Singlet carbene stability: linear free-energy analysis of substituent effects

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Table 1. M06-2X/cc-pVDZ Calculations for X-Substituted Methylcarbenes

Zero Point Energies are listed in Table 3

System	H	Δ(ΔH)/CH3	G	Δ(ΔG)/CH2	Δ(ΔG)/CH3
CH2;	39.087466		39.108961	0	
CH4	40.432482		40.453633		
CH3CF	177.63001	25.77118766	177.660107	39.44336464	25.29428044
CH3CH2F	178.91191		178.941922		
CH3CCL	538.000535	18.48391983	538.031733	32.10024847	17.95116427
CH3CH2CL	539.294048		539.32525		
CH3CNH2	133.765359	52.9881572	133.7952	66.12004851	51.9709643
CH3CH2NH2	135.003886		135.034503		
CH3COCH3	192.880827	41.48528055	192.914959	57.61603976	43.46695556
CH3CH2OCH3	194.137685		194.167814		
CH3CH	78.371354	0	78.398129	14.14908421	0
CH3CH3	79.694323		79.720253		
CH3CC6H5	309.28704	12.75162055	309.326997	26.36543915	12.21635495
CH3CH2C6H5	310.589688		310.629653		
CH3CCN	170.611345	9.417662576	170.64331	22.83318818	8.684103971
CH3CH2CN	171.919306		171.951595		
CH3CC=O(CH3)	230.944202	9.767812877	230.981178	24.06687185	9.917787648
CH3CH2C=O(CH3)	232.251605		232.287497		
CH3CNO2	282.836828	11.93648571	282.871627	25.59611251	11.4470283
CH3CH2NO2	284.140775		284.175509		
CH3CCOCH=O	266.912319	35.7943969	266.948128	49.05492765	34.90584345
CH3CH2OCH=O	268.178246		268.214626		
CH3CSCH3	515.860437	35.80004448	515.89631	48.49393416	34.34484995
CH3CH2SCH3	517.126355		517.163702		
CH3COH	153.6268	42.32802581	153.656895	55.62022351	41.4357073
CH3CH2OH	154.882315		154.912987		
CH3CCH3	117.653596	11.08558283	117.68432	24.48932243	10.41854023
CH3CH2CH3	118.958899		118.989841		
CH3CBr	90.942259	17.656862	90.974679	31.179344	17.0306078
CH3CH2Br	92.23709		92.269663		
CH3CSI(CH3)3	486.849624	1.967242282	486.896562	15.65949957	1.510415367
CH3CH2Si(CH3)3	488.169458		488.216279		
CH3CCF3	415.336537	1.148969894	415.37331	12.5037543	1.645329909
CH3CH2CF3	416.661337		416.698056		
CH3COC=O(CH3)	306.187766	29.45215838	306.227805	42.74469212	28.59560791
CH3CH2OC=O(CH3)	307.4638		307.504359		
tBuCCH3	235.450018	8.55985709	235.49091	22.09711953	7.948035327
tBuCH2CH3	236.759346		236.800368		
CH3CCCH	154.512937	18.63012955	154.546632	32.91614	18.76727
CH3CH2CCH	155.806217		155.838848		
CH3CN(CH3)3+	251.834509	4.883906438	251.875129	18.8344125	4.6855425
CH3CH2N(CH3)3+	253.149695		253.189786		
CH3CNHC=O(CH3)	286.335081	45.3657993	286.376412	61.2697275	47.1208575
CH3CH2NHC=O(CH3)	287.585755		287.623443		
CH3CN(CH3)2	212.281074	50.97887178	212.319701	65.5103725	51.3615025
CH3CH2N(CH3)2	213.522803		213.559974		
CH3CS(CH3)2+	555.412639	9.63854592	555.454263	23.94038	9.79151
CH3CH2S(CH3)2+	556.720248		556.760783		

