Table 1: Perfomance of tested density functionals for heat of formations in the test set G3/05. Given are the experimental values as well as the deviations (exp. - theo.) in kcal mol^{-1}.

	molecule	Exp.[a]	deviation				
			B-LYP	TPSS	B3-LYP	B2-PLYP	mPW2-PLYP
1	H_2	0.0	0.1	3.5	0.9	-0.8	-1.0
2	LiH	33.3	0.0	1.2	0.4	-0.9	-0.8
3	BeH	81.7	7.7	11.1	8.6	6.8	6.9
4	CH	142.5	1.9	3.6	1.5	-0.1	-0.1
5	$CH_2(^3B_1)$	93.7	0.3	8.8	2.2	0.6	0.9
6	$CH_2(^1A_1)$	102.8	-0.4	0.8	-0.1	-1.8	-1.7
7	CH_3	35.0	0.3	7.2	2.7	0.8	1.2
8	CH_4	-17.9	-2.3	5.7	1.0	-0.6	0.0
9	NH	85.2	5.9	6.7	4.1	1.4	1.3
10	NH_2	45.1	7.9	6.3	5.7	2.4	2.3
11	NH_3	-11.0	4.2	2.1	2.6	0.3	0.1
12	OH	9.4	4.1	0.5	2.2	0.8	0.5
13	H_2O	-57.8	1.0	-3.7	-1.4	-1.4	-2.2
14	HF	-65.1	1.0	-1.5	-1.2	-0.6	-1.3
15	$SiH_2(^3B_1)$	65.2	-0.1	4.8	1.3	-0.3	0.0
16	$SiH_2(^1A_1)$	86.2	-0.8	10.3	1.6	0.0	0.5
17	SiH_3	47.9	-1.4	11.6	2.5	0.5	1.3
18	SiH_4	8.2	-4.3	11.7	1.2	-0.4	0.6
19	PH_2	33.1	4.8	8.5	5.5	2.2	2.5
20	PH_3	1.3	1.0	7.6	2.7	-0.5	0.0
21	H_2S	-4.9	-0.4	3.7	0.6	-0.2	-0.1
22	HCl	-22.1	-0.4	1.8	0.0	0.4	0.3
23	Li_2	51.6	-3.8	-1.6	-3.6	-3.4	-2.7
24	LiF	-80.1	2.7	-1.7	-1.1	0.3	-0.2
25	C_2H_2	54.2	0.8	0.6	-2.2	-0.2	-0.9
26	$H_2C{=}CH_2$	12.5	-1.4	5.6	-0.1	-0.7	-0.3
27	$H_3C\text{-}CH_3$	-20.1	-6.1	7.8	-0.4	-1.4	-0.1
28	CN	104.9	10.1	1.8	-2.5	-0.4	-2.9
29	HCN	31.5	8.3	1.5	0.3	2.2	0.6
30	CO	-26.4	3.9	-4.5	-3.7	-0.1	-1.8
31	HCO	10.0	9.7	4.7	2.0	2.6	1.1
32	$H_2C{=}O$	-26.0	5.7	3.2	0.2	0.6	-0.5
33	CH_3OH	-48.0	0.1	3.0	-0.5	-1.1	-1.1
34	N_2	0.0	11.5	-0.9	-0.3	1.6	-0.7
35	$H_2N\text{-}NH_2$	22.8	9.9	5.6	4.9	0.9	0.6
36	NO	24.6	17.4	6.8	5.1	5.3	2.9
37	O_2	0.0	16.8	7.1	4.1	3.8	1.1
38	HO-OH	-32.5	9.3	0.5	-0.9	-1.8	-3.8
39	F_2	0.0	12.2	8.6	-0.1	-0.9	-3.4
40	CO_2	-94.0	13.0	1.1	-0.8	3.2	0.4
41	Na_2	34.0	0.6	2.0	-0.5	0.8	0.8
42	Si_2	139.9	-2.2	0.2	-5.8	-4.4	-5.2
43	P_2	34.3	4.4	-0.9	-2.3	-0.7	-2.0

44	S_2	30.7	8.2	9.0	3.1	3.4	2.4
45	Cl_2	0.0	3.3	5.8	0.0	0.6	0.0
