

Supplementary Information

Unraveling the α -Effect in α -Fluorinated Carbanionic Nucleophiles: Origins and Synthetic Implications

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Supplementary Computational Results

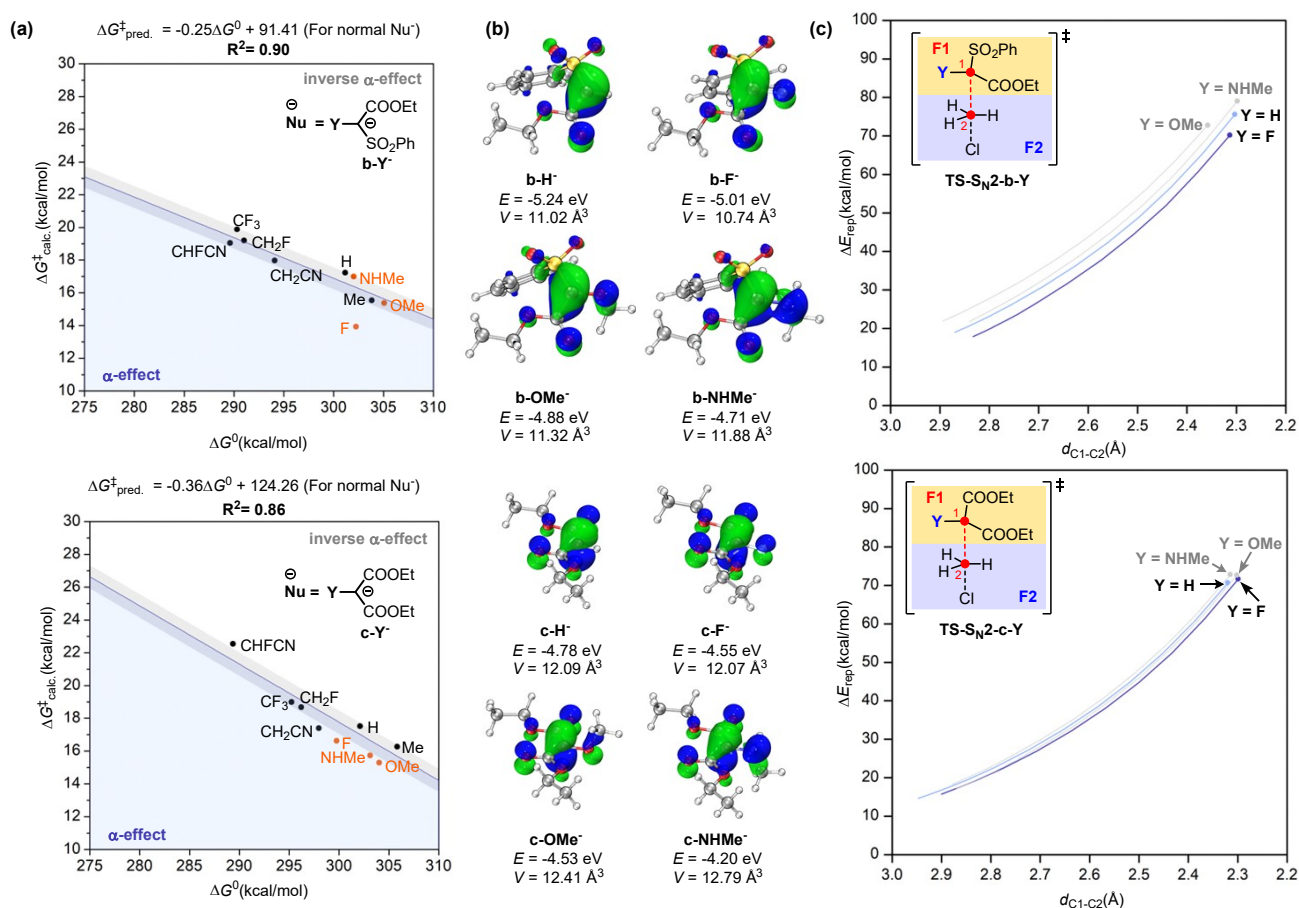


Figure S1. (a) Brønsted-type correlation between free energy barrier ($\Delta G^\ddagger$) and basicity (ΔG^0) for carbanions **b-Y**/**c-Y**. (b) Isosurfaces (isovalues = 0.05), energies, and volumes (isovalues = 0.05) of HOMO in **b-H**/**c-H** and α -nucleophiles **b-Y**/**c-Y**. (c) Pauli repulsion energy (ΔE_{rep}) between carbanion **b-Y**/**c-Y** and CH_3Cl along the IRC projected on the $\text{C1}\cdots\text{C2}$ distance ($d_{\text{C1-C2}}$).

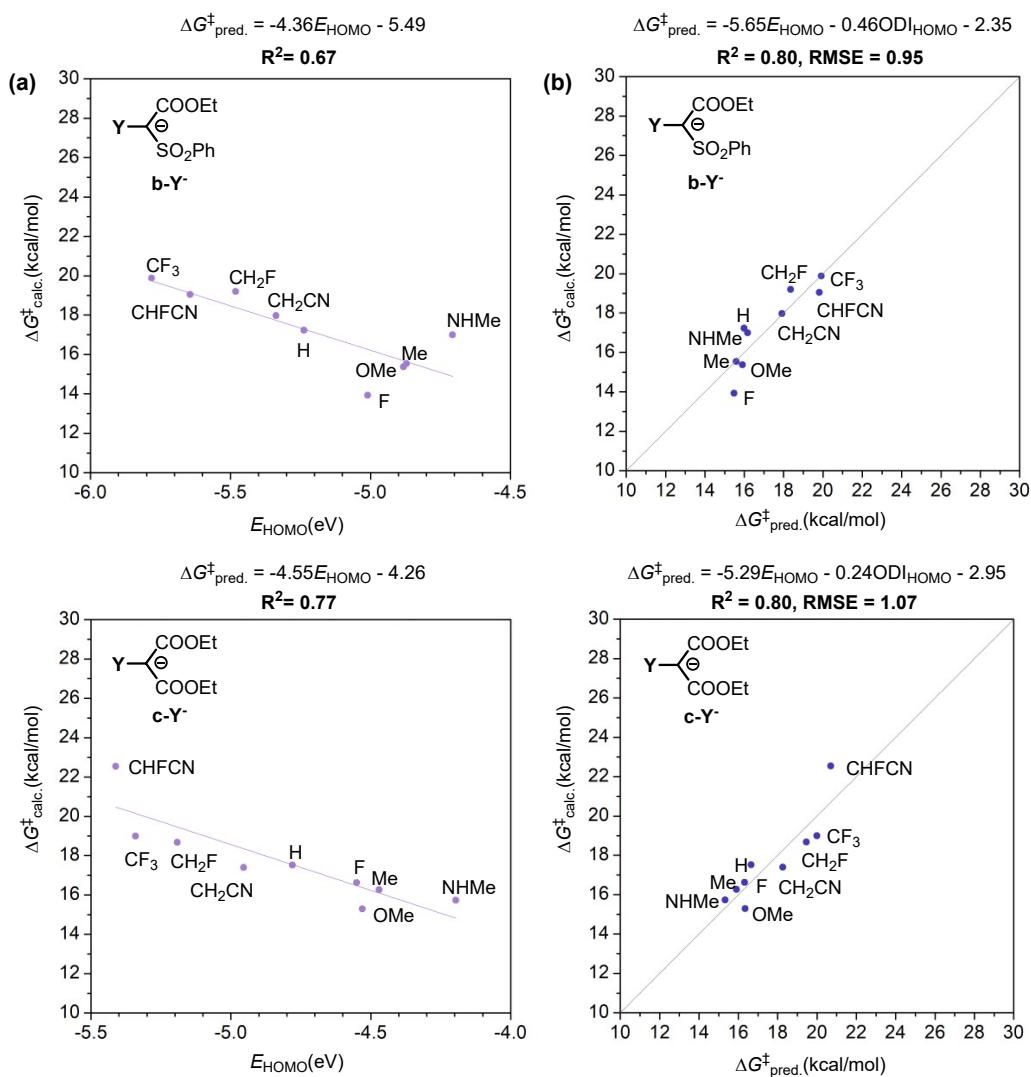


Figure S2. (a) Relationship between free energy barrier ($\Delta G^\ddagger$) of S_N2 reaction and E_{HOMO} of carbanions **b-Y⁻**/**c-Y⁻**. (c) Plot of computed vs. predicted free energy barrier of S_N2 reaction between **b-Y⁻**/**c-Y⁻** and CH_3Cl using the multivariate linear regression model.

