Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Stabilization of carbocations CH_3^+, $C_2H_5^+$, *i*-$C_3H_7^+$, *tert*-Bu^+, and *cyclo*-pentyl$^+$ in solid phases: empirical data versus calculations

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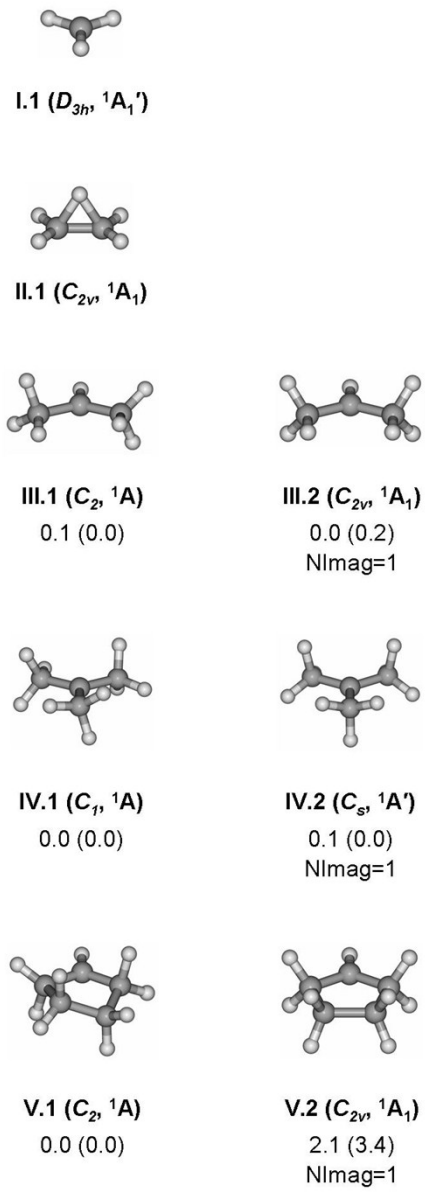

Figure S1. Representative structures of R^+ compounds (R = CH_3 (I), C_2H_5 (II), *i*-C_3H_7 (III), *t*-C_4H_9 (IV), *c*-C_5H_9 (V)), their point group symmetries and spectroscopic states. ZPE-corrected (B3LYP-D3/def2-TZVPD) relative energies (kcal/mol) are given at the B3LYP-D3/def2-TZVPD and CCSD(T)/def2-TZVPD theoretical levels (in parentheses).

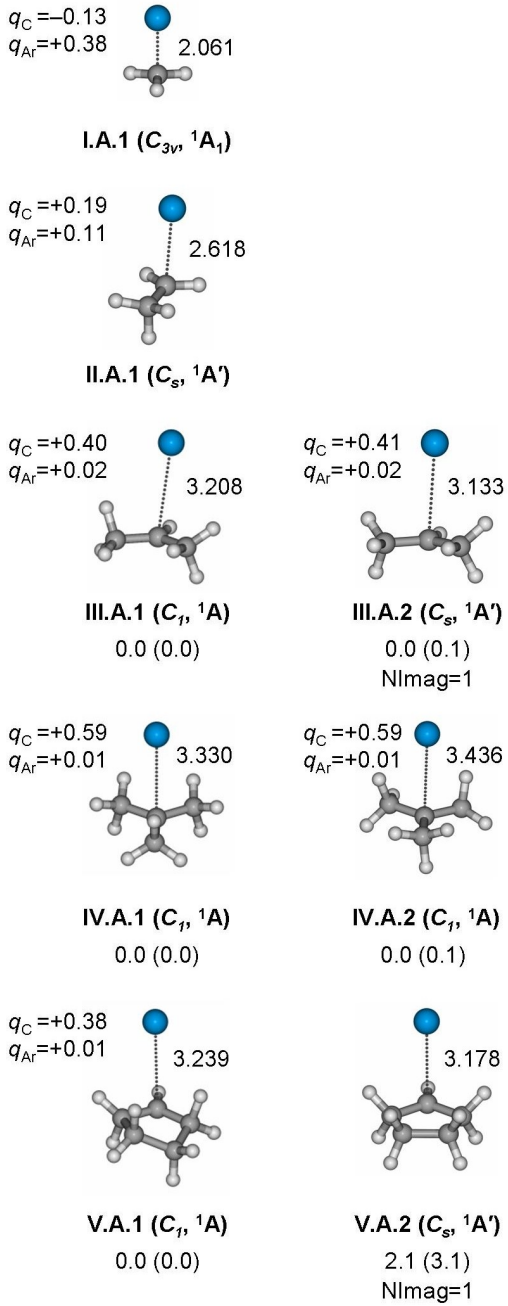

Figure S2. Representative structures of $R^+\cdots Ar$ compounds (R = CH_3 (I), C_2H_5 (II), *i*-C_3H_7 (III), *t*-C_4H_9 (IV), *c*-C_5H_9 (V)), their point group symmetries and spectroscopic states. C–Ar distances (Å) and NPA charges on the corresponding C and Ar atoms (q, $|e|$) are presented for the structures of interest. ZPE-corrected (B3LYP-D3/def2-TZVPD) relative energies (kcal/mol) are given at the B3LYP-D3/def2-TZVPD and CCSD(T)/def2-TZVPD theoretical levels (in parentheses).

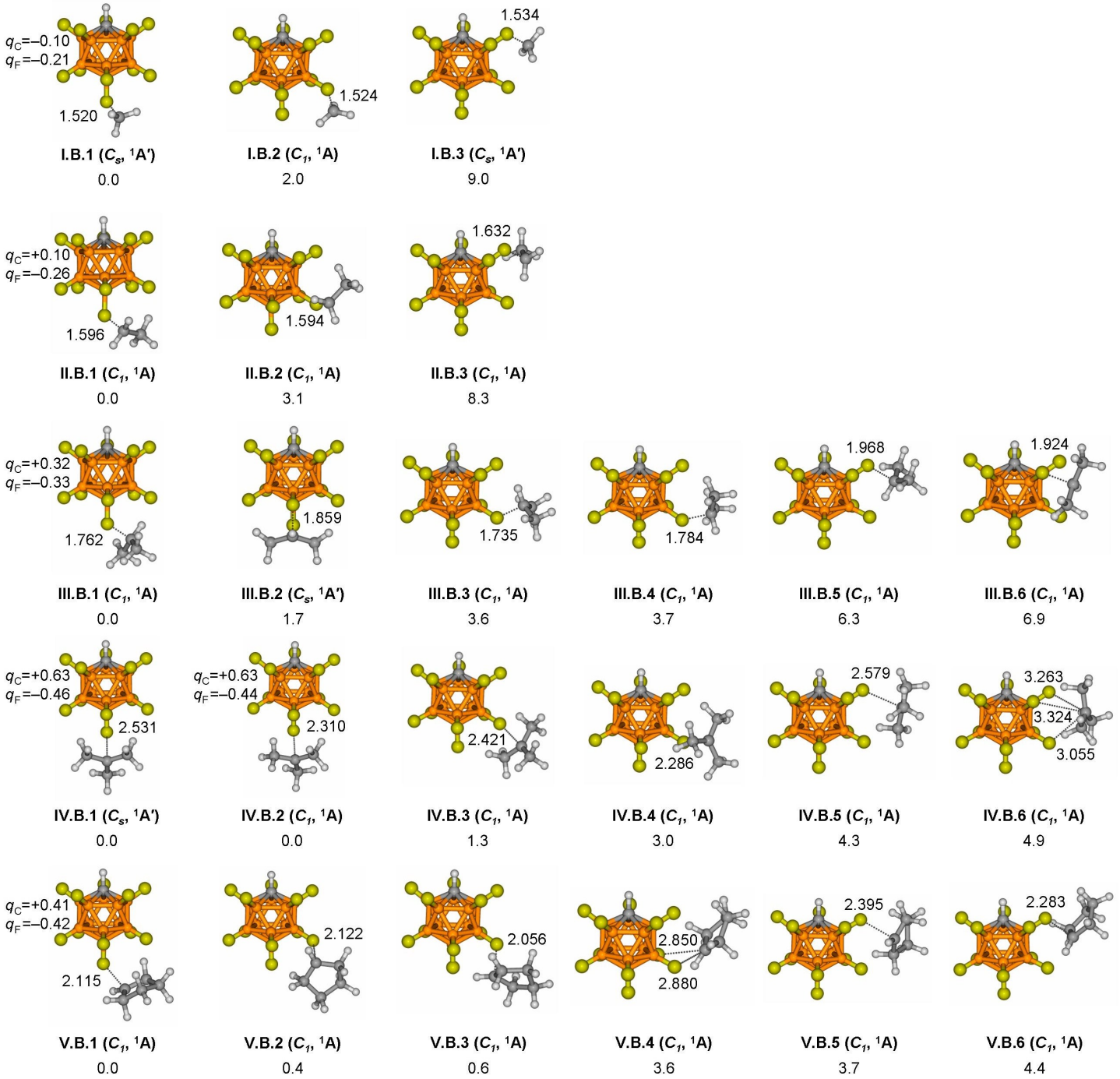

Figure S3. Representative structures of R{F_{11}} compounds (R = CH_3 (I), C_2H_5 (II), *i*-C_3H_7 (III), *t*-C_4H_9 (IV), *c*-C_5H_9 (V)), their point group symmetries and spectroscopic states. C–F distances (Å) and NPA charges on the corresponding C and F atoms (q, $|e|$) are presented for the structures of interest. ZPE-corrected (B3LYP-D3/def2-TZVPD) relative energies (kcal/mol) are given at the B3LYP-D3/def2-TZVPD level of theory.

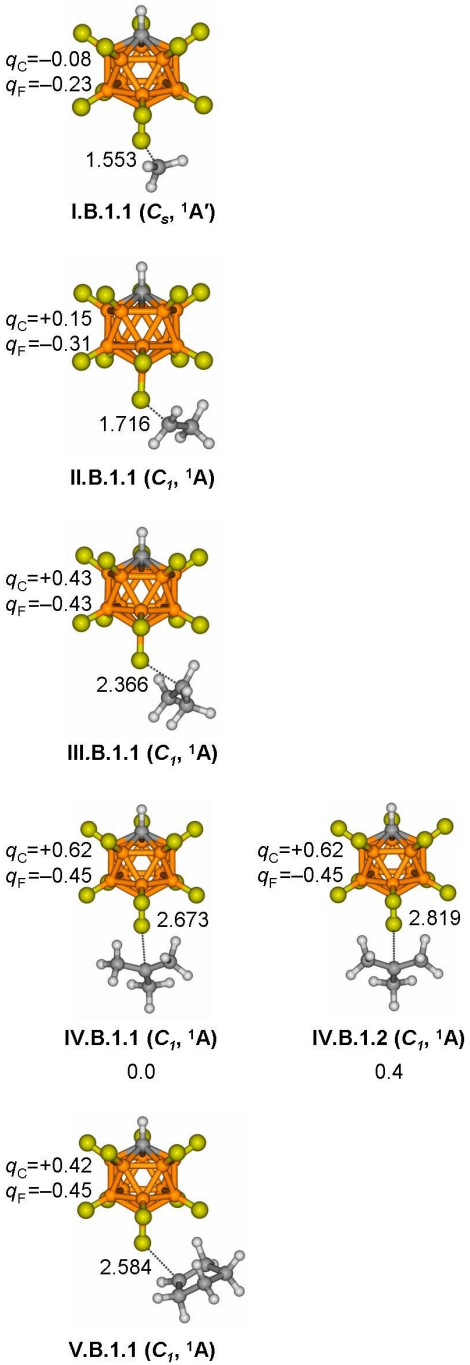

Figure S4. Representative structures of R{F_{11}} compounds optimized in dichloroethane solution (R = CH_3 (I), C_2H_5 (II), *i*-C_3H_7 (III), *t*-C_4H_9 (IV), *c*-C_5H_9 (V)), their point group symmetries and spectroscopic states. C–F distances (Å) and NPA charges on the corresponding C and F atoms (q, $|e|$) are presented for the structures of interest. ZPE-corrected (SMD-B3LYP-D3/def2-TZVPD) relative energies (kcal/mol) are given at the SMD-B3LYP-D3/def2-TZVPD level of theory.