46	NaCl	-43.6	-5.6	-0.8	-4.6	-2.0	-1.8
47	SiO	-24.6	3.6	-5.2	-5.0	-0.5	-2.4
48	CS	66.9	2.1	-0.7	-4.7	-0.8	-2.4
49	SO	1.2	12.1	6.5	2.8	3.6	1.8
50	ClO	24.2	12.6	8.8	3.1	1.1	-0.4
51	ClF	-13.2	8.4	7.2	1.2	1.2	-0.1
52	$H_3Si\text{-}SiH_3$	19.1	-10.9	17.7	-1.3	-2.5	-0.4
53	CH_3Cl	-19.6	-2.3	6.8	-0.4	0.1	0.6
54	H_3CSH	-5.5	-3.5	6.9	-0.8	-0.9	-0.3
55	HOCl	-17.8	6.9	3.7	0.1	0.3	-1.0
56	SO_2	-71.0	11.9	1.9	-5.4	0.9	-2.9
57	BF_3	-271.4	2.0	-3.8	-3.6	1.5	1.1
58	BCl_3	-96.3	-6.1	2.7	-5.6	1.7	2.2
59	AlF_3	-289.0	-1.0	-4.8	-7.2	0.4	-0.4
60	$AlCl_3$	-139.7	-11.7	2.0	-8.2	0.3	1.2
61	CF_4	-223.0	5.3	3.2	-5.2	-0.3	-1.4
62	CCl_4	-22.9	-6.9	4.3	-11.6	-1.9	-2.3
63	COS	-33.1	12.2	6.4	0.6	4.8	2.4
64	CS_2	27.9	9.7	9.9	0.2	5.1	3.0
65	COF_2	-149.1	7.2	-0.3	-5.9	-2.4	-4.5
66	SiF_4	-386.0	-9.8	-12.1	-15.5	-5.5	-5.8
67	$SiCl_4$	-158.4	-19.8	-0.8	-16.1	-4.2	-3.1
68	N_2O	19.6	27.3	12.0	4.7	6.7	2.2
69	ClNO	12.4	24.2	13.9	3.2	3.3	-0.6
70	NF_3	-31.6	27.7	19.9	4.6	2.3	-1.2
71	PF_3	-229.1	6.5	1.5	-3.8	-0.7	-1.7
72	O_3	34.1	25.4	9.4	-5.4	0.7	-6.4
73	F_2O	5.9	24.1	16.1	2.3	0.1	-3.8
74	ClF_3	-38.0	30.9	26.6	6.1	5.0	1.0
75	C_2F_4	-157.4	17.7	13.7	1.9	4.9	3.2
76	C_2Cl_4	-3.0	-3.3	8.7	-9.7	1.4	0.8
77	CF_3CN	-118.4	13.5	4.5	-4.5	2.3	-0.1
78	C_3H_4(propyne)	44.2	-1.6	4.3	-2.3	-0.1	0.0
79	C_3H_4(allene)	45.5	3.0	8.7	1.2	0.7	0.9
80	C_3H_4(cyclopropen)	66.2	-4.0	6.9	-4.0	-2.6	-2.4
81	C_3H_6(propylen)	4.8	-5.3	7.5	-1.8	-1.6	-0.4
82	C_3H_6(cyclopropane)	12.7	-8.8	9.2	-3.5	-2.3	-1.0
83	C_3H_8(propane)	-25.0	-11.0	8.8	-2.9	-2.8	-0.7
84	C_4H_6(butadiene)	26.3	-3.9	8.0	-2.9	-1.7	-0.7
85	C_4H_6(2-butyne)	34.8	-5.1	7.1	-3.4	-0.9	-0.1
86	C_4H_6(methylenecyclopropane)	47.9	-3.8	12.9	-1.4	0.2	1.2
87	C_4H_6(bicyclobutane)	51.9	-13.0	9.6	-8.7	-5.0	-3.8
88	C_4H_6(cyclobutene)	37.4	-10.6	7.3	-7.4	-4.5	-3.3
89	C_4H_8(cyclobutane)	6.8	-14.8	9.4	-6.9	-4.2	-2.0
90	C_4H_8(isobutene)	-4.0	-10.8	8.0	-4.7	-3.2	-1.2
