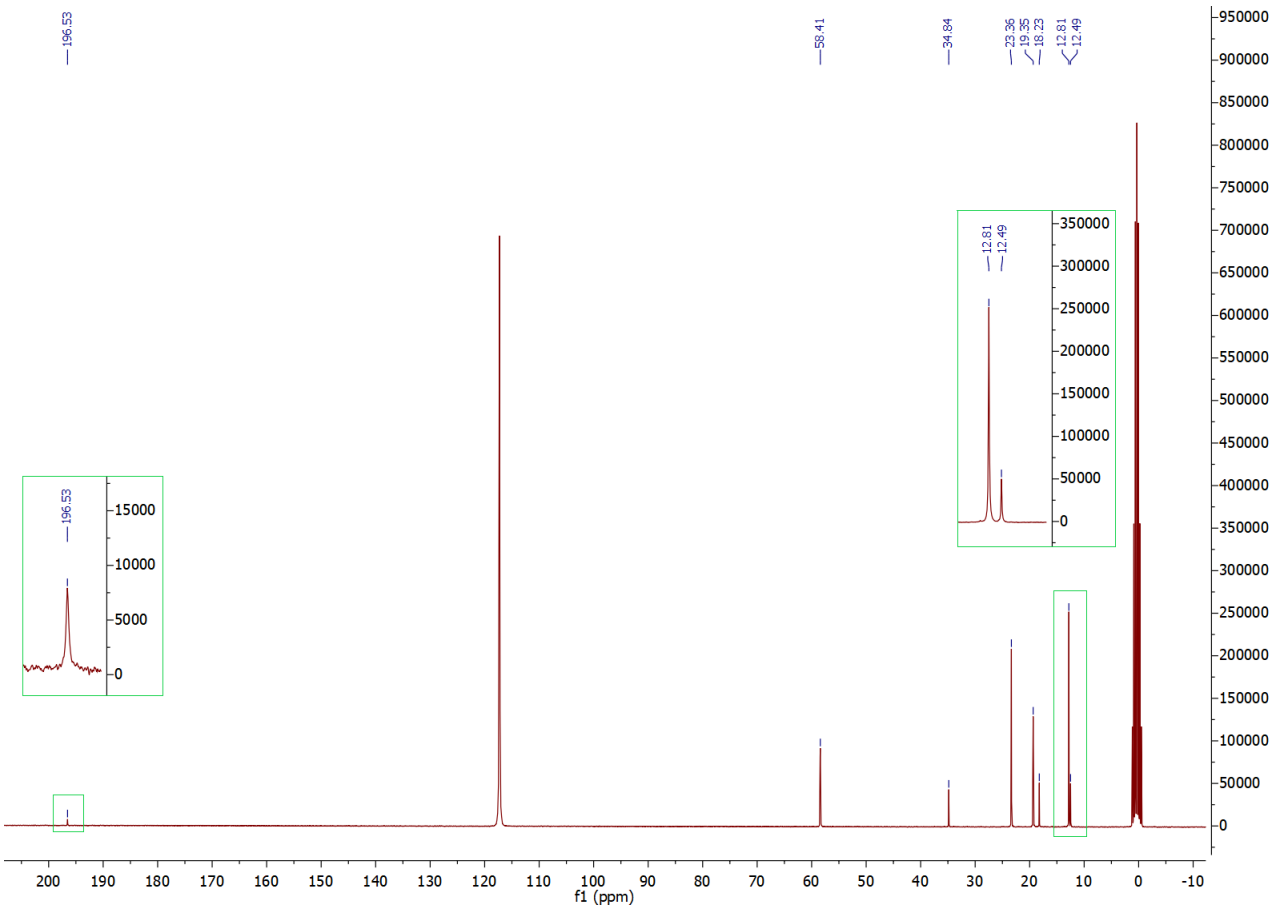


Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CC_3H_7]$

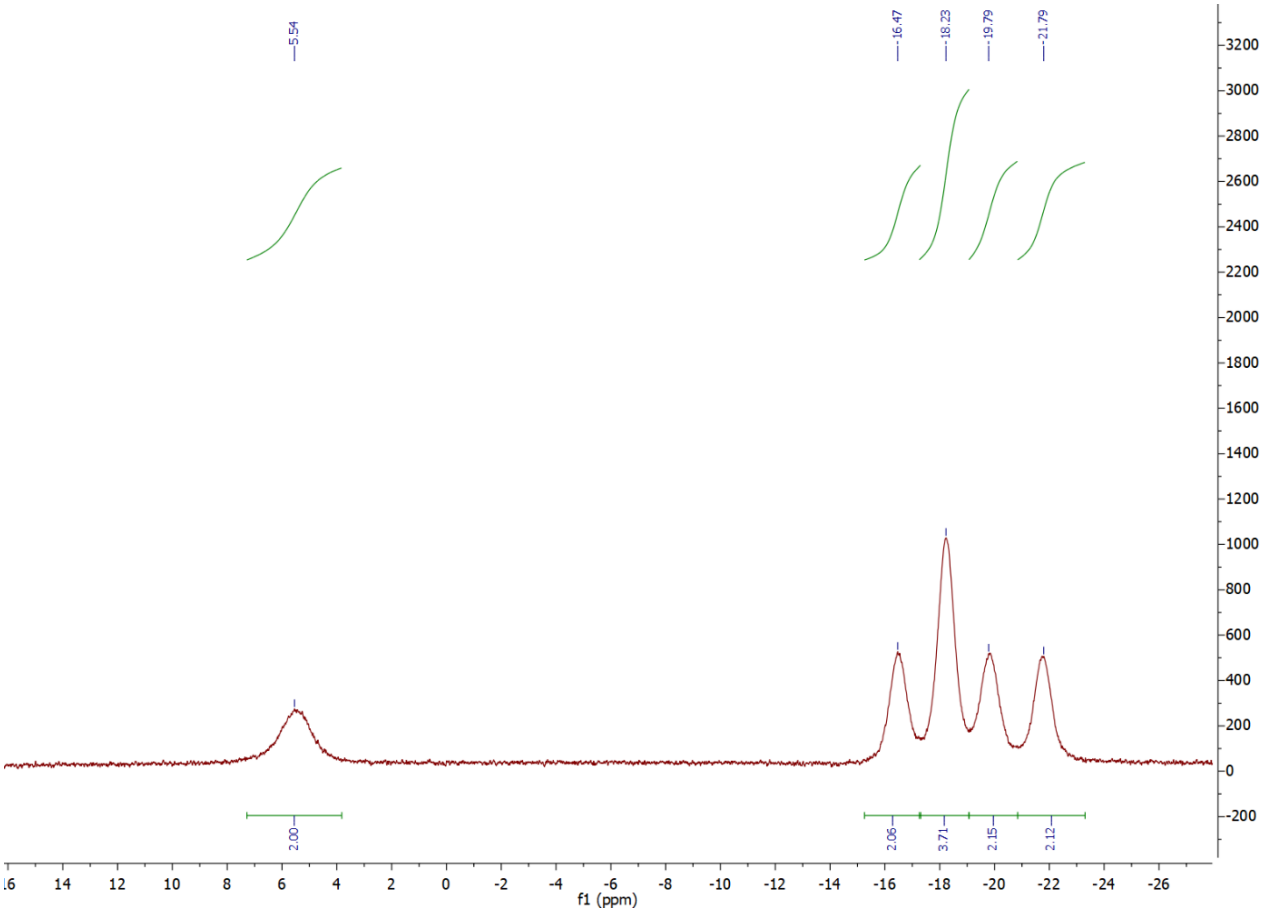


Figure S12. $^{11}B\{^{1}H\}$ NMR spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CC_6H_5]$

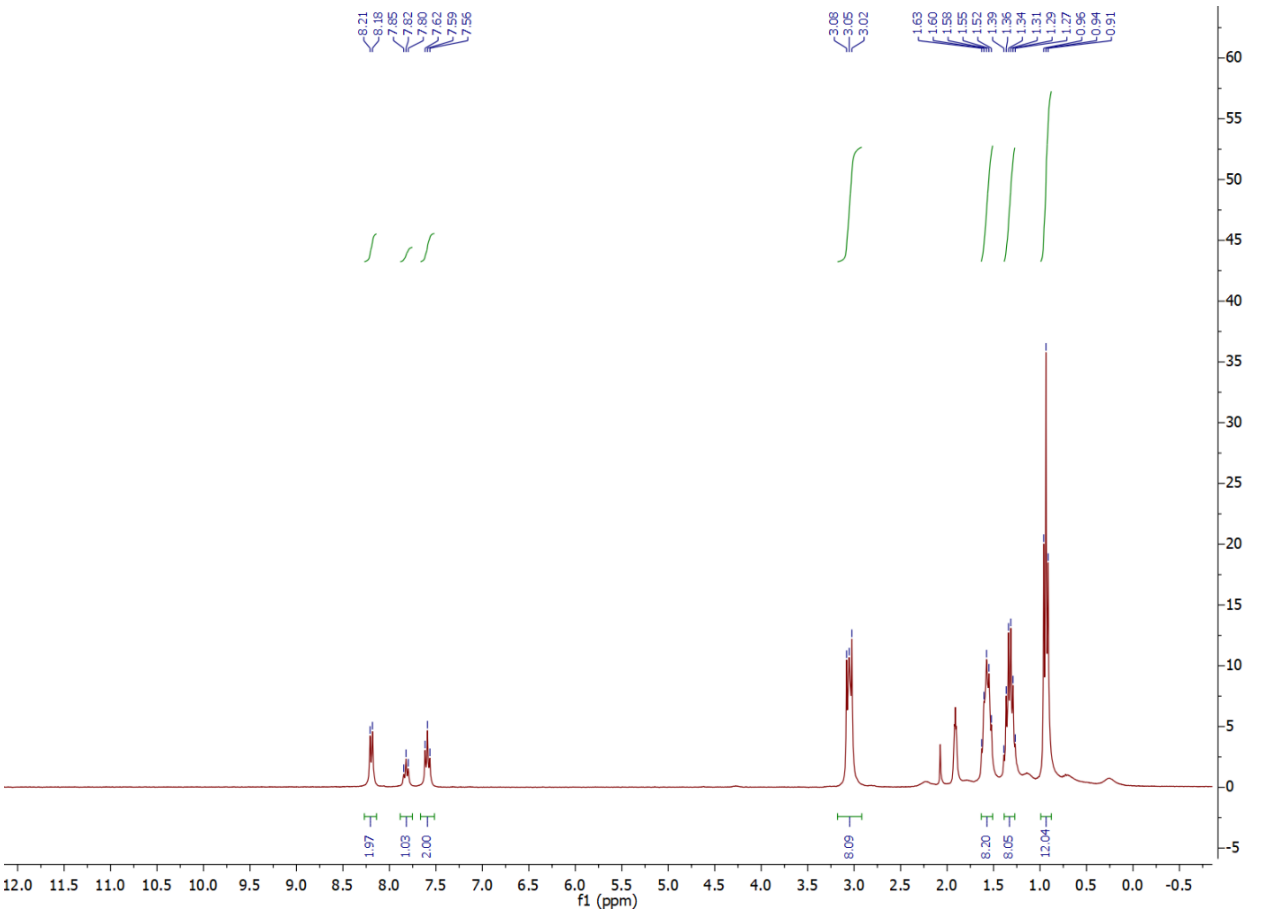


Figure S13. ^{1}H NMR spectrum of ((*n*-C_4H_9)$_4$N)[1,2-$B_{12}H_{10}O_2CC_6H_5$]

