ADDITIONS AND CORRECTIONS

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Correction to "Bond Dissociation Energies and Radical Stabilization
Energies: An Assessment of Contemporary Theoretical Procedures"

SUPPORTING INFORMATION

(Tables S1, S2 and S3. Total 10 Pages)

TABLE S1: Total Energies of Substituted Methyl Radicals ($\bullet\text{CH}_2\text{X}$) and Substituted Methanes (CH_3X) (0 K, Hartrees)^a

Species	UBMK ^{a,b}	RBMK ^{a,b}	UMPWB1K ^{a,b}	RMPWB1K ^{a,b}	UM05 ^{c,b}	UM05-2X ^{a,b}	UB2-PLYP ^{a,b}	RB2-PLYP ^{a,b}	UMPW2-PLYP ^{a,b}	RMPW2-PLYP ^{a,b}	G3(MP2)-RAD	G3X(MP2)-RAD	CBS-QB3	ROCBS-QB3	W1 ^c
CH_4	-40.44822	-40.44822	-40.45075	-40.45075	-40.44193	-40.47154	-40.44556	-40.44556	-40.44437	-40.44437	-40.42078	-40.42170	-40.40999	-40.40999	-40.47905
$\bullet\text{CH}_3$	-39.78558	-39.78402	-39.78902	-39.78751	-39.78223	-39.80941	-39.78573	-39.78428	-39.78479	-39.78328	-39.75592	-39.75649	-39.74479	-39.74510	-39.81440
CH_3NH_2	-95.76173	-95.76173	-95.76726	-95.76726	-95.75146	-95.80951	-95.75473	-95.75474	-95.75266	-95.75266	-95.68517	-95.68653	-95.66847	-95.66847	-95.82950
$\bullet\text{CH}_2\text{NH}_2$	-95.11970	-95.11823	-95.12629	-95.12469	-95.11139	-95.16701	-95.11456	-95.11321	-95.11256	-95.11108	-95.03716	-95.03853	-95.02214	-95.02244	-95.18362
CH_3OH	-115.64707	-115.64707	-115.65165	-115.65165	-115.64256	-115.69557	-115.63858	-115.63858	-115.63610	-115.63610	-115.55178	-115.55304	-115.53995	-115.53995	-115.73250
$\bullet\text{CH}_2\text{OH}$	-114.99933	-114.99790	-115.00488	-115.00330	-114.99679	-115.04691	-114.99269	-114.99134	-114.99027	-114.98881	-114.89894	-114.90019	-114.88814	-114.88835	-115.08129
CH_3OCH_3	-154.90282	-154.90282	-154.91164	-154.91164	-154.89179	-154.97448	-154.89058	-154.89059	-154.88811	-154.88811	-154.77068	-154.77276	-154.75222	-154.75222	-155.01220
$\bullet\text{CH}_2\text{OCH}_3$	-154.25518	-154.25378	-154.26414	-154.26318	-154.24603	-154.32563	-154.24482	-154.24351	-154.24233	-154.24089	-154.11764	-154.11972	-154.10026	-154.10047	-154.36094
CH_3F	-139.68541	-139.68541	-139.69377	-139.69377	-139.68761	-139.73578	-139.67463	-139.67463	-139.67259	-139.67259	-139.56943	-139.57075	-139.56384	-139.56384	-139.80024
$\bullet\text{CH}_2\text{F}$	-139.02900	-139.02762	-139.03871	-139.03728	-139.03357	-139.07880	-139.02072	-139.01936	-139.01877	-139.01732	-138.90931	-138.91052	-138.90421	-138.90445	-139.14121
CH_3CH_3	-79.71196	-79.71196	-79.71970	-79.71970	-79.69961	-79.75857	-79.70585	-79.70585	-79.70452	-79.70452	-79.64934	-79.65086	-79.63057	-79.63057	-79.76918
$\bullet\text{CH}_2\text{CH}_3$	-79.05598	-79.05429	-79.06523	-79.06363	-79.04850	-79.10309	-79.05262	-79.05113	-79.05149	-79.04990	-78.98986	-78.99118	-78.97155	-78.97183	-79.11056
$\text{CH}_3\text{CH}_2\text{CH}_3$	-118.97936	-118.97936	-118.99225	-118.99225	-118.96074	-119.05003	-118.97009	-118.97010	-118.96873	-118.96873	-118.88265	-118.88479	-118.85587	-118.85587	-119.06372
$\bullet\text{CH}_2\text{CH}_2\text{CH}_3$	-118.32224	-118.32058	-118.33626	-118.33479	-118.30830	-118.39330	-118.31568	-118.31423	-118.31444	-118.31290	-118.22255	-118.22385	-118.19574	-118.19603	-118.40391
CH_3CF_3	-377.49224	-377.49224	-377.52005	-377.52005	-377.50841	-377.62048	-377.46247	-377.46247	-377.45921	-377.45921	-377.16617	-377.16322	-377.16323	-377.16323	-377.80356
$\bullet\text{CH}_2\text{CF}_3$	-376.82736	-376.82574	-376.85626	-376.85514	-376.84858	-376.95619	-376.80107	-376.79961	-376.79787	-376.79634	-376.49835	-376.49584	-376.49553	-376.49584	-377.13658
$\text{CH}_3\text{CF}_2\text{CF}_3$	-615.26224	-615.26224	-615.30796	-615.30796	-615.29107	-615.46947	-615.21419	-615.21418	-615.20958	-615.20958	-614.72789	-614.73353	-614.72754	-614.72754	
$\bullet\text{CH}_2\text{CF}_2\text{CF}_3$	-614.59869	-614.59706	-614.64518	-614.64428	-614.63237	-614.80631	-614.55390	-614.55245	-614.54936	-614.54783	-614.06114	-614.06676	-614.06114	-614.02598	
CH_3PH_2	-382.30044	-382.30044	-382.43598	-382.43598	-382.39051	-382.40920	-382.31254	-382.31254	-382.31964	-382.31964	-381.92725	-381.92933	-381.90707	-381.90707	-383.05162 ^c