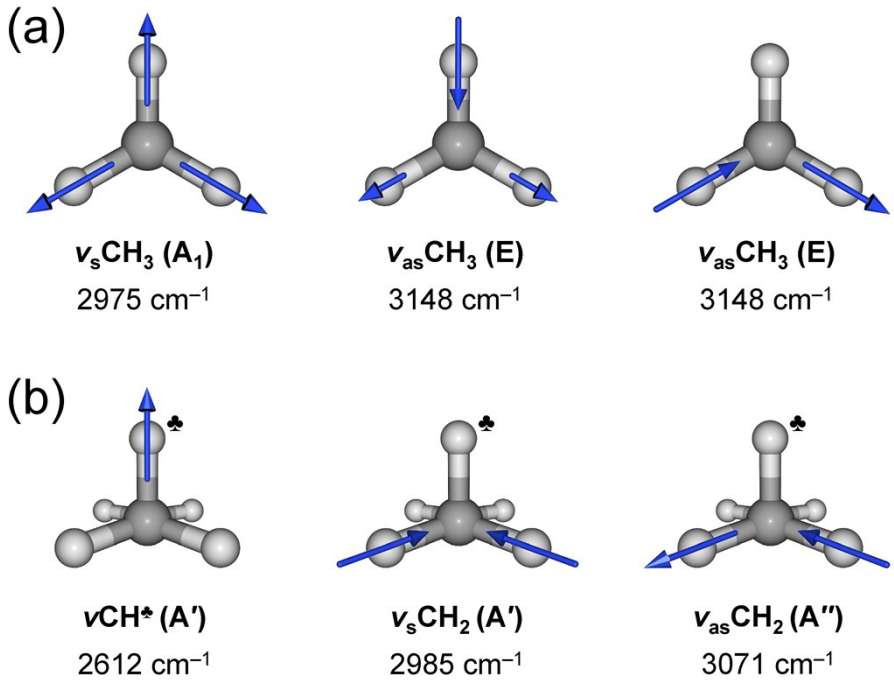

Figure S5. Relevant vibrational frequencies for the CH_3^+ (a) and $C_2H_5^+$–Ar (b; Ar atom is omitted for clarity) compounds, their assignments and scaled displacement vectors. A scaling factor (0.9674) was applied to B3LYP-D3/def2-TZVPD harmonic frequencies.

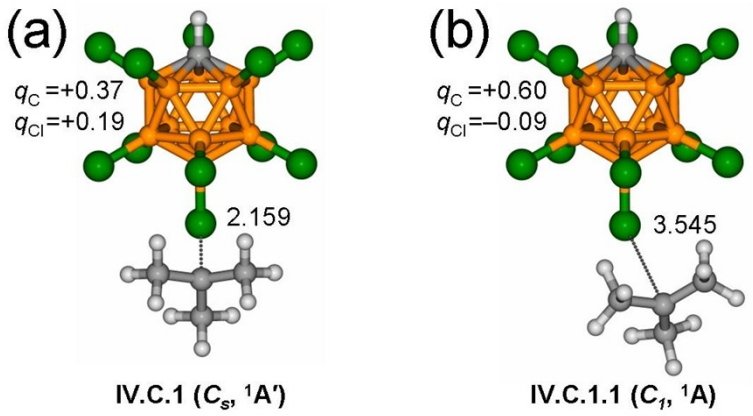

Figure S6. Representative structures of *t*-$C_4H_9\{Cl_{11}\}$ optimized in the gas phase (a) and in dichloroethane solution (b), their point group symmetries and spectroscopic states. C–Cl distances (Å) and NPA charges on the corresponding C and Cl atoms (q, $|e|$) are presented.

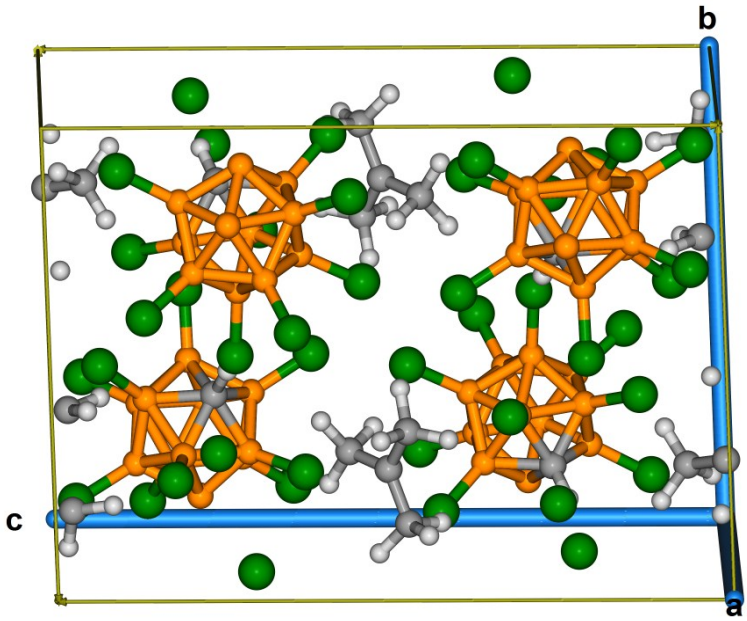

Figure S7. Crystallographic unit cell of *t*-$C_4H_9\{Cl_{11}\}$ [Stoyanov E. S., et al. *Angew. Chem. Int. Ed.* 2012, **51**, 9149] used for periodic calculations.

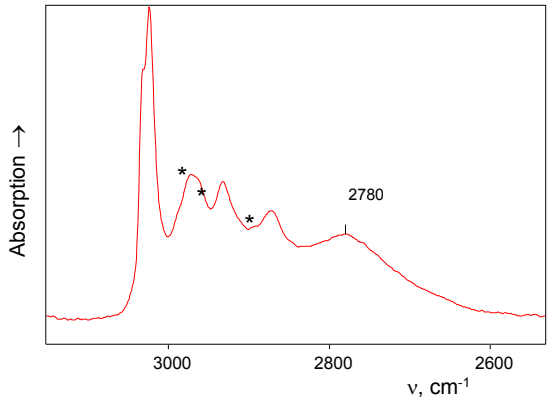

Figure S8. An IR spectrum of the mixture of *i*-$C_3H_7^+$ and chloronium cation $(C_3H_7)_2Cl^+$ (marked with an asterisk) with the $\{Cl_{11}^-\}$ counterion.

Table S1. Results of EDA (kcal/mol) for the relevant compounds under study computed at the SR-ZORA-B3LYP-D3/TZ2P level of theory.

Compound	Fragments	ΔE_{int} [a]	ΔE_{Pauli}	ΔE_{elstat} [b]	ΔE_{orb} [b]	ΔE_{disp} [b]	ΔE_{steric} [c]
I.A.1 [d]	CH_3^+ + Ar	-25.5	45.4	-10.4 (14.6%)	-59.5 (83.9%)	-1.0 (1.5%)	35.0
II.A.1 [d]	$C_2H_5^+$ + Ar	-5.1	10.1	-2.8 (18.3%)	-10.7 (70.6%)	-1.7 (11.0%)	7.3
III.A.1 [d]	*i*-$C_3H_7^+$ + Ar	-2.2	2.5	-0.7 (15.0%)	-2.2 (46.2%)	-1.8 (38.9%)	1.8
III.A.2 [d]	*i*-$C_3H_7^+$ + Ar	-2.3	2.8	-0.8 (15.4%)	-2.5 (48.3%)	-1.9 (36.3%)	2.1
IV.A.1 [d]	*t*-$C_4H_9^+$ + Ar	-2.1	2.3	-0.7 (14.6%)	-1.6 (36.3%)	-2.2 (49.1%)	1.7
IV.A.2 [d]	*t*-$C_4H_9^+$ + Ar	-2.0	2.2	-0.6 (14.9%)	-1.5 (35.3%)	-2.1 (49.8%)	1.6
V.A.1 [d]	*c*-$C_5H_9^+$ + Ar	-2.2	2.6	-0.7 (15.5%)	-1.9 (40.1%)	-2.1 (44.4%)	1.8
I.B.1 [d]	CH_3^+ + $\{F_{11}^-\}$	-153.0	110.7	-136.7 (51.9%)	-122.8 (46.6%)	-4.2 (1.6%)	-26.1
II.B.1 [d]	$C_2H_5^+$ + $\{F_{11}^-\}$	-121.8	112.7	-130.3 (55.5%)	-98.1 (41.8%)	-6.2 (2.6%)	-17.6
III.B.1 [d]	*i*-$C_3H_7^+$ + $\{F_{11}^-\}$	-99.1	78.3	-110.3 (62.2%)	-60.1 (33.9%)	-7.0 (4.0%)	-32.0
IV.B.1 [d]	*t*-$C_4H_9^+$ + $\{F_{11}^-\}$	-80.1	19.6	-78.2 (78.5%)	-12.7 (12.7%)	-8.7 (8.8%)	-58.6
IV.B.2 [d]	*t*-$C_4H_9^+$ + $\{F_{11}^-\}$	-80.5	24.7	-80.8 (76.8%)	-16.0 (15.2%)	-8.4 (8.0%)	-56.1
V.B.1 [d]	*c*-$C_5H_9^+$ + $\{F_{11}^-\}$	-83.8	32.7	-84.9 (72.9%)	-23.1 (19.9%)	-8.4 (7.2%)	-52.3
I.B.1.1 [e]	CH_3^+ + $\{F_{11}^-\}$	-145.7	96.3	-126.2 (52.1%)	-112.1 (46.3%)	-3.7 (1.5%)	-29.9
II.B.1.1 [e]	$C_2H_5^+$ + $\{F_{11}^-\}$	-110.4	76.9	-110.8 (59.2%)	-70.7 (37.7%)	-5.8 (3.1%)	-34.0
III.B.1.1 [e]	*i*-$C_3H_7^+$ + $\{F_{11}^-\}$	-81.6	13.0	-73.9 (78.2%)	-14.8 (15.6%)	-5.8 (6.1%)	-61.0
IV.B.1.1 [e]	*t*-$C_4H_9^+$ + $\{F_{11}^-\}$	-75.7	9.2	-69.1 (81.4%)	-9.2 (10.8%)	-6.6 (7.8%)	-59.9
IV.B.1.2 [e]	*t*-$C_4H_9^+$ + $\{F_{11}^-\}$	-75.9	8.8	-68.9 (81.4%)	-8.8 (10.4%)	-6.9 (8.2%)	-60.2
V.B.1.1 [e]	*c*-$C_5H_9^+$ + $\{F_{11}^-\}$	-76.5	9.5	-69.2 (80.5%)	-10.3 (12.0%)	-6.5 (7.5%)	-59.7
IV.C.1 [d]	*t*-$C_4H_9^+$ + $\{Cl_{11}^-\}$	-91.8	85.5	-97.8 (55.2%)	-69.3 (39.1%)	-10.2 (5.7%)	-12.4
IV.C.1.1 [e]	*t*-$C_4H_9^+$ + $\{Cl_{11}^-\}$	-69.7	6.8	-59.7 (78.0%)	-10.4 (13.6%)	-6.4 (8.4%)	-52.9

[a] $\Delta E_{int}=\Delta E_{Pauli}+\Delta E_{elstat}+\Delta E_{orb}+\Delta E_{disp}$.