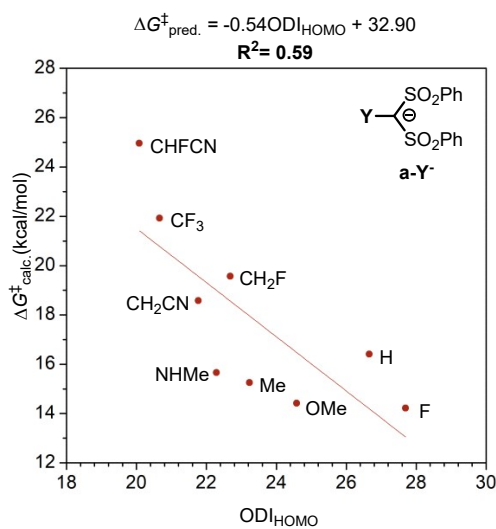


Figure S3. Relationship between free energy barrier ($\Delta G^\ddagger$) of S_N2 reaction and ODI_{HOMO} of carbanions **a-Y⁻**.

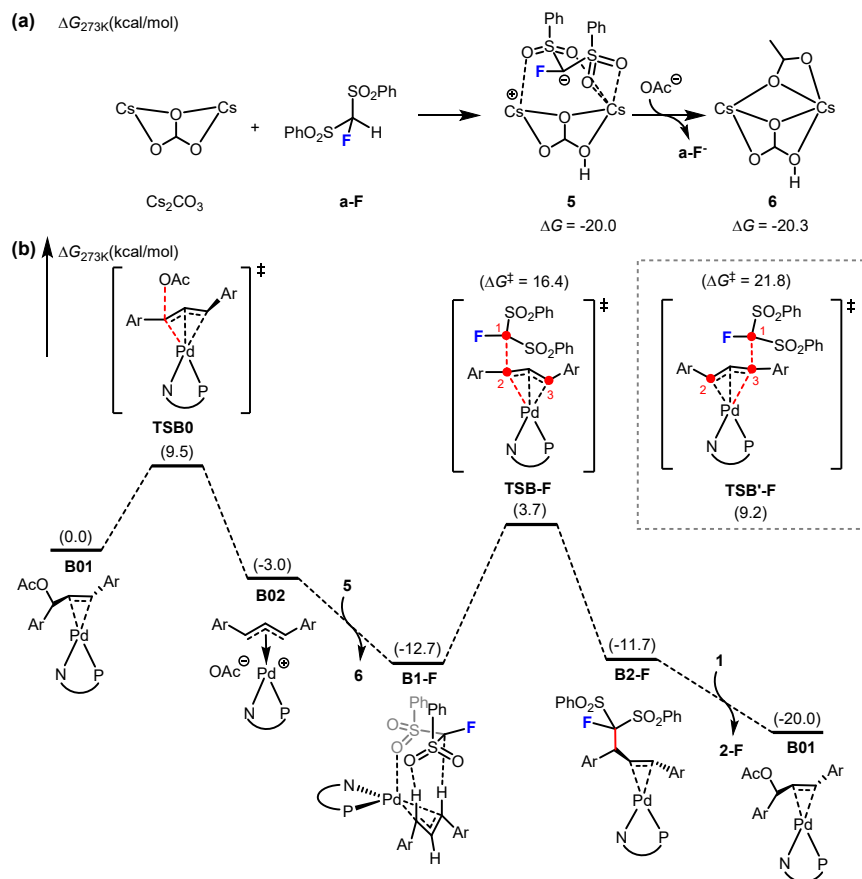


Figure S4. Calculated free energy profiles for overall catalytic cycle of palladium-catalyzed allylic monofluoromethylation reaction.

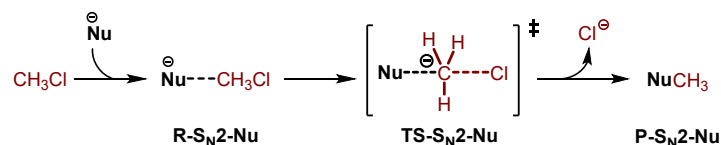
The nucleophile $(\text{PhSO}_2)_2\text{CFH}$ (**a-F**) could facilely react with strong base Cs_2CO_3 , yielding corresponding carbanion (**a-F**⁻). Then an oxidative addition with dissociation of the leaving group takes place, leading to Pd η^3 -allyl intermediate, which could yield an adduct **B1-F** with carbanion **a-F**⁻. Subsequently, the nucleophilic attack by carbanion to allyl group via **TSB-F** occurs, which is the rate-limiting step, giving methylation product (*R*)-**2-F** finally via ligand exchange with **1**. In addition, the energy barrier of nucleophilic attack yielding (*S*)-**2-F** is higher than that of (*R*)-**2-F** (21.9 kcal/mol for **TSB-F'** vs 16.4 kcal/mol for **TSB-F**), which is in line with the experimental observations.

Table S1. Free energy profile for reaction between nucleophile **a-Y**⁻ and quinone methide (energies in kcal/mol).

Species	ΔG^a	Species	ΔG^a
TSA-CF₃	22.0	A2-CF₃	14.5
TSA-CH₂CN	15.8	A2-CH₂CN	7.3
TSA-CH₂F	14.7	A2-CH₂F	6.0
TSA-CHFCN	26.2	A2-CHFCN	21.0
TSA-F	6.2	A2-F	-
			11.6
TSA-H	10.3	A2-H	-8.2
TSA-Me	9.3	A2-Me	-5.3
TSA-NHMe	10.6	A2-NHMe	-2.9
TSA-OMe	9.8	A2-OMe	-8.5

$a. \Delta G = G(\text{TSA}/\text{A2-Y}) - G(\text{A1-Y}).$

Table S2. Free energy profile for S_N2 reactions of various carbanions (energies in kcal/mol).