•CH ₂ PH ₂	-381.64959	-381.64776	-381.78600	-381.78403	-381.74365	-381.75778	-381.66364	-381.66197	-381.67090	-381.66907	-381.27125	-381.27322	-381.25270	-381.25267	-382.39723 ^c
CH ₃ SH	-438.53833	-438.53833	-438.70251	-438.70251	-438.65156	-438.66601	-438.56527	-438.56527	-438.57282	-438.57282	-438.16994	-438.17188	-438.15282	-438.15282	-439.57214 ^c
•CH ₂ SH	-437.89014	-437.88837	-438.05731	-438.05533	-438.00855	-438.01929	-437.92099	-437.91943	-437.92859	-437.92685	-437.51884	-437.52087	-437.50337	-437.50351	-438.92326 ^c
CH ₃ Cl	-499.94444	-499.94444	-500.13322	-500.13322	-500.07758	-500.08375	-499.96290	-499.96290	-499.97282	-499.97282	-499.57329	-499.57502	-499.56208	-499.56208	-501.31991 ^c
•CH ₂ Cl	-499.28969	-499.28794	-499.48153	-499.47973	-499.42820	-499.43036	-499.31191	-499.31035	-499.32193	-499.32024	-498.91647	-498.91832	-498.90592	-498.90605	-500.66404 ^c
CH ₃ Br	-2612.67435	-2612.67435	-2614.33712	-2614.33712	-2613.92922	-2613.96091	-2613.68177	-2613.68177	-2613.71474	-2613.71474			-2612.68925		
•CH ₂ Br	-2612.01850	-2612.01672	-2613.68321	-2613.68137	-2613.27816	-2613.30400	-2613.02840	-2613.02689	-2613.06149	-2613.05984			-2612.02790		
CH ₃ BH ₂	-65.85100	-65.85100	-65.85383	-65.85383	-65.84045	-65.88878	-65.84313	-65.84313	-65.84237	-65.84237	-65.78322	-65.78438	-65.76609	-65.76609	-65.89024
•CH ₂ BH ₂	-65.20658	-65.20539	-65.20897	-65.20799	-65.19736	-65.24295	-65.19959	-65.19856	-65.19904	-65.19796	-65.13362	-65.13473	-65.11716	-65.11705	-65.24117
CH ₃ CH=CH ₂	-117.77224	-117.77224	-117.78653	-117.78653	-117.75395	-117.84280	-117.76751	-117.76751	-117.76541	-117.76541	-117.67130	-117.67293	-117.64621	-117.64621	-117.85362
•CH ₂ CH=CH ₂	-117.13801	-117.13340	-117.15419	-117.14894	-117.12668	-117.20979	-117.13503	-117.13309	-117.13334	-117.13060	-117.03337	-117.03480	-117.00950	-117.00964	-117.21574
CH ₃ C=CH	-116.54903	-116.54903	-116.56475	-116.56475	-116.53654	-116.61915	-116.55048	-116.55048	-116.54733	-116.54733	-116.44388	-116.44525	-116.42172	-116.42172	-116.62846