[b] The percentage values in parentheses give the contribution to the total attractive interactions ($\Delta E_{elstat}+\Delta E_{orb}+\Delta E_{disp}$).

[c] $\Delta E_{steric}=\Delta E_{Pauli}+\Delta E_{elstat}$.

[d] Structural parameters were optimized in the gas phase.

[e] Structural parameters were optimized in the dichloroethane solution.

Table S2. Results of NBO analysis for the relevant compounds under study computed at the B3LYP-D3/def2-TZVPD level of theory.

Compound	X[a]	Bonding[b]	ON[c]	Contribution[d]	Configuration[e]	$\Delta E_{ij}^{(2)}$ [f]
I.A.1 [g]	Ar	Covalent	1.995	18.81%	[core]2s(1.29)2p(2.83)	–
II.A.1 [g]	Ar	Ionic			[core]2s(1.17)2p(2.62)4d(0.01)	49.6 [i]
III.A.1 [g]	Ar	Ionic			[core]2s(1.07)2p(2.51)3p(0.01)4d(0.01)	24.2 / 27.3 [i]
III.A.2 [g]	Ar	Ionic			[core]2s(1.07)2p(2.51)3p(0.01)3d(0.01)	20.9 / 20.9 [i]
IV.A.1 [g]	Ar	Ionic			[core]2s(1.00)2p(2.39)3p(0.01)	21.7 / 21.7 / 23.0 [i]
IV.A.2 [g]	Ar	Ionic			[core]2s(1.00)2p(2.39)3p(0.01)	18.5 / 20.7 / 21.8 [i]
V.A.1 [g]	Ar	Ionic			[core]2s(1.07)2p(2.53)3p(0.01)	29.2 / 30.5 [i]
I.B.1 [g]	F	Covalent	1.990	20.79%	[core]2s(1.19)2p(2.90)	–
II.B.1 [g]	F	Covalent	1.986	18.40%	[core]2s(1.12)2p(2.76)3d(0.01)	9.2 [j]
III.B.1 [g]	F	Covalent	1.978	13.64%	[core]2s(1.07)2p(2.59)3p(0.01)3d(0.01)	11.6 / 11.7 [j]
IV.B.1 [g]	F	Ionic			[core]2s(1.00)2p(2.35)3p(0.01)	19.2 / 19.2 / 19.3 [i]
IV.B.2 [g]	F	Ionic			[core]2s(1.00)2p(2.35)3p(0.01)3d(0.01)	16.6 / 18.9 / 19.5 [i]
V.B.1 [g]	F	Ionic			[core]2s(1.08)2p(2.50)3p(0.01)3d(0.01)	14.6 / 21.7 [i]
I.B.1.1 [h]	F	Covalent	1.987	18.79%	[core]2s(1.21)2p(2.86)	–
II.B.1.1 [h]	F	Covalent	1.980	13.99%	[core]2s(1.15)2p(2.69)4d(0.01)	13.2 [j]
III.B.1.1 [h]	F	Ionic			[core]2s(1.07)2p(2.49)3p(0.01)3d(0.01)	24.0 / 25.2 [i]
IV.B.1.1 [h]	F	Ionic			[core]2s(1.00)2p(2.37)3p(0.01)	21.7 / 21.8 / 22.0 [i]
IV.B.1.2 [h]	F	Ionic			[core]2s(0.99)2p(2.37)3p(0.01)	20.9 / 21.4 / 23.0 [i]
V.B.1.1 [h]	F	Ionic			[core]2s(1.07)2p(2.50)3p(0.01)	24.2 / 28.0 [i]
IV.C.1 [g]	Cl	Ionic			[core]2s(1.02)2p(2.59)3p(0.01)3d(0.01)	17.3 / 18.3 / 18.3 [i]
IV.C.1.1 [h]	Cl	Ionic			[core]2s(0.99)2p(2.39)3p(0.01)	21.4 / 22.0 / 23.2 [i]

[a] Atom which is interacted with the sp^2 C atom.
[b] Type of C–X bonding according to NBO analysis.
[c] Occupation number for the C–X covalent bond ($|e|$).
[d] Contribution of sp^2 C atom to the C–X covalent bond.
[e] Natural electron configuration of sp^2 C atom.
[f] Second-order perturbation interaction energies (kcal/mol) corresponding to hyperconjugative stabilization (B3LYP-D3/def2-TZVP level of theory).
[g] Structural parameters were optimized in the gas phase.
[h] Structural parameters were optimized in the dichloroethane solution.
[i] $\sigma(CH^{\clubsuit}) \rightarrow n^*(C)$ donor–acceptor interactions.
[j] $\sigma(CH^{\clubsuit}) \rightarrow \sigma^*(CF)$ donor–acceptor interactions.

Table S3. Selected frequencies (cm^{-1}, scaled by factor 0.9674) calculated at the (SMD-)B3LYP-D3/def2-TZVPD level of theory for the CH_3^+, CH_3^+–Ar, and $CH_3\{F_{11}\}$ compounds as compared with the frequencies from the empirical data. The most intense νCF band is marked in bold.

Compound	$\nu_{as}CH_3$		ν_sCH_3	$\delta_{as}CH_3$		δ_sCH_3	νCX (X = F, Ar)
CH_3^+, I.1 [a]	3108	3108	2922	1362	1362	1377	
CH_3^+–Ar, I.A.1 [a]	3148	3148	2975	1373	1373	1310	322
$CH_3\{F_{11}\}$, I.B.1 [a]	3138	3131	2999	1426	1413	1418	690 **704**
$CH_3\{F_{11}\}$, I.B.1.1 [b]	3160	3156	3011	1401	1396	1408	599 **631**
$CH_3\{F_{11}\}$ [c]	3111	3085	2975	1426	1418	1335	Not determined

[a] Gas. [b] Dichloroethane solution. [c] Experiment.

Table S4. CH stretch frequencies (cm^{-1}, scaled by factor 0.9674) and their IR intensities (km/mol, in parentheses) calculated at the (SMD-)B3LYP-D3/def2-TZVPD level of theory for the carbocations paired with $\{F_{11}^-\}$ anion. The frequencies of C–H bonds affected by hyperconjugation are marked in bold.

$C_2H_5\{F_{11}\}$				*i*-Pr$\{F_{11}\}$				*t*-Bu$\{F_{11}\}$								*c*-$C_5H_9\{F_{11}\}$			
II.B.1 [a]		II.B.1.1 [b]		III.B.1 [a]		III.B.1.1 [b]		IV.B.1 [a]		IV.B.2 [a]		IV.B.1.1 [b]		IV.B.1.2 [b]		V.B.1 [a]		V.B.1.1 [b]	
2930	(2.4)	**2892**	(24.6)	**2916**	(9.4)	**2817**	(120.4)	**2863**	(72.5)	**2874**	(28.5)	**2859**	(83.8)	**2855**	(93.7)	**2806**	(20.7)	**2742**	(101.7)
3006	(2.8)	3005	(2.3)	**2923**	(1.4)	**2833**	(62.2)	**2873**	(173.0)	**2885**	(79.5)	**2869**	(72.2)	**2880**	(87.7)	**2902**	(88.4)	**2857**	(131.7)
3034	(1.6)	3059	(1.1)	2998	(0.4)	2977	(7.6)	**2884**	(27.9)	**2894**	(27.8)	**2893**	(66.6)	**2894**	(85.9)	2933	(12.8)	2960	(24.5)
3053	(0.6)	3064	(0.5)	3001	(5.3)	2985	(5.2)	2962	(0.0)	2956	(4.5)	2987	(3.3)	2980	(2.6)	2953	(16.3)	2973	(22.1)
3116	(1.5)	3154	(5.1)	3045	(1.4)	3062	(5.6)	2964	(4.6)	2990	(24.7)	2992	(0.4)	2987	(3.3)	2983	(7.6)	2992	(4.6)
				3050	(0.5)	3065	(4.5)	2995	(1.2)	2999	(2.4)	2995	(12.9)	2989	(3.6)	3012	(1.4)	3013	(3.8)
				3083	(1.9)	3106	(2.6)	3055	(0.0)	3056	(0.6)	3056	(0.3)	3052	(0.3)	3030	(7.7)	3028	(16.0)
								3064	(1.3)	3065	(3.2)	3062	(2.2)	3057	(0.1)	3045	(1.3)	3035	(16.3)
								3070	(1.2)	3066	(4.5)	3068	(3.7)	3060	(2.0)	3109	(2.5)	3103	(4.3)

[a] Gas. [b] Dichloroethane solution.

Table S5. Correlation between calculated CH stretch frequencies (cm^{-1}) of *t*-Bu^+ in the gas phase (B3LYP-D3/def2-TZVPD level of theory; frequencies were scaled by factor 0.9674), dichloroethane solution (SMD-B3LYP-D3/def2-TZVPD level of theory; frequencies were scaled by factor 0.9674) and *t*-Bu$\{Cl_{11}\}$ crystal (PBE-D3 periodic calculations, E_{cut}=400 eV; the frequencies of the same type are averaged and not scaled). The frequencies of C–H bonds affected by hyperconjugation are marked in bold.

set 1	*t*-Bu^+, IV.2 (gas phase)	**2835**	**2838**	**2852**	2974	2975	2977	3044	3046	3052
set 2	*t*-Bu$\{Cl_{11}\}$ (gas phase)	**2915**	**2920**	**2932**	3001	3015	3017	3042	3068	3071
set 3	*t*-Bu$\{Cl_{11}\}$ (dichloroethane solution)	**2839**	**2847**	**2859**	2982	2987	2988	3056	3057	3062
set 4	*t*-Bu$\{Cl_{11}\}$ (solid phase, fully relaxed structure)	**2833**	**2846**	**2879**	2998	3010	3017	3100	3105	3106
set 5	*t*-Bu$\{Cl_{11}\}$ (solid phase, experimental structure)	**2818**	**2828**	**2850**	2960	2979	2985	3061	3070	3075
ratio 1	set 1 / set 4	1.00	1.00	0.99	0.99	0.99	0.99	0.98	0.98	0.98
ratio 2	set 1 / set 5	1.01	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.99
ratio 3	set 2 / set 4	1.03	1.03	1.02	1.00	1.00	1.00	0.98	0.99	0.99
ratio 4	set 3 / set 4	1.00	1.00	0.99	0.99	0.99	0.99	0.99	0.98	0.99
ratio 5	set 5 / set 4	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99

Table S6. Values of electron density (atomic units) calculated at the bond critical points for C–H bonds of selected compounds.

