W4-17: A diverse and high-confidence dataset of atomization energies for benchmarking high-level electronic structure methods

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Supplementary Data

(Tables S1–S7)

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Table S1. Geometries and reference data in the W4-17 database. CCSD(T)/cc-pV(Q+d)Z optimized geometries (Cartesian coordinates, in Å) and Gaussian input files for the species in the W4-17 database, and in the W4-17-nonMR and W4-17-MR subsets.

Link to a text file containing the reference TAEs used for the evaluation of the CCSD(T) composite methods and the DHDFT methods (in kcal/mol):

https://www.dropbox.com/s/lf4azi7tztblot3/W4-17_Ref.txt?dl=0

Link to a text file containing TAE0 values (in kcal/mol):[a]

https://www.dropbox.com/s/m3fodo4e21glqfe/W4-17_Ref_TAE0.txt?dl=0

Links to Cartesian coordinates in xyz format. The following folders are available:

- **W4-17 database (200 molecules)**
- **W4-17-nonMR database (183 molecules)**
- **W4-17-MR database (17 molecules)**

https://www.dropbox.com/sh/ucw0itall5t4k44/AAAwzcOhU6wLYwpplCR0shioa?dl=0

Links to Gaussian09 input files. The following folders are available:

- **W4-17 database (200 molecules):**
- **W4-17-nonMR database (183 molecules):**
- **W4-17-MR database (17 molecules):**
- **W4-17-Atoms (11 atoms):**

https://www.dropbox.com/sh/ep2hv0xbluymf38/AABwhf3vXoPgFAjIRWO5F14qa?dl=0

[a]Note that some of the ZPVE values used for converting the W4 TAEe to TAE0 values are obtained by scaling harmonic DSD-PBEP86-D3BJ/aug'-cc-pV(Q+d)Z frequencies rather than from high-level ab initio anharmonic force field calculations as prescribed in the W4 protocol

Table S2. Component breakdown of the 200 TAEs in the W4-17 database, which were obtained by means of W4 theories (kcal mol^{-1}).

Filename in Table S1	Protocol	SCF	CCSD	(T)	T3-(T)	T4	T5	T6	CV	Rel.	S-O	DBOC	M-A	TAEe	ZPVE (a)	TAE0
cyclobutene	W4lite	759.66	221.75	16.01	-1.39	0.89			4.62	-0.70	-0.34	0.19	0.08	1000.74	53.57	947.17
t-butadiene	W4lite	775.19	217.03	16.33	-1.17	0.92			4.76	-0.66	-0.34	0.20	0.08	1012.32	52.62	959.70
cyclobutane	W4lite	883.35	248.23	14.68	-1.15	0.66			4.63	-0.76	-0.34	0.21	0.08	1149.56	68.70	1080.86
n-pentane	W4lite	1239.83	334.44	17.62	-1.23	0.69			5.96	-0.96	-0.42	0.30	0.10	1596.28	99.45	1496.83
benzene	W4lite	1045.01	290.71	26.70	-2.62	1.63			7.37	-0.99	-0.51	0.23	0.13	1367.59	62.16	1305.43
acetic	W4lite	578.81	206.15	16.15	-1.13	1.08			2.91	-0.79	-0.62	0.21	0.09	802.82	38.46	764.36
hclo4	W4lite	80.52	227.34	26.50	-2.08	2.22			0.92	-2.72	-1.73	0.11	0.10	331.12	17.26	313.86
c2f6	W4lite	544.61	222.91	22.62	-1.65	1.32			2.13	-1.34	-2.48	0.12	0.08	788.29	18.32	769.97
c2cl6	W4lite	355.51	177.41	27.57	-3.07	1.36			2.53	-1.13	-5.21	0.07	0.09	555.08	11.63	543.45
n2o4	W4lite	112.87	313.27	42.85	-2.92	4.21			1.40	-1.00	-0.89	0.06	0.20	469.94	14.37	455.57
cloocl	W4lite	0.19	130.15	18.19	-1.29	1.80			0.09	-0.27	-2.13	0.01	0.06	146.77	4.27	142.50
clo3	W4lite	-26.01	170.84	23.84	-1.76	2.39			0.53	-1.64	-1.51	0.02	0.08	166.75	6.85	159.90
hoclo	W4lite	59.07	128.86	15.38	-0.91	1.52			0.37	-0.61	-1.29	0.07	0.06	202.49	10.43	192.06
pf5	W4lite	383.89	163.04	14.66	-1.41	1.17			0.22	-3.51	-1.93	0.05	0.04	556.20	10.47	545.73
sf6	W4lite	265.61	199.44	20.86	-1.69	1.56			-0.35	-3.19	-2.87	0.05	0.05	479.44	13.16	466.28
oxadiazole	W4lite	418.46	256.66	27.81	-2.54	2.50			3.18	-0.74	-0.39	0.14	0.17	705.16	28.30	676.86
dioxetan2one	W4lite	503.82	225.02	21.74	-1.80	1.59			2.74	-0.96	-0.84	0.13	0.11	751.50	28.21	723.29
dioxetane	W4lite	525.50	207.01	15.39	-1.26	0.97			2.39	-0.84	-0.62	0.11	0.09	748.70	39.25	709.45
dithiotane	W4lite	491.16	175.91	15.24	-1.45	0.84			2.68	-1.08	-1.29	0.10	0.07	682.16	35.59	646.57
borole	W4lite	813.78	218.97	19.38	-1.56	1.26			5.85	-0.72	-0.37	0.16	0.09	1056.79	47.50	1009.29
c2cl4	W4lite	311.52	137.62	20.86	-2.24	1.26			2.74	-1.09	-3.53	0.06	0.08	467.24	9.65	457.59
c2f4	W4lite	395.13	173.71	18.63	-1.30	1.26			2.64	-1.06	-1.71	0.10	0.07	587.42	13.44	573.98
cis-c2f2cl2	W4lite	351.49	155.59	19.71	-1.67	1.24			2.67	-1.09	-2.62	0.08	0.07	525.42	11.48	513.94
trans-c2f2cl2	W4lite	352.34	155.20	19.62	-1.67	1.23			2.67	-1.09	-2.62	0.08	0.07	525.79	11.49	514.30
cyclopentadiene	W4lite	897.13	258.05	21.36	-1.92	1.31			5.97	-0.84	-0.42	0.24	0.10	1180.93	57.23	1123.70
formic-anhydride	W4lite	509.47	222.55	22.05	-1.61	1.65			2.90	-0.91	-0.84	0.11	0.11	755.43	26.38	729.05
furan	W4lite	727.68	240.43	22.48	-2.12	1.55			5.11	-0.91	-0.56	0.21	0.11	993.91	43.34	950.57
oxetane	W4lite	701.86	228.02	15.09	-1.18	0.82			3.54	-0.80	-0.48	0.16	0.09	947.07	53.89	893.18
pyrrole	W4lite	782.11	262.95	22.81	-2.19	1.47			5.65	-0.96	-0.34	0.26	0.13	1071.82	51.13	1020.69
silole	W4lite	837.31	239.50	19.76	-1.77	1.28			4.83	-1.33	-0.77	0.16	0.09	1099.02	50.79	1048.23
thiophene	W4lite	713.56	224.35	22.77	-2.36	1.52			5.15	-1.06	-0.90	0.18	0.10	963.26	41.28	921.98
beta-lactim	W4lite	699.42	269.12	21.59	-1.87	1.43			4.18	-0.97	-0.48	0.24	0.14	992.72	49.96	942.76
clf5	w4lite	-36.36	194.85	27.67	-1.33	2.40			-0.43	-0.71	-2.77	0.02	0.04	183.36	8.51	174.85
pf3	W4	-5.50	116.97	16.51	-0.73	1.33	0.05		-0.09	-0.26	-2.00	0.01	0.03	126.31	4.39	121.92
pf3	W4	247.80	107.62	9.99	-0.91	0.50	-0.02		0.62	-0.98	-1.16	0.02	0.03	363.50	5.32	358.18
hoclo2	W4	67.58	182.33	22.37	-1.54	1.85	-0.03		0.61	-1.26	-1.51	0.09	0.08	270.54	13.29	257.25
h2no	W4	150.56	115.32	8.07	-0.38	0.55	0.03		0.83	-0.44	-0.22	0.07	0.07	274.42	16.15	258.27
nh2oh	W4	214.85	135.63	8.48	-0.49	0.51	0.03		0.71	-0.46	-0.22	0.15	0.07	359.22	25.09	334.13
cyclopropane	W4	655.52	184.21	10.82	-0.87	0.55	0.03		3.71	-0.58	-0.25	0.19	0.06	853.35	50.44	802.91
cyclopropene	W4	507.18	159.08	12.24	-1.09	0.85	0.06		3.62	-0.53	-0.25	0.14	0.06	681.33	34.69	646.64
ch3ph2	W4	403.08	128.88	5.82	-0.32	0.29	0.01		1.54	-0.67	-0.08	0.09	0.03	538.65	33.84	504.81
nh2f	W4	143.51	105.10	7.31	-0.31	0.43	0.02		0.41	-0.28	-0.39	0.09	0.06	255.92	17.15	238.77
cclh3	W4	303.87	85.73	5.28	-0.37	0.28	0.01		1.25	-0.42	-0.93	0.08	0.03	394.80	23.49	371.31
clno	W4	54.72	118.49	17.06	-0.64	1.95	0.11		0.25	-0.20	-1.06	0.00	0.08	190.74	3.95	186.79
tetrahedrane	W4	570.61	201.48	16.94	-1.86	1.17	0.07		5.08	-0.78	-0.34	0.23	0.08	792.64	36.85	755.79
n-butane	W4	1012.59	271.73	13.85	-0.93	0.57	0.03		4.79	-0.77	-0.34	0.25	0.08	1301.81	81.79	1220.02