•CH ₂ C=CH	-115.90894	-115.90503	-115.92655	-115.92221	-115.90264	-115.97946	-115.91192	-115.91070	-115.90903	-115.90717	-115.79906	-115.80019	-115.77866	-115.77819	-115.98424
CH ₃ C ₆ H ₅	-271.32470	-271.32470	-271.36758	-271.36758	-271.28053	-271.48964	-271.31867	-271.31867	-271.31476	-271.31476	-271.06697	-271.07059	-271.02044	-271.02044	-271.50079
•CH ₂ C ₆ H ₅	-270.68578	-270.68216	-270.73004	-270.72603	-270.64828	-270.85116	-270.67959	-270.67960	-270.67615	-270.67540	-270.42454	-270.42793	-270.37807	-270.37961	-270.85866
CH ₃ CHO	-153.73818	-153.73818	-153.74591	-153.74591	-153.72996	-153.80379	-153.72867	-153.72867	-153.72515	-153.72515	-153.59909	-153.60054	-153.58247	-153.58247	-153.84286
•CH ₂ CHO	-153.09103	-153.08764	-153.10055	-153.09670	-153.08663	-153.15759	-153.08285	-153.08191	-153.07970	-153.07820	-152.94754	-152.94904	-152.93284	-152.93225	-153.19213
CH ₃ COOH	-228.99069	-228.99069	-229.00088	-229.00088	-228.98531	-229.08121	-228.97474	-228.97474	-228.97006	-228.97006	-228.78232	-228.78436	-228.76536	-228.76536	-229.14894
•CH ₂ COOH	-228.33771	-228.33563	-228.34929	-228.34730	-228.33706	-228.42910	-228.32453	-228.32322	-228.32001	-228.31850	-228.12552	-228.12757	-228.10974	-228.10962	-228.49331
CH ₃ COOCH ₃	-268.24512	-268.24512	-268.25947	-268.25947	-268.23227	-268.35930	-268.22568	-268.22568	-268.22093	-268.22093	-268.00079	-268.00355	-267.97707	-267.97707	-268.42797
•CH ₂ COOCH ₃	-267.59225	-267.59024	-267.60795	-267.60610	-267.58430	-267.70726	-267.57568	-267.57438	-267.57106	-267.56956	-267.34412	-267.34701	-267.32156	-267.32146	-267.77219
•CH ₂ OCOCH ₃	-267.59214	-267.59073	-267.60740	-267.60602	-267.58267	-267.70516	-267.57463	-267.57329	-267.56990	-267.56845	-267.34279	-267.34602	-267.32022	-267.32057	-267.76997
CH ₃ CN	-132.66766	-132.66766	-132.67728	-132.67728	-132.65512	-132.73478	-132.66583	-132.66583	-132.66167	-132.66167	-132.54593	-132.54752	-132.52665	-132.52665	-132.75467
•CH ₂ CN	-132.01898	-132.01540	-132.03087	-132.02671	-132.01212	-132.08632	-132.01910	-132.01827	-132.01522	-132.01379	-131.89323	-131.89430	-131.87587	-131.87525	-132.10263