Compound	$\rho(\mathbf{r}_{bcp})$
CH_4 [a]	0.28 / 0.28 / 0.28 / 0.28
CH_3F [a]	0.29 / 0.29 / 0.29
CH_3Cl [a]	0.29 / 0.29 / 0.29
CH_3^+, I.1 [a]	0.30 / 0.30 / 0.30
CH_3^+–Ar, I.A.1 [a]	0.30 / 0.30 / 0.30
$CH_3\{F_{11}\}$, I.B.1 [a]	0.30 / 0.30 / 0.30
$CH_3\{F_{11}\}$, I.B.1.1 [b]	0.30 / 0.30 / 0.30

[a] Gas (ZORA-B3LYP-D3/TZ2P//B3LYP-D3/def2-TZVPD level of theory).

[b] Dichloroethane solution (COSMO-ZORA-B3LYP-D3/TZ2P//SMD-B3LYP-D3/def2-TZVPD level of theory).

Cartesian coordinates (Å) and total energies (a.u.) for the most relevant species under study.

CH3+ (I.1)
E(B3LYP-D3/def2-TZVPD)=-39.4951355736 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.031175 a.u.

6	0.000000000	0.000000000	0.000000000
1	0.000000000	1.092104000	0.000000000
1	0.945790000	-0.546052000	0.000000000
1	-0.945790000	-0.546052000	0.000000000

C2H5+ (II.1)
E(B3LYP-D3/def2-TZVPD)=-78.8931651662 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.060249 a.u.

6	0.000000000	0.688635000	-0.063995000
6	0.000000000	-0.688635000	-0.063995000
1	-0.933606000	-1.244458000	-0.073808000
1	0.933606000	-1.244458000	-0.073808000
1	0.000000000	0.000000000	1.063175000
1	0.933606000	1.244458000	-0.073808000
1	-0.933606000	1.244458000	-0.073808000

C3H7+ (III.1)
E(B3LYP-D3/def2-TZVPD)=-118.259959945 a.u.,
E(CCSD(T)/def2-TZVPD)=-117.9613412 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.087914 a.u.

6	0.000000000	1.276858000	-0.197298000
6	0.000000000	0.000000000	0.454605000
1	0.000000000	0.000000000	1.545807000
1	-1.044608000	1.629339000	-0.017627000
1	0.596396000	2.025145000	0.335372000
1	0.172711000	1.253512000	-1.270678000
6	0.000000000	-1.276858000	-0.197298000
1	-0.172711000	-1.253512000	-1.270678000
1	1.044608000	-1.629339000	-0.017627000
1	-0.596396000	-2.025145000	0.335372000

C3H7+ (III.2)
E(B3LYP-D3/def2-TZVPD)=-118.259741255 a.u.,
E(CCSD(T)/def2-TZVPD)=-117.9606783 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.087575 a.u.

6	0.000000000	1.280966000	-0.201532000
6	0.000000000	0.000000000	0.442802000
1	0.000000000	0.000000000	1.534097000
1	-0.850826000	1.862739000	0.200448000
1	0.850826000	1.862739000	0.200448000
1	0.000000000	1.261775000	-1.287155000
6	0.000000000	-1.280966000	-0.201532000
1	0.850826000	-1.862739000	0.200448000
1	-0.850826000	-1.862739000	0.200448000
1	0.000000000	-1.261775000	-1.287155000

C4H9+ (IV.1)
E(B3LYP-D3/def2-TZVPD)=-157.619431551 a.u.,
E(CCSD(T)/def2-TZVPD)=-157.224943 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.116118 a.u.

6	0.002312000	0.000084000	-0.003915000
6	1.437053000	0.256135000	-0.009019000
1	2.053714000	-0.632056000	-0.118696000
1	1.692050000	1.027073000	-0.744335000
1	1.663534000	0.734249000	0.960997000
6	-0.494060000	-1.369697000	0.013227000
1	0.114904000	-2.010438000	0.658175000
1	-1.556838000	-1.462354000	0.222798000
1	-0.301636000	-1.755601000	-1.005501000
6	-0.940407000	1.113042000	-0.007239000
1	-0.487181000	2.090794000	-0.144238000
1	-1.732847000	0.931123000	-0.744245000
1	-1.475085000	1.079825000	0.956719000

C4H9+ (IV.2)
E(B3LYP-D3/def2-TZVPD)=-157.6193402 a.u.,
E(CCSD(T)/def2-TZVPD)=-157.2250928 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.116233 a.u.

6	-0.018757000	-0.005105000	0.000000000
6	0.022474000	1.451020000	0.000000000
1	0.447916000	1.876724000	0.908520000
1	0.447916000	1.876724000	-0.908520000
1	-1.048625000	1.737032000	0.000000000
6	-0.018757000	-0.727054000	1.267019000
1	-0.421424000	-0.137759000	2.091956000
1	-0.456138000	-1.721813000	1.210003000
1	1.055349000	-0.861091000	1.502144000
6	-0.018757000	-0.727054000	-1.267019000
1	-0.456138000	-1.721813000	-1.210003000
1	-0.421424000	-0.137759000	-2.091956000
1	1.055349000	-0.861091000	-1.502144000

C5H9+ (V.1)
E(B3LYP-D3/def2-TZVPD)=-195.714828178 a.u.,
E(CCSD(T)/def2-TZVPD)=-195.241718 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.125247 a.u.

6	0.000000000	0.000000000	1.247381000
6	0.000000000	1.190315000	0.441681000
6	0.000000000	-1.190315000	0.441681000
1	0.000000000	0.000000000	2.335390000
1	1.083799000	1.462139000	0.562221000
1	-0.529551000	2.053197000	0.851369000
1	0.529551000	-2.053197000	0.851369000
1	-1.083799000	-1.462139000	0.562221000
6	0.259223000	-0.725250000	-1.005968000
1	-0.231132000	-1.360062000	-1.739058000
6	-0.259223000	0.725250000	-1.005968000
1	0.231132000	1.360062000	-1.739058000
1	1.333540000	-0.759591000	-1.198646000
1	-1.333540000	0.759591000	-1.198646000

C5H9+ (V.2)
E(B3LYP-D3/def2-TZVPD)=-195.710497179 a.u.,
E(CCSD(T)/def2-TZVPD)=-195.2354327 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.124301 a.u.

6	0.000000000	0.000000000	1.245205000
6	0.000000000	1.199654000	0.457061000
6	0.000000000	-1.199654000	0.457061000
1	0.000000000	0.000000000	2.333754000
1	0.847714000	1.828175000	0.793125000
1	-0.847714000	1.828175000	0.793125000
1	0.847714000	-1.828175000	0.793125000
1	-0.847714000	-1.828175000	0.793125000
6	0.000000000	-0.779176000	-1.026833000
1	-0.874574000	-1.179333000	-1.535055000
6	0.000000000	0.779176000	-1.026833000
1	0.874574000	1.179333000	-1.535055000
1	0.874574000	-1.179333000	-1.535055000
1	-0.874574000	1.179333000	-1.535055000

CH3+Ar (I.A.1)
E(B3LYP-D3/def2-TZVPD)=-567.079253412 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.036284 a.u.

6	0.000000000	0.000000000	-1.357249000
1	0.000000000	1.074475000	-1.509421000
1	0.930523000	-0.537237000	-1.509421000
1	-0.930523000	-0.537237000	-1.509421000
18	0.000000000	0.000000000	0.703986000

C2H5+Ar (II.A.1)
E(B3LYP-D3/def2-TZVPD)=-606.448245077 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.061684 a.u.

6	-1.412666000	1.298149000	0.000000000
6	0.000000000	1.269221000	0.000000000
1	0.562359000	1.353664000	0.926430000
1	0.562359000	1.353664000	-0.926430000
1	-1.441418000	2.437690000	0.000000000
1	-1.908956000	1.003507000	-0.922808000
1	-1.908956000	1.003507000	0.922808000
18	0.700589000	-1.253125000	0.000000000

C3H7+Ar (III.A.1)
E(B3LYP-D3/def2-TZVPD)=-645.814797034 a.u.,
E(CCSD(T)/def2-TZVPD)=-644.9991001 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.088528 a.u.

6	-1.438448000	1.295936000	-0.158204000
6	-1.201689000	0.006904000	0.424067000
1	-0.706536000	-0.017378000	1.394852000
1	-2.312506000	1.650950000	0.440981000
1	-0.659211000	2.025260000	0.076456000
1	-1.737933000	1.284624000	-1.203976000
6	-1.582819000	-1.253540000	-0.147289000
1	-2.213354000	-1.191394000	-1.030809000
1	-0.604000000	-1.698001000	-0.438065000
1	-1.948314000	-1.957732000	0.608528000
18	1.973310000	-0.021785000	-0.031078000

C3H7+Ar (III.A.2)
E(B3LYP-D3/def2-TZVPD)=-645.814625983 a.u.,
E(CCSD(T)/def2-TZVPD)=-644.9986876 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.088328 a.u.

6	0.106156000	-1.468223000	1.280321000
6	-0.462794000	-1.153906000	0.000000000
1	-1.450620000	-0.692731000	0.000000000
1	-0.052920000	-0.646434000	1.990925000
1	-0.558582000	-2.256733000	1.695664000
1	1.132860000	-1.822358000	1.260227000
6	0.106156000	-1.468223000	-1.280321000
1	-0.558582000	-2.256733000	-1.695664000
1	-0.052920000	-0.646434000	-1.990925000
1	1.132860000	-1.822358000	-1.260227000
18	0.106156000	1.926994000	0.000000000

C4H9+Ar (IV.A.1)
E(B3LYP-D3/def2-TZVPD)=-685.173977486 a.u.,
E(CCSD(T)/def2-TZVPD)=-684.2630566 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.116760 a.u.

6	1.160906000	0.000014000	-0.032196000
6	1.093287000	-1.266857000	-0.751061000
1	0.743254000	-2.089568000	-0.126595000
1	0.564297000	-1.208724000	-1.699712000
1	2.150225000	-1.503388000	-0.981882000
6	1.347496000	-0.000150000	1.412450000
1	1.813929000	-0.908565000	1.792742000
1	1.814240000	0.908060000	1.792869000
1	0.310072000	0.000043000	1.800647000
6	1.093234000	1.267040000	-0.750778000
1	0.563699000	1.209171000	-1.699149000
1	0.743818000	2.089780000	-0.126023000
1	2.150109000	1.503205000	-0.982284000
18	-2.167954000	-0.000016000	0.053272000

C4H9+Ar (IV.A.2)
E(B3LYP-D3/def2-TZVPD)=-685.173936445 a.u.,
E(CCSD(T)/def2-TZVPD)=-684.2627866 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.116641 a.u.