91	C_4H_{10}(butane)	-32.1	-18.3	7.4	-7.7	-6.4	-3.5
92	C_4H_{10}(isobutane)	-32.1	-17.5	8.2	-6.8	-5.1	-2.1
93	C_5H_8(spiropentane)	44.3	-14.5	13.3	-7.6	-3.7	-1.7

94	C_6H_6(benzene)	19.7	-7.9	8.2	-7.0	-0.3	1.0
95	H_2CF_2	-107.7	4.4	7.3	-0.3	0.7	0.3
96	CHF_3	-166.6	5.3	5.7	-2.6	0.2	-0.5
97	H_2CCl_2	-22.8	-3.2	6.6	-3.2	-0.2	0.1
98	$CHCl_3$	-24.7	-4.8	5.6	-7.1	-1.0	-1.0
99	CH_3NH_2	-5.5	1.2	6.1	1.8	-0.5	0.1
100	CH_3CN	18.0	5.7	4.9	0.0	1.9	1.1
101	CH_3NO_2	-17.8	19.8	12.7	1.6	2.5	-0.6
102	CH_3-O-N=O	-15.9	20.0	12.7	0.4	0.5	-2.7
103	H_3C-SiH_3	-7.0	-10.1	10.9	-2.3	-2.9	-1.1
104	HCOOH	-90.5	8.0	0.3	-1.6	0.3	-1.3
105	$HCOOCH_3$	-85.0	6.1	6.2	-1.7	0.6	-0.3
106	CH_3CONH_2	-57.0	5.1	4.9	-0.5	0.0	-0.1
107	CH_2-NH-CH_2 (aziran)	30.2	-0.2	10.1	-0.8	-1.1	-0.7
108	NC-CN	73.3	19.4	3.5	-0.1	5.0	1.5
109	$(CH_3)_2NH$	-4.4	-2.7	9.0	0.1	-1.5	-0.2
110	$C_2H_5NH_2$	-11.3	-2.7	8.0	0.3	-0.9	0.5
111	H_2C=C=O	-11.3	10.0	6.4	1.8	3.0	1.6
112	H_2C-O-CH_2	-12.6	0.0	8.7	-2.6	-1.4	-1.7
113	CH_3CHO	-39.7	2.1	5.0	-1.1	-0.3	-0.5
114	O=CH-CH=O	-50.7	10.2	2.3	-2.2	0.9	-1.1
115	C_2H_5OH	-56.2	-4.7	3.8	-3.0	-2.6	-1.8
116	CH_3-O-CH_3	-44.0	-2.5	7.9	-1.3	-1.6	-0.8
117	CH_2-S-CH_2(thiirane)	19.6	-4.8	10.1	-3.3	-0.7	-0.2
118	CH_3-SO-CH_3	-36.2	-3.2	9.0	-5.3	-2.6	-2.4
119	C_2H_5SH	-11.1	-8.2	8.1	-3.1	-2.1	-0.7
120	CH_3-S-CH_3	-8.9	-7.3	9.4	-2.7	-1.8	-0.5
121	H_2C=CHF	-33.2	4.0	8.1	0.8	1.0	0.9
122	C_2H_5Cl	-26.8	-7.1	7.8	-2.9	-1.4	-0.1
123	H_2C=CHCl	5.5	-1.0	6.9	-1.6	0.1	0.3
124	H_2C=CHCN	43.2	5.7	3.9	-2.8	0.1	-0.9
125	CH_3-CO-CH_3	-51.9	-2.9	5.7	-3.6	-1.7	-1.2
126	CH_3COOH	-103.4	2.8	0.8	-4.0	-1.3	-2.1
127	CH_3COF	-105.7	4.4	4.7	-3.0	-0.5	-1.3
128	CH_3COCl	-58.0	2.8	6.3	-3.4	-0.1	-0.8
129	C_3H_7Cl	-31.5	-12.0	8.8	-5.3	-2.6	-0.6
130	$(CH_3)_2CHOH$	-65.2	-10.4	3.9	-6.1	-4.2	-2.6
131	$C_2H_5OCH_3$	-51.7	-6.9	9.2	-3.3	-2.5	-0.9
132	$(CH_3)_3N$	-5.7	-7.2	11.4	-2.2	-2.4	-0.2
133	C_4H_4O(furan)	-8.3	-1.0	7.0	-6.1	-0.9	-1.1