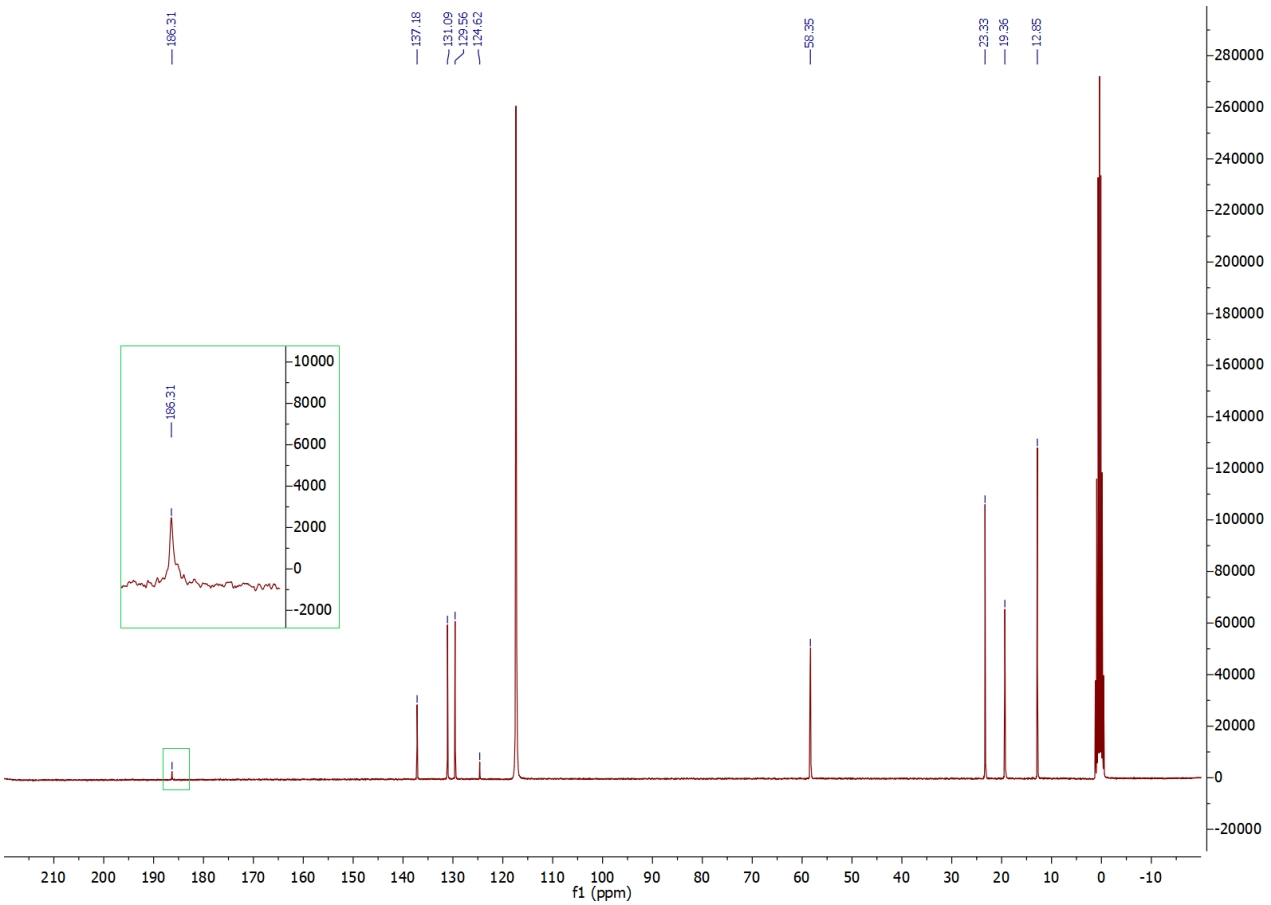


Figure S14. ^{13}C{^{1}H} NMR spectrum of ((*n*-C_4H_9)$_4$N)[1,2-$B_{12}H_{10}O_2CC_6H_5$]

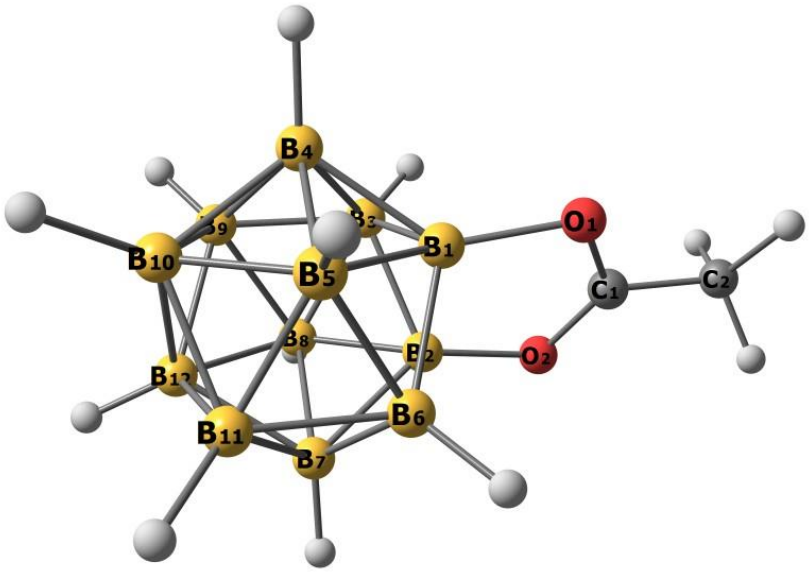
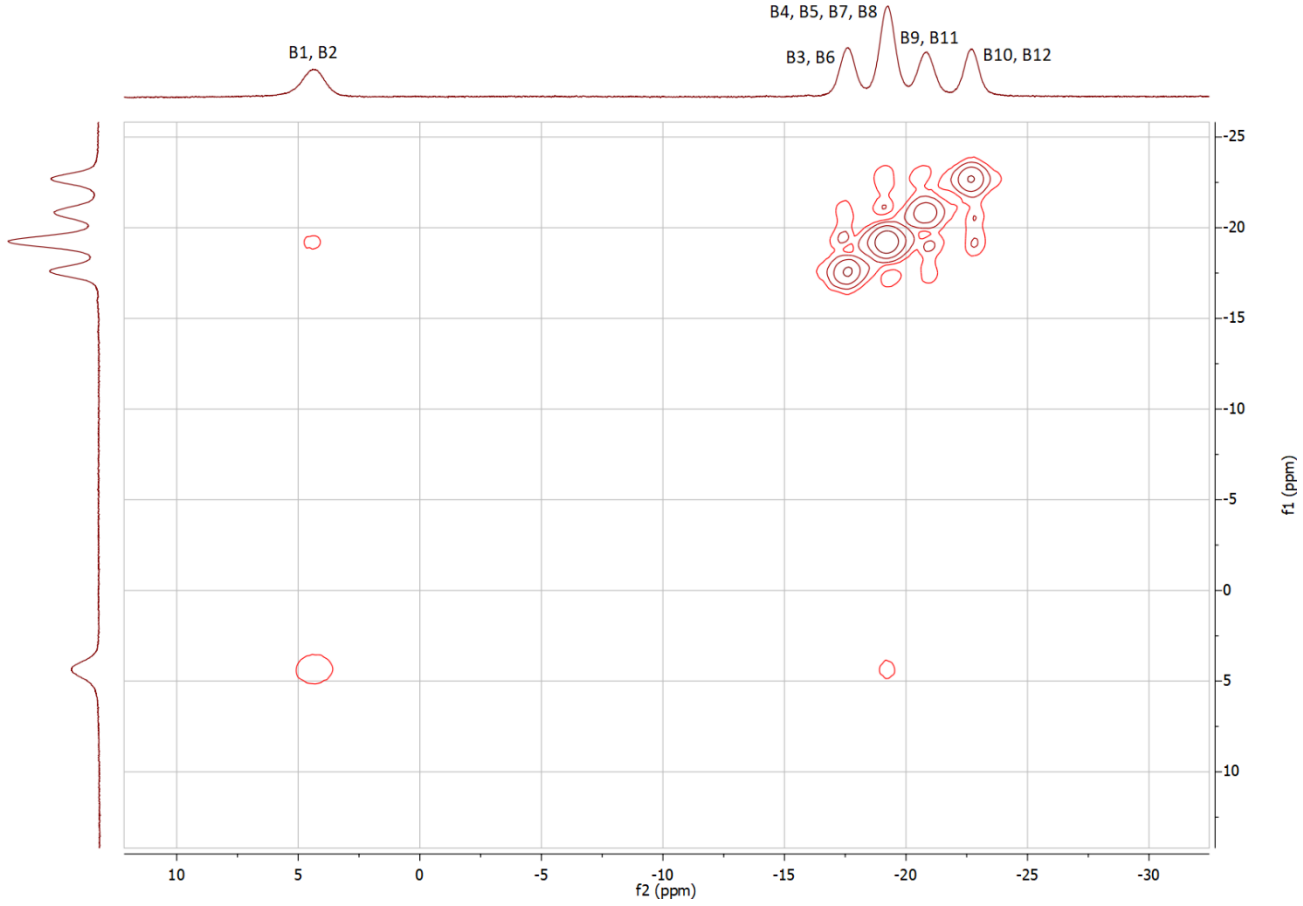


Figure S15. Atom numbering in $[1,2\text{-}B_{12}H_{10}O_2CCH_3]^-$ (for ^{11}B-^{11}B COSY spectrum below)