c2cl2	W4	232.31	101.26	14.28	-1.54	1.33	0.08	2.86	-0.83	-1.85	0.06	0.06	348.00	6.80	341.20
c2clh3	W4	409.00	122.54	10.38	-0.81	0.71	0.03	2.47	-0.55	-1.01	0.11	0.05	542.89	26.43	516.46
c2clh5	W4	533.29	148.28	9.09	-0.67	0.47	0.02	2.44	-0.59	-1.01	0.14	0.05	691.47	41.36	650.11
c2clh	W4	266.61	97.97	11.29	-1.11	1.01	0.08	2.67	-0.55	-1.01	0.09	0.05	377.07	11.73	365.34
ccl2h2	W4	273.32	89.00	8.28	-0.72	0.54	0.01	1.27	-0.56	-1.77	0.06	0.04	369.46	18.33	351.13
ccl2o	W4	221.70	108.81	15.08	-1.23	1.18	0.04	1.51	-0.60	-1.99	0.04	0.06	344.57	6.52	338.05
ccl3h	W4	238.45	94.15	11.80	-1.16	0.85	0.01	1.30	-0.64	-2.61	0.05	0.05	342.24	12.45	329.79
ccl4	W4	197.85	100.89	15.80	-1.69	1.22	0.02	1.34	-0.66	-3.45	0.04	0.06	311.37	6.03	305.34
cf2cl2	W4	259.11	117.75	14.58	-1.24	0.88	-0.02	1.17	-0.77	-2.54	0.05	0.05	389.01	8.19	380.82
fno	W4	66.29	131.30	16.66	-0.66	1.53	0.09	0.21	-0.24	-0.61	0.01	0.08	214.63	4.47	210.16
ch2clf	W4	294.42	99.23	8.16	-0.59	0.43	0.01	1.18	-0.55	-1.31	0.06	0.04	401.06	19.34	381.72
chf3	W4	325.94	122.16	10.70	-0.76	0.47	-0.01	1.06	-0.68	-1.24	0.07	0.04	457.73	15.75	441.98
clcof	W4	249.93	117.73	14.33	-1.10	0.98	0.03	1.47	-0.64	-1.53	0.05	0.06	381.28	7.57	373.71
formamide	W4	387.04	166.12	12.86	-0.81	0.77	0.03	2.14	-0.65	-0.31	0.17	0.10	567.41	28.11	539.30
cyclobutadiene	W4	597.99	199.69	18.45	-1.38	1.55	0.09	4.44	-0.65	-0.34	0.17	0.08	820.06	37.77	782.29
allyl	W4	584.27	167.81	11.23	-0.71	0.73	0.03	3.49	-0.50	-0.25	0.12	0.06	766.25	41.08	725.17
cyclopropyl	W4	562.53	161.69	10.12	-0.70	0.53	0.02	3.53	-0.56	-0.25	0.15	0.06	737.09	41.55	695.54
h2ccn	W4	357.01	139.91	12.56	-0.90	1.16	0.10	2.81	-0.40	-0.17	0.08	0.09	512.20	19.42	492.78
oxirene	W4	293.68	145.48	14.37	-1.17	1.19	0.09	2.39	-0.46	-0.39	0.11	0.07	455.33	18.05	437.28
oxirane	W4	471.05	166.38	11.81	-0.95	0.70	0.04	2.46	-0.56	-0.39	0.13	0.07	650.70	35.68	615.02
dioxirane	W4	239.56	154.29	14.72	-1.18	1.38	0.10	1.14	-0.40	-0.53	0.07	0.07	409.17	20.25	388.92
ketene	W4	381.75	135.76	13.04	-0.84	0.93	0.05	2.75	-0.47	-0.39	0.11	0.07	532.70	19.60	513.10
acetaldehyde	W4	501.58	162.09	11.63	-0.77	0.70	0.04	2.58	-0.53	-0.39	0.12	0.07	677.07	34.49	642.58
formic	W4	343.07	144.63	12.57	-0.89	0.81	0.03	1.65	-0.59	-0.53	0.13	0.07	500.90	21.10	479.80
methanol	W4	376.98	128.31	6.87	-0.44	0.31	0.01	1.43	-0.46	-0.31	0.13	0.04	512.86	31.92	480.94
ethanol	W4	607.58	190.64	10.56	-0.69	0.46	0.02	2.63	-0.65	-0.39	0.19	0.07	810.39	49.71	760.68
glyoxal	W4	436.32	178.80	17.15	-1.23	1.31	0.08	2.62	-0.65	-0.62	0.07	0.09	633.91	22.94	610.97
t-hcoh	W4	217.06	97.10	7.28	-0.29	0.44	0.01	0.86	-0.33	-0.31	0.04	0.04	321.87	16.60	305.27
c-hcoh	W4	211.87	97.39	7.40	-0.29	0.45	0.01	0.81	-0.32	-0.31	0.02	0.04	317.04	16.18	300.86
hcnh	W4	220.02	105.66	8.77	-0.43	0.63	0.05	1.51	-0.32	-0.08	0.05	0.07	335.90	16.01	319.89
hocn	W4	252.90	141.36	13.59	-1.14	1.16	0.11	2.04	-0.52	-0.31	0.12	0.10	409.36	13.38	395.98
honc	W4	192.93	141.31	14.06	-1.01	1.14	0.08	1.60	-0.50	-0.31	0.11	0.10	349.45	12.62	336.83
hnco	W4	277.92	139.88	14.60	-0.98	1.08	0.04	2.14	-0.54	-0.31	0.11	0.10	434.00	13.27	420.73
hcno	W4	192.35	152.35	17.53	-1.41	1.74	0.11	2.24	-0.56	-0.31	0.09	0.10	364.18	11.95	352.23
c-n2h2	W4	149.24	130.71	10.16	-0.64	0.83	0.07	0.71	-0.31	0.00	0.03	0.10	290.85	17.16	273.69
hnnn	W4	134.62	176.22	18.64	-1.35	1.94	0.18	1.47	-0.50	0.00	0.07	0.15	331.35	13.29	318.06
hnc	W4	194.77	93.05	8.79	-0.57	0.64	0.05	1.45	-0.26	-0.08	0.09	0.07	297.95	9.68	288.27
t-hono	W4	135.79	158.81	16.73	-0.84	1.50	0.10	0.52	-0.42	-0.45	0.08	0.10	311.87	12.13	299.74
c-hono	W4	136.24	158.11	16.65	-0.91	1.47	0.10	0.51	-0.42	-0.45	0.08	0.10	311.44	12.13	299.31
nh2cl	W4	147.94	92.63	6.85	-0.43	0.48	0.02	0.55	-0.39	-0.84	0.09	0.06	246.92	16.38	230.54
t-hooo	W4	58.53	153.82	18.44	-0.20	2.33	0.18	0.17	-0.31	-0.67	0.06	0.07	232.38	11.64	220.74
c-hooo	W4	62.62	151.22	17.20	-0.34	2.04	0.15	0.18	-0.31	-0.67	0.06	0.07	232.18	11.03	221.15
ch3f	W4	319.78	96.78	5.32	-0.29	0.19	0.01	1.17	-0.38	-0.47	0.08	0.03	422.19	24.51	397.68
ch2f2	W4	319.52	109.50	8.00	-0.51	0.33	0.01	1.09	-0.53	-0.85	0.07	0.03	436.63	20.63	416.00
cf4	W4	330.49	134.31	13.25	-1.02	0.62	0.02	1.07	-0.85	-1.63	0.07	0.04	476.36	10.86	465.50
sih3f	W4	302.49	77.36	3.09	-0.38	0.12	0.00	0.06	-0.95	-0.81	0.01	0.01	381.00	17.31	363.69
sif4	W4	448.41	119.07	10.12	-1.14	0.46	0.00	0.84	-1.90	-1.97	0.05	0.03	573.96	8.04	565.92
c2h3f	W4	428.27	132.97	10.23	-0.65	0.58	0.03	2.44	-0.51	-0.55	0.12	0.05	572.95	27.32	545.63
c2h5f	W4	551.42	158.87	8.97	-0.52	0.34	0.02	2.38	-0.56	-0.55	0.14	0.05	720.53	42.30	678.23