134	C_4H_4S(thiophene)	27.5	-6.8	8.0	-8.4	-0.8	-0.6
135	C_4H_4NH(pyrrole)	25.9	-0.5	9.1	-3.4	0.6	1.0
136	C_5H_5N(pryridine)	33.6	1.5	10.4	-3.4	1.9	2.2
137	SH	34.2	2.1	3.5	2.3	1.2	1.2
138	CCH	135.1	0.9	0.2	-3.4	-2.0	-2.9
139	C_2H_3	71.6	3.2	8.6	2.7	1.0	1.3
140	CH_3CO	-2.4	6.8	7.4	1.3	2.0	1.3
141	H_2COH	-4.1	4.5	5.3	2.0	0.6	0.4
142	CH_3O	4.1	6.0	8.5	3.9	0.7	0.9
143	C_2H_5O	-3.7	0.5	8.9	0.5	-1.8	-0.8

144	CH_3S	29.8	0.8	8.4	2.3	1.4	2.0
145	C_2H_5	28.9	-2.2	10.1	2.1	0.2	1.4
146	$(CH_3)_2CH$	21.5	-5.6	12.3	0.9	-0.5	1.4
147	$(CH_3)_3C$	12.3	-11.1	12.6	-2.5	-2.8	0.0
148	NO_2	7.9	28.6	13.8	5.3	6.0	1.4
149	CH_3-CH=C=CH_2	38.8	-1.5	10.2	-1.0	-0.6	0.3
150	C_5H_8(isoprene)	18.0	-10.1	8.0	-6.4	-3.6	-1.8
151	C_5H_{10}(cyclopentane)	-18.3	-22.4	7.6	-11.1	-6.4	-3.2
152	C_5H_{12}(n-pentane)	-35.1	-21.5	10.2	-8.4	-5.9	-2.2
153	C_5H_{12}(neopentane)	-40.2	-25.4	6.7	-11.9	-7.9	-4.1
154	C_6H_8(1,3-cyclohexadiene)	25.4	-16.0	5.8	-11.4	-5.3	-3.1
155	C_6H_8(1,4-cyclohexadiene)	25.0	-16.7	5.1	-11.6	-5.7	-3.5
156	C_6H_{12}(cyclohexane)	-29.5	-29.9	5.9	-15.4	-9.1	-4.9
157	C_6H_{14}(n-hexane)	-39.9	-26.5	11.1	-10.9	-7.3	-2.8
158	C_6H_{14}(3-methyl-pentane)	-41.1	-29.2	8.8	-13.4	-9.0	-4.4
159	$C_6H_5CH_3$(toluene)	12.0	-13.3	8.8	-10.0	-1.9	0.1
160	C_7H_{16}(n-heptane)	-44.9	-31.6	11.9	-13.6	-8.9	-3.6
161	C_8H_8(cyclooctatetraene)	70.7	-14.4	5.2	-14.6	-5.6	-3.8
162	C_8H_{18}(n-octane)	-49.9	-36.9	12.6	-16.4	-10.4	-4.3
163	$C_{10}H_8$(naphtalene)	35.9	-15.4	9.6	-15.5	-0.6	1.4
164	$C_{10}H_8$(azulene)	69.1	-11.9	12.4	-15.4	-1.0	0.2
165	CH_3COOCH_3	-98.4	-0.3	5.6	-5.2	-2.1	-2.1
166	$(CH_3)_3COH$	-74.7	-17.7	2.6	-10.8	-6.9	-4.4
167	$C_6H_5NH_2$	20.8	-3.8	9.2	-5.9	0.5	1.8
168	C_6H_5OH(phenol)	-23.0	-6.3	4.7	-9.7	-1.7	-1.0
169	C_4H_6O	-3.3	-0.4	7.8	-4.0	-2.0	-1.6
170	C_4H_8O(tetrahydrofuran)	-44.0	-14.1	6.4	-9.7	-5.7	-3.8
171	C_5H_8O(cyclopentanone)	-45.9	-13.3	5.5	-10.7	-4.5	-2.9