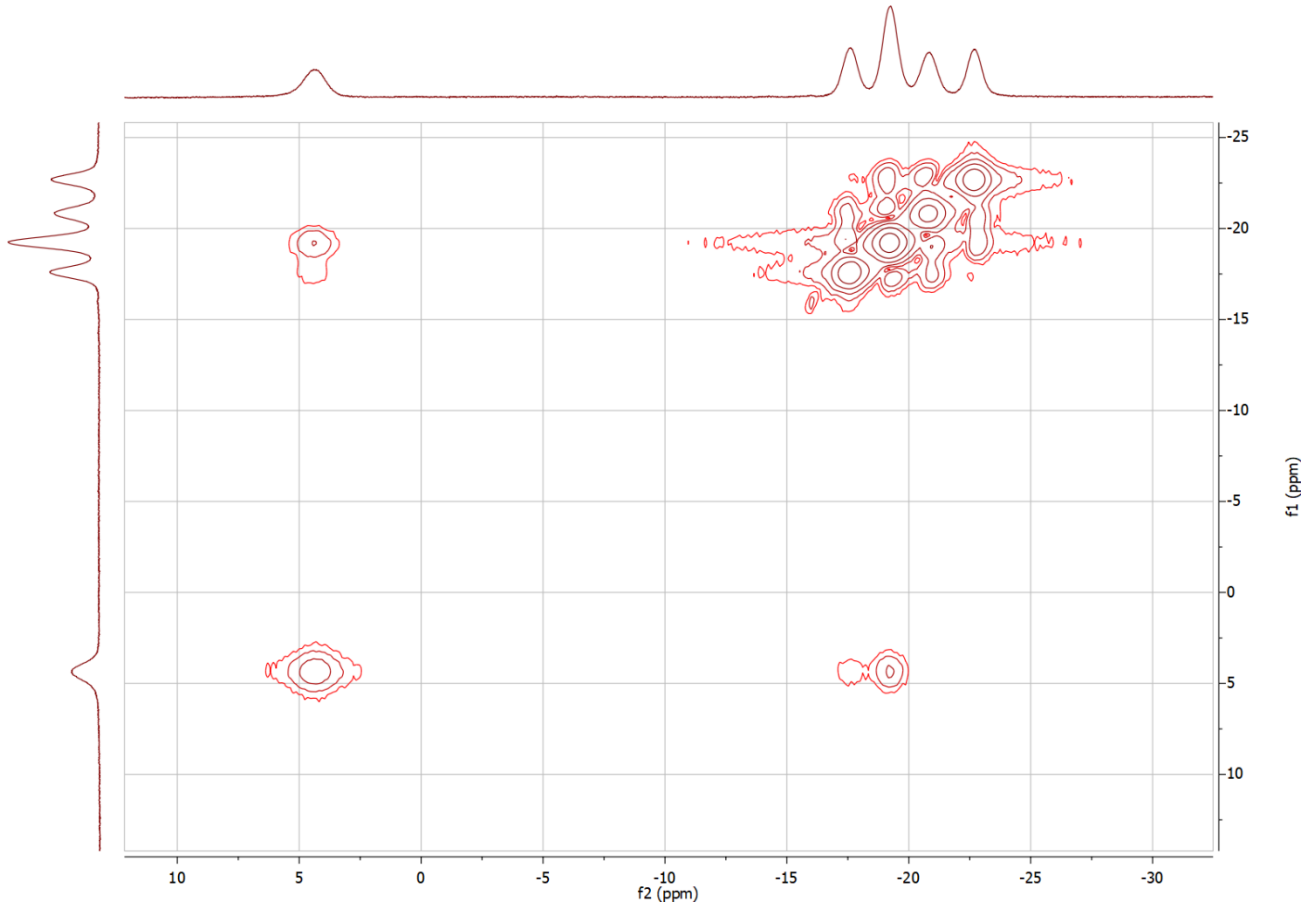


Figure S16. ^{11}B-^{11}B COSY spectrum of $[1,2\text{-}B_{12}H_{10}O_2CCH_3]^-$

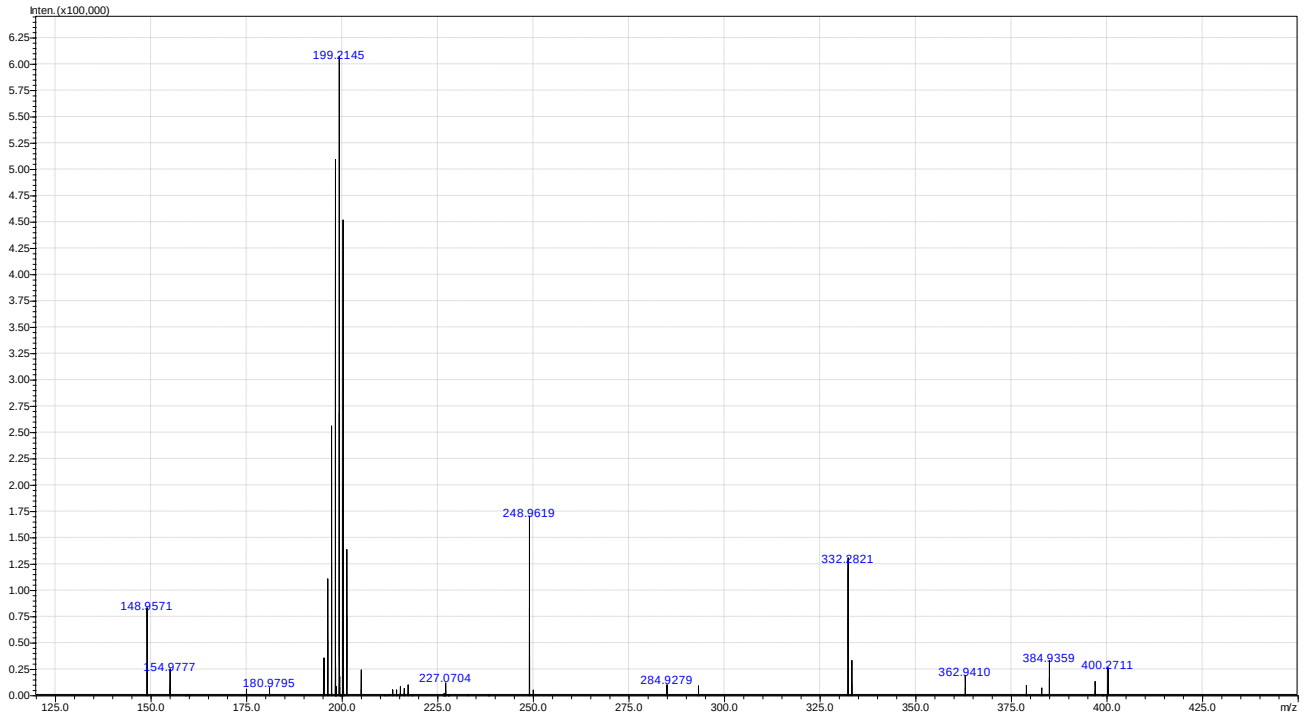


Figure S17. ESI-MS spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CCH_3]$ (negative area)

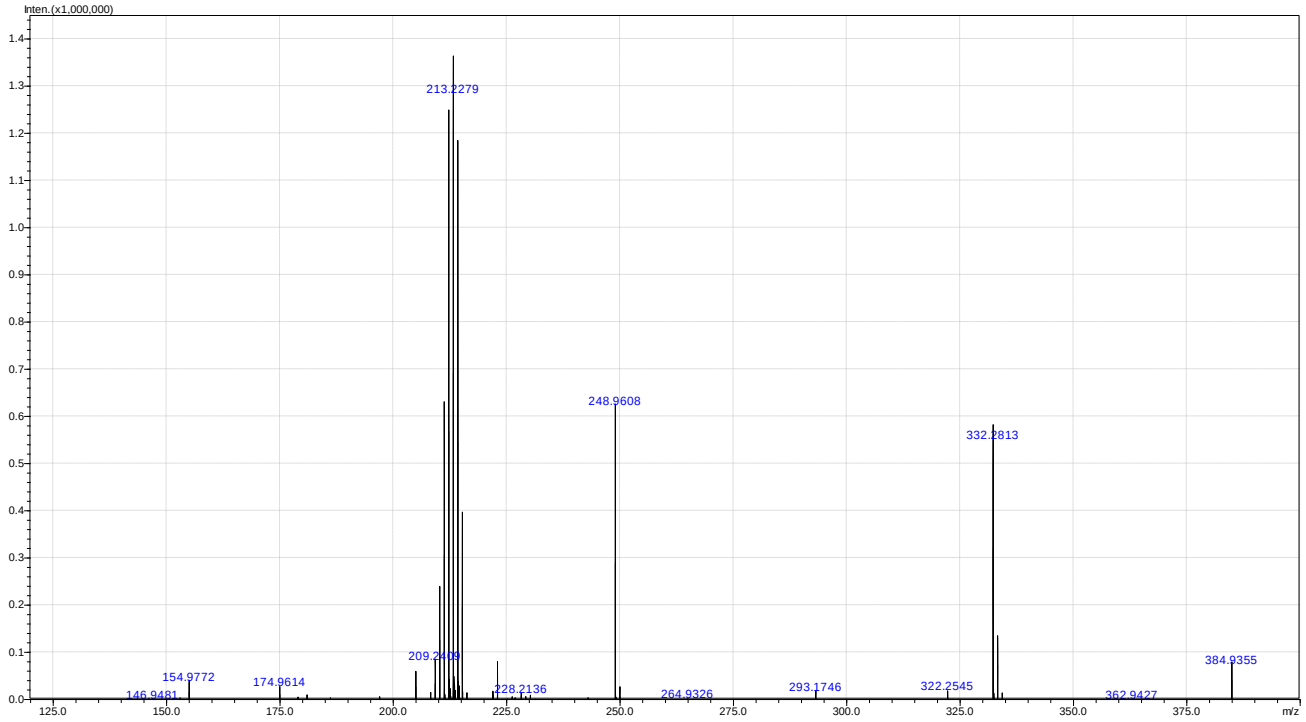


Figure S18. ESI-MS spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CC_2H_5]$ (negative area)

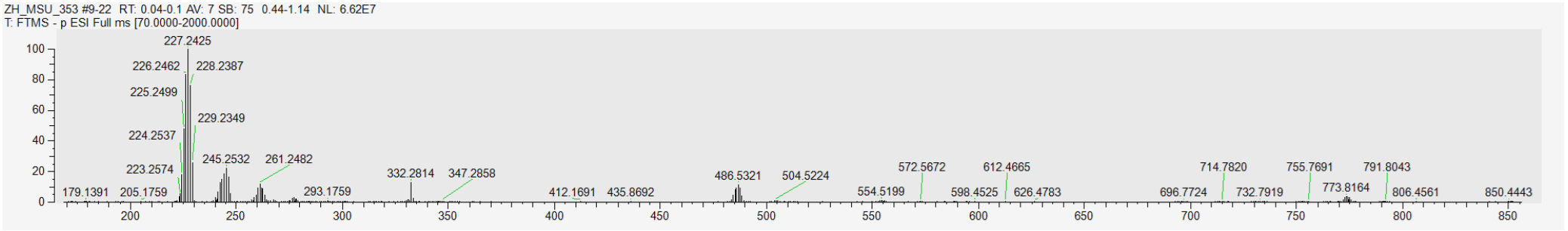


Figure S19. ESI-MS spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CC_3H_7]$ (negative area)

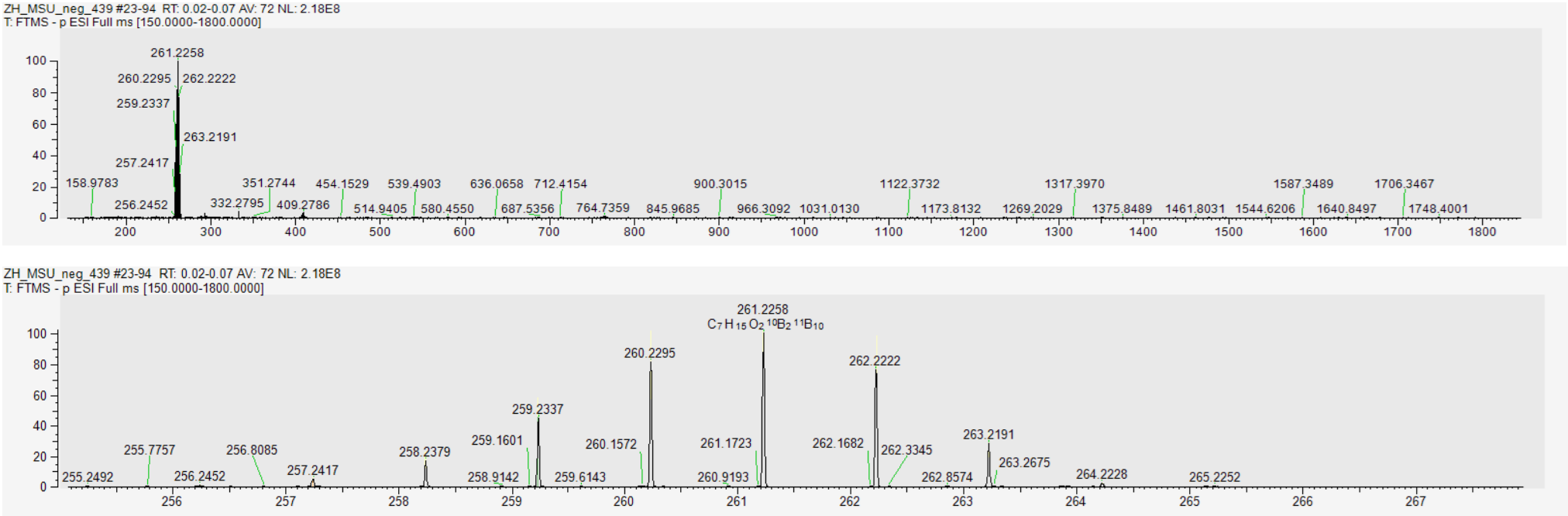


Figure S20. ESI-MS spectrum of $((n\text{-}C_4H_9)_4N)[1,2\text{-}B_{12}H_{10}O_2CC_6H_5]$ (negative area)