Species	ΔG^a	Species	ΔG^a	Species	ΔG^b
R-S _N 2-a-CF ₃	4.4	TS-S _N 2-a-CF ₃	21.9	P-S _N 2-a-CF ₃	-22.4
R-S _N 2-a-CH ₂ CN	5.1	TS-S _N 2-a-CH ₂ CN	18.6	P-S _N 2-a-CH ₂ CN	-30.7
R-S _N 2-a-CH ₂ F	5.9	TS-S _N 2-a-CH ₂ F	19.6	P-S _N 2-a-CH ₂ F	-25.7
R-S _N 2-a-CHFCN	4.1	TS-S _N 2-a-CHFCN	25.0	P-S _N 2-a-CHFCN	-18.2
R-S _N 2-a-F	4.9	TS-S _N 2-a-F	14.2	P-S _N 2-a-F	-42.4
R-S _N 2-a-H	5.2	TS-S _N 2-a-H	16.4	P-S _N 2-a-H	-37.6
R-S _N 2-a-Me	5.1	TS-S _N 2-a-Me	15.3	P-S _N 2-a-Me	-39.0
R-S _N 2-a-NHMe	5.2	TS-S _N 2-a-NHMe	15.7	P-S _N 2-a-NHMe	-40.3
R-S _N 2-a-OMe	3.6	TS-S _N 2-a-OMe	15.0	P-S _N 2-a-OMe	-41.7
R-S _N 2-b-CF ₃	4.5	TS-S _N 2-b-CF ₃	20.8	P-S _N 2-b-CF ₃	-28.1
R-S _N 2-b-CH ₂ CN	5.1	TS-S _N 2-b-CH ₂ CN	18.0	P-S _N 2-b-CH ₂ CN	-32.9
R-S _N 2-b-CH ₂ F	4.9	TS-S _N 2-b-CH ₂ F	19.2	P-S _N 2-b-CH ₂ F	-30.1
R-S _N 2-b-CHFCN	4.1	TS-S _N 2-b-CHFCN	19.0	P-S _N 2-b-CHFCN	-28.1
R-S _N 2-b-F	5.4	TS-S _N 2-b-F	13.9	P-S _N 2-b-F	-45.3
R-S _N 2-b-H	4.9	TS-S _N 2-b-H	17.2	P-S _N 2-b-H	-40.7
R-S _N 2-b-Me	5.4	TS-S _N 2-b-Me	15.5	P-S _N 2-b-Me	-42.8
R-S _N 2-b-NHMe	5.2	TS-S _N 2-b-NHMe	17.0	P-S _N 2-b-NHMe	-41.1
R-S _N 2-b-OMe	3.8	TS-S _N 2-b-OMe	15.4	P-S _N 2-b-OMe	-44.4
R-S _N 2-c-CF ₃	4.0	TS-S _N 2-c-CF ₃	19.0	P-S _N 2-c-CF ₃	-31.9
R-S _N 2-c-CH ₂ CN	3.7	TS-S _N 2-c-CH ₂ CN	17.2	P-S _N 2-c-CH ₂ CN	-35.2
R-S _N 2-c-CH ₂ F	4.6	TS-S _N 2-c-CH ₂ F	18.7	P-S _N 2-c-CH ₂ F	-33.1
R-S _N 2-c-CHFCN	5.1	TS-S _N 2-c-CHFCN	22.5	P-S _N 2-c-CHFCN	-26.3
R-S _N 2-c-F	5.5	TS-S _N 2-c-F	16.6	P-S _N 2-c-F	-42.6
R-S _N 2-c-H	3.7	TS-S _N 2-c-H	17.0	P-S _N 2-c-H	-39.5
R-S _N 2-c-Me	4.7	TS-S _N 2-c-Me	16.1	P-S _N 2-c-Me	-42.8
R-S _N 2-c-NHMe	4.9	TS-S _N 2-c-NHMe	15.7	P-S _N 2-c-NHMe	-41.3
R-S _N 2-c-OMe	3.8	TS-S _N 2-c-OMe	15.3	P-S _N 2-c-OMe	-42.2
R-S _N 2-d-F	4.5	TS-S _N 2-d-F	15.3	P-S _N 2-d-F	-44.1
R-S _N 2-d-H	4.8	TS-S _N 2-d-H	16.4	P-S _N 2-d-H	-40.2
R-S _N 2-e-F	5.0	TS-S _N 2-e-F	16.8	P-S _N 2-e-F	-35.8
R-S _N 2-e-H	5.5	TS-S _N 2-e-H	20.2	P-S _N 2-e-H	-30.4
R-S _N 2-f-F	4.7	TS-S _N 2-f-F	16.2	P-S _N 2-f-F	-41.7
R-S _N 2-f-H	4.5	TS-S _N 2-f-H	19.2	P-S _N 2-f-H	-33.6
R-S _N 2-g-F	4.7	TS-S _N 2-g-F	11.5	P-S _N 2-g-F	-55.4
R-S _N 2-g-H	4.0	TS-S _N 2-g-H	13.6	P-S _N 2-g-H	-51.6
R-S _N 2-CH ₃	8.4	TS-S _N 2-CH ₃	8.0	P-S _N 2-CH ₃ e	-82.5
R-S _N 2-CH ₂ F	7.0	TS-S _N 2-CH ₂ F	8.6	P-S _N 2-CH ₂ F	-85.3
R-S _N 2-CHF ₂	7.6	TS-S _N 2-CHF ₂	9.9	P-S _N 2-CHF ₂	-80.8
R-S _N 2-CF ₃	6.8	TS-S _N 2-CF ₃	11.3	P-S _N 2-CF ₃	-65.1

a. $\Delta G = G(\text{R/TS-S}_\text{N}2\text{-Nu}) - [G(\text{CH}_3\text{Cl}) + G(\text{Nu}^-)]$. *b.* $\Delta G = [G(\text{P-S}_\text{N}2\text{-Nu}) + G(\text{Cl}^-)] - [G(\text{CH}_3\text{Cl}) + G(\text{Nu}^-)]$.

Table S3. E_{HOMO} (in eV), ODI_{HOMO} , and volume of isosurface of HOMO (V in $\text{\AA}^3$, isovalues = 0.05) of carbanions **a-Y⁻**, **b-Y⁻**, and **c-Y⁻**.

anion	a-CF₃⁻	a-CH₂CN⁻	a-CH₂F⁻	a-CHFCN⁻	a-F⁻	a-H⁻	a-Me⁻	a-NHMe⁻	a-OMe⁻
E_{HOMO}	-6.07	-5.68	-5.90	-6.08	-5.62	-5.80	-5.37	-5.31	-5.41
ODI_{HOMO}	20.66	21.77	22.68	20.08	27.70	26.66	23.23	22.29	24.58
V	10.10	9.90	9.95	10.00	9.80	10.00	10.20	10.20	10.20
anion	b-CF₃⁻	b-CH₂CN⁻	b-CH₂F⁻	b-CHFCN⁻	b-F⁻	b-H⁻	b-Me⁻	b-NHMe⁻	b-OMe⁻
E_{HOMO}	-5.78	-5.34	-5.48	-5.64	-5.01	-5.24	-4.87	-4.71	-4.88
ODI_{HOMO}	22.81	21.66	22.49	21.31	22.95	24.64	20.99	17.70	20.42
V	11.11	10.75	11.08	11.59	10.74	11.02	11.33	11.88	11.32
anion	c-CF₃⁻	c-CH₂CN⁻	c-CH₂F⁻	c-CHFCN⁻	c-F⁻	c-H⁻	c-Me⁻	c-NHMe⁻	c-OMe⁻
E_{HOMO}	-5.34	-4.95	-5.19	-5.41	-4.55	-4.78	-4.47	-4.20	-4.53
ODI_{HOMO}	22.45	21.15	21.38	21.04	20.27	24.03	20.27	16.55	19.71
V	11.88	11.85	11.90	11.76	12.07	12.09	12.35	12.79	12.41

Table S4. Comparison of free energy barriers ($\Delta G^\ddagger$ in kcal/mol) of $\text{S}_\text{N}2$ reactions, E_{HOMO} (in eV) and ODI_{HOMO} for carbanions **a-H⁻ ~ g-H⁻**, **a-F⁻ ~ g-F⁻**, and (fluoro)methyl anions.

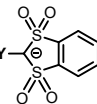
species		$\Delta G^\ddagger$	E_{HOMO}	ODI_{HOMO}	species		$\Delta G^\ddagger$	E_{HOMO}	ODI_{HOMO}
 a-Y⁻	Y =	16.4	-5.80	26.66	 e-Y⁻	Y =	20.2	-5.83	22.74
	H	14.2	-5.62	27.70		H	16.8	-5.65	21.37
	Y = F					Y = F			
 b-Y⁻	Y =	17.2	-5.24	24.64	 f-Y⁻	Y =	19.2	-5.37	23.19
	H	13.9	-5.01	22.95		H	16.2	-5.05	21.07
	Y = F					Y = F			
 c-Y⁻	Y =	17.0	-4.78	24.03	 g-Y⁻	Y =	13.6	-4.33	16.09
	H	16.6	-4.55	20.27		H	11.5	-4.37	18.09
	Y = F					Y = F			
 d-Y⁻	Y =	16.3	-6.03	32.84	 (Y = H or F)	CH ₃ ⁻	8.0	-2.79	64.87
	H	15.2	-6.00	35.68		CH ₂ F ⁻	8.6	-2.93	54.74
	Y = F					CHF ₂ ⁻	9.9	-3.22	47.58
						CF ₃ ⁻	11.3	-4.18	46.60

Table S5. Combining final single point energy with thermal corrections of stationary points created by Goodvibes. (energies in a.u., temperatures: $a = 293.15$ K, $b = 273.15$ K, $c = 195.15$ K)

Species	E_{SPC}	E	ZPE	H_{SPC}	$qh-H_{\text{SPC}}$	$T.S$	$T.qh-S$	$G(T)_{\text{SPC}}$	$qh-G(T)_{\text{SPC}}$	T
A1-CF₃	-3225.494	-3224.945	0.451918	-3225.005	-3225.013	0.106599	0.096902	-3225.111	-3225.109	<i>a</i>
A1-CH₂CN	-3020.109	-3019.632	0.474223	-3019.598	-3019.606	0.106359	0.096425	-3019.704	-3019.702	<i>a</i>
A1-CH₂F	-3027.123	-3026.632	0.468114	-3026.619	-3026.626	0.104368	0.094707	-3026.723	-3026.721	<i>a</i>
A1-CHFCN	-3119.274	-3118.763	0.466161	-3118.770	-3118.778	0.109891	0.098891	-3118.880	-3118.877	<i>a</i>
A1-F	-2987.818	-2987.336	0.438207	-2987.345	-2987.352	0.101300	0.092262	-2987.446	-2987.444	<i>a</i>
A1-H	-2888.663	-2888.214	0.446303	-2888.182	-2888.190	0.101356	0.091347	-2888.284	-2888.281	<i>a</i>
A1-Me	-2927.940	-2927.486	0.475135	-2927.429	-2927.437	0.103278	0.093649	-2927.533	-2927.530	<i>a</i>
A1-NHMe	-2983.240	-2982.773	0.492346	-2982.711	-2982.719	0.104529	0.095305	-2982.816	-2982.814	<i>a</i>
A1-OMe	-3003.096	-3002.619	0.481486	-3002.579	-3002.586	0.098539	0.091991	-3002.678	-3002.678	<i>a</i>
A2-CF₃	-3225.477	-3224.928	0.454031	-3224.987	-3224.993	0.099597	0.093125	-3225.087	-3225.086	<i>a</i>