fccf	W4	247.55	121.94	13.68	-1.12	1.02	0.08	2.91	-0.72	-0.94	0.08	0.05	384.50	8.30	376.20
hccf	W4	276.39	108.31	11.07	-0.93	0.86	0.07	2.68	-0.49	-0.55	0.10	0.05	397.53	12.45	385.08
hcof	W4	277.02	114.27	11.08	-0.74	0.69	0.03	1.37	-0.49	-0.69	0.06	0.05	402.62	13.07	389.55
f2co	W4	279.65	126.11	13.54	-1.01	0.82	0.03	1.47	-0.67	-1.08	0.06	0.06	418.95	8.91	410.04
ch2-sing	W4	130.07	48.76	1.90	0.20	0.12	0.00	0.39	-0.09	-0.08	-0.10	0.02	181.18	10.31	170.87
propane	W4	785.34	209.05	10.12	-0.63	0.38	0.02	3.61	-0.58	-0.25	0.12	0.06	1007.20	64.20	943.00
propene	W4	665.18	181.71	11.17	-0.76	0.60	0.04	3.61	-0.52	-0.25	0.12	0.06	860.92	49.36	811.56
propyne	W4	534.14	155.80	11.94	-1.01	0.87	0.07	3.76	-0.48	-0.25	0.12	0.06	704.99	34.52	670.47
allene	W4	532.55	155.63	12.27	-0.84	0.74	0.05	3.67	-0.47	-0.25	0.11	0.06	703.48	34.08	669.40
b2h6	W4	490.60	108.85	4.47	0.02	0.18	0.00	2.90	-0.18	-0.06	0.04	0.01	606.83	39.30	567.53
bhf2	W4	329.85	73.54	6.11	-0.48	0.27	0.01	1.66	-0.47	-0.80	0.04	0.02	409.75	11.02	398.73
bf3	W4	374.64	86.41	8.28	-0.72	0.39	0.02	1.94	-0.69	-1.18	0.06	0.02	469.15	7.83	461.32
c2h6	W4	558.01	146.34	6.37	-0.35	0.23	0.01	2.43	-0.39	-0.17	0.14	0.04	712.67	46.39	666.28
h2cn	W4	234.71	99.73	7.44	-0.21	0.52	0.03	1.49	-0.25	-0.08	0.04	0.07	343.45	15.50	327.95
nccn	W4	302.67	174.82	20.51	-1.91	2.25	0.24	3.38	-0.46	-0.17	-0.06	0.14	501.35	9.85	491.50
ch2nh2	W4	342.84	130.67	6.95	-0.34	0.31	0.01	1.80	-0.46	-0.08	0.14	0.07	481.87	30.85	451.02
ch3nh	W4	341.87	124.93	6.20	-0.19	0.26	0.01	1.52	-0.36	-0.08	0.06	0.07	474.24	30.02	444.22
ch3nh2	W4	422.57	150.70	7.31	-0.41	0.31	0.01	1.77	-0.46	-0.08	0.15	0.07	581.91	39.69	542.22
cf2	W4	168.55	80.52	9.15	-0.42	0.52	0.01	0.44	-0.32	-0.85	0.02	0.03	257.63	4.37	253.26
n2h	W4	104.63	109.49	9.51	-0.46	0.80	0.07	0.78	-0.26	0.00	-0.02	0.10	224.58	8.13	216.45
t-n2h2	W4	155.33	130.18	9.97	-0.62	0.82	0.06	0.75	-0.33	0.00	0.04	0.10	296.25	17.57	278.68
n2h4	W4	272.65	156.04	8.44	-0.46	0.43	0.02	1.12	-0.51	0.00	0.17	0.10	437.94	33.18	404.76
fo2	W4	-22.48	133.54	20.64	-0.12	2.91	0.23	-0.03	-0.17	-0.83	-0.02	0.05	133.71	3.56	130.15
foof	W4	-48.79	173.73	25.82	-0.74	2.29	0.27	-0.24	-0.16	-1.22	0.01	0.06	151.00	5.00	146.00
alf3	W4	334.44	88.98	7.91	-0.78	0.37	0.04	0.00	-1.31	-1.37	0.03	0.02	428.32	4.84	423.48
si2h6	W4	424.14	108.85	2.90	-0.13	0.16	0.00	-0.04	-1.32	-0.86	0.01	0.01	533.72	30.63	503.09
p4	W4	121.40	146.17	21.82	-3.28	2.57	0.13	1.76	-0.72	0.00	0.02	0.04	289.87	3.91	285.96
so2	W4	121.91	121.45	15.83	-1.28	1.56	0.14	0.97	-0.83	-1.01	0.02	0.06	258.80	4.38	254.42
so3	W4	159.72	165.45	20.28	-1.68	1.75	0.21	1.16	-1.85	-1.23	0.05	0.08	343.91	7.79	336.12
ocs	W4	218.25	101.32	14.47	-1.09	1.32	0.05	1.41	-0.54	-0.87	0.03	0.06	334.37	5.72	328.65
cs2	W4	175.21	87.63	15.71	-1.30	1.78	0.05	1.68	-0.62	-1.20	0.02	0.04	278.97	4.30	274.67
s2o	W4	84.73	105.57	16.83	-1.32	2.00	0.15	0.79	-0.68	-1.34	0.01	0.05	206.77	3.19	203.58
s3	W4	62.10	87.37	17.03	-1.32	2.42	0.13	0.62	-0.56	-1.68	0.01	0.04	166.13	2.16	163.97
s4-c2v	W4	73.29	129.53	28.47	-2.78	4.84	0.30	0.68	-0.67	-2.24	0.01	0.05	231.44	3.29	228.15
ccl2	W4	103.34	62.35	10.66	-0.48	0.94	-0.01	0.52	-0.27	-1.77	0.01	0.04	175.33	2.62	172.71
alcl3	W4	258.16	47.94	7.17	-0.83	0.52	-0.01	-0.31	-1.28	-2.74	0.02	0.03	308.65	3.05	305.60
clcn	W4	169.49	101.51	12.44	-1.15	1.24	0.11	1.78	-0.45	-0.93	0.04	0.08	284.12	5.33	278.79
oclo	W4	-10.77	120.52	17.30	-1.28	1.77	0.12	0.43	-0.76	-1.29	-0.08	0.05	125.99	3.67	122.32
cloo	W4	-13.00	116.56	19.41	0.10	3.13	0.22	-0.08	-0.13	-1.29	0.00	0.05	124.96	3.08	121.88
cl2o	W4	11.36	78.55	11.05	-0.88	1.16	0.04	0.15	-0.25	-1.90	0.01	0.04	99.31	2.37	96.94
bn3pi	W4.2	53.99	43.57	6.38	0.22	0.56	0.01	1.08	-0.13	0.04	-0.01	[0]	105.72	2.17	103.55
cf	W4.2	83.62	43.65	5.03	-0.15	0.24	-0.01	0.33	-0.16	-0.36	0.01	[0]	132.21	1.86	130.35
ch2c	W4.2	265.16	85.80	6.85	-0.20	0.49	0.02	1.80	-0.20	-0.17	0.06	[0]	359.63	14.53	345.10
ch2ch	W4.2	339.45	97.46	6.76	-0.26	0.42	0.02	2.23	-0.30	-0.17	0.08	[0]	445.68	22.62	423.06
c2h4	W4.2	434.97	119.32	7.40	-0.46	0.43	0.03	2.41	-0.33	-0.17	0.12	[0]	563.71	31.60	532.11
ch2nh	W4.2	305.41	123.85	8.49	-0.54	0.57	0.04	1.63	-0.34	-0.08	0.09	[0]	439.10	24.69	414.41
hco	W4.2	186.34	83.33	8.39	-0.48	0.60	0.06	1.19	-0.38	-0.31	-0.02	[0]	278.71	8.05	270.66
h2co	W4.2	264.83	100.53	7.92	-0.53	0.54	0.03	1.33	-0.34	-0.31	0.03	[0]	374.04	16.53	357.51
co2	W4.2	258.08	116.34	13.86	-1.03	1.04	0.05	1.80	-0.48	-0.53	0.05	[0]	389.18	7.24	381.94