Compound	**((*n*-C_4H_9)$_4$N)[1,2-$B_{12}H_{10}O_2CCH_3$]**	**((*n*-C_4H_9)$_4$N)[1,2-$B_{12}H_{10}O_2CC_2H_5$]**
Chemical formula	$C_{18}H_{49}B_{12}NO_2$	$C_{19}H_{51}B_{12}NO_2$
M_r	441.30	455.32
Temperature, K	100.00	100.00
Crystal system	orthorhombic	monoclinic
Space group	Pbca	$P2_1$, n
a, Å	17.10(3)	9.167(6)
b, Å	15.16(4)	21.48(3)
c, Å	22.21(4)	14.716(16)
β, °	90	95.05(4)
V, Å^3	5757(20)	2886(5)
Z	8	4
ρ_{calc}g, cm^3	1.018	1.048
μ, mm^{-1}	0.056	0.419
F(000)	1920.0	992.0
Radiation type	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2Θ range for data collection,	4.032 to 49.996	7.3 to 133.35
Reflections collected	19274	25006
Independent reflections	5050 [R_{int} = 0.0681, R_{sigma} = 0.0791]	5008 [R_{int} = 0.0323, R_{sigma} = 0.0306]
S	1.015	1.904
Final R indexes [I>=2σ (I)]	R_1 = 0.0621, wR_2 = 0.1461	R_1 = 0.1063, wR_2 = 0.3803
Final R indexes [all data]	R_1 = 0.1093, wR_2 = 0.1755	R_1 = 0.1103, wR_2 = 0.3888
Compound	**((*n*-C_4H_9)$_4$N)[1,2-$B_{12}H_{10}O_2CC_3H_7$]**	**((*n*-C_4H_9)$_4$N)[1,2-$B_{12}H_{10}O_2CC_6H_5$]**
Chemical formula	$C_{20}H_{52}B_{12}NO_2$	$C_{23}H_{51}B_{12}NO_2$
M_r	468.34	503.36
Temperature, K	100.00	100.00
Crystal system	monoclinic	monoclinic
Space group	$P2_1$, n	$P2_1$, c
a, Å	9.3412(9)	17.052(6)
b, Å	21.8620(17)	11.397(2)
c, Å	14.5823(15)	16.762(4)
β, °	95.341(4)	107.565(14)
V, Å^3	2965.0(5)	3105.9(15)
Z	4	4
ρ_{calc}g, cm^3	1.049	1.076
μ, mm^{-1}	0.058	0.059
F(000)	1020.0	1088.0
Radiation type	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection,	3.368 to 49.988	4.364 to 55.998
Reflections collected	23942	28719
Independent reflections	5196 [R_{int} = 0.0571, R_{sigma} = 0.0461]	7490 [R_{int} = 0.0356, R_{sigma} = 0.0358]
S	1.025	1.116
Final R indexes [I>=2σ (I)]	R_1 = 0.1037, wR_2 = 0.2612	R_1 = 0.0523, wR_2 = 0.1218
Final R indexes [all data]	R_1 = 0.1382, wR_2 = 0.2904	R_1 = 0.0637, wR_2 = 0.1270

Table S1. Crystal data and structure refinement for all compounds studied

Despite the good quality of the experiment for the structures of ((*n*-$C_4H_9)_4N$)[1,2-$B_{12}H_{10}O_2CC_2H_5$] and ((*n*-$C_4H_9)_4N$)[1,2-$B_{12}H_{10}O_2CC_3H_7$], their R1 was 10.6% and 10.4%, respectively, and for the structure of ((*n*-$C_4H_9)_4N$)[1,2-$B_{12}H_{10}O_2CC_2H_5$] GOOF was 1.904. The high value of these parameters was due to the high degree of disorder of *closo*-borate anions (See SI for more details) and tetrabutylammonium cations. Despite the high values of R1 and GOOF parameters, the structural models of these compounds were undoubtedly correct.

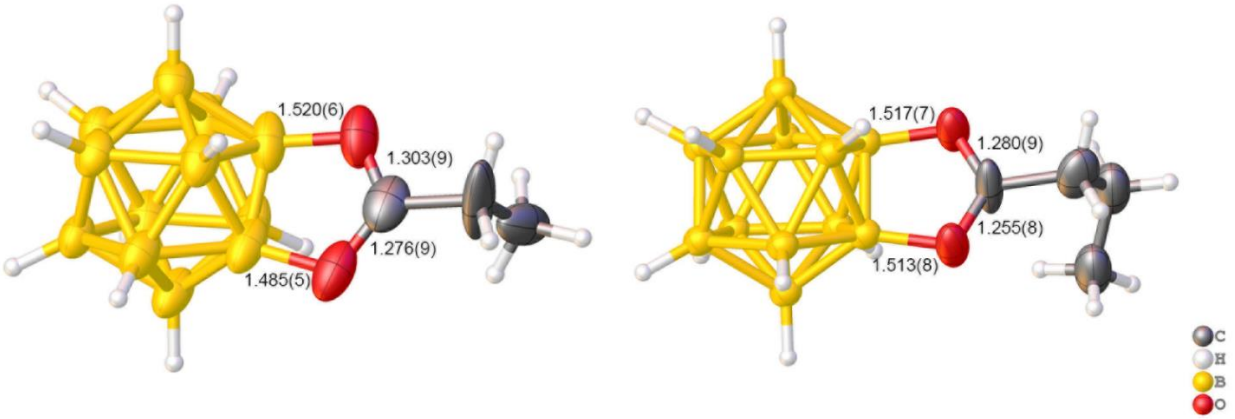


Figure S21. X-ray structures of [1,2-$B_{12}H_{10}O_2CC_2H_5$]$^-$ (left) and [1,2-$B_{12}H_{10}O_2CC_3H_7$]$^-$ (right). Length units – Å

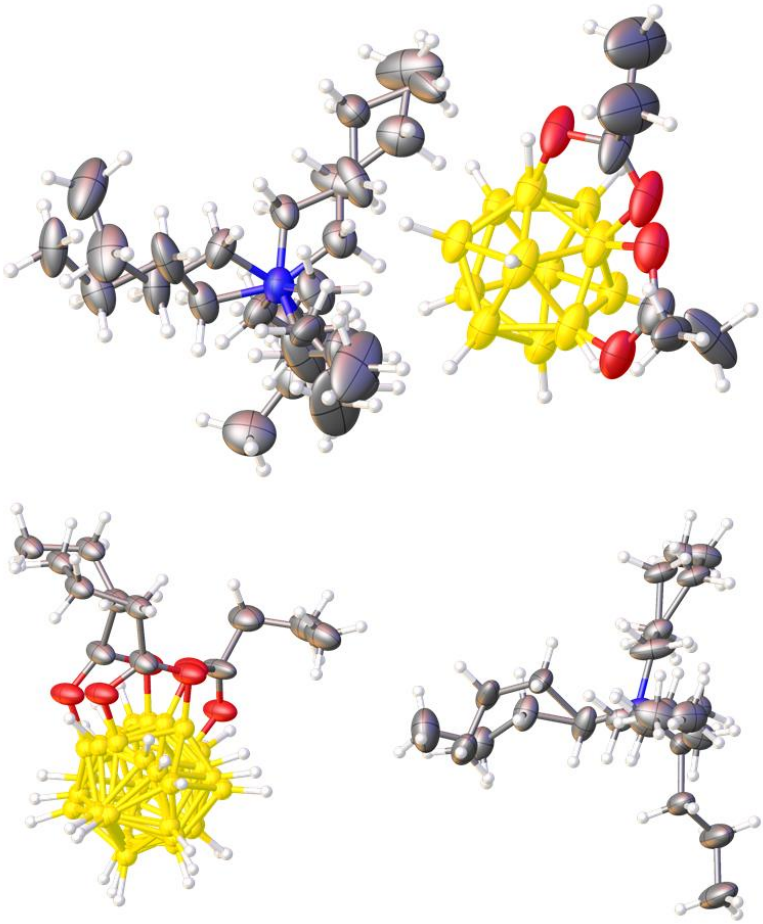


Figure S22. Disorder in the structures of ((*n*-$C_4H_9)_4N$)[1,2-$B_{12}H_{10}O_2CC_2H_5$] (top) and ((*n*-$C_4H_9)_4N$)[1,2-$B_{12}H_{10}O_2CC_3H_7$] (bottom). The thermal ellipsoids are shown at 50% probability level

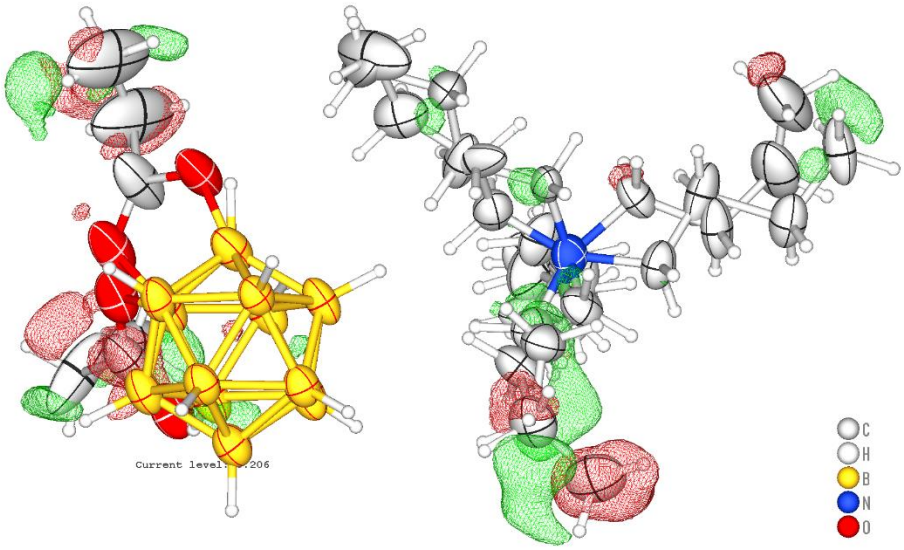


Figure S23. Residual density plot in the structure of ((*n*-C_4H_9)$_4$N)[1,2-$B_{12}H_{10}O_2CC_2H_5$]