172	$C_6H_4O_2$(benzochinone)	-29.4	2.0	2.0	-12.3	-2.8	-4.0
173	$C_4H_4N_2$	46.8	11.6	13.7	1.4	5.3	4.8
174	$C_2H_6O_2S$(dimethyl sulphone)	-89.2	-8.1	2.5	-13.2	-6.7	-7.1
175	C_6H_5Cl	12.4	-11.2	6.1	-12.2	-2.3	-1.3
176	NC-CH_2-CH_2-CN	50.1	7.4	3.8	-5.1	1.9	0.4
177	$C_4H_4N_2$	46.9	8.3	10.0	-2.5	1.3	0.6
178	CH_3COCCH(acetyl acetylene)	15.6	0.3	1.0	-7.7	-2.7	-3.6
179	CH_3-CH=CH-CHO	-24.0	0.7	8.6	-2.8	-0.1	0.1
180	$(CH_3CO)_2O$(acetic anhydride)	-136.8	4.3	4.8	-7.3	-1.0	-1.9
181	C_4H_6S	20.8	-12.4	7.7	-9.2	-3.4	-2.0
182	$(CH_3)_2CH$-CN	5.6	-6.8	4.4	-7.5	-3.0	-2.2
183	CH_3-CO-CH_2-CH_3	-57.1	-7.7	7.0	-5.8	-2.7	-1.3
184	$(CH_3)_2$-CH-CHO	-51.6	-9.8	5.2	-7.9	-4.3	-3.0
185	$C_4H_8O_2$	-75.5	-10.9	5.5	-10.8	-5.9	-4.4
186	C_4H_8S	-8.2	-20.2	6.9	-12.3	-6.4	-4.0
187	$(CH_3)_3C$-Cl	-43.5	-21.4	5.6	-12.0	-6.8	-3.8
188	C_4H_9Cl(n-butyl chloride)	-37.0	-17.8	9.1	-8.6	-4.7	-1.9
189	C_4H_8NH	-0.8	-13.8	8.3	-7.7	-4.8	-2.3
190	CH_3-$CH(OCH_3)_2$-NO_2	-39.1	2.5	13.4	-8.1	-2.9	-3.5
191	$(C_2H_5)_2O$(diethyl ether)	-60.3	-12.3	9.5	-6.2	-4.4	-2.0
192	CH_3-$CH(OCH_3)_2$	-93.1	-11.6	7.0	-9.7	-6.5	-4.6
193	$(CH_3)_3C$-SH	-26.2	-22.4	6.3	-12.1	-7.0	-4.0

194	CH_3-CH_2-S-S-CH_2-CH_3	-17.9	-19.2	12.1	-11.6	-6.8	-4.1
195	$(CH_3)_3$C-NH_2	-28.9	-17.0	5.7	-8.7	-6.2	-3.1
196	$Si(CH_3)_4$	-55.7	-32.2	3.7	-17.2	-13.5	-9.6
197	C_5H_6S	20.0	-11.8	8.9	-11.0	-2.2	-1.3
198	C_5H_7N	24.6	-5.1	11.3	-5.8	-0.7	0.4
199	$C_5H_{10}O$	-53.4	-20.6	5.4	-13.3	-7.7	-4.8
200	CH_3-CH_3CO-C_2-CH_3	-61.6	-12.4	8.4	-8.0	-3.6	-1.5
201	CH_3-C(=O)-O-$CH(CH_3)_2$	-115.1	-11.4	6.0	-11.4	-5.5	-3.9
202	$C_5H_{10}S$	-15.2	-26.3	6.4	-15.6	-8.2	-4.8
203	cyc-$C_5H_{10}NH$	-11.3	-21.0	6.5	-12.1	-7.6	-4.2
204	$(CH_3)_3$C-O-CH_3	-67.8	-21.7	6.7	-12.7	-8.1	-4.8
205	$C_6H_4F_2$	-73.9	0.2	10.6	-7.7	0.6	0.8
206	$C_6H_4F_2$	-73.3	0.2	10.6	-7.8	0.5	0.7
207	C_6H_5F	-27.7	-4.1	9.2	-7.6	0.0	0.7
208	$(CH_3)_2$CH-O-$CH(CH_3)_2$	-76.3	-25.4	8.3	-14.1	-8.9	-4.8