CH3CSH	476.588427	29.57013017	476.619893	42.90594	28.75707
CH3CH2SH	477.864273		477.896189		
CH3CC=O(H)	191.663876	8.240454754	191.698357	22.5881175	8.4392475
CH3CH2C=O(H)	192.973713		193.007032		
CH3CO-	153.05918	75.58853935	153.08943	89.55931	75.41044
CH3CH2O-	154.261691		154.291378		
CH3CS-	476.04138	47.01489427	476.072808	60.833615	46.684745
CH3CH2S-	477.289426		477.320534		
CH3CCH=CH2	155.723196	14.49546945	155.756893	28.1088625	13.9599925
CH3CH2CH=CH2	157.023065		157.05677		
CH3CSO(CH3)	590.985413	24.56636942	591.024149	38.349035	24.200165
CH3CH2SO(CH3)	592.269233		592.307707		
CH3CCO2CH3	306.147717	6.389929238	306.187412	20.0492525	5.9003825
CH3CH2CO2CH3	307.460503		307.500133		
CH3CC=O(CN)	283.884842	8.525971576	283.922914	22.2442475	8.0953775
CH3CH2C=O(CN)	285.194224		285.232137		
CH3CC=O(F)	290.913213	5.980165535	290.94835	19.498935	5.350065
CH3CH2C=O(F)	292.226652		292.261948		

Table 2. M06-2X/cc-pVDZ Calculations for X-Substituted Methylenes

Zero Point Energies are listed in Table 4

System	H	Δ(ΔH)/CH2	G	Δ(ΔG)/CH2
CH2;	39.087466	0	39.108961	0
CH4	40.432482		40.453633	
HCCF3	376.046519	-2.3550075	376.079656	-2.2151103
CH3CF3	377.395288		377.427858	
HCF	138.34491	31.3831575	138.370251	31.21436
CH3F	139.639913		139.665179	
HCCL	498.718702	24.016935	498.745379	23.86508
CH3CL	500.025444		500.052019	
HCNH2	94.487693	61.1630525	94.513559	60.09944
CH3NH2	95.735238		95.762455	
HCOCH3	153.601473	49.5078675	153.631257	48.8176175
CH3OCH3	154.867592		154.898132	
HCCH3	78.371354	13.826335	78.398129	13.09216
CH3CH3	79.694336		79.721937	
HCC6H5	270.010865	19.398535	270.046268	17.578785
CH3C6H5	271.324967		271.362926	
HCCN	131.329093	11.552275	131.35681	11.4474825
CH3CN	132.655699		132.683239	
HC=O(CH3)	191.663426	15.5751775	191.697105	15.2338175
CH3C=O(CH3)	192.983621		193.0175	
HCSCH3	476.588385	45.781145	476.61962	44.641
CH3SCH3	477.860443		477.893154	
HCOH	114.346267	49.7011375	114.37181	48.58105
CH3OH	115.612078		115.639062	
HCBr	51.661012	23.173575	51.688982	23.008543
CH3Br	52.969098		52.996987	
HCSI(CH3)3	447.566941	2.3838725	447.61027	4.652285

Si(CH3)4	448.908158		448.947528	
HCOC=O(CH3)	266.906478	35.98838	266.941186	34.649295
CH3OC=O(CH3)	268.194142		268.23064	
HCS(CH3)2+	516.126615	13.4655225	516.163444	13.9436775
CH3S(CH3)2+	517.450172		517.485895	
HCN(CH3)2	173.011509	62.5473175	173.044588	62.5096675
CH3N(CH3)2	174.256848		174.289643	
HCCCH	115.23376	22.6609075	115.262216	22.7374625
CH3CCH	116.542663		116.570653	
HCNHCH3(C=O)	247.056484	52.4018975	247.090948	51.4757075
CH3NHCH3(C=O)	248.317991		248.353587	
HCSH	437.319046	40.911745	437.346173	39.5632475
CH3SH	438.598864		438.627796	
HCCH=CH2	116.443738	18.8256275	116.473092	18.1818125
CH3CH=CH2	117.758753		117.788789	
HCSO(CH3)	551.717467	38.34025	551.751314	37.347545
CH3SO(CH3)	553.001383		553.036468	
HCCO2CH3	266.864201	9.4595625	266.899921	8.7555075
CH3CO2CH3	268.194142		268.23064	
HCC=O(CN)	244.595365	8.2158575	244.629627	7.76845
CH3C=O(CN)	245.927288		245.961919	
HCC=O(F)	251.626453	7.24637	251.657662	6.57369
CH3C=O(F)	252.959921		252.991858	