Species	E_{SPC}	E	ZPE	H_{SPC}	$qh-H_{\text{SPC}}$	$T.S$	$T.qh-S$	$G(T)_{\text{SPC}}$	$qh-G(T)_{\text{SPC}}$	T
A2-CH₂CN	-3020.104	-3019.623	0.476397	-3019.592	-3019.598	0.098584	0.092190	-3019.691	-3019.691	<i>a</i>
A2-CH₂F	-3027.120	-3026.629	0.470493	-3026.615	-3026.621	0.097079	0.090680	-3026.712	-3026.712	<i>a</i>
A2-CHFCN	-3119.248	-3118.738	0.468514	-3118.743	-3118.749	0.100769	0.093974	-3118.844	-3118.843	<i>a</i>
A2-F	-2987.841	-2987.362	0.440563	-2987.367	-2987.373	0.097467	0.089642	-2987.464	-2987.463	<i>a</i>
A2-H	-2888.682	-2888.232	0.449256	-2888.200	-2888.207	0.094790	0.087469	-2888.295	-2888.294	<i>a</i>
A2-Me	-2927.955	-2927.499	0.477841	-2927.443	-2927.449	0.096057	0.089236	-2927.539	-2927.539	<i>a</i>
A2-NHMe	-2983.251	-2982.779	0.494592	-2982.721	-2982.727	0.098111	0.091726	-2982.819	-2982.819	<i>a</i>
A2-OMe	-3003.076	-3002.600	0.479122	-3002.560	-3002.568	0.105736	0.095938	-3002.666	-3002.664	<i>a</i>
TSA-CF₃	-3225.462	-3224.915	0.452155	-3224.974	-3224.981	0.100374	0.093366	-3225.075	-3225.074	<i>a</i>
TSA-CH₂CN	-3020.088	-3019.609	0.474522	-3019.577	-3019.584	0.099903	0.092771	-3019.677	-3019.677	<i>a</i>
TSA-CH₂F	-3027.103	-3026.614	0.468458	-3026.600	-3026.606	0.098196	0.091200	-3026.698	-3026.698	<i>a</i>
TSA-CHFCN	-3119.237	-3118.725	0.466610	-3118.734	-3118.741	0.100806	0.093953	-3118.835	-3118.835	<i>a</i>
TSA-F	-2987.810	-2987.329	0.438224	-2987.338	-2987.344	0.097924	0.090138	-2987.436	-2987.434	<i>a</i>
TSA-H	-2888.650	-2888.201	0.446715	-2888.170	-2888.177	0.095295	0.087855	-2888.265	-2888.265	<i>a</i>
TSA-Me	-2927.929	-2927.476	0.475440	-2927.420	-2927.426	0.096316	0.089485	-2927.516	-2927.515	<i>a</i>
TSA-NHMe	-2983.227	-2982.759	0.492561	-2982.699	-2982.705	0.098957	0.091985	-2982.798	-2982.797	<i>a</i>
TSA-OMe	-3003.064	-3002.589	0.479350	-3002.550	-3002.556	0.099176	0.092205	-3002.649	-3002.649	<i>a</i>
CH₃Cl	-499.9343	-499.8936	0.038162	-499.8922	-499.8922	0.024124	0.024124	-499.9163	-499.9164	<i>a</i>
a-CF₃	-1935.688	-1935.325	0.237457	-1935.430	-1935.434	0.066732	0.063089	-1935.497	-1935.497	<i>a</i>
a-CH₂CN	-1730.312	-1730.020	0.259754	-1730.032	-1730.035	0.066997	0.062686	-1730.099	-1730.098	<i>a</i>
a-CH₂F	-1737.326	-1737.023	0.254055	-1737.053	-1737.056	0.062935	0.060033	-1737.116	-1737.116	<i>a</i>
a-CHFCN	-1829.470	-1829.143	0.252154	-1829.197	-1829.200	0.065726	0.063056	-1829.263	-1829.263	<i>a</i>
a-F	-1698.032	-1697.738	0.224231	-1697.790	-1697.793	0.062516	0.058652	-1697.852	-1697.851	<i>a</i>
a-H	-1598.872	-1598.612	0.232162	-1598.622	-1598.625	0.061075	0.057169	-1598.684	-1598.682	<i>a</i>
a-Me	-1638.155	-1637.890	0.260804	-1637.876	-1637.879	0.062256	0.058955	-1637.938	-1637.938	<i>a</i>
a-NHMe	-1693.454	-1693.172	0.277900	-1693.156	-1693.159	0.065965	0.062167	-1693.222	-1693.221	<i>a</i>
a-OMe	-1713.297	-1713.008	0.264885	-1713.012	-1713.015	0.066476	0.062305	-1713.079	-1713.078	<i>a</i>
a-CF₃⁻	-1935.224	-1934.859	0.224711	-1934.979	-1934.982	0.065622	0.062246	-1935.045	-1935.044	<i>a</i>
a-CH₂CN⁻	-1729.835	-1729.543	0.246966	-1729.568	-1729.571	0.064948	0.061533	-1729.633	-1729.633	<i>a</i>
a-CH₂F⁻	-1736.853	-1736.548	0.241044	-1736.593	-1736.596	0.061943	0.059234	-1736.655	-1736.655	<i>a</i>
a-CHFCN⁻	-1829.010	-1828.680	0.238859	-1828.750	-1828.754	0.066915	0.063304	-1828.817	-1828.817	<i>a</i>
a-F⁻	-1697.547	-1697.250	0.211091	-1697.318	-1697.320	0.059436	0.057061	-1697.377	-1697.377	<i>a</i>
a-H⁻	-1598.389	-1598.128	0.219228	-1598.153	-1598.156	0.058078	0.055327	-1598.211	-1598.211	<i>a</i>
a-Me⁻	-1637.665	-1637.398	0.247679	-1637.399	-1637.401	0.061918	0.058711	-1637.461	-1637.460	<i>a</i>
a-NHMe⁻	-1692.964	-1692.682	0.265019	-1692.679	-1692.682	0.063343	0.060521	-1692.742	-1692.742	<i>a</i>
a-OMe⁻	-1712.807	-1712.517	0.252075	-1712.535	-1712.538	0.063363	0.060451	-1712.599	-1712.599	<i>a</i>
P-S_N2-a-CF₃	-1974.97	-1974.602	0.265866	-1974.682	-1974.685	0.06712	0.064519	-1974.749	-1974.75	<i>a</i>
P-S_N2-a-CH₂CN	-1769.594	-1769.294	0.288324	-1769.284	-1769.287	0.067189	0.064043	-1769.351	-1769.351	<i>a</i>
P-S_N2-a-CH₂F	-1776.603	-1776.292	0.282119	-1776.301	-1776.304	0.065164	0.062295	-1776.366	-1776.366	<i>a</i>
P-S_N2-a-CHFCN	-1868.749	-1868.418	0.280213	-1868.447	-1868.45	0.06829	0.065423	-1868.515	-1868.515	<i>a</i>
P-S_N2-a-F	-1737.323	-1737.024	0.252218	-1737.052	-1737.054	0.062629	0.060075	-1737.114	-1737.115	<i>a</i>
P-S_N2-a-H	-1638.159	-1637.892	0.260997	-1637.88	-1637.882	0.060797	0.058343	-1637.94	-1637.94	<i>a</i>
P-S_N2-a-Me	-1677.437	-1677.165	0.289288	-1677.128	-1677.131	0.063573	0.060686	-1677.192	-1677.192	<i>a</i>
P-S_N2-a-NHMe	-1732.738	-1732.448	0.30637	-1732.41	-1732.413	0.066163	0.063366	-1732.476	-1732.476	<i>a</i>
P-S_N2-a-OMe	-1752.583	-1752.288	0.293274	-1752.269	-1752.272	0.065829	0.063179	-1752.335	-1752.335	<i>a</i>
R-S_N2-a-CF₃	-2435.164	-2434.762	0.263803	-2434.876	-2434.881	0.078924	0.072873	-2434.955	-2434.954	<i>a</i>