2. Computational data

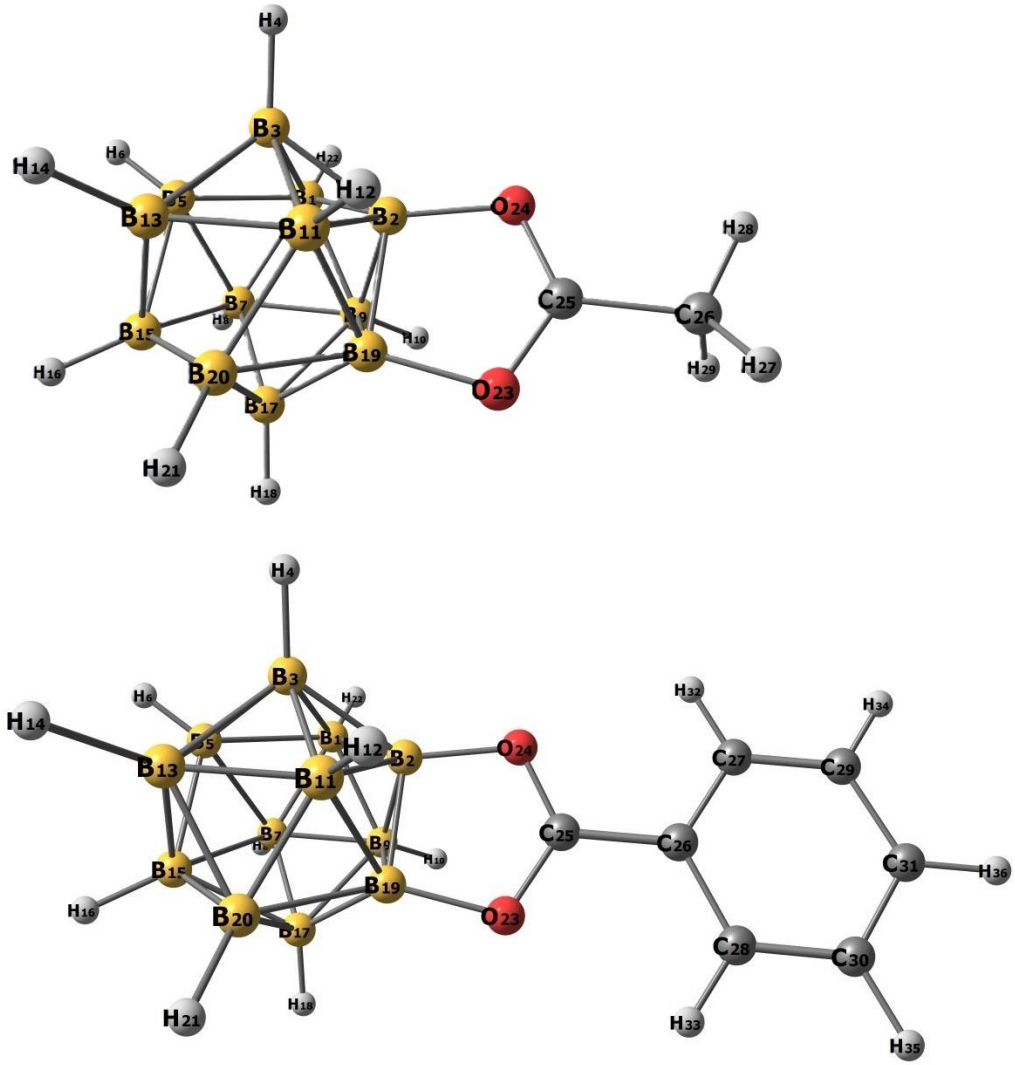


Figure S24. Automatically generated (using ChemCraft software) atom numbering in [1,2-$B_{12}H_{10}O_2CR$]$^-$ (for **Tables S2, S3, S6** and **S7** below)

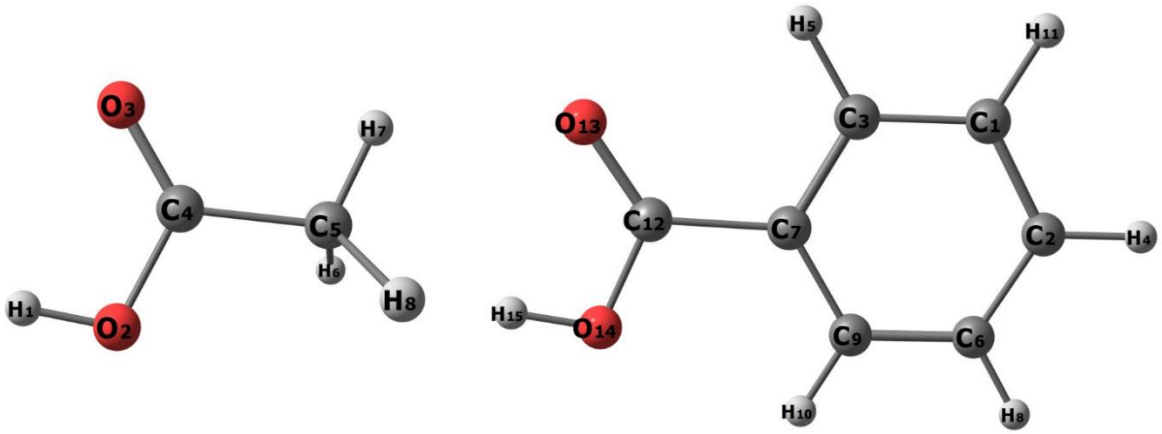


Figure S25. Automatically generated (using ChemCraft software) atom numbering in RCOOH (for **Tables S2, S3, S6** and **S7** below)

Bond type	Mayer BO	FBO
CH_3COOH		
C4–O3	2.059	2.038
C4–O2	1.169	1.376
C_6H_5COOH		
C12–O13	2.041	2.002
C12–O14	1.205	1.364
$[1,2\text{-}B_{12}H_{10}O_2CCH_3]^-$		
C25–O24	1.410	1.584
C25–O23	1.420	1.589
B2–O24	0.638	0.850
B19–O23	0.648	0.853
$[1,2\text{-}B_{12}H_{10}O_2CC_6H_5]^-$		
C25–O24	1.336	1.563
C25–O23	1.339	1.565
B2–O24	0.633	0.847
B19–O23	0.634	0.850

Table S2. The bond order (BO) values for selected bonds in RCOOH and $[1,2\text{-}B_{12}H_{10}O_2CR]^-$

CH_3COOH		**C_6H_5COOH**		**$[1,2\text{-}B_{12}H_{10}O_2CCH_3]^-$**		**$[1,2\text{-}B_{12}H_{10}O_2CC_6H_5]^-$**	
C4	0.218	C12	0.210	C25	0.274	C25	0.265
O3	–0.289	O13	–0.282	O24	–0.101	O24	–0.091
O2	–0.180	O14	–0.168	O23	–0.099	O23	–0.092

Table S3. The Hirshfeld charges for RCOOH and $[1,2\text{-}B_{12}H_{10}O_2CR]^-$

Model structure	NICS(0)	NICS(1)
[1,2-$B_{12}H_{10}O_2CCH_3$]$^-$	–4.469	–4.234
[1,2-$B_{12}H_{10}O_2CC_6H_5$]$^-$	–3.943	–4.118

Table S4. NICS(0) and NICS(1) values of [1,2-$B_{12}H_{10}O_2CR$]$^-$ in ppm (ωB97X-D3/def2-TZVPP level of theory)

Analysis of molecular orbitals.

MO analysis can be a useful, and visual, approach for understanding the structural features of borylated organic heterocycles. The canonical molecular orbitals of [1,2-$B_{12}H_{10}O_2CR$]$^-$ were considered. Orbital composition analysis was carried out using the Mulliken and Stout-Politzer partitions. Orbitals were selected based on cross-term values between two molecular fragments, (the values reflecting the contribution to chemical bonding between the fragments). In the compounds studied, as in the classical examples of carboxonium ions, an empty p-orbital of carbon overlapped with an oxygen electron pair. The orbitals corresponding to this interaction were the HOMO-23, HOMO-16 of [1,2-$B_{12}H_{10}O_2CCH_3$]$^-$ and the HOMO-30, HOMO-22 of [1,2-$B_{12}H_{10}O_2CC_6H_5$]$^-$. In addition, the interactions between the R substituents and O_2C-fragments were also observed. The HOMO-23 consisted of 37% oxygen p-orbitals (the sum of O1 and O2), 25% the p-orbital of C1, 14% the p-orbital of C2 and 9% the s-orbitals of three hydrogen atoms of the substituent (**Figure 2**). The HOMO-30 consisted of 47% oxygen p-orbitals (the sum of O1 and O2), 27% the p-orbital of C1 and 4% the p-orbital of C2. The remaining carbon atoms of the benzene ring contributed no more than 1% to this MO. The HOMO-23 and HOMO-30 had a bonding character for the interactions between the R substituents and O_2C-fragments. The cross-term values were equal to 7.9% (HOMO-23) and 4.4% (HOMO-30).

The HOMO-16 and HOMO-22 also contained the delocalised π-system of the O_2C-fragment, but the interaction with the R substituent had an antibonding character (**Figure 3**). The corresponding cross-values were equal to –4.9% (HOMO-16) and –1.6% (HOMO-22). In addition, interaction with the boron cage, which also had an antibonding character, was observed. In this case, the cross-term values were –8.7% (HOMO-16) and –6.7% (HOMO-22). The composition of the HOMO-16 was as follows: 17% p-orbitals of oxygen (the sum of O1 and O2), 6% the p-orbital of C1, 8% the p-orbital of C2 and 8% the s-orbitals of three hydrogen atoms. The B-H cluster fragments (consisting of only s-orbitals) contributed to this MO of 46%, (the sum of B3(7%)-H(4%), B6(7%)-H(4%) and B9(8%)-H(4%), B11(8%)-H(4%)). The HOMO-22 consisted of 9% oxygen p-orbitals (the sum of O1 and O2), 5% the p-orbital of C1 and 28% the p-orbitals from the C2-C7 atoms of the benzene ring (C2(1%), C3+C7(7%), C4+C6(13%) and C5(7%)). The contribution of the B-H fragments was close to the corresponding values for the HOMO-16 and differed by approximately 1% for all atoms.

The next MOs considered were formed by sigma overlaps between orbitals of the *exo*-polyhedral substituent and cluster. The HOMO-29 and HOMO-37 had a bonding character for the $B_{12}H_{10}$-O_2C interaction (**Figure 4**). The cross-term values were equal to 8.0% (HOMO-29) and 3.4% (HOMO-37). These MOs included overlaps between the p-orbitals of O1, O2, the s-orbital of C1 and sp-hybrids of the B1, B2 atoms. For the HOMO-29, the composition was as follows: 35% corresponding to the sum of O1

and O2, 13% C1 and 10% the sum of B1 and B2. For the HOMO-37, there was a reduction in the contributions of the atoms in the B_2O_2C-fragment. The values were equal to 16% (O1+O2), 5% (C1) and 5% (B1+B2). It may be concluded that this type of MO is beneficial for the $B_{12}H_{10}$-O_2C interaction only in the case of $[1,2\text{-}B_{12}H_{10}O_2CCH_3]^-$.

The most beneficial MOs for the $B_{12}H_{10}$-O_2C interaction were the HOMO-28 and HOMO-36 (**Figure 5**). These MOs had the largest cross-term values among all MOs (10.8% for the HOMO-28 and 8.9% for the HOMO-36). More cluster atoms were involved in the interaction and the C1 overlapped, with its p-orbital, with O1, O2. For the boron atoms, atomic s-orbitals of the unsubstituted positions and sp-hybrids (with a predominance of s-orbital) of the B1, B2 positions were involved. The HOMO-28 consisted of 34% oxygen (the sum of O1 and O2), 9% C1, 14% the substituted positions (the sum of B1 and B2) and 26% the unsubstituted positions (the sum of B4, B5, B7 and B8). In the case of the HOMO-36, the contribution of the O_2C-fragment decreased, while the contribution of B4, B5, B7 and B8 increased slightly. The corresponding values were equal to 27% (O1, O2), 7% (C1) and 29% (B4, B5, B7 and B8). The B1, B2 contribution remained the same as for the HOMO-28. The HOMO-25 and HOMO-32 were also the bonding MO for the $B_{12}H_{10}$-O_2C interaction (**Figure 5**). In this case, the B1, B2 positions overlapped by sp-hybrids, but with a predominance of the p-orbital. For the unsubstituted boron atoms, atomic s-orbitals of the B4, B5, B7 and B8, and sp-hybrids (with a predominance of s-orbital) of the B10, B12 positions, were involved. The cross-term values of these MO were equal to 3.4% (HOMO-25) and 4.1% (HOMO-32). The HOMO-25 was composed of 27% (the sum of O1, O2), 8% (C1), 40% (the sum of B1, B2 and B4, B5, B7, B8) and 9% (the sum of B10, B12). For the HOMO-32, the oxygen contribution increased to 29%, while the contribution of C1 remained the same. The boron contribution slightly decreased to 36% (for the B1, B2 and the B4, B5, B7, B8) and 8% (for the B10, B12).