Table 3. CCSD(T)/cc-pVDZ//M06-2X/cc-pVDZ Calculations for X-Substituted Methylcarbenes

System	E CCSD(T)	ZPEs	Corrected	Δ(ΔE)/CH3	Δ(ΔE)/CH2
CH2;	39.0225051	0.016943	39.0055621		0
CH4	40.387534	0.044946	40.342588		
CH3CF	177.3066984	0.041215	177.2654834	26.56742756	36.90582093
CH3CH2F	178.6118972	0.068201	178.5436962		
CH3CCL	537.325818	0.040352	537.285466	19.23945947	29.577847
CH3CH2CL	538.6419976	0.066641	538.5753566		
CH3CNH2	133.5251624	0.06801	133.4571524	51.66359697	62.00201034
CH3CH2NH2	134.7886619	0.09329	134.6953719		
CH3COCH3	192.5309716	0.083179	192.4477926	41.87805067	52.21645625
CH3CH2OCH3	193.8100594	0.108453	193.7016064		
CH3CH	78.2349866	0.04701	78.1879766	0	10.3383722
CH3CH3	79.58293427	0.074407	79.50852727		
CH3CC6H5	308.6547482	0.130877	308.5238712	12.56080683	22.89918905
CH3CH2C6H5	309.982041	0.157636	309.824405		
CH3CCN	170.2639501	0.047434	170.2165161	9.396345451	19.73472514
CH3CH2CN	171.5968627	0.07477	171.5220927		
CH3CC=O(CH3)	230.5043947	0.085881	230.4185137	8.782076401	19.1204556
CH3CH2C=O(CH3)	231.8372072	0.112138	231.7250692		
CH3CNO2	282.2895649	0.051998	282.2375669	13.52532031	23.86370329
CH3CH2NO2	283.6164026	0.079839	283.5365636		
CH3CSCH3	515.1603756	0.079186	515.0811896	36.12774187	46.46614286
CH3CH2SCH3	516.44813	0.103963	516.344167		
CH3COH	153.3463117	0.055454	153.2908577	42.70655774	53.04496397