Species	E_{SPC}	E	ZPE	H_{SPC}	$qh-H_{\text{SPC}}$	$T.S$	$T.qh-S$	$G(T)_{\text{SPC}}$	$qh-G(T)_{\text{SPC}}$	T
R-S_N2-a-CH₂CN	-2229.774	-2229.444	0.286131	-2229.463	-2229.469	0.07906	0.072416	-2229.542	-2229.541	<i>a</i>
R-S_N2-a-CH₂F	-2236.791	-2236.445	0.280041	-2236.487	-2236.492	0.076614	0.070604	-2236.563	-2236.562	<i>a</i>
R-S_N2-a-CHFCN	-2328.951	-2328.585	0.278111	-2328.647	-2328.652	0.081038	0.074278	-2328.728	-2328.727	<i>a</i>
R-S_N2-a-F	-2197.486	-2197.151	0.250217	-2197.213	-2197.218	0.073729	0.068152	-2197.287	-2197.286	<i>a</i>
R-S_N2-a-H	-2098.329	-2098.028	0.258442	-2098.048	-2098.053	0.071836	0.066225	-2098.12	-2098.119	<i>a</i>
R-S_N2-a-Me	-2137.604	-2137.299	0.28674	-2137.294	-2137.299	0.075592	0.06956	-2137.369	-2137.368	<i>a</i>
R-S_N2-a-NHMe	-2192.903	-2192.583	0.304253	-2192.574	-2192.579	0.076877	0.071245	-2192.651	-2192.651	<i>a</i>
R-S_N2-a-OMe	-2212.747	-2212.418	0.290858	-2212.432	-2212.437	0.078474	0.072125	-2212.511	-2212.509	<i>a</i>
TS-S_N2-a-CF₃	-2435.14	-2434.736	0.263729	-2434.852	-2434.856	0.07377	0.069722	-2434.926	-2434.926	<i>a</i>
TS-S_N2-a-CH₂CN	-2229.756	-2229.424	0.286102	-2229.447	-2229.451	0.072759	0.068836	-2229.519	-2229.519	<i>a</i>
TS-S_N2-a-CH₂F	-2236.772	-2236.428	0.280063	-2236.47	-2236.474	0.070753	0.067043	-2236.541	-2236.541	<i>a</i>
TS-S_N2-a-CHFCN	-2328.921	-2328.553	0.278028	-2328.619	-2328.623	0.074675	0.070576	-2328.693	-2328.693	<i>a</i>
TS-S_N2-a-F	-2197.473	-2197.138	0.249746	-2197.202	-2197.205	0.069842	0.065808	-2197.271	-2197.271	<i>a</i>
TS-S_N2-a-H	-2098.313	-2098.012	0.258229	-2098.034	-2098.038	0.067643	0.063615	-2098.102	-2098.101	<i>a</i>
TS-S_N2-a-Me	-2137.591	-2137.284	0.286756	-2137.282	-2137.286	0.070062	0.066057	-2137.352	-2137.352	<i>a</i>
TS-S_N2-a-NHMe	-2192.89	-2192.567	0.304143	-2192.562	-2192.566	0.071664	0.067952	-2192.634	-2192.634	<i>a</i>
TS-S_N2-a-OMe	-2212.733	-2212.403	0.290795	-2212.418	-2212.423	0.072941	0.068625	-2212.491	-2212.491	<i>a</i>
b-CF₃	-1423.484	-1423.17	0.217339	-1423.249	-1423.252	0.061578	0.058715	-1423.31	-1423.31	<i>a</i>
b-CH₂CN	-1218.102	-1217.86	0.23983	-1217.844	-1217.847	0.060511	0.057634	-1217.905	-1217.905	<i>a</i>
b-CH₂F	-1225.113	-1224.86	0.233631	-1224.862	-1224.865	0.05857	0.055962	-1224.921	-1224.921	<i>a</i>
b-CHFCN	-1317.261	-1316.985	0.231763	-1317.011	-1317.014	0.062633	0.059559	-1317.073	-1317.073	<i>a</i>
b-F	-1185.825	-1185.581	0.204248	-1185.605	-1185.608	0.056301	0.053656	-1185.662	-1185.661	<i>a</i>
b-H	-1086.663	-1086.453	0.212267	-1086.436	-1086.438	0.054548	0.051897	-1086.49	-1086.49	<i>a</i>
b-Me	-1125.943	-1125.728	0.240736	-1125.686	-1125.688	0.057121	0.054513	-1125.743	-1125.743	<i>a</i>
b-NHMe	-1181.238	-1181.007	0.258156	-1180.962	-1180.965	0.059635	0.05709	-1181.022	-1181.022	<i>a</i>
b-OMe	-1201.084	-1200.845	0.244795	-1200.822	-1200.825	0.060954	0.057671	-1200.883	-1200.882	<i>a</i>
b-CF₃⁻	-1423.009	-1422.692	0.203797	-1422.787	-1422.79	0.063029	0.059122	-1422.85	-1422.849	<i>a</i>
b-CH₂CN⁻	-1217.619	-1217.376	0.226107	-1217.374	-1217.378	0.063104	0.058735	-1217.438	-1217.436	<i>a</i>
b-CH₂F⁻	-1224.635	-1224.378	0.220222	-1224.398	-1224.401	0.059493	0.056307	-1224.457	-1224.457	<i>a</i>
b-CHFCN⁻	-1316.786	-1316.507	0.218191	-1316.549	-1316.552	0.062839	0.059573	-1316.612	-1316.612	<i>a</i>
b-F⁻	-1185.33	-1185.081	0.190377	-1185.124	-1185.126	0.057536	0.054255	-1185.181	-1185.18	<i>a</i>
b-H⁻	-1086.169	-1085.958	0.198366	-1085.956	-1085.958	0.054687	0.051974	-1086.01	-1086.01	<i>a</i>
b-Me⁻	-1125.444	-1125.228	0.226458	-1125.201	-1125.203	0.05844	0.055374	-1125.259	-1125.259	<i>a</i>
b-NHMe⁻	-1180.743	-1180.51	0.244228	-1180.481	-1180.484	0.060378	0.057288	-1180.541	-1180.541	<i>a</i>
b-OMe⁻	-1200.585	-1200.345	0.231232	-1200.336	-1200.339	0.060405	0.057288	-1200.396	-1200.396	<i>a</i>
P-S_N2-b-CF₃	-1462.765	-1462.446	0.245304	-1462.499	-1462.502	0.063904	0.061108	-1462.563	-1462.563	<i>a</i>
P-S_N2-b-CH₂CN	-1257.383	-1257.134	0.267709	-1257.095	-1257.098	0.062738	0.06002	-1257.158	-1257.158	<i>a</i>
P-S_N2-b-CH₂F	-1264.394	-1264.135	0.261534	-1264.114	-1264.116	0.060888	0.058398	-1264.174	-1264.175	<i>a</i>
P-S_N2-b-CHFCN	-1356.541	-1356.26	0.259816	-1356.261	-1356.264	0.0646	0.06176	-1356.326	-1356.326	<i>a</i>
P-S_N2-b-F	-1225.113	-1224.863	0.231909	-1224.863	-1224.866	0.058754	0.056224	-1224.922	-1224.922	<i>a</i>
P-S_N2-b-H	-1125.944	-1125.728	0.240534	-1125.687	-1125.69	0.057707	0.054897	-1125.745	-1125.745	<i>a</i>
P-S_N2-b-Me	-1165.224	-1165.002	0.268668	-1164.937	-1164.94	0.059431	0.056886	-1164.997	-1164.997	<i>a</i>
P-S_N2-b-NHMe	-1220.519	-1220.281	0.285931	-1220.214	-1220.216	0.061965	0.059455	-1220.276	-1220.276	<i>a</i>
P-S_N2-b-OMe	-1240.366	-1240.122	0.272905	-1240.074	-1240.077	0.062031	0.059404	-1240.136	-1240.136	<i>a</i>
R-S_N2-b-CF₃	-1922.949	-1922.594	0.242909	-1922.683	-1922.688	0.077605	0.070428	-1922.76	-1922.759	<i>a</i>
R-S_N2-b-CH₂CN	-1717.558	-1717.277	0.265152	-1717.269	-1717.275	0.077431	0.069958	-1717.347	-1717.345	<i>a</i>