CH ₃ NO ₂	-244.91797	-244.91797	-244.93025	-244.93025	-244.92728	-245.01220	-244.91446	-244.91446	-244.90641	-244.90641	-244.70583	-244.70837	-244.69274	-244.69274	-245.09607
•CH ₂ NO ₂	-244.26218	-244.26020	-244.27500	-244.27289	-244.27554	-244.35579	-244.26042	-244.25913	-244.25244	-244.25095	-244.04539	-244.04748	-244.03385	-244.03381	-244.43655
•H	-0.49862	-0.49862	-0.49782	-0.49782	-0.49766	-0.49921	-0.49861	-0.49861	-0.49818	-0.49818	-0.50171	-0.50179	-0.49982	-0.49982	-0.49999

^a Including scaled (by 0.9806) RB3-LYP/6-31G(d) ZPVEs.

^b Energy calculations carried out with the 6-311+G(3df,2p) basis set on RB3-LYP/6-31G(d) geometries.

^c W1' calculations for systems containing second- and third-row elements.

TABLE S2: Comparison of Calculated Bond Dissociation Energies for $\text{CH}_3\text{X} \rightarrow \bullet\text{CH}_2\text{X} + \bullet\text{H}$ with Experimental Values (0 K, kJ mol^{-1})

Radical($\bullet\text{CH}_2\text{X}$)	UBMK	RBMK	UMPWBIK	RMPWBIK	UM05	UM05-2X	UB2-PLYP	RB2-PLYP	UMPW2-PLYP	RMPW2-PLYP	G3(MP2)-RAD	G3X(MP2)-RAD	CBS-QB3	ROCBS-QB3	W1 ^a	Experiment ^b
$\bullet\text{CH}_3$	430.6	434.7	430.4	434.3	425.4	427.8	423.3	427.1	423.8	427.7	428.4	429.1	434.2	433.4	432.3	432.4 ± 0.4
$\bullet\text{CH}_2\text{NH}_2$	376.5	380.4	375.8	380.1	373.9	376.2	371.6	375.2	372.6	376.5	384.1	383.9	384.6	383.9	383.0	386.8 ± 8.4
$\bullet\text{CH}_2\text{OH}$	391.5	395.3	391.1	395.2	388.8	392.4	386.7	390.2	387.6	391.5	396.8	396.6	399.1	398.5	397.0	395.8 ± 0.63
$\bullet\text{CH}_2\text{OCH}_3$	391.3	394.9	393.0	395.5	388.8	392.9	386.4	389.8	387.5	391.3	397.3	397.1	399.4	398.9	397.1	395.7^c
$\bullet\text{CH}_2\text{F}$	414.3	417.9	412.8	416.6	410.6	414.2	407.7	411.3	408.6	412.4	415.9	416.0	419.6	419.0	417.5	417.4 ± 4.2
$\bullet\text{CH}_2\text{CH}_3$	413.1	417.6	411.3	415.5	402.9	410.3	405.9	409.9	406.6	410.7	414.2	414.5	418.0	417.3	416.5	413.0 ± 1.3
$\bullet\text{CH}_2\text{CH}_2\text{CH}_3$	416.2	420.5	415.3	419.1	406.4	413.6	409.1	412.9	409.8	413.9	415.9	417.8	420.9	420.1	419.6	414.8 ± 2.1
$\bullet\text{CH}_2\text{CF}_3$	436.5	440.8	435.8	438.7	425.8	433.4	427.4	431.2	428.4	432.4	436.1	434.8	440.8	440.0	438.4	439.3 ± 4.5
$\bullet\text{CH}_2\text{CF}_2\text{CF}_3$	433.0	437.3	433.1	435.5	422.8	430.5	424.5	428.3	425.5	429.5	433.3	433.2	437.3			
$\bullet\text{CH}_2\text{PH}_2$	399.7	404.5	399.5	404.7	391.7	399.6	394.6	399.0	395.3	400.1	405.1	405.2	405.8	405.9	405.4 ^a	
$\bullet\text{CH}_2\text{SH}$	392.7	397.4	387.0	392.1	381.6	387.3	382.5	386.5	383.5	388.0	392.2	391.8	392.8	392.5	390.9 ^a	386.3 ± 8.4
$\bullet\text{CH}_2\text{Cl}$	409.9	414.5	404.0	408.7	398.4	404.8	400.1	404.2	400.9	405.4	407.2	406.7	410.5	410.1	409.3 ^a	411.9 ± 2.3
$\bullet\text{CH}_2\text{Br}$	412.8	417.5	409.8	414.6	402.7	414.1	406.3	410.3	407.1	411.4			424.1			410.3 ± 2.4
$\bullet\text{CH}_2\text{BH}_2$	382.8	385.9	386.0	388.6	381.8	385.0	380.5	383.2	381.1	383.9	388.3	388.2	391.5	391.8	391.4	
$\bullet\text{CH}_2\text{CH}=\text{CH}_2$	356.0	368.2	353.2	367.0	340.3	351.3	351.5	356.6	351.5	358.7	357.7	358.0	359.4	359.0	362.0	363.5 ± 3