CH3CH2OH	154.6236422	0.080291	154.5433512		
CH3CCH3	117.4480129	0.075403	117.3726099	9.867046602	20.20542667
CH3CH2CH3	118.7813474	0.103911	118.6774364		
CH3CBr	90.7651772	0.039533	90.7256442	18.47038382	28.80877075
CH3CH2Br	92.05964141	0.065872	91.99373741		
CH3CSI(CH3)3	486.0783531	0.14932	485.9290331	1.28262879	11.62100202
CH3CH2Si(CH3)3	487.4232458	0.175706	487.2475398		
CH3CCF3	414.5653447	0.054262	414.5110827	-1.362279826	8.976091293
CH3CH2CF3	415.9158113	0.082007	415.8338043		
CH3COC=O(CH3)	305.6023061	0.092231	305.5100751	29.25479347	39.59318898
CH3CH2OC=O(CH3)	306.9025233	0.118518	306.7840053		
tBuCCH3	235.0453391	0.160622	234.8847171	7.421064772	17.75943697
tBuCH2CH3	236.3809166	0.187475	236.1934416		
CH3CNHC=O(CH3)	285.7911797	0.105175	285.6860047	46.1699622	56.5083344
CH3CH2NHC=O(CH3)	287.0630657	0.130088	286.9329777		
CH3CN(CH3)3+	251.4100334	0.163425	251.2466084	4.305195298	14.6435675
CH3CH2N(CH3)3+	252.7526742	0.192376	252.5602982		
CH3CN(CH3)2	211.9052428	0.124061	211.7811818	50.2824968	60.620869
CH3CH2N(CH3)2	213.170613	0.149012	213.021601		
CH3CS(CH3)2+	554.658938	0.116493	554.542445	8.985153048	19.32352525
CH3CH2S(CH3)2+	555.9923527	0.143676	555.8486767		
CH3CCCH	154.195406	0.057387	154.138019	18.58966805	28.92804025
CH3CH2CCH	155.5143317	0.085387	155.4289447		
CH3CSH	475.9577989	0.051473	475.9063259	30.23694655	40.57531875
CH3CH2SH	477.2541612	0.075471	477.1786902		
CH3CC=O(H)	191.292609	0.057175	191.235434	7.384086798	17.722459
CH3CH2C=O(H)	192.6288232	0.084606	192.5442172		
CH3CCH=CH2	155.4309743	0.081917	155.3490573	14.3150753	24.6534475
CH3CH2CH=CH2	156.7554521	0.108657	156.6467951		
CH3CSO(CH3)	590.1391644	0.084009	590.0551554	26.9093768	37.247749
CH3CH2SO(CH3)	591.4407866	0.107964	591.3328226		
CH3CCO2CH3	305.5620865	0.092102	305.4699845	6.617363372	16.95573557
CH3CH2CO2CH2	306.8991216	0.119132	306.7799896		
CH3CC=O(CN)	283.303662	0.056806	283.246856	7.259528047	17.59790025
CH3CH2C=O(CN)	284.6397397	0.083902	284.5558377		
CH3CC=O(F)	290.3549286	0.051191	290.3037376	5.761522397	16.0998946
CH3CH2C=O(F))	291.6932636	0.078157	291.6151066		

Table 4. CCSD(T)/cc-pVDZ//M06-2X/cc-pVDZ Calculations for X-Substituted Methylenes

System	ECCSD(T)	ZPEs	Sum	Δ(ΔE)/CH2
CH2;	39.0225051	0.016943	39.0055621	0
CH4	40.387534	0.044946	40.342588	
HCCF3	375.3479687	0.026309	375.3216597	-3.051658
CH3CF3	376.7163898	0.052841	376.6635488	
HCF	138.0921467	0.012534	138.0796127	30.5874122
CH3F	139.4073767	0.039483	139.3678937	
HCCL	498.1145718	0.011416	498.1031558	23.71536478
CH3CL	499.4402133	0.037825	499.4023883	
HCNH2	94.3168631	0.039802	94.2770611	57.4705915
CH3NH2	95.5867254	0.064225	95.5225004	