Species	E_{SPC}	E	ZPE	H_{SPC}	$qh-H_{\text{SPC}}$	$T.S$	$T.qh-S$	$G(T)_{\text{SPC}}$	$qh-G(T)_{\text{SPC}}$	T
R-S_N2-b-CH₂F	-1724.574	-1724.278	0.259367	-1724.293	-1724.298	0.073741	0.067594	-1724.367	-1724.366	<i>a</i>
R-S_N2-b-CHFCN	-1816.728	-1816.412	0.2578	-1816.447	-1816.452	0.075147	0.06957	-1816.522	-1816.522	<i>a</i>
R-S_N2-b-F	-1685.268	-1684.981	0.229556	-1685.018	-1685.023	0.071853	0.065521	-1685.09	-1685.088	<i>a</i>
R-S_N2-b-H	-1586.108	-1585.858	0.237482	-1585.851	-1585.855	0.069432	0.063545	-1585.92	-1585.919	<i>a</i>
R-S_N2-b-Me	-1625.383	-1625.128	0.265768	-1625.095	-1625.1	0.07221	0.066327	-1625.168	-1625.167	<i>a</i>
R-S_N2-b-NHMe	-1680.682	-1680.41	0.283651	-1680.376	-1680.381	0.073173	0.067821	-1680.45	-1680.449	<i>a</i>
R-S_N2-b-OMe	-1700.527	-1700.248	0.270576	-1700.234	-1700.239	0.073681	0.067832	-1700.307	-1700.306	<i>a</i>
TS-S_N2-b-CF₃	-1922.927	-1922.571	0.242878	-1922.661	-1922.666	0.071406	0.066806	-1922.733	-1922.732	<i>a</i>
TS-S_N2-b-CH₂CN	-1717.541	-1717.259	0.265294	-1717.254	-1717.258	0.070717	0.065971	-1717.325	-1717.324	<i>a</i>
TS-S_N2-b-CH₂F	-1724.555	-1724.259	0.259226	-1724.275	-1724.279	0.068728	0.064357	-1724.343	-1724.343	<i>a</i>
TS-S_N2-b-CHFCN	-1816.706	-1816.39	0.257486	-1816.426	-1816.43	0.072401	0.067662	-1816.499	-1816.498	<i>a</i>
TS-S_N2-b-F	-1685.256	-1684.968	0.228934	-1685.007	-1685.011	0.068807	0.063376	-1685.076	-1685.075	<i>a</i>
TS-S_N2-b-H	-1586.092	-1585.842	0.237678	-1585.835	-1585.839	0.064572	0.060308	-1585.9	-1585.899	<i>a</i>
TS-S_N2-b-Me	-1625.37	-1625.114	0.26581	-1625.084	-1625.087	0.067222	0.063153	-1625.151	-1625.15	<i>a</i>
TS-S_N2-b-NHMe	-1680.666	-1680.394	0.283204	-1680.361	-1680.365	0.069541	0.06522	-1680.431	-1680.43	<i>a</i>
TS-S_N2-b-OMe	-1700.51	-1700.23	0.270066	-1700.218	-1700.222	0.070588	0.065713	-1700.289	-1700.288	<i>a</i>
c-CF₃	-911.272	-911.0059	0.196821	-911.0585	-911.0616	0.059401	0.055785	-911.1179	-911.1174	<i>a</i>
c-CH₂CN	-705.8857	-705.6928	0.219245	-705.6502	-705.6533	0.058598	0.054873	-705.7088	-705.7082	<i>a</i>
c-CH₂F	-712.8972	-712.6912	0.212978	-712.6688	-712.6717	0.056166	0.052941	-712.725	-712.7246	<i>a</i>
c-CHFCN	-805.0483	-804.8211	0.211222	-804.8199	-804.8232	0.060754	0.056753	-804.8807	-804.8799	<i>a</i>
c-F	-673.6101	-673.4139	0.183952	-673.4121	-673.4145	0.053289	0.050198	-673.4654	-673.4647	<i>a</i>
c-H	-574.4447	-574.2841	0.191558	-574.2398	-574.2421	0.051668	0.048614	-574.2914	-574.2907	<i>a</i>
c-Me	-613.7227	-613.5567	0.219976	-613.4879	-613.4904	0.05487	0.051525	-613.5428	-613.5419	<i>a</i>
c-NHMe	-669.0158	-668.8336	0.237687	-668.7622	-668.7649	0.057601	0.054147	-668.8198	-668.8191	<i>a</i>
c-OMe	-688.8639	-688.6743	0.224529	-688.6235	-688.6263	0.05718	0.053826	-688.6807	-688.6802	<i>a</i>
c-CF₃⁻	-910.7886	-910.518	0.18316	-910.5891	-910.592	0.058092	0.054901	-910.6472	-910.6469	<i>a</i>
c-CH₂CN⁻	-705.3981	-705.2048	0.205562	-705.1766	-705.1795	0.056776	0.053846	-705.2334	-705.2333	<i>a</i>
c-CH₂F⁻	-712.4123	-712.2003	0.199512	-712.1977	-712.2005	0.054726	0.052113	-712.2524	-712.2526	<i>a</i>
c-CHFCN⁻	-804.5749	-804.3431	0.197898	-804.3603	-804.3633	0.058304	0.055531	-804.4186	-804.4188	<i>a</i>
c-F⁻	-673.1184	-672.9175	0.169924	-672.9345	-672.9369	0.051775	0.049557	-672.9863	-672.9864	<i>a</i>
c-H⁻	-573.9494	-573.7855	0.178148	-573.7582	-573.7603	0.049195	0.047354	-573.8074	-573.8077	<i>a</i>
c-Me⁻	-613.2213	-613.0535	0.205717	-613.0009	-613.0034	0.053809	0.051147	-613.0547	-613.0546	<i>a</i>
c-NHMe⁻	-668.5197	-668.3353	0.223719	-668.2803	-668.283	0.055383	0.05296	-668.3357	-668.336	<i>a</i>
c-OMe⁻	-688.3662	-688.1758	0.210597	-688.14	-688.1427	0.055405	0.052994	-688.1954	-688.1956	<i>a</i>
P-S_N2-c-CF₃	-950.5489	-950.2783	0.22487	-950.306	-950.3091	0.06185	0.058253	-950.3678	-950.3673	<i>a</i>
P-S_N2-c-CH₂CN	-745.1635	-744.965	0.247208	-744.8986	-744.9017	0.060762	0.057226	-744.9594	-744.9589	<i>a</i>
P-S_N2-c-CH₂F	-752.1746	-751.9635	0.241033	-751.9167	-751.9196	0.058265	0.055314	-751.975	-751.9749	<i>a</i>
P-S_N2-c-CHFCN	-844.3258	-844.0933	0.239276	-844.0681	-844.0714	0.062544	0.058946	-844.1306	-844.1303	<i>a</i>
P-S_N2-c-F	-712.8953	-712.6925	0.21149	-712.6681	-712.6708	0.05615	0.052989	-712.7243	-712.7238	<i>a</i>
P-S_N2-c-H	-613.7213	-613.555	0.220118	-613.4864	-613.4889	0.054239	0.051257	-613.5407	-613.5402	<i>a</i>
P-S_N2-c-Me	-653.0002	-652.8278	0.24804	-652.7361	-652.7386	0.056811	0.053724	-652.7929	-652.7923	<i>a</i>
P-S_N2-c-NHMe	-708.2951	-708.1071	0.265421	-708.0123	-708.0151	0.059299	0.056239	-708.0716	-708.0713	<i>a</i>
P-S_N2-c-OMe	-728.1428	-727.9471	0.252387	-727.8732	-727.8761	0.059629	0.056266	-727.9328	-727.9324	<i>a</i>
R-S_N2-c-CF₃	-1410.729	-1410.421	0.222387	-1410.486	-1410.491	0.072599	0.066165	-1410.558	-1410.557	<i>a</i>
R-S_N2-c-CH₂CN	-1205.34	-1205.107	0.244798	-1205.074	-1205.079	0.070811	0.064883	-1205.145	-1205.144	<i>a</i>
R-S_N2-c-CH₂F	-1212.354	-1212.103	0.23916	-1212.095	-1212.099	0.067399	0.062372	-1212.162	-1212.162	<i>a</i>