hno	W4.2	85.45	109.46	10.08	-0.60	0.99	0.07		0.45	-0.27	-0.22	-0.05	[0]	205.34	8.56	196.78
no2	W4.2	59.55	147.16	19.36	-1.08	1.96	0.19		0.73	-0.43	-0.45	0.00	[0]	227.01	5.40	221.61
n2o	W4.2	95.13	155.03	18.81	-1.51	1.98	0.19		1.22	-0.46	-0.22	0.04	[0]	270.21	6.78	263.43
o3	W4.2	-45.09	163.94	25.62	-1.34	3.81	0.41		0.08	-0.25	-0.67	-0.03	[0]	146.48	4.15	142.33
hoo	W4.2	75.70	90.94	8.11	-0.17	0.65	0.04		0.27	-0.27	-0.45	0.01	[0]	174.82	8.85	165.97
hooh	W4.2	142.62	116.90	8.98	-0.55	0.72	0.03		0.38	-0.37	-0.45	0.11	[0]	268.39	16.31	252.08
f2o	W4.2	-30.21	109.52	13.71	-0.59	1.38	0.10		-0.13	-0.11	-0.99	0.01	[0]	92.68	3.26	89.42
hocl	W4.2	86.70	72.35	6.77	-0.47	0.58	0.02		0.28	-0.33	-1.06	0.07	[0]	164.91	8.18	156.73
ssh	W4.2	101.22	56.93	6.29	-0.33	0.57	0.01		0.45	-0.49	-1.12	-0.01	[0]	163.51	5.83	157.68
b2	W4.3	20.49	34.96	9.77	0.06	1.29	0.08	0.00	0.82	-0.06	-0.06	0.01	[0]	67.35	1.50	65.85
bh	W4.3	64.31	20.01	0.41	0.00	0.05	0.00	0.00	0.20	-0.02	-0.03	-0.10	[0]	84.84	3.35	81.49
bh3	W4.3	234.35	44.97	0.79	-0.02	0.04	0.00	0.00	1.15	-0.07	-0.03	-0.02	[0]	281.17	16.36	264.81
bn	W4.3	-11.35	96.17	19.58	-2.63	2.12	0.16	0.04	1.15	-0.17	-0.03	0.01	[0]	105.05	2.43	102.62
bf	W4.3	143.09	34.76	4.00	-0.32	0.28	-0.01	0.00	0.73	-0.16	-0.41	0.01	[0]	181.95	2.00	179.95
nh	W4.3	48.64	33.06	1.18	0.05	0.05	0.00	0.00	0.11	-0.07	0.00	-0.05	[0]	82.98	4.64	78.34
nh2	W4.3	116.87	62.75	2.51	-0.01	0.12	0.01	0.00	0.33	-0.16	0.00	-0.01	[0]	182.43	11.85	170.58
hcn	W4.3	204.39	97.85	9.20	-0.77	0.93	0.10	0.01	1.71	-0.22	-0.08	0.08	[0]	313.19	9.98	303.21
hof	W4.3	62.13	87.80	8.16	-0.39	0.77	0.04	0.01	0.14	-0.21	-0.61	0.07	[0]	157.90	8.58	149.32
alh	W4.3	55.09	18.52	0.07	-0.06	0.05	0.00	0.00	-0.09	-0.08	-0.21	-0.06	[0]	73.22	2.38	70.84
alh3	W4.3	171.26	42.39	0.17	-0.02	0.04	0.00	0.00	-0.67	-0.42	-0.21	-0.02	[0]	212.52	11.61	200.91
alf	W4.3	125.45	34.72	3.27	-0.41	0.22	-0.01	-0.01	0.56	-0.29	-0.60	0.01	[0]	162.90	1.14	161.76
alcl	W4.3	98.81	20.57	2.97	-0.38	0.31	0.00	0.00	0.34	-0.24	-1.05	0.00	[0]	121.32	0.69	120.63
sih	W4.3	52.26	21.12	0.39	0.04	0.07	0.03	0.00	0.02	-0.11	-0.22	-0.05	[0]	73.54	2.89	70.65
sih4	W4.3	259.83	64.18	0.81	0.04	0.08	0.03	0.00	-0.02	-0.67	-0.43	0.00	[0]	323.85	19.69	304.16
sio	W4.3	117.78	65.67	8.35	-0.73	0.89	0.02	0.00	1.06	-0.28	-0.65	0.01	[0]	192.14	1.77	190.37
sif	W4.3	102.24	36.55	3.55	-0.34	0.25	0.02	0.00	0.45	-0.29	-0.58	0.00	[0]	141.84	1.22	140.62
cs	W4.3	104.16	57.06	9.68	-0.61	1.05	0.05	0.00	0.82	-0.16	-0.64	0.01	[0]	171.42	1.83	169.59
h2	W4.4	83.85	25.65	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	[0]	109.51	6.23	103.28
oh	W4.4	69.37	35.95	1.68	-0.04	0.09	0.00	0.00	0.15	-0.12	-0.02	0.00	[0]	107.05	5.29	101.76
hf	W4.4	100.05	39.31	2.14	-0.16	0.11	0.00	0.00	0.19	-0.20	-0.39	0.06	[0]	141.12	5.85	135.27
h2o	W4.4	160.02	69.08	3.51	-0.24	0.21	0.01	0.00	0.39	-0.27	-0.22	0.09	[0]	232.58	13.26	219.32
ch	W4.4	57.22	25.83	0.88	0.10	0.04	0.00	0.00	0.15	-0.04	-0.04	-0.11	[0]	84.03	4.04	79.99
ch2-trip	W4.4	154.77	34.15	0.97	-0.01	0.03	0.00	0.00	0.83	-0.15	-0.08	0.01	[0]	190.53	10.67	179.86
ch3	W4.4	243.40	61.46	1.90	-0.05	0.07	0.00	0.00	1.09	-0.17	-0.08	0.01	[0]	307.63	18.55	289.08
ch4	W4.4	331.55	84.71	2.89	-0.10	0.10	0.01	0.00	1.28	-0.19	-0.08	0.05	[0]	420.20	27.74	392.46
cch	W4.4	181.72	74.08	7.82	-0.49	0.77	0.08	0.01	2.18	-0.28	-0.17	0.01	[0]	265.73	8.69	257.04
c2h2	W4.4	299.87	94.71	8.33	-0.74	0.75	0.08	0.01	2.53	-0.28	-0.17	0.09	[0]	405.16	16.46	388.70
nh3	W4.4	203.28	90.16	3.88	-0.17	0.19	0.01	0.00	0.66	-0.25	0.00	0.10	[0]	297.86	21.33	276.53
c2	W4.4	18.38	107.57	19.32	-2.28	2.35	0.32	0.07	1.30	-0.17	-0.17	0.02	[0]	146.71	2.64	144.07
n2	W4.4	119.69	98.09	9.46	-0.79	1.06	0.11	0.02	0.84	-0.14	0.00	0.01	[0]	228.36	3.36	225.00
co	W4.4	181.58	69.07	7.99	-0.58	0.64	0.03	0.00	1.00	-0.16	-0.31	0.01	[0]	259.26	3.11	256.15
cn	W4.4	85.03	83.79	10.47	-0.37	1.12	0.12	0.01	1.19	-0.16	-0.08	0.02	[0]	181.13	2.95	178.18
no	W4.4	54.92	87.50	9.45	-0.56	0.89	0.08	0.01	0.46	-0.19	-0.05	0.01	[0]	152.51	2.71	149.80
o2	W4.4	26.78	83.94	9.25	-0.69	1.15	0.10	0.02	0.27	-0.18	-0.45	0.01	[0]	120.21	2.25	117.96
of	W4.4	-12.23	57.59	6.85	0.28	0.57	0.03	0.00	-0.02	-0.08	-0.33	0.00	[0]	52.67	1.50	51.17
f2	W4.4	-31.08	61.92	7.61	-0.31	0.92	0.04	0.01	-0.06	-0.03	-0.77	0.00	[0]	38.25	1.30	36.95
ph3	W4.4	173.22	66.53	1.99	0.06	0.11	0.00	0.00	0.36	-0.46	0.00	-0.01	[0]	241.80	14.44	227.36
hs	W4.4	61.34	25.08	1.08	-0.01	0.07	0.00	0.00	0.17	-0.19	-0.02	-0.03	[0]	87.49	3.81	83.68
h2s	W4.4	133.63	47.65	2.22	-0.09	0.16	0.00	0.00	0.34	-0.40	-0.56	0.03	[0]	182.98	9.40	173.58

hcl	W4.4	80.85	24.99	1.47	-0.12	0.11	0.00	0.00	0.19	-0.25	-0.84	0.03	[0]	106.44	4.24	102.20
so	W4.4	53.14	64.15	8.43	-0.79	0.91	0.06	0.01	0.56	-0.34	-0.78	0.00	[0]	125.34	1.64	123.70
clo	W4.4	9.48	48.68	6.31	0.03	0.67	0.04	0.00	0.23	-0.24	-0.61	-0.01	[0]	64.59	1.22	63.37
clf	W4.4	15.41	41.85	5.23	-0.29	0.50	0.02	0.00	0.08	-0.18	-1.23	0.00	[0]	61.40	1.12	60.28
p2	W4.4	38.93	67.43	9.66	-0.96	1.52	0.13	0.03	0.87	-0.28	0.00	0.01	[0]	117.33	1.11	116.22
s2	W4.4	49.65	46.13	7.69	-0.74	0.96	0.06	0.00	0.50	-0.32	-1.12	0.00	[0]	102.81	1.04	101.77
cl2	W4.4	26.82	28.08	4.56	-0.41	0.51	0.02	0.00	0.17	-0.20	-1.68	0.00	[0]	57.87	0.80	57.07