•CH ₂ C≡CH	371.4	381.7	368.5	380.0	357.7	368.8	367.4	370.6	367.9	372.8	375.7	376.2	376.1	377.3	378.7	377.7 ± 4.2 ^d
•CH ₂ C ₆ H ₅	368.4	377.9	366.8	377.4	353.4	365.7	368.8	368.8	368.7	370.7	369.5	369.8	374.3	370.2	373.2	370.7 ± 5.0
•CH ₂ CHO	390.0	398.9	387.4	397.5	382.4	385.9	386.5	389.0	386.6	390.6	393.4	393.1	393.3	394.9	395.8	392.6 ^{c, e}
•CH ₂ COOH	405.3	410.7	403.7	409.0	395.4	401.4	398.0	401.4	398.7	402.7	407.2	406.9	409.1	409.4	408.6	407.7 ± 3.3 ^f
•CH ₂ COOCH ₃	405.0	410.3	403.5	408.4	394.6	401.3	397.5	400.9	398.3	402.2	406.8	406.3	408.8	409.0	409.0	401.1 ± 10.5 ^g
•CH ₂ OCOCH ₃	405.3	409.0	405.0	408.6	398.8	406.7	400.2	403.7	401.3	405.1	410.3	408.9	412.3	411.4	414.8	398.4 ^c
•CH ₂ CN	394.0	403.4	390.1	401.1	381.6	391.9	388.9	391.0	389.3	393.0	396.4	397.6	396.4	398.0	399.2	399.5 ± 4.2
•CH ₂ NO ₂	412.6	417.8	413.3	418.9	404.6	412.8	408.1	411.5	409.0	412.9	416.8	417.7	417.7	417.8	418.8	409.7 ^c
MD (W1) ^h	-4.5	1.1	-6.0	-0.1	-13.0	-6.4	-10.3	-6.9	-9.6	-5.5	-2.1	-2.0	0.3	0.0		
MAD (W1) ^h	4.8	3.0	6.0	1.8	13.0	6.4	10.3	6.9	9.6	5.5	2.3	2.2	1.7	1.3		
LD (W1) ^h	-9.6	6.5	-10.1	-6.2	-21.7	-10.8	-11.5	-11.1	-13.5	-9.7	-4.5	-5.9	-2.8	-3.5		
MD (Expt) ^{c, g, h}	-2.5	3.4	-4.8	1.5	-12.2	-4.9	-8.8	-5.3	-8.1	-3.9	-1.3	-1.2	2.4	0.8	0.7	
MAD (Expt) ^{c, g, h}	3.9	4.3	4.9	3.1	12.2	5.5	8.8	5.4	8.1	4.3	2.8	2.8	4.0	2.5	2.1	
LD (Expt) ^{c, g, h}	-10.2	11.1	-10.9	6.6	-23.2	-12.2	-15.1	-11.6	-14.1	-10.3	5.9	±5.5	13.8	6.2	4.8	

^a W1' calculations for systems containing second- and third-row elements. ^b Bond dissociation energies at 0 K calculated using experimental BDEs at 298 K from ref 1, unless otherwise noted, with the thermal corrections to 0 K obtained at the RB3-LYP/6-31G(d) level.