HCOCH3	153.3207286	0.055444	153.2652846	47.4556915
CH3OCH3	154.6068139	0.08013	154.5266839	
HCCH3	78.2349866	0.04701	78.1879766	10.33601371
CH3CH3	79.58293777	0.074407	79.50853077	
HCC6H5	269.4482251	0.103286	269.3449391	17.156101
CH3C6H5	270.7829996	0.128375	270.6546246	
HCCN	131.0526328	0.018594	131.0340388	10.8890075
CH3CN	132.3991437	0.045432	132.3537117	
HC=O(CH3)	191.2960637	0.058272	191.2377917	13.510326
CH3C=O(CH3)	192.6373102	0.084023	192.5532872	
HCSCH3	475.9577864	0.051575	475.9062114	43.9289156
CH3SCH3	477.2490911	0.07586	477.1732311	
HCOH	114.1355449	0.027106	114.1084389	47.99126275
CH3OH	115.4205827	0.051598	115.3689847	
HCBr	51.553937	0.011107	51.54283	22.370419
CH3Br	52.8583971	0.037166	52.8212361	
HCSI(CH3)3	446.8662576	0.121382	446.7448756	0.64789375
Si(CH3)4	448.228754	0.147885	448.080869	
HCOC=O(CH3)	266.3903387	0.06486	266.3254787	33.46526525
CH3OC=O(CH3)	267.6995025	0.090329	267.6091735	
HCN(CH3)2	515.4437687	0.089737	515.3540317	10.60907975
CH3N(CH3)2	516.7892777	0.115127	516.6741507	
HCCCH	172.7047739	0.096958	172.6078159	58.92921525
CH3CCH	173.9710257	0.120095	173.8509307	
HCNHCH3(C=O)	114.9853833	0.028884	114.9564993	20.72337575
CH3NHCH3(C=O)	116.3164399	0.05594	116.2604999	
HCSH	436.756529	0.021872	436.734657	39.2493092
CH3SH	438.756529	0.046031	438.710498	
HCCH=CH2	116.2206713	0.053762	116.1669093	16.6274448
CH3CH=CH2	117.5572963	0.079859	117.4774373	
HCSO(CH3)	550.9395944	0.055936	550.8836584	37.8705286
CH3SO(CH3)	552.2394099	0.079077	552.1603329	
HCCO2CH3	266.3509753	0.064254	266.2867213	9.14499675
CH3CO2CH3	267.6995025	0.090329	267.6091735	
HCC=O(CN)	244.0892422	0.028629	244.0606132	8.1776804
CH3C=O(CN)	245.4396839	0.055077	245.3846069	
HCC=O(F)	251.1409725	0.023238	251.1177345	6.69435825
CH3C=O(F)	252.4934711	0.049379	252.4440921	

Regression Analysis of Substituted Methylenes *vs.* Swain F and R From Table V Taft: Chem Reviews[5]

$$Y = 3.7 + F \times 32.6 + R \times -31.8$$

Average value of the dependent variable Var38:	26.8865
Number of observations:	20

The least squares estimates of your multiple-regression equation:

variable	coefficient	std. error	t value	one-sided p value
intercept	3.6969	3.1031	1.1914	0.1249
Var39	32.5952	9.4394	3.4531	0.0015
Var40	-31.7995	2.5854	12.2995	0.0000

standard error of estimate (SEE):	6.4704
coefficient of determination (R-squared):	0.9024
(adjusted for degrees of freedom)	0.8909

The computer will use the observed values of x to calculate the
MEAN: average value of x
VARIANCE: average squared deviation of x about its mean
STANDARD DEVIATION: square root of the variance
SKEWNESS COEFFICIENT: average cubed deviation of x about its mean, divided by the standard deviation cubed.

y-yHat, row 1 to row 22, number of actual observations:	20
Number of missing observations:	2
The mean:	-0.0000
The variance:	37.4588
The standard deviation:	6.1204
The skewness coefficient:	0.2024

	Δ(ΔE)	F	R	
H	0	0	0	-3.696934
F	30.59	0.45	-0.52	-4.310519
Cl	23.72	0.42	-0.31	-3.524769
Br	22.37	0.44	-0.03	3.377183
CF3	-3.05	0.23	0.27	-5.657973
NH2	57.47	0.08	-1.38	7.282154
OCH3	47.46	0.29	-1.07	0.284999
CH3	10.34	0.01	-0.32	-3.858722
C6H5	17.16	0.12	-0.3	0.011793
CN	10.89	0.51	0.15	-4.660575
SCH3	43.93	0.23	-0.83	6.342589
OH	47.99	0.33	-1.25	-6.212718
Si(CH3)3	0.65	0.01	0.01	-3.054891
N(CH3)2	58.93	0.15	-1.85	-8.485271
CCH	20.72	0.22	-0.04	8.580137
SH	39.25	0.3	-0.33	15.280668
CH=CH2	16.63	0.13	-0.29	-0.526165
CO2CH3	9.14	0.34	0.14	-1.187382
OC=O(CH3)	33.46	0.42	-0.61	-3.324616
NHC=O(CH3)	50.08	0.31	-0.91	7.341012