(a) The ZPVE values with a green background were taken from the W4-11 database [A. Karton, S. Daon, J. M. L. Martin, Chem. Phys. Lett. 2011, 510, 165]. The ZPVE values with a yellow background are harmonic DSD-PBEP86-D3BJ/aug'-cc-pV(Q+d)Z values scaled by 0.9831 as recommended in ref. [M. K. Kesharwani, B. Brauer, J. M. L. Martin, J. Phys. Chem. A 2015, 119, 1701]. The later values should be treated with some caution.

Table S3. List of 200 species in the W4-17 database.

Molecular Formula	Molecule Name	Filename in Table S1	Protocol
C4H6	cyclobutene	cyclobutene	W4lite
C4H6	trans-butadiene	t-butadiene	W4lite
C4H8	cyclobutane	cyclobutane	W4lite
C5H12	n-pentane	n-pentane	W4lite
C6H6	benzene	benzene	W4lite
CH3COOH	acetic acid	acetic	W4lite
HClO4	perchloric acid	hclo4	W4lite
C2F6	hexafluoroethane	c2f6	W4lite
C2Cl6	hexachloroethane	c2cl6	W4lite
N2O4	dinitrogen tetraoxide	n2o4	W4lite
ClOOCl	dioxygen dichloride	cloocl	W4lite
OClOO	chlorine trioxide	clo3	W4lite
HOClO	chlorous acid	hoclo	W4lite
PF5	phosphorus pentafluoride	pf5	W4lite
SF6	sulfur hexafluoride	sf6	W4lite
H2C2N2O	1,2,5-oxadiazole	oxadiazole	W4lite
H2C2O3	1,3-dioxetan-2-one	dioxetan2one	W4lite
H4C2O2	1,3-dioxetane	dioxetane	W4lite
H4C2S2	1,3-dithiotane	dithiotane	W4lite
H5BC4	borole	borole	W4lite
C2Cl4	tetrachloroethylene	c2cl4	W4lite
C2F4	perfluoroethene	c2f4	W4lite
cis-C2F2Cl2	cis-dichlorodifluoroethene	cis-c2f2cl2	W4lite
trans-C2F2Cl2	trans-dichlorodifluoroethene	trans-c2f2cl2	W4lite
H6C5	cyclopentadiene	cyclopentadiene	W4lite
H2C2O3	formic_anhydride	formic-anhydride	W4lite
H4C4O	furan	furan	W4lite
H6C3O	oxetane	oxetane	W4lite
H5C4N	pyrrole	pyrrole	W4lite
H6C4Si	silole	silole	W4lite
H4C4S	thiophene	thiophene	W4lite
H5C3NO	beta-lactim	beta-lactim	W4lite
ClF5	chlorine pentafluoride	clf5	W4lite
ClF3	phosphorus trifluoride	pf3	W4
PF3	phosphorus trifluoride	pf3	W4
HOClO2	chloric acid	hoclo2	W4
H2NO	dihydronitroxide radical	h2no	W4
NH2OH	hydroxylamine	nh2oh	W4
C3H6	cyclopropane	cyclopropane	W4
C3H4	cyclopropene	cyclopropene	W4
CH3PH2	methylphosphine	ch3ph2	W4
NH2F	fluoroamine	nh2f	W4
CClH3	chloromethane	cclh3	W4
ClNO	nitrosyl chloride	clno	W4

C4H4	tetrahedrane	tetrahedrane	W4
C4H10	n-butane	n-butane	W4
C2Cl2	dichloroacetylene	c2cl2	W4
C2ClH3	vinyl chloride	c2clh3	W4
C2ClH5	chloroethane	c2clh5	W4
C2ClH	chloroethyne	c2clh	W4
CCl2H2	dichloromethane	ccl2h2	W4
CCl2O	phosgene	ccl2o	W4
CCl3H	chloroform	ccl3h	W4
CCl4	carbon tetrachloride	ccl4	W4
CF2Cl2	dichlorodifluoromethane	cf2cl2	W4
FNO	nitrosyl fluoride	fno	W4
CH2ClF	chlorofluoromethane	ch2clf	W4
CHF3	fluoroform	chf3	W4
ClCOF	carbonyl chloride fluoride	clcof	W4
CH3NO	formamide	formamide	W4
C4H4	cyclobutadiene	cyclobutadiene	W4
C3H5	allyl radical	allyl	W4
C3H5	cyclopropyl radical	cyclopropyl	W4
H2CCN	cyanomethyl	h2ccn	W4
H2C2O	oxirene	oxirene	W4
C2H4O	oxirane	oxirane	W4
H2CO2	dioxirane	dioxirane	W4
H2C2O	ketene	ketene	W4
H4C2O	acetaldehyde	acetaldehyde	W4
HCOOH	formic acid	formic	W4
CH3OH	methanol	methanol	W4
C2H5OH	ethanol	ethanol	W4
H2C2O2	glyoxal	glyoxal	W4
trans-H(HO)C	hydroxymethylene	t-hcoh	W4
cis-H(HO)C	hydroxymethylene	c-hcoh	W4
HNCH	iminometyl radical	hcnh	W4
HOCN	cyanic acid	hocn	W4
HONC	isofulminic acid	honc	W4
HNCO	isocyanic acid	hnco	W4
HCNO	formonitrile oxide	hcno	W4
cis-H2N2	diazene	c-n2h2	W4
HN3	hydrogen azide	hnnn	W4
HNC	hydrogen isocyanide	hnc	W4
trans-HONO	nitrous acid	t-hono	W4
cis-HONO	nitrous acid	c-hono	W4
H2NCl	chloramine	nh2cl	W4
trans-HO3	hydrotrioxy radical	t-hooo	W4
cis-HO3	hydrotrioxy radical	c-hooo	W4
CH3F	fluoromethane	ch3f	W4
CF2H2	difluoromethane	ch2f2	W4

CF4	tetrafluoromethane	cf4	W4
SiH3F	fluorosilane	sih3f	W4
SiF4	tetrafluorosilane	sif4	W4
C2H3F	fluoroethylene	c2h3f	W4
C2H5F	fluoroethane	c2h5f	W4
C2F2	difluoroacetylene	fccf	W4
HC2F	fluoroacetylene	hccf	W4
HCOF	formylfluoride	hcof	W4
F2CO	carbonyl fluoride	f2co	W4
H2C ($^1A_1$)	singlet methylene	ch2-sing	W4
C3H8	propane	propane	W4
C3H6	propene	propene	W4
C3H4	propyne	propyne	W4
C3H4	allene	allene	W4
B2H6	diborane	b2h6	W4
HBF2	difluoroborane	bhf2	W4
BF3	trifluoroborane	bf3	W4
C2H6	ethane	c2h6	W4
H2CN	methanimine radical	h2cn	W4
C2N2	cyanogen	nccn	W4
H2NCH2	aminomethyl radical	ch2nh2	W4
H3CNH	methylamine radical	ch3nh	W4
CH3NH2	methylamine	ch3nh2	W4
F2C	carbon difluoride	cf2	W4
HN2	dinitrogen monohydride	n2h	W4
trans-N2H2	trans-diazene	t-n2h2	W4
N2H4	hydrazine	n2h4	W4
FO2	dioxygen fluoride	fo2	W4
F2O2	dioxygen difluoride	foof	W4
AlF3	aluminium fluoride	alf3	W4
Si2H6	disilane	si2h6	W4
P4	tetraphosphorus	p4	W4
SO2	sulfur dioxide	so2	W4
SO3	sulfur trioxide	so3	W4
OCS	carbon oxide sulfide	ocs	W4
CS2	carbon disulfide	cs2	W4
SSO	disulfur oxide	s2o	W4
S3	trisulfur	s3	W4
S4	tetrasulfur	s4-c2v	W4
CCl2	carbon dichloride	ccl2	W4
AlCl3	aluminium chloride	alcl3	W4
ClCN	cyanogen chloride	clcn	W4
O2Cl	chlorine dioxide	oclo	W4
OOCl	dioxygen chloride	cloo	W4
ClOCl	dichlorine monoxide	cl2o	W4
BN ($^3\mathbf{\Pi}$)	boron nitride	bn3pi	W4.2