^c Species without experimental error bars are not included in the statistics. ^d Calculated using the experimental BDE for propyne reported by Tsang.² ^e Calculated using the experimental BDE for acetaldehyde reported by Cummings and Kebarle.³ ^f Calculated using the experimental

BDE for acetic acid reported by Lagoa et al.^{4 g} Species with experimental uncertainties greater than $\pm 10 \text{ kJ mol}^{-1}$ are not included in the statistics. ^h MD, MAD and LD are mean deviation, mean absolute deviation and largest deviation, respectively, from W1 and experimental values.

TABLE S3: Comparison of Calculated Radical Stabilization Energies with Experimental Values (0 K, kJ mol⁻¹)

Radical($\bullet$ CH ₂ X)	UBMK	RBMK	UMPWB1K	RMPWB1K	UM05	UM05-2X	UB2-PLYP	RB2-PLYP	UMPW2-PLYP	RMPW2-PLYP	G3(MP2)-RAD	G3X(MP2)-RAD	CBS-QB3	ROCBS-QB3	W1 ^a	Experiment ^b
$\bullet$ CH ₂ NH ₂	54.1	54.4	54.5	54.3	51.5	51.6	51.6	51.9	51.1	51.2	44.2	45.2	49.5	49.5	49.3	45.6 ± 8.4
$\bullet$ CH ₂ OH	39.1	39.4	39.3	39.1	36.6	35.4	36.6	36.9	36.1	36.2	31.6	32.5	35.1	34.9	35.3	36.5 ± 0.63
$\bullet$ CH ₂ OCH ₃	39.4	39.8	37.4	38.8	36.6	35.0	36.9	37.3	36.2	36.4	31.0	32.0	34.7	34.5	35.2	36.6 ^c
$\bullet$ CH ₂ F	16.4	16.8	17.5	17.7	14.9	13.5	15.6	15.8	15.1	15.3	12.4	14.5	14.6	14.5	14.8	15.0 ± 4.2
$\bullet$ CH ₂ CH ₃	17.5	17.1	19.1	18.8	22.5	17.5	17.4	17.2	17.2	17.0	14.1	14.5	16.2	16.2	15.8	19.3 ± 1.3
$\bullet$ CH ₂ CH ₂ CH ₃	14.5	14.2	15.1	15.2	19.0	14.2	14.2	14.2	13.9	13.8	12.5	13.3	13.3	13.3	12.7	17.6 ± 2.1
$\bullet$ CH ₂ CF ₃	-5.9	-6.1	-5.4	-4.4	-0.4	-5.6	-4.1	-4.1	-4.6	-4.7	-7.7	-5.7	-6.6	-6.6	-6.1	-6.9 ± 4.5
$\bullet$ CH ₂ CF ₂ CF ₃	-2.4	-2.6	-2.8	-1.2	2.6	-2.6	-1.2	-1.2	-1.7	-1.7	-4.9		-3.1			
$\bullet$ CH ₂ PH ₂	30.9	30.2	30.8	29.6	33.7	28.1	28.7	28.1	28.5	27.6	23.3	23.9	28.4	27.5	27.0	
$\bullet$ CH ₂ SH	37.9	37.4	43.4	42.2	44.0	40.5	40.8	40.5	40.3	39.7	36.1	37.3	41.4	40.9	41.4	46.1 ± 8.4
$\bullet$ CH ₂ Cl	20.7	20.2	26.4	25.6	27.1	22.9	23.2	22.9	22.8	22.4	21.1	22.4	23.7	23.3	23.0	20.5 ± 2.3
$\bullet$ CH ₂ Br	17.8	17.2	20.5	19.7	22.8	13.9	17.0	16.8	16.6	16.3			10.1			22.1 ± 2.4
$\bullet$ CH ₂ BH ₂	47.8	48.8	44.3	45.7	43.7	42.8	42.8	43.9	42.7	43.8	40.1	40.9	42.7	41.6	40.9	
$\bullet$ CH ₂ CH=CH ₂	74.6	66.6	77.2	67.3	85.2	76.6	71.8	70.5	72.2	69.0	70.7	71.1	74.8	74.4	70.3	68.9 ± 3
$\bullet$ CH ₂ C≡CH	59.2	53.0	61.8	54.3	67.7	58.9	55.9	56.5	55.9	55.0	52.6	52.9	58.1	56.1	53.6	54.7 ± 4.2 ^d
$\bullet$ CH ₂ C ₆ H ₅	62.3	56.8	63.5	57.0	72.1	62.0	54.5	58.3	55.1	57.1	58.9	59.2	59.9	63.2	59.1	61.6 ± 5.0