6	1.220827000	-0.001614000	0.019172000
6	1.081390000	-0.189086000	1.456986000
1	0.511934000	0.612423000	1.931002000
1	0.733508000	-1.178534000	1.746075000
1	2.113642000	-0.072939000	1.841489000
6	1.285243000	1.343977000	-0.535601000
1	1.453442000	2.122681000	0.205172000
1	1.972176000	1.413769000	-1.381361000
1	0.280553000	1.508569000	-0.969775000
6	1.267790000	-1.165219000	-0.858776000
1	1.592909000	-0.953473000	-1.873635000
1	1.840378000	-1.980902000	-0.406076000
1	0.232379000	-1.548546000	-0.886644000
18	-2.214579000	0.008256000	-0.038718000

C5H9+Ar (V.A.1)
E(B3LYP-D3/def2-TZVPD)=-723.269665349 a.u.,
E(CCSD(T)/def2-TZVPD)=-722.2796998 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.125762 a.u.

6	-0.433640000	0.339037000	1.066740000
6	-1.036640000	1.261248000	0.141578000
6	-0.776112000	-1.023547000	0.762875000
1	0.198223000	0.636673000	1.900034000
1	-0.129311000	1.502180000	-0.470553000
1	-1.335043000	2.227542000	0.554568000
1	-0.020838000	-1.775708000	0.996741000
1	-1.560227000	-1.170251000	1.553857000
6	-1.446497000	-0.991990000	-0.625400000
1	-2.193572000	-1.772313000	-0.742964000
6	-2.029288000	0.431786000	-0.699160000
1	-2.125866000	0.807091000	-1.714397000
1	-0.679262000	-1.143581000	-1.387390000
1	-3.014325000	0.477914000	-0.230317000
18	2.510738000	0.006181000	-0.241076000

C5H9+Ar (V.A.2)
E(B3LYP-D3/def2-TZVPD)=-723.265488936 a.u.,
E(CCSD(T)/def2-TZVPD)=-722.2739738 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.124990 a.u.

6	-0.930338000	-0.922401000	0.000000000
6	-1.046280000	-0.139298000	1.199051000
6	-1.046280000	-0.139298000	-1.199051000
1	-0.825947000	-2.005419000	0.000000000
1	-0.318263000	-0.456463000	1.959558000
1	-1.996245000	-0.491708000	1.660260000
1	-0.318263000	-0.456463000	-1.959558000
1	-1.996245000	-0.491708000	-1.660260000
6	-1.046280000	1.344479000	-0.779250000
1	-1.912243000	1.862317000	-1.185083000
6	-1.046280000	1.344479000	0.779250000
1	-0.162525000	1.841030000	1.174691000
1	-0.162525000	1.841030000	-1.174691000
1	-1.912243000	1.862317000	1.185083000
18	2.238735000	-0.690705000	0.000000000

CH3{F11} (I.B.1)
E(B3LYP-D3/def2-TZVPD)=-1451.53428550 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.137804 a.u.

5	-0.681804000	0.117244000	1.492100000
5	-0.681804000	0.117244000	-1.492100000
5	-0.678243000	-1.566413000	-0.909061000
5	-1.648477000	-0.373888000	0.000000000
5	-0.678243000	-1.566413000	0.909061000
5	0.872048000	0.908615000	0.918866000
5	1.809665000	-0.292691000	0.000000000
5	0.872048000	0.908615000	-0.918866000
5	0.859218000	-0.781939000	-1.470643000
5	-0.634059000	1.078977000	0.000000000
5	0.859218000	-0.781939000	1.470643000
6	0.784045000	-1.674820000	0.000000000
1	1.277060000	-2.640276000	0.000000000
9	-1.142886000	-2.647678000	-1.563869000
9	-1.142886000	-2.647678000	1.563869000
9	1.512341000	-1.285568000	-2.535806000
9	3.149196000	-0.438858000	0.000000000
9	1.512341000	-1.285568000	2.535806000
9	-1.304492000	0.563021000	-2.612999000
9	1.406430000	1.963949000	-1.604487000
9	1.406430000	1.963949000	1.604487000
9	-1.304492000	0.563021000	2.612999000
9	-3.003006000	-0.318172000	0.000000000
9	-1.350250000	2.414062000	0.000000000
6	-0.594034000	3.732290000	0.000000000
1	-0.005169000	3.703363000	-0.909348000
1	-1.403165000	4.451352000	0.000000000
1	-0.005169000	3.703363000	0.909348000

C2H5{F11} (II.B.1)
E(B3LYP-D3/def2-TZVPD)=-1490.88082500 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.165627 a.u.

5	0.291576000	0.769712000	1.474283000
5	-0.178166000	-1.517318000	-0.364544000
5	1.577256000	-1.331269000	-0.124568000
5	0.504994000	-1.051564000	1.273145000
5	1.863298000	0.068570000	0.998174000
5	-0.518419000	1.414997000	-0.044546000
5	0.570783000	1.106512000	-1.423145000
5	-0.798629000	0.003319000	-1.175739000
5	0.776845000	-0.689354000	-1.620079000
5	-0.898143000	-0.202953000	0.586638000
5	1.240337000	1.574479000	0.194618000
6	1.889062000	0.259383000	-0.715200000
1	2.862361000	0.421228000	-1.164062000
9	2.518526000	-2.288525000	-0.240740000
9	3.014565000	0.127019000	1.695961000
9	1.123406000	-1.181471000	-2.826603000
9	0.770010000	1.910876000	-2.486832000
9	1.939755000	2.720487000	0.311168000
9	-0.850182000	-2.692184000	-0.540881000
9	-1.913765000	-0.047163000	-1.970267000
9	-1.421285000	2.434243000	0.011064000
9	0.023367000	1.310320000	2.689560000
9	0.386867000	-1.887139000	2.336096000
9	-2.208540000	-0.444700000	1.252679000
6	-4.197886000	0.483448000	0.133718000
6	-3.546222000	-0.803916000	0.459241000
1	-3.151336000	-1.377914000	-0.372118000
1	-4.014858000	-1.415282000	1.222260000
1	-5.113886000	0.226807000	-0.411760000
1	-4.475350000	1.037092000	1.028937000
1	-3.579826000	1.093060000	-0.521849000

C3H7{F11} (III.B.1)
E(B3LYP-D3/def2-TZVPD)=-1530.22751924 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.192220 a.u.

5	0.117934000	1.432940000	-0.701300000
5	-0.321635000	-0.919630000	1.040805000
5	0.955066000	0.088054000	1.761999000
5	-0.407358000	0.903854000	0.963716000
5	1.230695000	1.529593000	0.691155000
5	0.539188000	-0.074746000	-1.662973000
5	1.902501000	-0.883406000	-0.838937000
5	0.265229000	-1.533413000	-0.576052000
5	1.373551000	-1.403567000	0.816646000
5	-0.774300000	-0.090879000	-0.465452000
5	1.813525000	0.929336000	-0.916039000
6	2.176291000	0.098360000	0.552731000
1	3.201060000	0.162796000	0.899767000
9	1.285728000	0.162429000	3.068417000
9	1.766766000	2.648668000	1.221087000
9	2.018561000	-2.414655000	1.434209000
9	2.939429000	-1.513786000	-1.427273000
9	2.786021000	1.606933000	-1.559379000
9	-1.269861000	-1.608473000	1.753634000
9	-0.200897000	-2.708517000	-1.078279000
9	0.305717000	-0.142605000	-2.998862000
9	-0.466600000	2.512367000	-1.291739000
9	-1.409070000	1.568143000	1.627853000
9	-2.146427000	-0.193309000	-0.936648000
6	-4.019069000	1.302751000	-0.221852000
6	-3.548402000	-0.051557000	0.121703000
1	-3.003811000	-0.135025000	1.056348000
1	-4.832568000	1.522423000	0.482060000
1	-3.241284000	2.045691000	-0.056408000
1	-4.413528000	1.359313000	-1.234913000
6	-4.297498000	-1.256130000	-0.283023000
1	-4.669503000	-1.187762000	-1.304022000
1	-3.705881000	-2.158525000	-0.140250000
1	-5.158705000	-1.314885000	0.395044000

C4H9{F11} (IV.B.1)
E(B3LYP-D3/def2-TZVPD)=-1569.57421592 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.217607 a.u.

5	1.122115000	0.394533000	0.000000000
5	-1.396908000	-0.822037000	0.916321000
5	-0.029001000	-1.827910000	1.468685000
5	0.164165000	-0.058381000	1.468382000
5	1.515929000	-1.076048000	0.906593000
5	0.164165000	-0.058381000	-1.468382000
5	-0.029001000	-1.827910000	-1.468685000
5	-1.396908000	-0.822037000	-0.916321000
5	-0.982158000	-2.296415000	0.000000000
5	-0.669397000	0.532939000	0.000000000
5	1.515929000	-1.076048000	-0.906593000
6	0.741233000	-2.309828000	0.000000000
1	1.213860000	-3.284875000	0.000000000
9	-0.009254000	-2.653630000	2.538082000
9	2.668892000	-1.329298000	1.567396000
9	-1.657428000	-3.466475000	0.000000000
9	-0.009254000	-2.653630000	-2.538082000
9	2.668892000	-1.329298000	-1.567396000
9	-2.547789000	-0.667626000	1.626743000
9	-2.547789000	-0.667626000	-1.626743000
9	0.225840000	0.742579000	-2.585097000
9	1.921404000	1.520766000	0.000000000
9	0.225840000	0.742579000	2.585097000
9	-1.263561000	1.794292000	0.000000000
6	-0.066371000	4.024805000	0.000000000
6	-1.440893000	4.534953000	0.000000000
1	-1.986808000	4.259187000	-0.899960000
1	-1.986808000	4.259187000	0.899960000
1	-1.332825000	5.632265000	0.000000000
6	0.607195000	3.814870000	-1.274303000
1	0.264128000	4.529920000	-2.026030000
1	1.688412000	3.761762000	-1.198657000
1	0.260282000	2.833802000	-1.642836000
6	0.607195000	3.814870000	1.274303000
1	1.688412000	3.761762000	1.198657000
1	0.264128000	4.529920000	2.026030000
1	0.260282000	2.833802000	1.642836000

C4H9{F11} (IV.B.2)
E(B3LYP-D3/def2-TZVPD)=-1569.57449525 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.217910 a.u.

5	0.680149000	-1.041419000	-1.302052000
5	0.116330000	1.510735000	0.077238000
5	1.867721000	1.411700000	-0.239141000
5	0.744426000	0.782408000	-1.474285000
5	2.211965000	-0.155601000	-1.081886000
5	0.014414000	-1.418164000	0.352417000
5	1.145909000	-0.778286000	1.570547000
5	-0.318399000	0.151580000	1.198230000
5	1.211477000	1.025273000	1.399381000
5	-0.582351000	-0.005598000	-0.567770000
5	1.763522000	-1.509769000	0.036303000
6	2.352033000	-0.000238000	0.628705000
1	3.358335000	0.001466000	1.030555000
9	2.730647000	2.441958000	-0.377751000
9	3.327303000	-0.266368000	-1.835807000
9	1.573970000	1.775137000	2.464919000
9	1.460451000	-1.341307000	2.759355000
9	2.547487000	-2.608468000	0.098483000
9	-0.618737000	2.666621000	0.091018000
9	-1.378450000	0.275364000	2.074406000
9	-0.811179000	-2.497702000	0.565455000
9	0.407805000	-1.844708000	-2.367220000
9	0.527999000	1.386327000	-2.674945000
9	-1.879386000	-0.022854000	-1.097354000
6	-3.953571000	0.016837000	-0.080406000
6	-3.771739000	1.404462000	0.341244000
1	-3.720636000	2.110114000	-0.482479000
1	-4.657067000	1.630130000	0.959537000
1	-2.918684000	1.507083000	1.012600000
6	-4.529492000	-0.281238000	-1.397261000
1	-4.182001000	0.410917000	-2.160922000
1	-4.375349000	-1.315553000	-1.697508000
1	-5.613432000	-0.122753000	-1.278864000
6	-3.775026000	-1.073262000	0.876663000
1	-3.607127000	-0.737399000	1.895002000
1	-4.600542000	-1.786648000	0.798375000
1	-2.883745000	-1.637001000	0.560112000

C5H9{F11} (V.B.1)
E(B3LYP-D3/def2-TZVPD)=-1607.67217545 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.227497 a.u.