Regression Analysis of Substituted Methylcarbenes *vs.* Swain 1983 Constants[12a]

$$Y = 8.7 + 12.3 \times F - 12.6 \times R$$

The computer will use the observed values of x to calculate the
MEAN: average value of x
VARIANCE: average squared deviation of x about its mean
STANDARD DEVIATION: square root of the variance
SKEWNESS COEFFICIENT: average cubed deviation of x about its mean, divided by the standard deviation cubed.

y-yHat, row 1 to row 22, number of actual observations:	22
Number of missing observations:	0
The mean:	0.0000
The variance:	53.8920
The standard deviation:	7.3411
The skewness coefficient:	-0.0523

	Δ(ΔE)	F	R	
H	0	0	0	-8.720418
F	26.57	0.74	-0.6	1.217669
Cl	19.24	0.72	-0.24	-1.339343
Br	18.47	0.72	-0.18	-1.354773
CF3	-1.36	0.64	0.76	-8.380895
NH2	51.67	0.38	-2.52	6.591778
OCH3	41.89	0.54	-1.68	5.411159
CH3	9.87	-0.01	-0.41	-3.883854
C5H6	12.56	0.25	-0.37	-3.883264
CN	9.4	0.9	0.71	-1.442159
C=O(CH3)	8.78	0.5	0.9	5.238781
SCH3	36.13	0.68	-1.3	2.711082
OH	42.71	0.46	-1.89	4.572461
Si(CH3)3	1.28	-0.1	0.16	-4.200366
NHC=O(CH3)	46.17	0.77	-1.43	10.011101
S(CH3)2+	8.99	1.62	0.52	-13.082276
N(CH3)2	50.28	0.69	-3.81	-14.827849
OC=O(CH3)	29.25	0.7	-0.04	11.431462
SH	30.24	0.52	-0.26	11.86487
C(CH3)3	7.42	-0.11	-0.29	-3.596848
NO2	13.53	1	1	5.107058
CO2CH3	6.62	0.47	0.67	0.554626

Regression Analysis of Substituted Methylcarbenes *vs.* Swain 1968 Constants[12b]

$$Y = 8.2 + 3.9 \times F - 53.8 \times R$$

Average value of the dependent variable Var28: 16.7411

Number of observations: 19

The least squares estimates of your multiple-regression equation:

variable	coefficient	std. error	t value	one-sided p value
intercept	8.2065	3.0741	2.6696	0.0084
Var34	3.9473	3.8815	1.0170	0.1621
Var35	-53.8171	7.4108	7.2620	0.0000

standard error of estimate (SEE): 7.9738

coefficient of determination (R-squared): 0.7715

(adjusted for degrees of freedom) 0.7429

The computer will use the observed values of x to calculate the
MEAN: average value of x
VARIANCE: average squared deviation of x about its mean
STANDARD DEVIATION: square root of the variance
SKEWNESS COEFFICIENT: average cubed deviation of x about its mean, divided by the standard deviation cubed.