Model structure	Type of interaction	№ Orbital	Cross-term value, %
[1,2-$B_{12}H_{10}O_2CCH_3$]$^-$	$O_2C–CH_3$	HOMO-23	7.9
		HOMO-16	–4.9
	$B_{12}H_{10}–O_2CCH_3$	HOMO-29	8.0
		HOMO-28	10.8
		HOMO-25	3.4
		HOMO-16	–8.7
[1,2-$B_{12}H_{10}O_2CC_6H_5$]$^-$	$O_2C–C_6H_5$	HOMO-30	4.4
		HOMO-22	–1.6
	$B_{12}H_{10}–O_2CC_6H_5$	HOMO-37	3.4
		HOMO-36	8.9
		HOMO-32	4.1
		HOMO-22	–6.7

Table S5. The cross-term values of selected occupied orbitals in [1,2-$B_{12}H_{10}O_2CR$]$^-$

Model structure	№ Orbital	Approach	№ Atom	Shell Type	Contribution, %
[1,2-$B_{12}H_{10}O_2CCH_3$]$^-$	HOMO-29	Mulliken	2B	S	1.58
			2B	S	4.88
			2B	S	–2.95
			2B	P	1.08
			2B	P	1.16
			5B	S	1.08
			5B	S	1.64
			7B	S	0.70
			7B	S	1.45
			7B	S	–0.72
			9B	P	0.57
			11B	P	0.57
			13B	S	0.70
			13B	S	1.51
			13B	S	–0.83
			15B	S	1.08
			15B	S	1.67
			19B	S	1.54
			19B	S	4.67
			19B	S	–2.84
			19B	P	1.06

			19B	P	1.02
			23O	S	0.72
			23O	S	1.33
			23O	S	0.85
			23O	P	6.04
			23O	P	6.62
			23O	P	1.75
			24O	S	0.75
			24O	S	1.38
			24O	S	0.86
			24O	P	6.30
			24O	P	6.90
			24O	P	1.77
			25C	S	7.03
			25C	S	6.35
			26C	S	3.22
			26C	S	4.65
			26C	S	0.88
			26C	P	2.65
			26C	P	1.68
			26C	P	0.60
			27H	S	1.02
			27H	S	2.01
			28H	S	1.00
			28H	S	2.12
			29H	S	1.02
			29H	S	1.91
	HOMO-29	Stout-Politzer	1B	S	0.57
			2B	S	0.90
			2B	S	8.66
			2B	S	–6.94
			2B	P	1.08
			2B	P	1.68
			3B	S	0.56
			5B	S	1.11
			5B	S	1.96
			7B	S	0.64
			7B	S	1.99
			7B	S	–0.70
			9B	S	0.76

			11B	S	0.71
			13B	S	0.64
			13B	S	2.13
			13B	S	–0.95
			15B	S	1.13
			15B	S	2.03
			17B	S	0.62
			19B	S	0.84
			19B	S	8.25
			19B	S	–6.69
			19B	P	1.05
			19B	P	1.39
			20B	S	0.57
			23O	S	0.81
			23O	S	3.01
			23O	S	1.79
			23O	P	6.28
			23O	P	5.40
			24O	S	0.83
			24O	S	3.10
			24O	S	1.76
			24O	P	6.60
			24O	P	5.73
			25C	S	0.85
			25C	S	5.23
			25C	S	3.66
			26C	S	4.29
			26C	S	8.62
			26C	S	0.67
			26C	P	2.64
			26C	P	0.65
			27H	S	0.77
			27H	S	2.01
			28H	S	0.71
			28H	S	2.17
			29H	S	0.88
			29H	S	2.01
	HOMO-28	Mulliken	1B	S	2.08
			1B	S	4.32
			1B	S	–1.26

			2B	S	3.70
			2B	S	4.82
			2B	S	–4.67
			2B	P	0.76
			2B	P	1.93
			3B	S	2.07
			3B	S	4.39
			3B	S	–1.25
			5B	S	0.56
			5B	S	0.76
			5B	P	0.57
			7B	P	0.74
			9B	P	0.76
			9B	P	1.42
			11B	P	0.76
			11B	P	1.43
			13B	P	0.74
			15B	S	0.55
			15B	S	0.74
			15B	P	0.56
			17B	S	2.09
			17B	S	4.38
			17B	S	–1.14
			19B	S	3.74
			19B	S	4.95
			19B	S	–4.83
			19B	P	0.79
			19B	P	1.89
			20B	S	2.08
			20B	S	4.37
			20B	S	–1.10
			23O	P	6.82
			23O	P	7.31
			23O	P	2.00
			24O	P	6.67
			24O	P	7.13
			24O	P	2.07
			25C	P	6.18
			25C	P	3.03
			26C	P	0.64
			26C	P	0.70

	HOMO-28	Stout-Politzer	1B	S	2.14
			1B	S	6.23
			1B	S	–1.02
			2B	S	4.81
			2B	S	7.48
			2B	S	–8.57
			2B	P	0.60
			2B	P	2.07
			3B	S	2.09
			3B	S	6.35
			3B	S	–0.98
			5B	S	0.57
			9B	P	0.60
			9B	P	0.81
			11B	P	0.59
			11B	P	0.83
			15B	S	0.54
			17B	S	2.12
			17B	S	6.35
			17B	S	–0.82
			19B	S	4.86
			19B	S	7.79
			19B	S	–9.10
			19B	P	0.64
			19B	P	2.18
			20B	S	2.12
			20B	S	6.37
			20B	S	–0.79
			23O	S	0.83
			23O	P	7.64
			23O	P	7.75
			23O	P	1.06
			24O	S	0.84
			24O	P	7.47
			24O	P	7.50
			24O	P	1.12
			25C	P	7.40
			25C	P	1.73
			26C	P	0.74
			26C	P	0.52

	HOMO-25	Mulliken	1B	S	2.97
			1B	S	4.76
			1B	S	–2.17
			1B	P	0.51
			1B	P	0.52
			2B	S	1.98
			2B	P	2.67
			2B	P	1.28
			3B	S	2.99
			3B	S	4.70
			3B	S	–2.17
			3B	P	0.51
			3B	P	0.52
			5B	S	1.39
			5B	S	2.39
			5B	S	–0.81
			5B	P	0.72
			5B	P	0.63
			7B	P	0.82
			7B	P	0.80
			13B	P	0.82
			13B	P	0.79
			15B	S	1.45
			15B	S	2.48
			15B	S	–0.80
			15B	P	0.71
			15B	P	0.62
			17B	S	2.97
			17B	S	4.78
			17B	S	–2.32
			17B	P	0.51
			17B	P	0.53
			19B	S	1.95
			19B	P	2.65
			19B	P	1.39
			20B	S	2.97
			20B	S	4.62
			20B	S	–2.31
			20B	P	0.51
			20B	P	0.50

			22H	S	0.50
			23O	S	0.62
			23O	P	5.51
			23O	P	5.65
			23O	P	0.93
			24O	S	0.62
			24O	P	5.51
			24O	P	5.62
			24O	P	0.99
			25C	P	4.97
			25C	P	2.47
			26C	P	0.99
			26C	P	1.01
			28H	S	0.55
	HOMO-25	Stout-Politzer	1B	S	2.94
			1B	S	5.84
			1B	S	–1.86
			2B	S	2.23
			2B	P	2.98
			2B	P	1.51
			3B	S	3.04
			3B	S	5.78
			3B	S	–1.88
			5B	S	1.25
			5B	S	2.71
			5B	S	–0.54
			7B	P	0.66
			13B	P	0.68
			15B	S	1.37
			15B	S	2.93
			15B	S	–0.61
			17B	S	2.98
			17B	S	5.93
			17B	S	–2.17
			19B	S	2.27
			19B	P	2.92
			19B	P	1.69
			20B	S	3.10
			20B	S	5.75
			20B	S	–2.24

			23O	S	1.25
			23O	P	6.15
			23O	P	6.01
			24O	S	1.28
			24O	S	0.55
			24O	P	6.16
			24O	P	5.97
			25C	P	5.87
			25C	P	1.46
			26C	P	1.21
			26C	P	0.89
			28H	S	0.56
	HOMO-23	Mulliken	2B	P	0.71
			2B	P	–0.64
			7B	S	0.93
			7B	S	2.37
			7B	S	–1.36
			9B	P	0.52
			9B	P	1.39
			11B	P	0.52
			11B	P	1.32
			13B	S	0.93
			13B	S	2.32
			13B	S	–1.45
			19B	P	0.79
			19B	P	–0.62
			23O	P	6.73
			23O	P	7.64
			23O	P	4.12
			24O	P	6.62
			24O	P	7.53
			24O	P	3.95
			25C	P	9.97
			25C	P	12.63
			25C	P	2.62
			26C	P	5.50
			26C	P	5.98
			26C	P	2.07
			27H	S	1.11
			27H	S	2.07

			29H	S	1.51
			29H	S	2.72
			29H	S	0.58
	HOMO-23	Stout-Polizter	1B	S	0.52
			1B	S	–0.63
			3B	S	0.53
			3B	S	–0.93
			7B	S	1.09
			7B	S	4.01
			7B	S	–2.44
			9B	P	0.52
			9B	P	1.48
			11B	P	0.51
			11B	P	1.11
			13B	S	1.10
			13B	S	4.08
			13B	S	–2.88
			17B	S	0.56
			17B	S	–0.51
			20B	S	0.58
			20B	S	–0.71
			23O	P	7.48
			23O	P	8.17
			23O	P	2.79
			24O	P	7.38
			24O	P	8.06
			24O	P	2.60
			25C	P	11.90
			25C	P	15.24
			25C	P	0.97
			26C	P	6.57
			26C	P	6.12
			26C	P	0.84
			27H	S	0.88
			27H	S	2.38
			29H	S	1.16
			29H	S	2.69
	HOMO-16	Mulliken	1B	P	0.65
			1B	P	0.53

			2B	P	1.25
			3B	P	0.63
			3B	P	0.53
			5B	P	1.66
			5B	P	0.83
			7B	S	2.09
			7B	S	6.78
			7B	S	–1.07
			7B	P	0.75
			7B	P	–0.99
			7B	P	0.57
			8H	S	0.82
			8H	S	2.13
			8H	S	1.02
			9B	S	2.12
			9B	S	5.59
			9B	P	0.56
			9B	P	–0.80
			10H	S	0.80
			10H	S	2.03
			10H	S	1.00
			11B	S	2.16
			11B	S	5.59
			11B	P	0.55
			11B	P	–0.79
			12H	S	0.81
			12H	S	2.09
			12H	S	1.00
			13B	S	2.10
			13B	S	6.55
			13B	S	–0.99
			13B	P	0.77
			13B	P	–0.84
			13B	P	0.55
			14H	S	0.81
			14H	S	2.08
			14H	S	1.01
			15B	P	1.76
			15B	P	0.89
			15B	P	0.51
			17B	P	0.65

			19B	P	1.24
			20B	P	0.66
			20B	P	0.51
			23O	P	3.22
			23O	P	3.17
			23O	P	0.91
			24O	P	3.93
			24O	P	3.88
			24O	P	1.22
			25C	P	2.91
			25C	P	2.63
			26C	P	3.65
			26C	P	3.42
			26C	P	0.87
			27H	S	0.99
			27H	S	1.49
			29H	S	1.61
			29H	S	2.65
			29H	S	0.61
	HOMO-16	Stout-Politzer	2B	P	0.95
			5B	P	1.48
			7B	S	1.43
			7B	S	9.67
			7B	S	–0.99
			8H	S	1.67
			9B	S	1.38
			9B	S	7.99
			10H	S	1.49
			11B	S	1.43
			11B	S	8.04
			12H	S	1.47
			13B	S	1.54
			13B	S	9.54
			13B	S	–0.91
			13B	P	0.50
			14H	S	0.51
			14H	S	1.75
			14H	S	0.58
			15B	P	1.61
			19B	P	0.92