5	1.012404000	-0.723158000	-1.478333000
5	0.215443000	1.469395000	0.347160000
5	1.994391000	1.435812000	0.236226000
5	1.049949000	1.094553000	-1.238614000
5	2.481663000	0.090097000	-0.880273000
5	0.159234000	-1.452268000	-0.043135000
5	1.112993000	-1.095806000	1.417422000
5	-0.320324000	-0.103808000	1.079238000
5	1.152230000	0.700601000	1.656747000
5	-0.352188000	0.128563000	-0.693332000
5	1.935281000	-1.474567000	-0.149940000
6	2.405169000	-0.133463000	0.826780000
1	3.354011000	-0.220923000	1.342823000
9	2.842691000	2.468043000	0.432475000
9	3.683033000	0.148481000	-1.493894000
9	1.366352000	1.193900000	2.896719000
9	1.293019000	-1.910012000	2.481731000
9	2.731345000	-2.562988000	-0.228907000
9	-0.540744000	2.595242000	0.511349000
9	-1.484546000	-0.187626000	1.808779000
9	-0.656730000	-2.551890000	-0.171716000
9	0.885748000	-1.269959000	-2.719188000
9	0.963119000	1.945272000	-2.296342000
9	-1.573029000	0.262234000	-1.391948000
6	-3.574958000	-0.407526000	-1.269360000
6	-3.668527000	-1.251896000	-0.088729000
6	-4.123342000	0.918970000	-1.022649000
1	-3.345869000	-0.787140000	-2.256929000
1	-2.644107000	-1.536768000	0.195877000
1	-4.127431000	-2.215362000	-0.340406000
1	-3.664955000	1.710725000	-1.613505000
1	-5.160847000	0.810942000	-1.404364000
6	-4.133955000	1.055115000	0.510240000
1	-4.895580000	1.749310000	0.858414000
6	-4.365089000	-0.390518000	0.987722000
1	-3.954463000	-0.574271000	1.975843000

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1       -3.162012000      1.419098000      0.842955000
1       -5.432246000     -0.623026000      1.007922000

C4H9{Cl11} (IV.C.1)
E(B3LYP-D3/def2-TZVPD)=-5533.25403355 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.205467 a.u.
5       -1.330773000     -0.483592000      0.910283000
5        0.289061000      0.106115000     -1.466188000
5       -0.094266000     -1.640875000     -1.458631000
5       -1.330773000     -0.483592000     -0.910283000
5       -1.090044000     -1.997864000      0.000000000
5        0.289061000      0.106115000      1.466188000
5        1.511135000     -1.065729000      0.901798000
5        1.292694000      0.457055000      0.000000000
5        1.511135000     -1.065729000     -0.901798000
5       -0.456902000      0.782452000      0.000000000
5       -0.094266000     -1.640875000      1.458631000
6        0.612124000     -2.213746000      0.000000000
1        0.977864000     -3.230945000      0.000000000
17      -0.223569000     -2.659893000     -2.900385000
17      -2.206369000     -3.371622000      0.000000000
17       2.979137000     -1.510153000     -1.788052000
17       2.979137000     -1.510153000      1.788052000
17      -0.223569000     -2.659893000      2.900385000
17       0.481714000      1.043478000     -2.974501000
17       2.610663000      1.673130000      0.000000000
17       0.481714000      1.043478000      2.974501000
17      -2.813525000     -0.159620000      1.844157000
17      -2.813525000     -0.159620000     -1.844157000
17      -1.327439000      2.426303000      0.000000000
6       -0.276100000      4.312160000      0.000000000
6        0.496010000      4.281962000     -1.277956000
1       -0.151794000      4.165250000     -2.143570000
1        0.996538000      5.255542000     -1.350352000
1        1.259854000      3.511364000     -1.283675000
6       -1.500164000      5.180831000      0.000000000
1       -2.107136000      5.041987000     -0.892769000
1       -2.107136000      5.041987000      0.892769000
1       -1.134625000      6.213838000      0.000000000
6        0.496010000      4.281962000      1.277956000
1        1.259854000      3.511364000      1.283675000
1        0.996538000      5.255542000      1.350352000
1       -0.151794000      4.165250000      2.143570000
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CH3{F11} (I.B.1.1)
E(SMD-B3LYP-D3/def2-TZVPD)=-1451.56646531 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.137565 a.u.

5	-0.661553000	0.163821000	1.484590000
5	-0.661553000	0.163821000	-1.484590000
5	-0.750074000	-1.520757000	-0.904087000
5	-1.648021000	-0.271549000	0.000000000
5	-0.750074000	-1.520757000	0.904087000
5	0.932471000	0.868278000	0.918688000
5	1.789339000	-0.398413000	0.000000000
5	0.932471000	0.868278000	-0.918688000
5	0.820047000	-0.828644000	-1.461084000
5	-0.571306000	1.152543000	0.000000000
5	0.820047000	-0.828644000	1.461084000
6	0.696474000	-1.723754000	0.000000000
1	1.134805000	-2.716877000	0.000000000
9	-1.292159000	-2.568427000	-1.571547000
9	-1.292159000	-2.568427000	1.571547000
9	1.442916000	-1.359930000	-2.541039000
9	3.127469000	-0.613112000	0.000000000
9	1.442916000	-1.359930000	2.541039000
9	-1.263382000	0.606916000	-2.625137000
9	1.575237000	1.841732000	-1.629223000
9	1.575237000	1.841732000	1.629223000
9	-1.263382000	0.606916000	2.625137000
9	-3.007791000	-0.164759000	0.000000000
9	-1.257536000	2.464867000	0.000000000
6	-0.550824000	3.847892000	0.000000000
1	0.025593000	3.835726000	-0.916758000
1	-1.405144000	4.512492000	0.000000000
1	0.025593000	3.835726000	0.916758000

C2H5{F11} (II.B.1.1)
E(SMD-B3LYP-D3/def2-TZVPD)=-1490.91551550 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.164491 a.u.

5	-0.243563000	0.899584000	-1.384260000
5	0.113238000	-1.564730000	0.216943000
5	-1.632196000	-1.271016000	-0.006946000
5	-0.531398000	-0.911406000	-1.362309000
5	-1.848359000	0.229305000	-0.986080000
5	0.576289000	1.359900000	0.184958000
5	-0.542937000	0.967029000	1.516102000
5	0.794634000	-0.163178000	1.172827000
5	-0.822972000	-0.816290000	1.537560000
5	0.928385000	-0.204589000	-0.609690000
5	-1.175990000	1.614255000	-0.043023000
6	-1.893561000	0.257855000	0.730962000
1	-2.864267000	0.416759000	1.190638000
9	-2.611039000	-2.209474000	0.000663000
9	-2.988563000	0.397141000	-1.701481000
9	-1.196947000	-1.417209000	2.694755000
9	-0.713175000	1.677804000	2.658624000
9	-1.817534000	2.809354000	-0.060904000
9	0.668933000	-2.810336000	0.301078000
9	1.872309000	-0.325381000	2.001038000
9	1.486841000	2.376656000	0.244070000
9	0.033271000	1.558388000	-2.547607000
9	-0.477637000	-1.649907000	-2.509227000
9	2.186285000	-0.413170000	-1.291536000
6	4.246662000	0.464111000	-0.108694000
6	3.667275000	-0.810290000	-0.521036000
1	3.262439000	-1.465640000	0.241117000
1	4.088667000	-1.314326000	-1.382180000
1	5.199669000	0.169204000	0.360684000
1	4.477780000	1.112800000	-0.951420000
1	3.653109000	0.972034000	0.648098000

C3H7{F11} (III.B.1.1)
E(SMD-B3LYP-D3/def2-TZVPD)=-1530.26955513 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.189425 a.u.

5	0.312736000	-1.483419000	0.662847000
5	-0.435353000	0.900358000	-0.890918000
5	0.829779000	0.015842000	-1.780449000
5	-0.411120000	-0.917535000	-0.905070000
5	1.289710000	-1.442463000	-0.829805000
5	0.736743000	-0.012447000	1.649181000
5	1.967322000	0.913187000	0.746448000
5	0.271817000	1.461587000	0.686034000
5	1.249603000	1.471039000	-0.806873000
5	-0.738448000	-0.024542000	0.621440000
5	1.992545000	-0.888300000	0.731881000
6	2.171711000	0.026346000	-0.710380000
1	3.159256000	0.042175000	-1.159733000
9	1.023730000	0.029616000	-3.125928000
9	1.828878000	-2.515762000	-1.466360000
9	1.758215000	2.568213000	-1.427260000
9	3.014409000	1.594152000	1.282625000
9	3.059201000	-1.547983000	1.256567000
9	-1.430519000	1.604870000	-1.523368000
9	-0.167908000	2.607731000	1.294702000
9	0.671041000	-0.023900000	3.017220000
9	-0.093878000	-2.650945000	1.253606000
9	-1.388909000	-1.638897000	-1.545842000
9	-2.002037000	-0.045139000	1.196413000
6	-4.480348000	-1.269183000	0.334733000
6	-3.957542000	-0.014406000	-0.134980000
1	-3.286547000	-0.046598000	-0.989613000
1	-5.213484000	-1.535446000	-0.454919000
1	-3.734818000	-2.064961000	0.283098000
1	-4.994405000	-1.214474000	1.290589000
6	-4.404349000	1.281461000	0.297261000
1	-4.895322000	1.287896000	1.266998000
1	-3.632562000	2.044267000	0.189001000
1	-5.155612000	1.537688000	-0.480176000

C4H9{F11} (IV.B.1.1)
E(SMD-B3LYP-D3/def2-TZVPD)=-1569.62223900 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.216440 a.u.