Species	E_{SPC}	E	ZPE	H_{SPC}	qh- H_{SPC}	$T.S$	$T.\text{qh-}S$	$G(T)_{\text{SPC}}$	qh- $G(T)_{\text{SPC}}$	T
R-S_N2-c-CHFCN	-1304.515	-1304.247	0.237504	-1304.256	-1304.261	0.071095	0.065718	-1304.327	-1304.327	<i>a</i>
R-S_N2-c-F	-1173.057	-1172.819	0.209329	-1172.829	-1172.833	0.066087	0.06084	-1172.895	-1172.894	<i>a</i>
R-S_N2-c-H	-1073.891	-1073.688	0.217402	-1073.655	-1073.659	0.063645	0.058654	-1073.719	-1073.718	<i>a</i>
R-S_N2-c-Me	-1113.163	-1112.957	0.245572	-1112.898	-1112.902	0.065311	0.060982	-1112.964	-1112.963	<i>a</i>
R-S_N2-c-NHMe	-1168.46	-1168.239	0.263363	-1168.177	-1168.181	0.068035	0.063226	-1168.245	-1168.244	<i>a</i>
R-S_N2-c-OMe	-1188.308	-1188.079	0.250046	-1188.038	-1188.043	0.068384	0.063279	-1188.106	-1188.106	<i>a</i>
TS-S_N2-c-CF₃	-1410.708	-1410.4	0.222126	-1410.466	-1410.47	0.067862	0.063273	-1410.534	-1410.533	<i>a</i>
TS-S_N2-c-CH₂CN	-1205.32	-1205.087	0.244553	-1205.056	-1205.06	0.067343	0.062496	-1205.123	-1205.122	<i>a</i>
TS-S_N2-c-CH₂F	-1212.332	-1212.083	0.23858	-1212.075	-1212.079	0.0647	0.060602	-1212.139	-1212.139	<i>a</i>
TS-S_N2-c-CHFCN	-1304.488	-1304.221	0.23673	-1304.231	-1304.235	0.068515	0.063952	-1304.3	-1304.299	<i>a</i>
TS-S_N2-c-F	-1173.041	-1172.802	0.208773	-1172.814	-1172.818	0.06235	0.058369	-1172.877	-1172.876	<i>a</i>
TS-S_N2-c-H	-1073.871	-1073.67	0.217069	-1073.637	-1073.64	0.060359	0.056477	-1073.697	-1073.697	<i>a</i>
TS-S_N2-c-Me	-1113.146	-1112.94	0.24516	-1112.883	-1112.886	0.062341	0.058939	-1112.945	-1112.945	<i>a</i>
TS-S_N2-c-NHMe	-1168.444	-1168.222	0.262699	-1168.162	-1168.166	0.06531	0.061405	-1168.227	-1168.227	<i>a</i>
TS-S_N2-c-OMe	-1188.291	-1188.062	0.249517	-1188.022	-1188.026	0.065462	0.061572	-1188.088	-1188.088	<i>a</i>
P-S_N2-d-F	-1505.266	-1505.017	0.149004	-1505.104	-1505.105	0.049595	0.048794	-1505.153	-1505.154	<i>a</i>
R-S_N2-d-F	-1965.426	-1965.14	0.146599	-1965.263	-1965.266	0.060802	0.057161	-1965.323	-1965.323	<i>a</i>
d-F⁻	-1465.487	-1465.239	0.107603	-1465.367	-1465.368	0.046269	0.045639	-1465.413	-1465.414	<i>a</i>
TS-S_N2-d-F	-1965.411	-1965.125	0.146204	-1965.248	-1965.251	0.057567	0.054974	-1965.306	-1965.306	<i>a</i>
P-S_N2-d-H	-1406.103	-1405.887	0.157688	-1405.932	-1405.934	0.047706	0.047007	-1405.98	-1405.981	<i>a</i>
R-S_N2-d-H	-1866.269	-1866.019	0.155239	-1866.098	-1866.101	0.057527	0.054661	-1866.156	-1866.156	<i>a</i>
d-H⁻	-1366.33	-1366.118	0.116041	-1366.202	-1366.203	0.044037	0.043604	-1366.246	-1366.247	<i>a</i>
TS-S_N2-d-H	-1866.252	-1866.002	0.154812	-1866.082	-1866.084	0.054816	0.052657	-1866.137	-1866.137	<i>a</i>
P-S_N2-e-F	-1162.48	-1162.24	0.162888	-1162.303	-1162.305	0.052296	0.050091	-1162.355	-1162.355	<i>a</i>
R-S_N2-e-F	-1622.654	-1622.377	0.161341	-1622.475	-1622.479	0.062829	0.058006	-1622.538	-1622.537	<i>a</i>
e-F⁻	-1122.714	-1122.476	0.121955	-1122.58	-1122.581	0.048518	0.046878	-1122.628	-1122.628	<i>a</i>
TS-S_N2-e-F	-1622.636	-1622.359	0.160608	-1622.459	-1622.462	0.059405	0.055804	-1622.519	-1622.518	<i>a</i>
P-S_N2-e-H	-1063.311	-1063.104	0.171622	-1063.126	-1063.128	0.051002	0.048698	-1063.177	-1063.177	<i>a</i>
R-S_N2-e-H	-1523.494	-1523.253	0.16957	-1523.308	-1523.311	0.05938	0.05555	-1523.367	-1523.366	<i>a</i>
e-H⁻	-1023.554	-1023.352	0.129949	-1023.412	-1023.414	0.046416	0.045081	-1023.459	-1023.459	<i>a</i>
TS-S_N2-e-H	-1523.472	-1523.23	0.169272	-1523.287	-1523.29	0.056289	0.053395	-1523.343	-1523.343	<i>a</i>
P-S_N2-f-F	-1302.219	-1301.96	0.251675	-1301.949	-1301.952	0.060481	0.057598	-1302.01	-1302.009	<i>a</i>
R-S_N2-f-F	-1762.383	-1762.089	0.249963	-1762.112	-1762.116	0.071824	0.066069	-1762.183	-1762.182	<i>a</i>
f-F⁻	-1262.443	-1262.188	0.210734	-1262.216	-1262.218	0.058244	0.055183	-1262.274	-1262.273	<i>a</i>
TS-S_N2-f-F	-1762.366	-1762.072	0.249384	-1762.097	-1762.1	0.06823	0.063661	-1762.165	-1762.164	<i>a</i>
P-S_N2-f-H	-1203.048	-1202.822	0.260383	-1202.77	-1202.773	0.060199	0.056884	-1202.83	-1202.829	<i>a</i>
R-S_N2-f-H	-1663.225	-1662.966	0.257807	-1662.946	-1662.951	0.070928	0.064868	-1663.017	-1663.015	<i>a</i>
f-H⁻	-1163.284	-1163.064	0.218567	-1163.05	-1163.053	0.056894	0.053804	-1163.107	-1163.106	<i>a</i>
TS-S_N2-f-H	-1663.205	-1662.945	0.257948	-1662.927	-1662.931	0.065263	0.061294	-1662.993	-1662.992	<i>a</i>
P-S_N2-g-F	-1188.985	-1188.758	0.24185	-1188.727	-1188.729	0.056482	0.053904	-1188.783	-1188.783	<i>a</i>
R-S_N2-g-F	-1649.126	-1648.86	0.239259	-1648.868	-1648.872	0.067823	0.062393	-1648.935	-1648.934	<i>a</i>
g-F⁻	-1149.186	-1148.958	0.200016	-1148.972	-1148.974	0.054356	0.051535	-1149.026	-1149.025	<i>a</i>
TS-S_N2-g-F	-1649.116	-1648.851	0.238489	-1648.859	-1648.862	0.065878	0.06083	-1648.925	-1648.923	<i>a</i>
P-S_N2-g-H	-1089.811	-1089.618	0.250377	-1089.545	-1089.548	0.055345	0.052596	-1089.601	-1089.6	<i>a</i>
R-S_N2-g-H	-1549.96	-1549.73	0.247247	-1549.694	-1549.698	0.065895	0.060577	-1549.76	-1549.758	<i>a</i>
g-H⁻	-1050.019	-1049.828	0.208102	-1049.797	-1049.799	0.05175	0.049491	-1049.849	-1049.848	<i>a</i>