y-yhat, row 1 to row 22, number of actual observations: 19

Number of missing observations: 3

The mean: -0.0000

The variance: 56.5163

The standard deviation: 7.5177

The skewness coefficient: 0.1139

	ΔΔ(E)	F	R	
H	0	0	0	-8.206499
F	26.57	0.708	-0.336	-2.51378
Cl	19.24	0.69	-0.161	-0.354727
Br	18.47	0.727	-0.176	-2.078036
CF3	-1.36	0.631	0.186	-2.047283
NH2	51.67	0.037	-0.681	6.667971
OCH3	41.89	0.413	-0.5	5.144674
CH3	9.87	-0.052	-0.141	-5.719455
C5H6	12.56	0.139	-0.088	-0.931089
CN	9.4	0.847	0.184	7.752456
C=O(CH3)	8.78	0.534	0.202	9.336684
SCH3	36.13	0.332	-0.186	16.602993
OH	42.71	0.487	-0.643	-2.023282
Si(CH3)3	1.28	-0.093	-0.047	-9.088802
S(CH3)2+	8.99	1.687	-0.042	-8.135988
N(CH3)3+	4.31	1.46	0	-9.659621
C(CH3)3	7.42	-0.104	-0.138	-7.802742
NO2	13.53	1.109	0.155	9.287555
CO2CH3	6.62	0.552	0.14	3.768968

Regression Analysis of Substituted Methylenes *vs.* Swain F and R From Table I Taft: Chem Reviews[5]

$$Y = 11.5 + F \times 9.9 + R \times -53.5$$

Average value of the dependent variable Var13: 24.7191

Number of observations: 23

The least squares estimates of your multiple-regression equation:

variable	coefficient	std. error	t value	one-sided p value
intercept	11.4964	4.4352	2.5921	0.0087
Var14	9.8792	10.7578	0.9183	0.1847
Var15	-53.5366	7.4802	7.1571	0.0000

standard error of estimate (SEE): 10.5699

coefficient of determination (R-squared): 0.7218

(adjusted for degrees of freedom) 0.6940

Average value of the dependent variable Var13: 24.7191

Number of observations: 23

The least squares estimates of your multiple-regression equation:

variable	coefficient	std. error	t value	one-sided p value
intercept	11.4964	4.4352	2.5921	0.0087
Var14	9.8792	10.7578	0.9183	0.1847
Var15	-53.5366	7.4802	7.1571	0.0000

standard error of estimate (SEE): 10.5699

coefficient of determination (R-squared): 0.7218

(adjusted for degrees of freedom) 0.6940

	Δ(ΔE)	F	R	
H	0	0	0	
F	30.59	0.45	-0.39	-6.231312
Cl	23.72	0.42	-0.19	-2.097622
Br	22.37	0.45	-0.22	-5.350094
CF3	-3.05	0.38	0.16	-9.734653
NH2	57.47	0.08	-0.74	5.566186
OCH3	47.46	0.29	-0.56	3.11814
CH3	10.34	0.01	-0.18	-10.891788
C6H5	17.16	0.12	-0.13	-2.48167
CN	10.89	0.51	0.15	2.385687
S(CH3)2+	10.61	0.98	-0.08	-14.850944
SCH3	43.93	0.23	-0.23	17.847961
OH	47.99	0.33	-0.7	-4.242148
Si(CH3)3	0.65	0.01	-0.08	-15.228131
N(CH3)2	58.93	0.15	-0.98	-6.514135
CCH	20.72	0.22	0.01	7.585531
SH	39.25	0.3	-0.15	16.759344
CH=CH2	16.63	0.13	-0.17	-5.251925
CO2CH3	9.14	0.34	0.11	0.173686
C=O(F)	6.69	0.48	0.22	2.229623
OC=O(CH3)	33.46	0.42	-0.11	11.925304
NHC=O(CH3)	50.08	0.31	-0.31	18.9247
C=O(CH3)	13.51	0.33	0.17	7.854672

Results for Fluorocarbene at : CCSD(T)/cc-pVQZ//M06-2X/cc-pVQZ

System	CCSD(T)/pp-vqz	Zero-Pt. Corr.	Corrected E	E Relative
CH2	-39.0719035	0.016997	-39.0549065	0
CH4	-40.4508724	0.045167	-40.4057054	
CHF	-138.2709321	0.012566	-138.2583661	-28.4885
CH3F	-139.603396	0.039631	-139.563765	