5	0.761027000	-0.965826000	-1.348840000
5	0.158047000	1.503539000	0.134715000
5	1.921596000	1.407688000	-0.123797000
5	0.834877000	0.850676000	-1.421782000
5	2.289550000	-0.103931000	-1.030027000
5	0.039092000	-1.431181000	0.252091000
5	1.136484000	-0.853464000	1.533449000
5	-0.328205000	0.091728000	1.168782000
5	1.209606000	0.943755000	1.461433000
5	-0.550112000	0.029632000	-0.619766000
5	1.802964000	-1.501903000	-0.005905000
6	2.381669000	-0.037862000	0.683215000
1	3.374328000	-0.060620000	1.120758000
9	2.787203000	2.454600000	-0.190957000
9	3.426766000	-0.179600000	-1.771530000
9	1.536996000	1.644804000	2.580145000
9	1.406880000	-1.486889000	2.706539000
9	2.577133000	-2.619609000	0.018107000
9	-0.528928000	2.690279000	0.179569000
9	-1.386811000	0.164011000	2.041168000
9	-0.742272000	-2.551801000	0.391940000
9	0.552083000	-1.718980000	-2.474893000
9	0.681791000	1.524565000	-2.605312000
9	-1.802284000	0.058448000	-1.197715000
6	-4.231691000	0.022549000	-0.083105000
6	-3.988720000	1.368324000	0.412473000
1	-3.808132000	2.097329000	-0.372758000
1	-4.936841000	1.635533000	0.914957000
1	-3.230094000	1.387362000	1.194337000
6	-4.741121000	-0.189910000	-1.429812000
1	-4.470663000	0.601329000	-2.124362000
1	-4.513045000	-1.185016000	-1.810373000
1	-5.838428000	-0.155718000	-1.298051000
6	-4.044395000	-1.118052000	0.799720000
1	-4.076487000	-0.855285000	1.855106000
1	-4.692888000	-1.956316000	0.545678000
1	-3.013849000	-1.450901000	0.584443000

C4H9{F11} (IV.B.1.2)
E(SMD-B3LYP-D3/def2-TZVPD)=-1569.62175527 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.216636 a.u.

5	1.106146000	0.390336000	-0.006304000
5	-1.376372000	-0.875101000	0.927134000
5	0.005293000	-1.868007000	1.458105000
5	0.170291000	-0.090639000	1.471392000
5	1.522988000	-1.093812000	0.884979000
5	0.138597000	-0.083135000	-1.467037000
5	-0.027131000	-1.860190000	-1.459098000
5	-1.396698000	-0.870204000	-0.892267000
5	-0.953010000	-2.343723000	0.008591000
5	-0.692299000	0.516016000	0.012871000
5	1.503395000	-1.088949000	-0.914939000
6	0.762693000	-2.342500000	-0.010289000
1	1.254291000	-3.309865000	-0.018426000
9	0.039303000	-2.691708000	2.539251000
9	2.691833000	-1.331178000	1.539166000
9	-1.633314000	-3.520729000	0.013078000
9	-0.017139000	-2.678262000	-2.545038000
9	2.657745000	-1.322735000	-1.595504000
9	-2.532327000	-0.757958000	1.654022000
9	-2.568714000	-0.748802000	-1.592126000
9	0.180369000	0.665375000	-2.616868000
9	1.923407000	1.493710000	-0.009480000
9	0.236897000	0.653995000	2.622480000
9	-1.328695000	1.737576000	0.022373000
6	-0.075271000	4.262296000	-0.000954000
6	-1.471359000	4.664682000	-0.041079000
1	-1.972977000	4.393640000	-0.968222000
1	-2.025264000	4.367707000	0.848076000
1	-1.411771000	5.769454000	-0.018939000
6	0.643448000	4.040864000	-1.245864000
1	0.240059000	4.641463000	-2.062492000
1	1.722837000	4.122656000	-1.149933000
1	0.410933000	2.994056000	-1.509320000
6	0.576264000	4.065751000	1.283799000
1	1.649943000	4.239434000	1.253514000
1	0.078184000	4.600187000	2.092173000
1	0.435666000	2.990107000	1.493174000

C5H9{F11} (V.B.1.1)
E(SMD-B3LYP-D3/def2-TZVPD)=-1607.72030103 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.225493 a.u.

5	-1.045990000	1.003128000	-1.295935000
5	-0.392945000	-1.550556000	0.012576000
5	-2.165783000	-1.357520000	-0.010932000
5	-1.226120000	-0.802610000	-1.420810000
5	-2.565094000	0.205314000	-0.811540000
5	-0.102416000	1.368937000	0.213995000
5	-1.052367000	0.792719000	1.607445000
5	0.299589000	-0.210008000	1.021807000
5	-1.232780000	-0.993594000	1.484006000
5	0.291363000	-0.082915000	-0.773853000
5	-1.877006000	1.533233000	0.189660000
6	-2.439743000	0.074735000	0.896598000
1	-3.364869000	0.128951000	1.461372000
9	-3.085840000	-2.358502000	0.000980000
9	-3.782123000	0.365761000	-1.395891000
9	-1.454099000	-1.723517000	2.609997000
9	-1.143284000	1.394435000	2.823586000
9	-2.578023000	2.686948000	0.352442000
9	0.229008000	-2.769591000	-0.071689000
9	1.464062000	-0.380297000	1.728784000
9	0.741689000	2.451076000	0.282956000
9	-0.938890000	1.793724000	-2.410804000
9	-1.264167000	-1.436006000	-2.635427000
9	1.462790000	-0.155167000	-1.501363000
6	3.902799000	0.632322000	-1.177820000
6	3.916026000	1.210907000	0.138556000
6	4.385706000	-0.720684000	-1.171983000
1	3.600625000	1.165035000	-2.072593000
1	2.825181000	1.203861000	0.362901000
1	4.184866000	2.268256000	0.174083000
1	3.938641000	-1.387473000	-1.908532000
1	5.419922000	-0.522107000	-1.553064000
6	4.447208000	-1.136989000	0.307478000
1	5.237298000	-1.858433000	0.501069000
6	4.651341000	0.201971000	1.038380000
1	4.262712000	0.199221000	2.053525000

```
1        3.492528000     -1.585787000      0.585386000
1        5.710697000      0.464498000      1.074368000

C4H9{Cl11} (IV.C.1.1)
E(SMD-B3LYP-D3/def2-TZVPD)=-5533.30961797 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.202470 a.u.
5        0.667648000     -1.293973000     -0.958492000
5        0.267975000      1.529377000     -0.346200000
5        2.015507000      1.176533000     -0.254932000
5        1.027590000      0.383805000     -1.512466000
5        2.260263000     -0.558623000     -0.631827000
5       -0.311316000     -1.181799000      0.548906000
5        0.683740000     -0.382362000      1.794243000
5       -0.556192000      0.559682000      0.927163000
5        1.041187000      1.284953000      1.243630000
5       -0.563847000     -0.001237000     -0.776989000
5        1.437073000     -1.521988000      0.635057000
6        2.146848000     -0.000537000      0.986549000
1        3.054234000     -0.001423000      1.576780000
17       3.313567000      2.354363000     -0.565779000
17       3.802700000     -1.115543000     -1.323659000
17       1.357921000      2.572038000      2.431819000
17       0.638338000     -0.763576000      3.532690000
17       2.151910000     -3.046132000      1.213251000
17      -0.342949000      3.134211000     -0.853632000
17      -2.026260000      1.150072000      1.768674000
17      -1.527718000     -2.426368000      0.982943000
17       0.478537000     -2.653276000     -2.107622000
17       1.220648000      0.786418000     -3.245591000
17      -2.065977000     -0.006145000     -1.763933000
6       -5.317513000      0.011856000     -0.353853000
6       -5.193351000      1.434036000     -0.082997000
1       -4.107515000      1.620515000     -0.190256000
1       -5.683366000      2.053418000     -0.833118000
1       -5.455230000      1.705387000      0.937819000
6       -5.593072000     -0.441272000     -1.706935000
1       -5.278765000      0.268545000     -2.470811000
1       -5.258914000     -1.459596000     -1.898553000
1       -6.699901000     -0.456850000     -1.738180000
6       -5.117767000     -0.965003000      0.702237000
1       -5.273761000     -0.572921000      1.703849000
1       -5.660110000     -1.892985000      0.515149000
1       -4.047871000     -1.233494000      0.611091000
```