209	PF_5	-381.1	-5.2	-5.0	-15.6	-6.5	-7.1
210	SF_6	-291.7	3.6	9.4	-14.9	-5.2	-7.3
211	P_4	14.1	-7.1	6.0	-14.8	-7.6	-9.1
212	SO_3	-94.6	10.8	0.5	-10.6	-2.5	-7.0
213	SCl_2	-4.2	2.1	6.7	-3.5	-2.2	-2.9
214	$POCl_3$	-133.8	-4.4	1.8	-12.0	-3.2	-4.1
215	PCl_5	-86.1	-10.2	9.0	-14.5	-3.7	-3.5
216	Cl_2O_2S	-84.8	5.1	4.7	-12.5	-4.2	-7.4
217	PCl_3	-69.0	-0.6	6.5	-5.4	-2.0	-2.2
218	Cl_2S_2	-4.0	11.1	17.4	1.1	2.9	1.6
219	$SiCl_2$	-40.3	-5.3	-0.3	-6.9	-3.3	-3.3
220	CF_3Cl	-169.5	3.6	4.4	-6.2	-1.0	-1.9
221	C_2F_6	-321.3	6.2	4.1	-10.3	-1.8	-2.9
222	CF_3	-111.3	11.7	10.2	1.4	3.2	2.1
223	C_6H_5	81.2	-2.8	12.2	-4.1	1.5	2.5
224	AlF	-63.5	2.9	-1.2	-0.5	1.7	1.3
225	Al_2Cl_6	-309.7	-36.1	0.2	-26.1	-4.7	-1.9
226	$ClNO_2$	2.9	32.9	19.3	5.4	6.6	1.4
227	NaF	-69.4	0.5	-1.2	-3.6	-5.7	-1.8
228	$ClFO_3$	-5.1	20.9	13.1	-10.0	-2.9	-9.0
229	N_2O_3	19.8	46.9	21.1	5.1	6.2	-1.7
230	N_2O_4	2.2	57.7	28.6	7.7	10.6	0.9
231	C_6F_6	-228.4	17.0	16.4	-8.6	2.8	0.7
232	C_6F_5Cl	-194.1	10.4	13.9	-12.5	1.3	-0.4
233	$COCl_2$	-52.4	8.2	6.7	-2.6	2.4	0.6
234	LiNa	43.4	-1.4	0.6	-1.8	-1.5	-0.7
235	BeF_2	-190.3	8.4	1.4	3.1	-3.6	4.8
236	ClCN	32.9	10.8	5.4	0.3	4.1	2.1
237	$MgCl_2$	-93.8	-7.9	4.1	-5.0	0.1	0.6
238	K_2	12.6	0.4	-2.0	1.2	0.8	0.1
239	KBr	90.5	3.6	-5.3	2.3	-2.5	-2.5
240	KCl	101.0	4.2	-1.6	3.4	1.6	1.5
241	KF	117.6	-1.5	-1.0	2.9	1.6	2.4
242	GeH_4	270.5	0.6	-14.7	-4.8	-3.9	-4.9
243	AsH	64.6	-2.8	-3.4	-2.6	-0.1	-0.3

244	AsH_2	131.1	-5.8	-8.3	-5.8	-2.2	-2.5
245	AsH_3	206.0	-2.6	-8.3	-3.4	0.4	0.0
246	SeH	74.3	-1.5	-3.4	-1.5	-0.3	-0.3
247	SeH_2	153.2	-1.1	-6.1	-1.6	-0.6	-0.6
248	HBr	86.5	-1.6	-4.5	-1.9	-4.9	-4.6
249	GaCl	109.9	-0.4	-3.2	0.3	-1.8	-1.8
250	GeO	155.2	-11.8	-4.1	-0.6	-6.9	-4.2
251	As_2	91.3	-8.4	-2.1	0.0	-1.5	0.0
252	BrCl	51.5	-4.9	-7.7	-1.6	-5.0	-4.3
253	BrF	58.9	-10.3	-9.1	-3.0	-5.8	-4.3
254	BrO	55.3	-14.8	-10.9	-4.4	-5.1	-3.3
255	Br_2	45.4	-6.2	-9.3	-3.1	-9.2	-8.4