FC	fluoromethylidyne	cf	W4.2
H2CC	vinylidene	ch2c	W4.2
H2CHC	vinyl radical	ch2ch	W4.2
C2H4	ethene	c2h4	W4.2
H2CNH	methanimine	ch2nh	W4.2
HOC	formyl radical	hco	W4.2
H2CO	formaldehyde	h2co	W4.2
CO2	carbon dioxide	co2	W4.2
HNO	nitrosyl hydride	hno	W4.2
O2N	nitrogen dioxide	no2	W4.2
NNO	nitrous oxide	n2o	W4.2
O3	ozone	o3	W4.2
HO2	hydroperoxy radical	hoo	W4.2
H2O2	hydrogen peroxide	hooh	W4.2
FOF	difluorine monoxide	f2o	W4.2
HOCl	hypochlorous acid	hocl	W4.2
HSS	hydrogen disulfide radical	ssh	W4.2
B2	diboron	b2	W4.3
BH	boron monohydride	bh	W4.3
BH3	borane	bh3	W4.3
BN ($^1\Sigma^+$)	boron nitride	bn	W4.3
BF	boron monofluoride	bf	W4.3
NH	imidogen radical	nh	W4.3
H2N	amino radical	nh2	W4.3
HCN	hydrogen cyanide	hcn	W4.3
HOF	hypofluorous acid	hof	W4.3
AlH	aluminum hydride	alh	W4.3
AlH3	aluminum trihydride	alh3	W4.3
AlF	aluminum monofluoride	alf	W4.3
AlCl	aluminum monochloride	alcl	W4.3
HSi	silicon hydride	sih	W4.3
SiH4	silane	sih4	W4.3
SiO	silicon monoxide	sio	W4.3
FSi	silicon fluoride	sif	W4.3
CS	carbon sulfide	cs	W4.3
H2	dihydrogen	h2	W4.4
HO	hydroxyl radical	oh	W4.4
HF	hydrogen fluoride	hf	W4.4
H2O	water	h2o	W4.4
HC	methylidyne	ch	W4.4
H2C ($^3B_1$)	triplet methylene	ch2-trip	W4.4
H3C	methyl radical	ch3	W4.4
CH4	methane	ch4	W4.4
HC≡C	ethynyl radical	cch	W4.4
C2H2	acetylene	c2h2	W4.4
NH3	ammonia	nh3	W4.4

C2	dicarbon	c2	W4.4
N2	dinitrogen	n2	W4.4
CO	carbon monoxide	co	W4.4
CN	cyano radical	cn	W4.4
NO	nitric oxide	no	W4.4
O2	dioxygen	o2	W4.4
FO	oxygen monofluoride	of	W4.4
F2	difluoride	f2	W4.4
PH3	phosphine	ph3	W4.4
HS	mercapto radical	hs	W4.4
H2S	hydrogen sulfide	h2s	W4.4
HCl	hydrogen chloride	hcl	W4.4
SO	sulfur monoxide	so	W4.4
ClO	chlorine monoxide	clo	W4.4
ClF	chlorine monofluoride	clf	W4.4
P2	diphosphorus	p2	W4.4
S2	disulfur	s2	W4.4
Cl2	dichlorine	cl2	W4.4

Table S4. %TAE[(T)] diagnostics for the systems in the W4-17 database. The %TAE[(T)] values are taken from W4 theory.

Molecular Formula	Molecule Name	%TAE[(T)] diagnostic	subset
BN (1Σ+)	boron nitride	18.81	W4-17-MR
O3	ozone	17.39	W4-17-MR
F2O2	dioxygen difluoride	16.92	W4-17-MR
OOCl•	dioxygen chloride	15.35	W4-17-MR
OOF•	dioxygen fluoride	15.32	W4-17-MR
ClF5	chlorine pentafluoride	14.78	W4-17-MR
B2	diboron	14.66	W4-17-MR
FOF	difluorine monoxide	14.60	W4-17-MR
OClOO	chlorine trioxide	14.08	W4-17-MR
O2Cl•	chlorine dioxide	13.55	W4-17-MR
C2	dicarbon	13.26	W4-17-MR
FO•	oxygen monofluoride	12.90	W4-17-MR
ClF3	phosphorus trifluoride	12.83	W4-17-MR
ClOOCl	dioxygen dichloride	12.20	W4-17-MR
S4	tetrasulfur	12.18	W4-17-MR
ClOCl	dichlorine monoxide	10.91	W4-17-MR
S3	trisulfur	10.15	W4-17-MR
F2	difluoride	19.46	W4-17-nonMR
ClO•	chlorine monoxide	9.68	W4-17-nonMR
N2O4	dinitrogen tetraoxide	9.11	W4-17-nonMR
ClNO	nitrosyl chloride	8.90	W4-17-nonMR
O2N•	nitrogen dioxide	8.52	W4-17-nonMR
ClF	chlorine monofluoride	8.34	W4-17-nonMR
P2	diphosphorus	8.27	W4-17-nonMR
HOClO2	chloric acid	8.21	W4-17-nonMR
SSO	disulfur oxide	8.09	W4-17-nonMR
HClO4	perchloric acid	7.92	W4-17-nonMR
trans-HO3•	hydrotrioxy radical	7.91	W4-17-nonMR
FNO	nitrosyl fluoride	7.74	W4-17-nonMR
O2	dioxygen	7.67	W4-17-nonMR
Cl2	dichlorine	7.65	W4-17-nonMR
P4	tetraphosphorus	7.56	W4-17-nonMR
HOClO	chlorous acid	7.54	W4-17-nonMR
S2	disulfur	7.41	W4-17-nonMR
cis-HO3•	hydrotrioxy radical	7.39	W4-17-nonMR
N≡N-O	nitrous oxide	6.98	W4-17-nonMR
SO	sulfur monoxide	6.70	W4-17-nonMR
ON•	nitric oxide	6.21	W4-17-nonMR
SO2	sulfur dioxide	6.10	W4-17-nonMR
BN (3**Π**)	boron nitride	6.09	W4-17-nonMR
Cl2C:	carbon dichloride	6.03	W4-17-nonMR

SO3	sulfur trioxide	5.87	W4-17-nonMR
N≡C•	cyano radical	5.81	W4-17-nonMR
CS	carbon sulfide	5.65	W4-17-nonMR
HN3	hydrogen azide	5.64	W4-17-nonMR
CS2	carbon disulfide	5.63	W4-17-nonMR
trans-HON=O	nitrous acid	5.36	W4-17-nonMR
cis-HON=O	nitrous acid	5.34	W4-17-nonMR
HOF	hypofluorous acid	5.15	W4-17-nonMR
CCl4	carbon tetrachloride	5.03	W4-17-nonMR
C2Cl6	hexachloroethane	4.93	W4-17-nonMR
HN=O	nitrosyl hydride	4.91	W4-17-nonMR
HCNO	formonitrile oxide	4.77	W4-17-nonMR
HOO•	hydroperoxy radical	4.63	W4-17-nonMR
C2Cl4	tetrachloroethylene	4.45	W4-17-nonMR
ClC≡N	cyanogen chloride	4.39	W4-17-nonMR
CCl2O	phosgene	4.36	W4-17-nonMR
SiO	silicon monoxide	4.35	W4-17-nonMR
OCS	carbon oxide sulfide	4.33	W4-17-nonMR
SF6	sulfur hexafluoride	4.29	W4-17-nonMR
HN≡N•	dinitrogen monohydride	4.24	W4-17-nonMR
N2	dinitrogen	4.16	W4-17-nonMR
N≡C–C≡N	cyanogen	4.11	W4-17-nonMR
C2Cl2	dichloroacetylene	4.11	W4-17-nonMR
HOCl	hypochlorous acid	4.08	W4-17-nonMR
HONC:	isofulminic acid	4.03	W4-17-nonMR
H2C2N2O	1,2,5-oxadiazole	3.96	W4-17-nonMR
HSS•	hydrogen disulfide radical	3.82	W4-17-nonMR
FC•	fluoromethylidyne	3.80	W4-17-nonMR
ClCOF	carbonyl chloride fluoride	3.75	W4-17-nonMR
cis-C2F2Cl2	cis-dichlorodifluoroethene	3.74	W4-17-nonMR
CF2Cl2	dichlorodifluoromethane	3.73	W4-17-nonMR
trans-C2F2Cl2	trans-dichlorodifluoroethene	3.73	W4-17-nonMR
H2CO2	dioxirane	3.60	W4-17-nonMR
FC≡CF	difluoroacetylene	3.57	W4-17-nonMR
CO2	carbon dioxide	3.57	W4-17-nonMR
F2C:	carbon difluoride	3.54	W4-17-nonMR
cis-H2N2	diazene	3.50	W4-17-nonMR
CCl3H	chloroform	3.43	W4-17-nonMR
HNCO	isocyanic acid	3.38	W4-17-nonMR
trans-N2H2	trans-diazene	3.37	W4-17-nonMR
H2O2	hydrogen peroxide	3.34	W4-17-nonMR
HOCN	cyanic acid	3.33	W4-17-nonMR
F2C=O	carbonyl fluoride	3.23	W4-17-nonMR
C2F4	perfluoroethene	3.17	W4-17-nonMR
H2C2O	oxirene	3.17	W4-17-nonMR
CO	carbon monoxide	3.09	W4-17-nonMR