Species	E_{SPC}	E	ZPE	H_{SPC}	qh- H_{SPC}	$T.S$	$T.\text{qh-}S$	$G(T)_{\text{SPC}}$	qh- $G(T)_{\text{SPC}}$	T
TS-S_N2-g-H	-1549.947	-1549.718	0.247001	-1549.682	-1549.685	0.062324	0.058275	-1549.744	-1549.743	<i>a</i>
CH₄	-40.47002	-40.463	0.045012	-40.42127	-40.42127	0.017761	0.017761	-40.43903	-40.43903	<i>a</i>
CH₃F	-139.6416	-139.5911	0.039568	-139.5983	-139.5983	0.021823	0.021823	-139.6201	-139.6201	<i>a</i>
CH₂F₂	-238.8298	-238.7427	0.033159	-238.7926	-238.7926	0.024489	0.02449	-238.8171	-238.8171	<i>a</i>
CF₃H	-338.0244	-337.908	0.025654	-337.9944	-337.9944	0.025928	0.025929	-338.0203	-338.0203	<i>a</i>
CF₃⁻	-337.4995	-337.3479	0.009617	-337.4854	-337.4854	0.027252	0.027254	-337.5127	-337.5127	<i>a</i>
CH₂F⁻	-139.0792	-138.9925	0.02318	-139.0522	-139.0522	0.022715	0.022715	-139.0749	-139.0749	<i>a</i>
CH₃⁻	-39.90263	-39.85395	0.028804	-39.87008	-39.87008	0.019566	0.019566	-39.88964	-39.88964	<i>a</i>
CHF₂⁻	-238.2794	-238.158	0.016801	-238.2585	-238.2585	0.025309	0.02531	-238.2838	-238.2838	<i>a</i>
CH₃CF₂H	-278.1199	-278.0261	0.061106	-278.0537	-278.0538	0.02826	0.028265	-278.082	-278.082	<i>a</i>
CH₃CF₃	-377.3146	-377.1922	0.05291	-377.2561	-377.2561	0.02983	0.029836	-377.2859	-377.286	<i>a</i>
CH₃CFH₂	-178.9272	-178.8684	0.068528	-178.854	-178.854	0.026341	0.026345	-178.8803	-178.8803	<i>a</i>
CH₃CH₃	-79.74606	-79.72981	0.075114	-79.66662	-79.66663	0.024006	0.024008	-79.69063	-79.69064	<i>a</i>
R-S_N2-CF₃	-837.4341	-837.2523	0.048858	-837.3759	-837.378	0.043005	0.040242	-837.4189	-837.4182	<i>a</i>
R-S_N2-CH₂F	-639.0132	-638.8982	0.062493	-638.9428	-638.9442	0.037537	0.035979	-638.9803	-638.9801	<i>a</i>
R-S_N2-CH₃	-539.8329	-539.761	0.067739	-539.7576	-539.7585	0.034802	0.034144	-539.7924	-539.7927	<i>a</i>
R-S_N2-CHF₂	-738.2131	-738.0651	0.056313	-738.1484	-738.1499	0.040281	0.038086	-738.1886	-738.188	<i>a</i>
TS-S_N2-CH₃	-539.8332	-539.755	0.067302	-539.7584	-539.7594	0.034734	0.033802	-539.7931	-539.7932	<i>a</i>
TS-S_N2-CH₂F	-639.0111	-638.897	0.061985	-638.9416	-638.9424	0.036158	0.035113	-638.9778	-638.9775	<i>a</i>
TS-S_N2-CHF₂	-738.2107	-738.0615	0.055738	-738.1472	-738.1481	0.037154	0.036207	-738.1844	-738.1843	<i>a</i>
TS-S_N2-CF₃	-837.4276	-837.2482	0.048027	-837.371	-837.3724	0.040745	0.038622	-837.4117	-837.411	<i>a</i>
B1-F	-4117.884	-4117.136	1.102180	-4116.721	-4116.736	0.156292	0.138968	-4116.878	-4116.875	<i>b</i>
TSB-F	-4117.857	-4117.109	1.101376	-4116.696	-4116.710	0.155611	0.138277	-4116.852	-4116.848	<i>b</i>
B2-F	-4117.886	-4117.143	1.104057	-4116.722	-4116.736	0.153933	0.137383	-4116.876	-4116.873	<i>b</i>
B1-H	-4018.727	-4018.014	1.110548	-4017.557	-4017.571	0.153459	0.136758	-4017.711	-4017.708	<i>b</i>
TSB-H	-4018.696	-4017.981	1.110002	-4017.527	-4017.541	0.153812	0.136543	-4017.681	-4017.678	<i>b</i>
B2-H	-4018.722	-4018.011	1.112787	-4017.551	-4017.565	0.152755	0.136064	-4017.704	-4017.701	<i>b</i>
Cs₂CO₃	-304.081	-303.957	0.015872	-304.058	-304.059	0.039012	0.037750	-304.097	-304.097	<i>b</i>
1	-1121.439	-1121.172	0.514694	-1120.899	-1120.905	0.079538	0.072258	-1120.979	-1120.977	<i>b</i>
2-F	-2590.582	-2590.096	0.676487	-2589.869	-2589.877	0.104523	0.094300	-2589.974	-2589.971	<i>b</i>
2-H	-2491.419	-2490.964	0.686005	-2490.697	-2490.705	0.102251	0.092331	-2490.8	-2490.797	<i>b</i>
5	-2002.164	-2001.767	0.240751	-2001.899	-2001.905	0.077304	0.071271	-2001.976	-2001.976	<i>b</i>
6	-533.051	-532.869	0.078514	-532.959	-532.963	0.055158	0.050800	-533.014	-533.014	<i>b</i>
a-F(DCM)	-1698.032	-1697.736	0.224269	-1697.792	-1697.795	0.056224	0.052827	-1697.848	-1697.848	<i>b</i>
a-F⁻(DCM)	-1697.541	-1697.240	0.211096	-1697.314	-1697.316	0.053385	0.051326	-1697.367	-1697.367	<i>b</i>
OAc⁻	-228.432	-228.344	0.049006	-228.378	-228.378	0.026456	0.026112	-228.405	-228.405	<i>b</i>
B01	-2648.754	-2648.232	0.942008	-2647.764	-2647.775	0.130646	0.116571	-2647.894	-2647.892	<i>b</i>
TSB0	-2648.737	-2648.210	0.939874	-2647.748	-2647.760	0.130552	0.116741	-2647.879	-2647.877	<i>b</i>
B02	-2648.759	-2648.236	0.941207	-2647.769	-2647.780	0.129001	0.116527	-2647.898	-2647.897	<i>b</i>
TSB'-F	-4117.849	-4117.102	1.101568	-4116.687	-4116.701	0.155773	0.138410	-4116.843	-4116.840	<i>b</i>
C1-F	-2923.810	-2923.318	0.568980	-2923.219	-2923.225	0.061153	0.056734	-2923.281	-2923.282	<i>c</i>
TSC-F	-2923.806	-2923.317	0.569267	-2923.216	-2923.222	0.058853	0.055035	-2923.275	-2923.277	<i>c</i>
C2-F	-2923.817	-2923.330	0.570731	-2923.225	-2923.231	0.058965	0.055079	-2923.284	-2923.286	<i>c</i>
C1-H	-2824.656	-2824.197	0.577152	-2824.058	-2824.064	0.061290	0.056327	-2824.119	-2824.120	<i>c</i>
TSC-H	-2824.646	-2824.190	0.577729	-2824.048	-2824.054	0.057763	0.054061	-2824.106	-2824.108	<i>c</i>
C2-H	-2824.654	-2824.197	0.579373	-2824.054	-2824.059	0.058000	0.054184	-2824.112	-2824.114	<i>c</i>

Species	E_{SPC}	E	ZPE	H_{SPC}	qh- H_{SPC}	$T.S$	$T.\text{qh-}S$	$G(T)_{\text{SPC}}$	qh- $G(T)_{\text{SPC}}$	T
C1-Cl	-3284.113	-3283.623	0.568106	-3283.523	-3283.529	0.062550	0.057624	-3283.585	-3283.586	c
TSC-Cl	-3284.101	-3283.613	0.568461	-3283.511	-3283.517	0.058840	0.055093	-3283.570	-3283.572	c
C2-Cl	-3284.103	-3283.616	0.569578	-3283.513	-3283.518	0.058894	0.055128	-3283.572	-3283.573	c