256	BBr	103.5	0.7	-0.2	2.9	-1.6	-1.1
257	NaBr	86.2	3.6	-4.2	2.5	-2.7	-2.8
258	CH_3Br	358.2	1.2	-8.3	-0.6	-1.2	-1.7
259	GeS_2	191.7	-2.4	-9.6	3.1	-2.6	-1.5
260	KrF_2	21.9	-25.2	-20.0	-5.3	-4.0	-0.5
261	CF_3Br	-155.0	4.9	5.7	-5.7	0.8	-0.4
262	CCl_3Br	-10.0	-7.8	3.7	-12.9	-1.5	-2.1
263	C_2H_3Br	18.9	-0.3	8.1	-1.1	2.2	2.3
264	C_2H_5Br	-14.8	-6.8	8.5	-2.8	0.4	1.5
265	C_3H_7Br	-23.8	-13.9	7.4	-7.4	-2.7	-0.8
266	C_6H_5Br	25.2	-11.4	6.5	-12.5	-0.8	0.0
267	C_6H_13Br	-35.4	-28.0	11.0	-14.2	-6.3	-2.0
268	C_3H_6Br	-17.1	-14.4	8.5	-9.8	-0.6	1.1
269	CHF_2Br	-101.6	4.6	8.1	-2.6	1.9	1.1
270	$COBr_2$	-27.1	9.7	8.4	-2.3	5.5	3.3
271	$C_5H_8Br_2$	-13.1	-27.4	6.0	-19.6	-4.8	-2.1

[a] Taken from J. Chem. Phys. 106, 1063 (1997) for molecules 1 - 148,
from J. Chem. Phys. 112, 7374 (2000) for molecules 149 - 223,
and from J. Chem. Phys. 123, 124107 (2005) for molecules 224 - 271.
See also references therein.

Table 2: Perfomance of tested density functionals for ionization potentials in the test set G3/05. Given are the experimental values as well as the deviations (exp. - theo.) in kcal mol^{-1}.

			deviation				
	molecule	Exp.[a]	B-LYP	TPSS	B3-LYP	B2-PLYP	mPW2-PLYP
1	He	567.1	-5.1	-3.6	-6.0	-2.1	-1.8
2	Ne	497.1	-3.0	1.8	-1.4	0.1	0.5
3	Ar	363.4	3.7	1.7	1.5	1.3	1.1
4	BF_3	358.8	3.5	1.8	12.6	3.1	0.2
5	BCl_3	267.5	0.7	-4.0	-9.9	5.5	3.8
6	B_2F_4	278.3	21.7	19.5	15.4	13.3	12.2
7	CO_2	317.6	8.6	7.9	4.1	-0.6	-0.8
8	CF_2	263.4	6.3	7.2	4.3	4.4	4.0
9	COS	257.6	4.8	2.0	2.8	1.3	1.3
10	CS_2	232.2	6.4	2.4	3.9	-0.2	0.1
11	CH_2	239.8	3.1	-0.6	1.9	2.8	2.7
12	CH_3	227.0	0.2	-2.2	-0.5	0.6	0.6
13	C_2H_5	187.1	1.8	-0.4	-0.4	0.4	-0.1
14	C_3H_4	222.9	10.9	9.4	8.5	5.2	5.2
15	$H_2C{=}C{=}CH_2$	223.5	10.2	8.8	7.7	4.3	4.3
16	*sec*-C_3H_7	169.9	7.0	2.9	4.0	3.0	2.6
17	C_6H_6	213.2	8.6	7.2	6.5	3.0	3.1
18	$C_6H_5CH_3$	203.6[b]	10.4	8.3	7.6	3.5	3.6
19	CH_3F	287.6	11.6	9.9	6.3	3.4	2.6
20	CH_2S	216.2	6.3	4.2	4.5	2.8	2.9