•CH ₂ CHO	40.7	35.8	43.0	36.8	43.0	41.8	36.8	38.1	37.1	37.2	34.9	36.0	40.9	38.5	36.6	39.8 ^{c,e}
•CH ₂ COOH	25.4	24.0	26.6	25.4	30.1	26.3	25.3	25.6	25.0	25.0	21.2	22.1	25.1	24.0	23.7	24.7 ± 3.3 ^f
•CH ₂ COOCH ₃	25.7	24.4	26.8	25.9	30.8	26.5	25.8	26.2	25.5	25.6	21.5	22.8	25.4	24.4	23.3	31.3 ± 10.5 ^g
•CH ₂ OCOCH ₃	25.4	25.7	25.4	25.7	26.6	21.1	23.1	23.4	22.5	22.6	18.0	20.2	21.9	22.0	17.5	34.0 ^c
•CH ₂ CN	36.7	31.3	40.2	33.2	43.8	36.0	34.4	36.1	34.5	34.7	31.9	31.5	37.8	35.4	33.1	32.8 ± 4.2
•CH ₂ NO ₂	18.0	16.9	17.0	15.4	20.9	15.0	15.2	15.6	14.7	14.8	11.6	11.4	16.5	15.6	13.5	22.7 ^c
MD (W1) ^h	3.0	1.5	4.1	2.3	6.5	1.9	1.4	1.8	1.1	1.0	-2.0	-1.1	1.6	1.1		
MAD (W1) ^h	3.6	3.1	4.1	2.8	6.5	2.1	1.9	1.9	1.7	1.6	2.1	1.6	1.7	1.4		
LD (W1) ^h	-3.5	-4.0	8.2	8.2	14.9	6.3	5.6	5.9	-4.1	5.2	-5.3	-4.1	4.7	4.6		
MD (Expt) ^{c, g, h}	0.8	-1.1	3.0	0.5	5.6	0.4	-0.3	0.1	-0.5	-0.7	-2.8	-1.9	-0.4	0.2	-0.8	
MAD (Expt) ^{c, g, h}	3.3	3.2	4.0	2.7	5.9	3.5	3.0	2.8	2.9	2.6	3.2	2.8	3.6	2.6	2.1	
LD (Expt) ^{c, g, h}	-8.2	-8.7	8.9	8.7	16.3	-8.2	-7.1	6.3	-6.6	-5.8	-9.9	-8.8	-12.0	5.5	-4.9	

^a W1' calculations for systems containing second- and third-row elements. ^b Bond dissociation energies at 0 K calculated using experimental BDEs at 298 K from ref 1, unless otherwise noted, with the thermal corrections to 0 K obtained at the RB3-LYP/6-31G(d) level. ^c Species without experimental error bars are not included in the statistics. ^d Calculated using the experimental BDE for propyne reported by Tsang.² ^e Calculated using the experimental BDE for acetaldehyde reported by Cummings and Kebarle.³ ^f Calculated using the experimental BDE for acetic acid reported by Lagoa et al.⁴ ^g For all species with experimental uncertainties less than ± 10 kJ mol⁻¹. ^h MD, MAD and LD are mean deviation, mean absolute deviation and largest deviation, respectively, from W1 and experimental values.

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