			23O	P	3.59
			23O	P	3.46
			23O	P	0.66
			24O	P	4.41
			24O	P	4.27
			24O	P	0.91
			25C	P	3.26
			25C	P	2.70
			26C	P	4.36
			26C	P	3.82
			27H	S	0.86
			27H	S	1.71
			29H	S	1.33
			29H	S	3.05
[1.2–$B_{12}H_{10}O_2CC_6H_5$]$^-$	HOMO-37	Mulliken	2B	S	0.89
			2B	S	2.30
			2B	S	–1.17
			5B	S	0.59
			5B	S	0.94
			7B	S	0.82
			13B	S	0.83
			13B	S	–0.52
			15B	S	0.59
			15B	S	0.94
			19B	S	0.91
			19B	S	2.33
			19B	S	–1.17
			23O	S	0.52
			23O	P	2.93
			23O	P	3.13
			23O	P	0.96
			24O	S	0.52
			24O	P	2.87
			24O	P	3.07
			24O	P	0.94
			25C	S	2.52
			25C	S	2.28
			26C	S	3.22
			26C	S	4.23
			26C	P	1.37

			26C	P	0.72
			27C	P	4.13
			27C	P	4.03
			27C	P	1.14
			28C	P	4.13
			28C	P	4.02
			28C	P	1.14
			29C	S	1.67
			29C	S	1.90
			29C	S	0.66
			29C	P	2.75
			29C	P	2.75
			30C	S	1.69
			30C	S	1.93
			30C	S	0.66
			30C	P	2.73
			30C	P	2.74
			31C	S	2.35
			31C	S	2.73
			32H	S	0.57
			33H	S	0.56
			34H	S	1.00
			34H	S	1.73
			35H	S	1.01
			35H	S	1.75
			36H	S	0.63
			36H	S	1.04
	HOMO-37	Stout-Polizter	2B	S	0.59
			2B	S	3.58
			2B	S	–1.94
			5B	S	0.62
			5B	S	1.18
			7B	S	1.14
			7B	S	–0.63
			13B	S	1.18
			13B	S	–0.69
			15B	S	0.62
			15B	S	1.19
			19B	S	0.59
			19B	S	3.58

			19B	S	–1.94
			23O	S	1.02
			23O	S	0.86
			23O	P	3.13
			23O	P	2.73
			24O	S	1.02
			24O	S	0.85
			24O	P	3.02
			24O	P	2.56
			25C	S	2.10
			25C	S	2.23
			26C	S	2.94
			26C	S	5.24
			26C	P	1.18
			27C	S	0.83
			27C	P	4.61
			27C	P	3.22
			28C	S	0.74
			28C	P	4.54
			28C	P	3.21
			29C	S	2.04
			29C	S	2.91
			29C	S	0.83
			29C	P	3.01
			29C	P	2.11
			30C	S	2.13
			30C	S	3.02
			30C	S	0.85
			30C	P	3.03
			30C	P	2.06
			31C	S	2.47
			31C	S	3.37
			34H	S	0.80
			34H	S	1.65
			35H	S	0.83
			35H	S	1.72
			36H	S	0.51
			36H	S	0.85
	HOMO-36	Mulliken	1B	S	2.38
			1B	S	4.89

			1B	S	–1.29
			2B	S	3.57
			2B	S	4.82
			2B	S	–4.47
			2B	P	0.71
			2B	P	1.79
			3B	S	2.41
			3B	S	4.95
			3B	S	–1.37
			5B	S	0.66
			5B	S	0.89
			5B	P	0.64
			7B	P	0.84
			9B	P	0.83
			9B	P	1.44
			11B	P	0.83
			11B	P	1.46
			13B	P	0.84
			15B	S	0.68
			15B	S	0.91
			15B	P	0.64
			17B	S	2.43
			17B	S	4.94
			17B	S	–1.33
			19B	S	3.52
			19B	S	4.82
			19B	S	–4.50
			19B	P	0.73
			19B	P	1.82
			20B	S	2.39
			20B	S	4.92
			20B	S	–1.32
			23O	P	5.54
			23O	P	5.88
			23O	P	1.63
			24O	P	5.56
			24O	P	5.90
			24O	P	1.64
			25C	P	5.02
			25C	P	2.17
			31C	P	0.57

			31C	P	0.52
	HOMO-36	Stout-Politzer	1B	S	2.42
			1B	S	6.98
			1B	S	–0.96
			2B	S	4.54
			2B	S	7.33
			2B	S	–7.87
			2B	P	0.56
			2B	P	1.82
			3B	S	2.48
			3B	S	7.11
			3B	S	–1.11
			5B	S	0.70
			9B	P	0.64
			9B	P	0.79
			11B	P	0.64
			11B	P	0.81
			15B	S	0.51
			15B	S	0.69
			17B	S	2.51
			17B	S	7.11
			17B	S	–1.04
			19B	S	4.41
			19B	S	7.34
			19B	S	–8.04
			19B	P	0.58
			19B	P	1.95
			20B	S	2.43
			20B	S	7.07
			20B	S	–1.00
			23O	P	6.24
			23O	P	6.19
			23O	P	0.77
			24O	P	6.14
			24O	P	5.97
			24O	P	0.78
			25C	P	5.95
			25C	P	0.93
			27C	S	0.61
			28C	S	0.63

			31C	P	0.72
			31C	P	0.54
	HOMO-32	Mulliken	1B	S	2.61
			1B	S	4.13
			1B	S	–1.88
			2B	S	1.52
			2B	P	2.58
			2B	P	1.38
			3B	S	2.63
			3B	S	4.11
			3B	S	–1.86
			5B	S	1.28
			5B	S	2.21
			5B	S	–0.74
			5B	P	0.65
			5B	P	0.54
			7B	P	0.75
			7B	P	0.66
			13B	P	0.75
			13B	P	0.65
			15B	S	1.31
			15B	S	2.23
			15B	S	–0.74
			15B	P	0.65
			15B	P	0.54
			17B	S	2.63
			17B	S	4.14
			17B	S	–1.87
			19B	S	1.48
			19B	P	2.57
			19B	P	1.37
			20B	S	2.61
			20B	S	4.10
			20B	S	–1.82
			23O	S	0.58
			23O	P	6.09
			23O	P	6.19
			23O	P	1.03
			24O	S	0.61
			24O	P	6.14

			24O	P	6.25
			24O	P	1.03
			25C	P	5.47
			25C	P	2.52
			29C	P	0.65
			29C	P	0.52
			30C	P	0.65
			30C	P	0.52
			31C	P	0.67
			31C	P	0.56
	HOMO-32	Stout-Polizter	1B	S	2.57
			1B	S	5.01
			1B	S	–1.57
			2B	S	1.50
			2B	P	2.88
			2B	P	1.61
			3B	S	2.68
			3B	S	5.06
			3B	S	–1.62
			5B	S	1.18
			5B	S	2.55
			5B	S	–0.53
			7B	P	0.60
			13B	P	0.61
			15B	S	1.22
			15B	S	2.60
			15B	S	–0.54
			17B	S	2.64
			17B	S	5.13
			17B	S	–1.69
			19B	S	1.70
			19B	P	2.76
			19B	P	1.57
			20B	S	2.66
			20B	S	5.09
			20B	S	–1.60
			23O	S	1.15
			23O	S	0.64
			23O	P	6.86
			23O	P	6.69

			24O	S	1.23
			24O	S	0.69
			24O	P	6.80
			24O	P	6.50
			24O	P	0.50
			25C	P	6.40
			25C	P	1.29
			29C	P	0.75
			30C	P	0.79
			31C	P	0.85
			31C	P	0.62
	HOMO-30	Mulliken	2B	P	1.27
			2B	P	–0.81
			7B	S	1.16
			7B	S	2.78
			7B	S	–1.68
			9B	P	0.72
			9B	P	1.83
			11B	P	0.71
			11B	P	1.90
			13B	S	1.23
			13B	S	2.99
			13B	S	–1.90
			19B	P	1.28
			19B	P	–0.81
			23O	P	8.43
			23O	P	9.50
			23O	P	5.06
			24O	P	8.40
			24O	P	9.47
			24O	P	5.04
			25C	P	10.69
			25C	P	13.06
			25C	P	2.96
			26C	P	1.48
			26C	P	2.19
			26C	P	0.67
	HOMO-30	Stout-Politzer	1B	S	0.70
			1B	S	–0.87

			2B	P	0.82
			3B	S	0.64
			3B	S	–1.10
			7B	S	1.36
			7B	S	4.85
			7B	S	–3.20
			9B	P	0.74
			9B	P	1.89
			11B	S	0.55
			11B	P	0.68
			11B	P	1.91
			13B	S	1.43
			13B	S	5.23
			13B	S	–3.75
			17B	S	0.69
			17B	S	–0.90
			19B	P	0.84
			20B	S	0.61
			20B	S	–1.04
			23O	P	9.44
			23O	P	10.31
			23O	P	3.60
			24O	P	9.40
			24O	P	10.34
			24O	P	3.67
			25C	P	12.55
			25C	P	15.26
			25C	P	1.34
			26C	P	1.58
			26C	P	2.06
	HOMO-22	Mulliken	1B	P	0.61
			1B	P	0.51
			2B	P	1.36
			3B	P	0.61
			5B	P	1.57
			5B	P	0.78
			7B	S	2.13
			7B	S	6.55
			7B	S	–1.31
			7B	P	0.59

			7B	P	–0.89
			7B	P	0.61
			8H	S	0.82
			8H	S	2.10
			8H	S	1.02
			9B	S	1.78
			9B	S	4.71
			9B	P	0.65
			10H	S	0.61
			10H	S	1.56
			10H	S	0.71
			11B	S	2.02
			11B	S	5.58
			11B	S	–0.71
			11B	P	0.64
			11B	P	–0.78
			12H	S	0.85
			12H	S	2.12
			12H	S	1.00
			13B	S	1.90
			13B	S	5.74
			13B	S	–0.95
			13B	P	0.61
			13B	P	–0.67
			13B	P	0.58
			14H	S	0.62
			14H	S	1.64
			14H	S	0.77
			15B	P	1.57
			15B	P	0.78
			17B	P	0.62
			17B	P	0.52
			19B	P	1.36
			20B	P	0.60
			23O	P	2.03
			23O	P	1.99
			23O	P	0.56
			24O	P	2.06
			24O	P	2.02
			24O	P	0.57
			25C	P	2.34

			25C	P	2.26
			26C	P	0.56
			27C	P	1.19
			27C	P	1.60
			27C	P	0.57
			28C	P	1.19
			28C	P	1.60
			28C	P	0.57
			29C	P	2.11
			29C	P	2.78
			29C	P	1.29
			30C	P	2.11
			30C	P	2.78
			30C	P	1.29
			31C	P	2.55
			31C	P	3.35
			31C	P	1.44
	HOMO-22	Stout-Politzer	2B	P	1.12
			5B	P	1.42
			7B	S	1.61
			7B	S	9.51
			7B	S	–1.34
			8H	S	1.76
			8H	S	0.56
			9B	S	1.25
			9B	S	6.84
			10H	S	1.21
			11B	S	1.31
			11B	S	7.72
			12H	S	1.63
			13B	S	1.54
			13B	S	8.74
			13B	S	–1.06
			14H	S	1.39
			15B	P	1.44
			19B	P	1.10
			23O	P	2.25
			23O	P	2.10
			24O	P	2.29
			24O	P	2.16

			25C	P	2.66
			25C	P	2.40
			26C	P	0.62
			27C	P	1.35
			27C	P	1.80
			28C	P	1.34
			28C	P	1.77
			29C	P	2.43
			29C	P	3.20
			29C	P	0.88
			30C	P	2.43
			30C	P	3.17
			30C	P	0.86
			31C	P	2.96
			31C	P	3.92
			31C	P	0.96

Table S6. Composition of selected occupied orbitals in [1,2-$B_{12}H_{10}O_2CR]^-$