H(O=)C•	formyl radical	3.02	W4-17-nonMR
C2ClH	chloroethyne	3.00	W4-17-nonMR
HNC:	hydrogen isocyanide	2.96	W4-17-nonMR
HC≡C•	ethynyl radical	2.96	W4-17-nonMR
HCN	hydrogen cyanide	2.95	W4-17-nonMR
H2NO	dihydronitroxide radical	2.95	W4-17-nonMR
H2C2O3	formic_anhydride	2.92	W4-17-nonMR
H2C2O3	1,3-dioxetan-2-one	2.90	W4-17-nonMR
C2F6	hexafluoroethane	2.86	W4-17-nonMR
NH2F	fluoroamine	2.85	W4-17-nonMR
HC≡CF	fluoroacetylene	2.80	W4-17-nonMR
CF4	tetrafluoromethane	2.77	W4-17-nonMR
H2NCl	chloramine	2.77	W4-17-nonMR
HC(=O)F	formylfluoride	2.75	W4-17-nonMR
PF3	phosphorus trifluoride	2.74	W4-17-nonMR
H(O=)C–C(=O)H	glyoxal	2.71	W4-17-nonMR
HN=CH•	iminometyl radical	2.62	W4-17-nonMR
PF5	phosphorus pentafluoride	2.61	W4-17-nonMR
HC(=O)OH	formic acid	2.51	W4-17-nonMR
FSi•	silicon fluoride	2.50	W4-17-nonMR
H2CCN•	cyanomethyl	2.46	W4-17-nonMR
H2C=C=O	ketene	2.46	W4-17-nonMR
AlCl	aluminum monochloride	2.43	W4-17-nonMR
H4C4S	thiophene	2.37	W4-17-nonMR
NH2OH	hydroxylamine	2.36	W4-17-nonMR
cis-H(HO)C:	hydroxymethylene	2.34	W4-17-nonMR
CHF3	fluoroform	2.33	W4-17-nonMR
AlCl3	aluminium chloride	2.29	W4-17-nonMR
CH3NO	formamide	2.27	W4-17-nonMR
H4C4O	furan	2.27	W4-17-nonMR
trans-H(HO)C:	hydroxymethylene	2.26	W4-17-nonMR
C4H4	cyclobutadiene	2.26	W4-17-nonMR
H4C2S2	1,3-dithiotane	2.24	W4-17-nonMR
CCl2H2	dichloromethane	2.23	W4-17-nonMR
BF	boron monofluoride	2.20	W4-17-nonMR
H5C3NO	beta-lactim	2.18	W4-17-nonMR
H2C=N•	methanimine radical	2.17	W4-17-nonMR
C4H4	tetrahedrane	2.15	W4-17-nonMR
H5C4N	pyrrole	2.14	W4-17-nonMR
H2C=O	formaldehyde	2.12	W4-17-nonMR
C2H2	acetylene	2.07	W4-17-nonMR
H4C2O2	1,3-dioxetane	2.06	W4-17-nonMR
CH2ClF	chlorofluoromethane	2.03	W4-17-nonMR
CH3C(=O)OH	acetic acid	2.02	W4-17-nonMR
AlF	aluminum monofluoride	2.00	W4-17-nonMR
C6H6	benzene	1.96	W4-17-nonMR

H2C=NH	methanimine	1.94	W4-17-nonMR
N2H4	hydrazine	1.93	W4-17-nonMR
C2ClH3	vinyl chloride	1.92	W4-17-nonMR
H2C=C:	vinylidene	1.91	W4-17-nonMR
H5BC4	borole	1.84	W4-17-nonMR
AlF3	aluminium fluoride	1.84	W4-17-nonMR
CF2H2	difluoromethane	1.83	W4-17-nonMR
C2H4O	oxirane	1.82	W4-17-nonMR
H6C5	cyclopentadiene	1.82	W4-17-nonMR
C3H4	cyclopropene	1.80	W4-17-nonMR
H6C4Si	silole	1.80	W4-17-nonMR
C2H3F	fluoroethylene	1.79	W4-17-nonMR
BF3	trifluoroborane	1.77	W4-17-nonMR
SiF4	tetrafluorosilane	1.75	W4-17-nonMR
C3H4	allene	1.75	W4-17-nonMR
H3C–C(=O)H	acetaldehyde	1.72	W4-17-nonMR
C3H4	propyne	1.70	W4-17-nonMR
C4H6	trans-butadiene	1.62	W4-17-nonMR
C4H6	cyclobutene	1.61	W4-17-nonMR
H6C3O	oxetane	1.60	W4-17-nonMR
HO•	hydroxyl radical	1.57	W4-17-nonMR
H2C=HC•	vinyl radical	1.52	W4-17-nonMR
HF	hydrogen fluoride	1.51	W4-17-nonMR
H2O	water	1.51	W4-17-nonMR
HBF2	difluoroborane	1.49	W4-17-nonMR
C3H5•	allyl radical	1.47	W4-17-nonMR
H2N–CH2•	aminomethyl radical	1.45	W4-17-nonMR
NH	imidogen radical	1.42	W4-17-nonMR
C3H5•	cyclopropyl radical	1.38	W4-17-nonMR
H2N•	amino radical	1.38	W4-17-nonMR
HCl	hydrogen chloride	1.37	W4-17-nonMR
CH3OH	methanol	1.34	W4-17-nonMR
CClH3	chloromethane	1.34	W4-17-nonMR
C2H4	ethene	1.32	W4-17-nonMR
C2ClH5	chloroethane	1.32	W4-17-nonMR
H3C–NH•	methylamine radical	1.31	W4-17-nonMR
C2H5OH	ethanol	1.31	W4-17-nonMR
NH3	ammonia	1.30	W4-17-nonMR
C3H6	propene	1.30	W4-17-nonMR
C4H8	cyclobutane	1.28	W4-17-nonMR
C3H6	cyclopropane	1.27	W4-17-nonMR
CH3F	fluoromethane	1.26	W4-17-nonMR
CH3NH2	methylamine	1.26	W4-17-nonMR
C2H5F	fluoroethane	1.25	W4-17-nonMR
HS•	mercapto radical	1.23	W4-17-nonMR
H2S	hydrogen sulfide	1.21	W4-17-nonMR

C5H12	n-pentane	1.11	W4-17-nonMR
CH3PH2	methylphosphine	1.08	W4-17-nonMR
C4H10	n-butane	1.07	W4-17-nonMR
H2C: (1A1)	singlet methylene	1.05	W4-17-nonMR
HC•	methylidyne	1.05	W4-17-nonMR
C3H8	propane	1.01	W4-17-nonMR
C2H6	ethane	0.90	W4-17-nonMR
PH3	phosphine	0.82	W4-17-nonMR
SiH3F	fluorosilane	0.81	W4-17-nonMR
B2H6	diborane	0.74	W4-17-nonMR
CH4	methane	0.69	W4-17-nonMR
H3C•	methyl radical	0.62	W4-17-nonMR
Si2H6	disilane	0.54	W4-17-nonMR
HSi•	silicon hydride	0.53	W4-17-nonMR
H2C: (3B1)	triplet methylene	0.51	W4-17-nonMR
BH	boron monohydride	0.48	W4-17-nonMR
BH3	borane	0.28	W4-17-nonMR
SiH4	silane	0.25	W4-17-nonMR
AlH	aluminum hydride	0.10	W4-17-nonMR
AlH3	aluminum trihydride	0.08	W4-17-nonMR
H2	dihydrogen	0.00	W4-17-nonMR

Table S5. Deviations larger than 2 kcal mol^{-1} for the CCSD(T) composite thermochemical procedures for the 183 atomization reactions in the W4-17-nonMR dataset.