C4H9{Cl11} (VASP, experimental structure)
E(PBE-D3, Ecut=400 eV)=-780.30711 eV

1	4.536750000	1.348690000	3.185140000
1	6.186300000	10.569090000	11.860240000
1	4.536750000	4.610190000	11.683630000
1	6.186300000	7.307600000	3.361750000
1	7.294190000	3.672480000	0.231390000
1	3.428860000	8.245310000	14.813990000
1	7.294190000	2.286420000	8.729890000
1	3.428860000	9.631370000	6.315490000
1	7.977930000	1.964160000	0.260620000
1	2.745120000	9.953630000	14.784760000
1	7.977930000	3.994750000	8.759120000
1	2.745120000	7.923040000	6.286260000
1	6.668020000	2.357470000	-0.823100000
1	4.055030000	9.560320000	15.868480000
1	6.668020000	3.601430000	7.675390000
1	4.055030000	8.316360000	7.369990000
1	7.720430000	4.572130000	14.357080000
1	3.002610000	7.345660000	0.688300000
1	7.720430000	1.386780000	5.858580000
1	3.002610000	10.531010000	9.186800000
1	9.494340000	4.561700000	14.373950000
1	1.228710000	7.356090000	0.671430000
1	9.494340000	1.397190000	5.875450000
1	1.228710000	10.520600000	9.169930000
1	8.514400000	5.195300000	-1.191230000
1	2.208650000	6.722490000	16.236610000
1	8.514400000	0.763600000	7.307240000
1	2.208650000	11.154190000	7.738140000
1	9.407320000	2.165030000	13.815880000
1	1.315730000	9.752760000	1.229500000
1	9.407320000	3.793860000	5.317380000
1	1.315730000	8.123930000	9.728000000
1	8.779110000	0.997440000	15.098770000
1	1.943940000	10.920350000	-0.053390000
1	8.779110000	4.961450000	6.600280000
1	1.943940000	6.956340000	8.445100000
1	10.196040000	2.047420000	-1.618720000
1	0.527010000	9.870370000	16.664100000
1	10.196040000	3.911480000	6.879770000
1	0.527010000	8.006310000	8.165610000
5	2.524210000	1.438360000	4.532950000
5	8.198840000	10.479430000	10.512430000
5	2.524210000	4.520540000	13.031440000
5	8.198840000	7.397250000	2.013940000
5	2.312430000	2.310500000	2.987370000
5	8.410620000	9.607290000	12.058010000
5	2.312430000	3.648390000	11.485870000
5	8.410620000	8.269400000	3.559510000
5	3.590180000	3.567350000	2.874650000
5	7.132860000	8.350440000	12.170730000
5	3.590180000	2.391540000	11.373140000
5	7.132860000	9.526250000	3.672240000
5	4.584100000	3.474750000	4.360820000
5	6.138950000	8.443040000	10.684560000
5	4.584100000	2.484140000	12.859310000
5	6.138950000	9.433650000	2.186070000
5	3.926780000	2.161650000	5.383840000
5	6.796270000	9.756140000	9.661540000
5	3.926780000	3.797250000	13.882340000
5	6.796270000	8.120540000	1.163040000
5	2.270710000	2.593070000	5.863890000
5	8.452340000	9.324720000	9.181490000
5	2.270710000	3.365820000	14.362380000
5	8.452340000	8.551970000	0.683000000
5	1.263180000	2.699020000	4.379850000
5	9.459870000	9.218770000	10.665530000
5	1.263180000	3.259870000	12.878350000
5	9.459870000	8.657920000	2.167030000
5	1.926400000	4.012600000	3.345560000
5	8.796650000	7.905190000	11.699820000
5	1.926400000	1.946290000	11.844050000
5	8.796650000	9.971500000	3.201330000
5	3.333150000	4.731840000	4.197390000
5	7.389900000	7.185950000	10.847990000
5	3.333150000	1.227060000	12.695890000
5	7.389900000	10.690730000	2.349490000
5	3.551470000	3.859340000	5.759450000
5	7.171580000	8.058450000	9.285930000

```
5        3.551470000      2.099560000     14.257950000
5        7.171580000      9.818230000      0.787430000
5        1.906560000      4.189220000      5.139460000
5        8.816490000      7.728570000      9.905920000
5        1.906560000      1.769670000     13.637960000
5        8.816490000     10.148120000      1.407420000
6        3.871130000      2.072980000      3.670980000
6        6.851920000      9.844810000     11.374400000
6        3.871130000      3.885910000     12.169480000
6        6.851920000      8.031880000      2.875900000
6        8.464240000      3.080510000     -1.482880000
6        2.258810000      8.837280000     16.528260000
6        8.464240000      2.878380000      7.015610000
6        2.258810000      9.039410000      8.029770000
6        7.590100000      2.794840000     -0.358700000
6        3.132950000      9.122950000     15.404080000
6        7.590100000      3.164050000      8.139800000
6        3.132950000      8.753740000      6.905580000
6        8.612750000      4.428290000     15.019320000
6        2.110300000      7.489500000      0.026060000
6        8.612750000      1.530600000      6.520820000
6        2.110300000     10.387190000      8.524560000
6        9.190400000      1.994560000     14.883590000
6        1.532650000      9.923230000      0.161790000
6        9.190400000      3.964330000      6.385100000
6        1.532650000      7.953460000      8.660280000
17       2.248070000     11.614760000      4.612340000
17       8.474980000      0.303030000     10.433040000
17       2.248070000      6.261930000     13.110830000
17       8.474980000      5.655860000      1.934550000
17       1.824420000      1.428840000      1.533900000
17       8.898630000     10.488950000     13.511480000
17       1.824420000      4.530060000     10.032390000
17       8.898630000      7.387730000      5.012990000
17       4.355400000      3.943410000      1.332430000
17       6.367650000      7.974380000     13.712950000
17       4.355400000      2.015490000      9.830920000
17       6.367650000      9.902300000      5.214460000
17       6.329730000      3.767460000      4.278370000
17       4.393320000      8.150330000     10.767010000
17       6.329730000      2.191430000     12.776860000
17       4.393320000      9.726360000      2.268520000
17       5.006620000      1.125990000      6.327620000
17       5.716430000     10.791800000      8.717760000
17       5.006620000      4.832900000     14.826110000
17       5.716430000      7.084890000      0.219270000
17       1.585990000      2.044480000      7.409350000
17       9.137060000      9.873310000      7.636030000
17       1.585990000      3.914410000     15.907850000
17       9.137060000      8.003380000     -0.862470000
17      10.247120000      2.332090000      2.464820000
17       0.475930000      9.585700000     12.580560000
17      10.247120000      3.626810000     10.963320000
17       0.475930000      8.290980000      4.082060000
17       0.876170000      4.950670000      2.258490000
17       9.846880000      6.967120000     12.786890000
17       0.876170000      1.008220000     10.756990000
17       9.846880000     10.909570000      4.288390000
17       3.753400000      6.456370000      4.003560000
17       6.969650000      5.461420000     11.041820000
17       3.753400000     11.420320000     12.502050000
17       6.969650000      0.497470000      2.543330000
17       4.216800000      4.684790000      7.186240000
17       6.506250000      7.233000000      7.859140000
17       4.216800000      1.274110000     15.684740000
17       6.506250000     10.643680000     -0.639360000
17       0.843420000      5.338180000      5.979330000
17       9.879630000      6.579610000      9.066050000
17       0.843420000      0.620710000     14.477830000
17       9.879630000     11.297080000      0.552550000

C4H9{Cl11} (VASP, full relaxation)
E(PBE-D3, Ecut=400 eV)=-780.28108 eV
1        4.516610000      1.348370000      3.161760000
1        6.101780000     10.529260000     11.799000000
1        4.501970000      4.597870000     11.615070000
1        6.116420000      7.279770000      3.345680000
1        7.207000000      3.646960000      0.227120000
1        3.411390000      8.230680000     14.733640000
1        7.193630000      2.292330000      8.678780000
```

1	3.424760000	9.585310000	6.281980000
1	7.847600000	1.931450000	0.250770000
1	2.770790000	9.946190000	14.709990000
1	7.833230000	4.008190000	8.703880000
1	2.785150000	7.869450000	6.256870000
1	6.583280000	2.377430000	-0.864100000
1	4.035110000	9.500210000	15.824860000
1	6.569530000	3.562190000	7.588220000
1	4.048860000	8.315450000	7.372540000
1	7.617000000	4.567510000	14.290740000
1	3.001380000	7.310130000	0.670020000
1	7.633530000	1.376720000	5.836980000
1	2.984850000	10.500920000	9.123780000
1	9.390200000	4.553320000	14.269110000
1	1.228180000	7.324320000	0.691640000
1	9.406750000	1.391160000	5.816340000
1	1.211640000	10.486480000	9.144410000
1	8.472500000	5.192360000	-1.200300000
1	2.145880000	6.685280000	16.161060000
1	8.459310000	0.748500000	7.249450000
1	2.159070000	11.129140000	7.711310000
1	9.378730000	2.153100000	13.779420000
1	1.239660000	9.724540000	1.181340000
1	9.395260000	3.791600000	5.329340000
1	1.223130000	8.086040000	9.631410000
1	8.750720000	0.990460000	15.056650000
1	1.867660000	10.887180000	-0.095890000
1	8.765600000	4.952890000	6.606950000
1	1.852780000	6.924750000	8.353800000
1	10.167760000	2.061540000	-1.551630000
1	0.450630000	9.816100000	16.512380000
1	10.154100000	3.881070000	6.902820000
1	0.464290000	7.996570000	8.057930000
5	2.513430000	1.427280000	4.512420000
5	8.104950000	10.450360000	10.448330000
5	2.498030000	4.519660000	12.965230000
5	8.120350000	7.357980000	1.995520000
5	2.299560000	2.298640000	2.967080000
5	8.318830000	9.579000000	11.993670000
5	2.284790000	3.648020000	11.419970000
5	8.333600000	8.229620000	3.540790000
5	3.573750000	3.559310000	2.852160000
5	7.044640000	8.318330000	12.108590000
5	3.559110000	2.387020000	11.305700000
5	7.059280000	9.490620000	3.655060000
5	4.570550000	3.468060000	4.337450000
5	6.047840000	8.409580000	10.623310000
5	4.555350000	2.478100000	12.791140000
5	6.063040000	9.399540000	2.169620000
5	3.915180000	2.155760000	5.358370000
5	6.703210000	9.721880000	9.602380000
5	3.899860000	3.790970000	13.811450000
5	6.718530000	8.086670000	1.149300000
5	2.257220000	2.583170000	5.843750000
5	8.361170000	9.294470000	9.117000000
5	2.241920000	3.363910000	14.296640000
5	8.376470000	8.513730000	0.664120000
5	1.246250000	2.688750000	4.361620000
5	9.372140000	9.188890000	10.599130000
5	1.231050000	3.257860000	12.814180000
5	9.387340000	8.619780000	2.146580000
5	1.905400000	4.002340000	3.323330000
5	8.712990000	7.875300000	11.637420000
5	1.890710000	1.944230000	11.776450000
5	8.727680000	9.933410000	3.184300000
5	3.315220000	4.727160000	4.176600000
5	7.303170000	7.150480000	10.784160000
5	3.300080000	1.219380000	12.630220000
5	7.318310000	10.658270000	2.330540000
5	3.536780000	3.853780000	5.737650000
5	7.081610000	8.023860000	9.223100000
5	3.521310000	2.093200000	14.191170000
5	7.097080000	9.784440000	0.769590000
5	1.891500000	4.183050000	5.119680000
5	8.726890000	7.694590000	9.841070000
5	1.876350000	1.763820000	13.572640000
5	8.742030000	10.113820000	1.388110000
6	3.854400000	2.067480000	3.650650000
6	6.763990000	9.810160000	11.310110000
6	3.839450000	3.878950000	12.103870000

6	6.778940000	7.998690000	2.856880000
6	8.414220000	3.067360000	-1.459730000
6	2.204170000	8.810290000	16.420490000
6	8.400970000	2.873910000	6.992600000
6	2.217420000	9.003740000	7.968160000
6	7.502890000	2.776170000	-0.366840000
6	3.115500000	9.101470000	15.327590000
6	7.489190000	3.163720000	8.085540000
6	3.129200000	8.713920000	6.875220000
6	8.523210000	4.420290000	14.925720000
6	2.095180000	7.457350000	0.035040000
6	8.539390000	1.523250000	6.472660000
6	2.079000000	10.354400000	8.488090000
6	9.145570000	1.989720000	14.841050000
6	1.472810000	9.887920000	0.119710000
6	9.161300000	3.954040000	6.390910000
6	1.457080000	7.923600000	8.569850000
17	2.245540000	11.547030000	4.603640000
17	8.372850000	0.330610000	10.357120000
17	2.229910000	6.263490000	13.055220000
17	8.388470000	5.614150000	1.905530000
17	1.819940000	1.411130000	1.509630000
17	8.798450000	10.466510000	13.451130000
17	1.805490000	4.535380000	9.962120000
17	8.812900000	7.342260000	4.998640000
17	4.343450000	3.937360000	1.310490000
17	6.274940000	7.940280000	13.650260000
17	4.328900000	2.008290000	9.764320000
17	6.289490000	9.869350000	5.196430000
17	6.318630000	3.769440000	4.255750000
17	4.299760000	8.108200000	10.705000000
17	6.303490000	2.176370000	12.709920000
17	4.314900000	9.701270000	2.250840000
17	4.999600000	1.122860000	6.302500000
17	5.618790000	10.754780000	8.658250000
17	4.984010000	4.824410000	14.754990000
17	5.634380000	7.053230000	0.205760000
17	1.569800000	2.027240000	7.387630000
17	9.048590000	9.850400000	7.573120000
17	1.554340000	3.920120000	15.840190000
17	9.064050000	7.957520000	-0.879440000
17	10.139630000	2.332360000	2.454370000
17	0.478760000	9.545280000	12.506390000
17	10.124300000	3.614500000	10.906910000
17	0.494090000	8.263140000	4.053850000
17	0.850400000	4.937200000	2.238020000
17	9.767990000	6.940440000	12.722730000
17	0.835810000	1.009310000	10.691220000
17	9.782580000	10.868330000	4.269530000
17	3.727860000	6.454930000	3.981050000
17	6.890530000	5.422710000	10.979700000
17	3.713390000	11.355050000	12.435700000
17	6.905000000	0.522590000	2.525060000
17	4.205290000	4.677750000	7.168010000
17	6.413090000	7.199890000	7.792740000
17	4.189030000	1.269880000	15.622390000
17	6.429350000	10.607770000	-0.661630000
17	0.831530000	5.331560000	5.968770000
17	9.786850000	6.546090000	8.991990000
17	0.816580000	0.614760000	14.421520000
17	9.801800000	11.262880000	0.524240000