Bond type	Length	$\rho(r)$	$\nabla^2\rho(r)$	$G(r)$	$V(r)$	$\lvert V(r)\rvert/G(r)$	$H(r)$	δ
[1,2-$B_{12}H_{10}O_2CCH_3]^-$								
C25–O24	1.270	0.371	–0.527	0.516	–1.164	2.255	–0.648	1.016
C25–O23	1.270	0.371	–0.535	0.514	–1.163	2.260	–0.648	1.012
B2–O24	1.535	0.128	0.547	0.226	–0.316	1.394	–0.090	0.481
B19–O23	1.532	0.140	–0.190	0.043	–0.134	1.395	–0.089	0.482
B2–B19	1.709	0.124	–0.146	0.044	–0.124	3.104	–0.091	0.572
B2–B1	1.746	0.124	–0.145	0.044	–0.124	2.835	–0.080	0.542
B2–B3	1.747	0.124	–0.147	0.044	–0.124	2.830	–0.080	0.542
B19–B17	1.745	0.124	–0.147	0.044	–0.124	2.838	–0.081	0.542
B19–B20	1.745	0.128	0.547	0.226	–0.316	2.838	–0.081	0.542
B2–B9	1.757	0.126	–0.136	0.044	–0.121	2.776	–0.078	0.472
B2–B11	1.757	0.126	–0.136	0.044	–0.121	2.778	–0.078	0.474
B19–B9	1.758	0.127	–0.137	0.044	–0.122	2.783	–0.078	0.474
B19–B11	1.757	0.126	–0.136	0.044	–0.121	2.778	–0.078	0.473
B9–B1	1.778	0.120	–0.118	0.039	–0.107	2.759	–0.068	0.438
B9–B17	1.780	0.119	–0.117	0.039	–0.107	2.754	–0.068	0.436
B11–B3	1.780	0.119	–0.117	0.039	–0.107	2.758	–0.068	0.437
B11–B20	1.779	0.120	–0.117	0.039	–0.107	2.756	–0.068	0.437
B9–B7	1.743	0.124	–0.145	0.040	–0.116	2.914	–0.076	0.514
B11–B13	1.744	0.124	–0.144	0.040	–0.115	2.911	–0.076	0.512
B1–B3	1.801	0.116	–0.106	0.037	–0.100	2.715	–0.063	0.403

B17–B20	1.802	0.116	–0.105	0.037	–0.100	2.710	–0.063	0.402
B1–B5	1.775	0.119	–0.124	0.037	–0.106	2.830	–0.068	0.476
B3–B5	1.776	0.119	–0.124	0.037	–0.105	2.829	–0.068	0.476
B17–B15	1.776	0.119	–0.124	0.037	–0.106	2.830	–0.068	0.476
B20–B15	1.776	0.119	–0.124	0.037	–0.105	2.829	–0.068	0.475
B1–B7	1.793	0.117	–0.109	0.038	–0.103	2.726	–0.065	0.435
B3–B13	1.793	0.117	–0.109	0.038	–0.102	2.729	–0.065	0.436
B17–B7	1.793	0.117	–0.110	0.038	–0.103	2.728	–0.065	0.437
B20–B13	1.793	0.117	–0.110	0.038	–0.103	2.729	–0.065	0.437
B5–B7	1.778	0.119	–0.124	0.037	–0.105	2.838	–0.068	0.466
B5–B13	1.778	0.119	–0.123	0.037	–0.104	2.839	–0.068	0.466
B15–B7	1.778	0.119	–0.123	0.037	–0.104	2.835	–0.068	0.467
B15–B13	1.779	0.119	–0.123	0.037	–0.104	2.835	–0.068	0.465
B5–B15	1.788	0.117	–0.116	0.037	–0.103	2.790	–0.066	0.451
$[1.2\text{–}B_{12}H_{10}O_2CC_6H_5]^-$								
C25–O24	1.271	0.370	–0.540	0.511	–1.157	2.264	–0.646	1.007
C25–O23	1.272	0.370	–0.541	0.510	–1.155	2.265	–0.645	1.005
B2–O24	1.534	0.128	0.554	0.227	–0.315	1.390	–0.089	0.480
B19–O23	1.531	0.129	0.561	0.229	–0.318	1.389	–0.089	0.481
B2–B19	1.708	0.140	–0.191	0.043	–0.134	3.109	–0.091	0.573
B2–B1	1.746	0.124	–0.147	0.044	–0.124	2.835	–0.080	0.542
B2–B3	1.746	0.124	–0.147	0.044	–0.125	2.838	–0.081	0.543
B19–B17	1.745	0.124	–0.147	0.044	–0.124	2.839	–0.081	0.542
B19–B20	1.746	0.124	–0.146	0.044	–0.124	2.834	–0.080	0.542
B2–B9	1.758	0.126	–0.136	0.044	–0.122	2.774	–0.078	0.472
B2–B11	1.756	0.126	–0.136	0.044	–0.122	2.775	–0.078	0.473
B19–B9	1.758	0.126	–0.135	0.044	–0.122	2.771	–0.078	0.470
B19–B11	1.757	0.126	–0.136	0.044	–0.122	2.775	–0.078	0.472
B9–B1	1.780	0.119	–0.117	0.039	–0.107	2.756	–0.068	0.435
B9–B17	1.780	0.120	–0.118	0.039	–0.107	2.758	–0.068	0.436
B11–B3	1.781	0.119	–0.117	0.039	–0.107	2.753	–0.068	0.435
B11–B20	1.780	0.119	–0.117	0.039	–0.107	2.755	–0.068	0.436
B9–B7	1.743	0.124	–0.145	0.040	–0.116	2.912	–0.076	0.513
B11–B13	1.744	0.124	–0.144	0.040	–0.115	2.909	–0.076	0.512
B1–B3	1.802	0.116	–0.106	0.037	–0.100	2.713	–0.063	0.402
B17–B20	1.801	0.116	–0.106	0.037	–0.100	2.713	–0.063	0.402
B1–B5	1.776	0.119	–0.124	0.037	–0.105	2.831	–0.068	0.475
B3–B5	1.776	0.119	–0.124	0.037	–0.105	2.830	–0.068	0.474
B17–B15	1.776	0.119	–0.124	0.037	–0.106	2.831	–0.068	0.475
B20–B15	1.775	0.119	–0.124	0.037	–0.106	2.830	–0.068	0.476
B1–B7	1.793	0.117	–0.109	0.038	–0.102	2.726	–0.065	0.437

B3–B13	1.793	0.117	–0.110	0.038	–0.102	2.731	–0.065	0.437
B17–B7	1.793	0.117	–0.109	0.038	–0.102	2.726	–0.065	0.436
B20–B13	1.793	0.117	–0.109	0.038	–0.103	2.728	–0.065	0.437
B5–B7	1.779	0.119	–0.123	0.037	–0.104	2.838	–0.068	0.466
B5–B13	1.779	0.119	–0.123	0.037	–0.104	2.835	–0.067	0.465
B15–B7	1.778	0.119	–0.123	0.037	–0.104	2.837	–0.068	0.466
B15–B13	1.779	0.119	–0.123	0.037	–0.104	2.835	–0.068	0.466
B5–B15	1.788	0.117	–0.116	0.037	–0.103	2.788	–0.066	0.451
CH_3COOH								
C4–O2	1.347	0.308	–0.684	0.320	–0.811	2.534	–0.491	0.843
C4–O3	1.200	0.436	–0.162	0.762	–1.564	2.053	–0.802	1.264
C_6H_5COOH								
C12–O14	1.346	0.310	–0.681	0.324	–0.818	2.526	–0.494	0.841
C12–O13	1.203	0.434	–0.196	0.748	–1.545	2.065	–0.797	1.245

Table S7. Topological parameters of electron density at bond critical points (BCPs) of $[1,2\text{-}B_{12}H_{10}O_2CR]^-$ and RCOOH. $\nabla^2\rho(r)$ – Laplacian of electron density at BCPs; *G(r)* – Lagrangian kinetic energy at BCPs; *H(r)* – total energy at BCPs; δ – delocalisation index.

Model structure	Atom	x	y	z
CH_3COOH	H	10.515734	15.155856	28.516072
	O	10.551744	14.663517	29.343318
	O	10.267593	16.734228	30.125868
	C	10.407553	15.561566	30.337409
	C	10.447557	14.909604	31.686713
	H	11.396205	14.389039	31.813837
	H	10.327353	15.663272	32.458004
	H	9.653903	14.166936	31.761498
	H	10.515734	15.155856	28.516072
C_6H_5COOH	C	26.580921	18.918706	27.434950
	C	25.308225	18.430536	27.696538
	C	27.425674	19.241252	28.482202
	H	24.647027	18.177828	26.877129
	H	28.421534	19.623577	28.301970
	C	24.880429	18.265964	29.005850
	C	26.999919	19.074612	29.795681
	H	23.887037	17.887356	29.208772

	C	25.723835	18.586334	30.056787
	H	25.397230	18.459253	31.079355
	H	26.913567	19.047688	26.413210
	C	27.945575	19.431003	30.886911
	O	29.052629	19.870577	30.720796
	O	27.442072	19.212914	32.115651
	H	28.125951	19.473446	32.741121
[1,2-$B_{12}H_{10}O_2CCH_3$]$^-$	B	9.009119	11.269517	21.023174
	B	9.568366	9.715777	20.455800
	B	8.802501	10.780221	19.301516
	H	7.724457	10.578192	18.828005
	B	9.406267	12.398973	19.712447
	H	8.748909	13.376774	19.515482
	B	10.481600	12.287900	21.123640
	H	10.567567	13.169118	21.926093
	B	10.558724	10.612403	21.597459
	H	10.697972	10.166058	22.701448
	B	10.227714	9.824386	18.830733
	H	10.150389	8.863575	18.117984
	B	10.151522	11.504360	18.368090
	H	10.008617	11.834696	17.228803
	B	11.180225	12.420228	19.493672
	H	11.748288	13.411083	19.143602
	B	11.908756	11.304054	20.666734
	H	12.989309	11.463251	21.150827
	B	11.264034	9.737533	20.247150
	B	11.702286	10.813723	18.944760
	H	12.637635	10.633366	18.223367
	H	8.075422	11.408794	21.755668
	O	11.589544	8.290012	20.628484
	O	9.384438	8.258028	20.898761
	C	10.516959	7.685176	20.940331
	C	10.601946	6.270234	21.392267
	H	11.237724	5.706810	20.712203

	H	9.611304	5.830004	21.447703
	H	11.065949	6.252894	22.378863
[1,2-$B_{12}H_{10}O_2CC_6H_5$]$^-$	B	8.732650	11.129533	20.595041
	B	9.556548	9.627318	20.259804
	B	9.079171	10.616375	18.902934
	H	8.206958	10.321041	18.141800
	B	9.404979	12.283108	19.423699
	H	8.758918	13.199702	19.012299
	B	10.025979	12.268510	21.090282
	H	9.806680	13.158232	21.856625
	B	10.094806	10.607892	21.615374
	H	9.944287	10.181284	22.724801
	B	10.651853	9.781639	18.895483
	H	10.861781	8.811371	18.224429
	B	10.580437	11.447019	18.382233
	H	10.749780	11.759638	17.241733
	B	11.158182	12.451680	19.731276
	H	11.722087	13.485832	19.532958
	B	11.598448	11.406418	21.097366
	H	12.472350	11.661214	21.871146
	B	11.231658	9.788860	20.554314
	B	11.944751	10.893900	19.405482
	H	13.061876	10.791919	18.994653
	H	7.617679	11.190672	21.019534
	O	11.543496	8.375556	21.053473
	O	9.365539	8.161148	20.667791
	C	10.478111	7.681466	21.052571
	C	10.535746	6.283639	21.519031
	C	9.382684	5.506470	21.528757
	C	11.743504	5.752651	21.958632
	C	9.440442	4.198611	21.978515
	C	11.795237	4.444685	22.408115
	C	10.645134	3.667994	22.417892
	H	8.453238	5.936953	21.182143

	H	12.628837	6.373305	21.944520
	H	8.543486	3.592726	21.987742
	H	12.733591	4.031198	22.754755
	H	10.687489	2.644580	22.769793

Table S8. Cartesian atomic coordinates of the calculated optimized model structures. All coordinates are given in Angstrom units, Å.