	G4		**G3B3**		**G3 cont.**		**CBS-QB3 cont.**		**ccCA-PS3**
hclo4	-2.52	sf6	-10.85	tetrahedrane	-2.13	cf2cl2	5.61	cf2cl2	2.06
hoclo2	-2.44	hclo4	-9.98	cyclopropyl	-2.07	cis-c2f2cl2	5.74	ccl3h	2.12
so3	-2.40	pf5	-8.41	cyclobutadiene	-2.03	trans-c2f2cl2	5.82	cis-c2f2cl2	2.15
s2o	-2.04	hoclo2	-6.10	cn	-2.03	c2f6	6.30	trans-c2f2cl2	2.19
c2cl4	2.48	pf3	-5.53	s2	-2.02	alcl3	6.43	ccl4	3.05
n2o4	2.49	so3	-5.30	n2h	-2.00	c2cl4	8.34	c2cl4	3.59
c2cl6	5.73	p4	-4.04	trans-c2f2cl2	2.00	ccl4	8.36	c2cl6	5.81
	G4(MP2)	s2o	-3.53	c2cl4	2.92	c2cl6	15.88		**W1X-1**
b2h6	-4.46	so2	-3.25	ccl4	3.15		**ROCBS-QB3**	so3	-2.30
hclo4	-2.95	sif4	-3.21	c2f6	3.16	sf6	-6.10	si2h6	-2.27
bf3	-2.63	b2h6	-2.83	c2cl6	8.65	borole	-4.19	c2cl6	3.49
bhf2	-2.40	n-pentane	-2.79		**G3(MP2)**	hclo4	-3.80		**W1X-2**
c-hooo	-2.20	ssh	-2.75	sf6	-10.56	cyclobutadiene	-3.33	hclo4	-2.53
so3	-2.07	hoclo	-2.62	hclo4	-10.55	b2h6	-3.09	si2h6	-2.15
hoclo2	-2.03	clo	-2.50	pf5	-7.93	bn3pi	-2.90	so3	-2.10
bh3	-2.03	si2h6	-2.43	so3	-6.73	cyclopentadiene	-2.79	p2	-2.04
dithiotane	2.16	n-butane	-2.41	hoclo2	-6.05	n-pentane	-2.38	c2f6	2.89
p4	2.30	cyclobutane	-2.31	b2h6	-6.05	cyclobutene	-2.35	c2cl6	3.23
ocs	2.43	s2	-2.29	pf3	-4.83	tetrahedrane	-2.32		**W2X**
ccl2	2.45	borole	-2.24	so2	-4.28	cyclobutane	-2.21	t-hooo	-2.23
thiophene	2.77	ch3ph2	-2.24	n-pentane	-3.59	hoclo2	-2.18	c2cl6	3.25
c2cl2	2.93	c-hooo	-2.16	sif4	-3.24	cyclopropyl	-2.18		
cs	3.39	pyrrole	-2.03	t-hooo	-3.21	t-butadiene	-2.10		
ccl4	3.44	n2o4	2.01	n-butane	-3.12	pf5	-2.02		
cs2	4.13	nccn	2.04	si2h6	-2.89	n-butane	-2.00		
c2cl4	4.91	c2cl6	5.39	hoclo	-2.80	ccl2h2	2.01		
c2cl6	7.53		**G3(MP2)B3**	cyclobutane	-2.66	no2	2.15		
	ROG4(MP2)-6X	hclo4	-12.94	n2h4	-2.62	dioxetan2one	2.17		
b2h6	-3.19	sf6	-12.53	bh3	-2.61	clcof	2.18		
c2f4	2.00	pf5	-8.73	propane	-2.52	s2	2.32		
s2	2.01	hoclo2	-7.15	s2o	-2.40	cf4	2.43		
co	2.06	so3	-6.18	borole	-2.33	ccl2o	2.71		
thiophene	2.13	b2h6	-5.76	clo	-2.32	p4	2.81		

clcof	2.16	pf3	-5.27	cyclopropane	-2.27	c2f4	2.89
cf2	2.17	sif4	-3.44	n2h	-2.18	c2cl2	2.98
sf6	2.19	so2	-3.25	n2o	-2.17	n2o4	4.03
cf4	2.24	hoclo	-3.00	ch2nh2	-2.15	ccl3h	4.03
clcn	2.25	c-hooo	-2.96	ch3nh2	-2.12	cf2cl2	4.38
alcl3	2.30	n-pentane	-2.85	sih3f	-2.06	cis-c2f2cl2	4.41
alf3	2.56	clo	-2.58	ch3ph2	-2.03	trans-c2f2cl2	4.50
pf5	2.79	si2h6	-2.53	hnnn	-2.03	c2f6	4.87
ocs	2.79	n-butane	-2.50	n2o4	-2.02	alcl3	5.17
ccl2o	2.83	bh3	-2.47	cis-c2f2cl2	2.14	c2cl4	6.70
ccl2	2.86	n2h4	-2.25	trans-c2f2cl2	2.17	ccl4	6.83
cf2cl2	2.93	cyclobutane	-2.16	ocs	2.31	c2cl6	13.52
cs	3.02	propane	-2.03	c2cl2	2.87		**CBS-APNO**
sif4	3.04	nh	2.06	cs	3.13	c-hooo	-3.86
ccl3h	3.28	ocs	2.66	ccl4	3.76	n-pentane	2.06
c2f6	3.30	c2cl2	2.74	cs2	3.97	no2	2.18
trans-c2f2cl2	3.60	ccl4	2.92	c2cl4	4.47	benzene	2.28
c2cl2	3.66	cs	3.18	c2cl6	8.93	dioxetan2one	2.32
cs2	3.70	c2cl4	3.82		**CBS-QB3**	chf3	2.35
cis-c2f2cl2	3.72	cs2	4.02	sf6	-4.41	c2f4	2.61
ccl4	5.12	c2cl6	7.45	borole	-3.70	cf4	3.13
c2cl4	6.39		**G3**	bn3pi	-3.15	n2o4	3.61
c2cl6	9.86	sf6	-7.52	cyclobutadiene	-2.96	c2f6	4.81
	G4(MP2)-6X	hclo4	-6.62	b2h6	-2.85		**W1**
b2h6	-3.52	pf5	-6.56	hclo4	-2.48	c2cl6	2.22
cf2	2.03	so3	-5.51	cyclopentadiene	-2.33	c2f6	2.25
dithiotane	2.07	pf3	-4.45	ccl2	2.01		**W2**
alf3	2.12	p4	-4.25	ch2f2	2.04	t-hooo	-2.52
alcl3	2.13	hoclo2	-4.22	dioxirane	2.15	c-hooo	-2.06
clcn	2.13	so2	-4.16	dioxetane	2.21	n2o4	-2.00
clcof	2.17	s2o	-3.79	ch2clf	2.25	c2cl6	2.71
thiophene	2.42	n-pentane	-3.36	no2	2.34		**W1-F12(1st)**
sf6	2.51	b2h6	-3.05	p4	2.36	s2o	-2.72
sif4	2.55	n-butane	-2.89	ocs	2.39	so3	-2.41
pf5	2.57	si2h6	-2.68	fccf	2.43	p4	-2.37
ocs	2.86	cyclobutane	-2.66	f2co	2.46	hclo4	-2.27
c2f6	2.97	pyrrole	-2.52	alcl	2.50	alcl3	-2.23
cf2cl2	2.98	borole	-2.50	cs2	2.59	t-hooo	-2.13
ccl2o	2.99	ch3ph2	-2.46	chf3	2.69		**W1-F12(all)**

ccl2	3.03	cyclobutene	-2.37	formic-anhydride	2.76	s2o	-2.60
cs	3.20	cyclopentadiene	-2.33	ccl2h2	2.83	p4	-2.48
ccl3h	3.36	propane	-2.27	dioxetan2one	3.07	so3	-2.31
c2cl2	3.62	ssh	-2.27	clcof	3.09	t-hooo	-2.20
trans-c2f2cl2	3.67	cyclopropane	-2.23	cf4	3.36	alcl3	-2.17
cis-c2f2cl2	3.78	sif4	-2.22	ccl2o	3.77	hclo4	-2.12
cs2	3.99	silole	-2.21	c2cl2	3.89	p2	-2.02
ccl4	5.29	t-hooo	-2.20	c2f4	3.91		**W2-F12**
c2cl4	6.65	n2h4	-2.20	n2o4	4.86	t-hooo	-2.07
c2cl6	10.24	benzene	-2.14	ccl3h	5.21	c2cl6	3.30

Table S6. This table includes raw data used for calculating the CV corrections in Table 6 of the main text and is provided as a separate excel spreadsheet.

Table S7. Full References for Gaussian 09 (ref 77), Q-Chem (ref 78), and Molpro (ref 88).

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