21	$HSCH_2$	173.8	2.2	-1.3	-1.1	0.1	-0.6
22	CH_3SH	217.7	8.3	6.2	5.6	3.9	3.8
23	CH_3Cl	258.8	9.9	7.1	5.6	2.9	2.6
24	C_2H_5OH	241.5	16.1	15.7	11.1	7.6	6.9
25	CH_3CHO	235.9	9.0	9.0	5.9	2.2	2.2
26	CH_3OF	261.5	13.1	12.8	7.2	3.4	2.8
27	C_2H_4S	208.7	7.3	4.9	5.1	3.2	3.1
28	NCCN	308.3	16.3	14.5	10.5	2.5	2.3
29	C_4H_4O	203.6	5.7	5.6	4.6	1.8	2.0
30	C_4H_4N	189.3	5.7	5.4	4.8	2.1	2.4
31	C_6H_5OH	196.2[b]	9.6	8.1	6.8	3.0	3.0
32	$C_6H_5NH_2$	178.0[b]	8.8	7.5	6.4	2.3	2.4
33	B_2H_4	223.6	7.6	7.3	6.6	5.7	5.7
34	NH	311.1	-0.6	-3.4	-2.0	-1.0	-1.2
35	NH_2	256.9	-2.8	3.3	-1.6	-0.3	-0.1
36	N_2H_2	221.1	6.4	5.8	3.9	4.1	3.7
37	N_2H_3	175.4	-1.9	-2.8	-4.1	-2.0	-2.7
38	HOF	293.1	8.1	9.8	4.2	2.8	2.2
39	SiH_2	211.0	5.6	5.7	4.5	4.6	4.6
40	SiH_3	187.6	2.3	-2.0	0.9	1.8	1.6
41	Si_2H_2	189.1	9.0	4.7	6.4	4.3	4.2
42	Si_2H_5	175.2	2.7	-2.5	0.5	0.5	0.3
43	Si_2H_6	224.6	7.4	3.8	3.8	2.0	1.7

44	H	314.9	2.5	1.0	1.8	1.9	2.2
45	Li	123.3	-4.2	-3.6	-4.7	-3.0	-3.4
46	Be	214.9	7.9	5.9	6.7	7.2	6.7
47	B	190.4	-8.4	-11.8	-9.1	-5.8	-6.2
48	C	259.6	-3.5	-4.6	-4.7	-2.2	-2.5
49	N	335.3	0.8	-2.9	-0.9	0.5	0.4
50	O	313.8	-11.9	-9.8	-9.3	-3.9	-3.9
51	F	401.7	-6.8	-0.1	-4.8	-1.2	-1.0
52	Na	118.5	-5.0	-0.9	-4.8	-2.5	-3.1
53	Mg	176.3	0.4	2.2	0.1	1.4	0.8
54	Al	138.0	2.6	-3.9	1.0	1.9	1.9
55	Si	188.0	4.9	-1.3	2.8	3.1	3.0
56	P	241.9	7.1	-0.3	4.4	3.6	3.5
57	S	239.0	-1.0	-2.1	-1.9	0.9	0.6
58	Cl	299.1	1.5	0.6	0.1	1.5	1.3
59	CH_4	291.0	9.4	7.1	5.7	2.6	2.2
60	NH_3	234.7	1.6	4.9	2.2	1.8	2.1
61	OH	300.0	-3.3	2.6	-2.1	-0.2	0.0
62	OH_2	291.0	2.4	6.0	2.9	2.0	2.5
63	FH	369.8	0.9	4.7	1.9	1.4	1.9
64	SiH_4	253.7	7.9	4.1	4.2	2.8	2.3
65	PH	234.1	4.2	-2.3	1.7	1.6	1.4
66	PH_2	226.4	1.9	-3.8	-0.4	0.1	-0.2
67	PH_3	227.6	4.0	3.8	3.2	3.2	3.3
68	SH	237.0	1.5	1.0	0.2	1.2	1.0
69	$SH(^2B_1)$	241.4	4.3	2.7	2.7	2.1	2.0
70	HCl	294.0	4.7	2.8	2.9	2.3	2.2
71	C_2H_2	262.9	7.4	7.8	6.8	4.0	4.3
72	C_2H_4	242.3	7.8	7.9	7.1	4.6	4.9
73	CO	323.1	2.6	3.4	-1.4	-0.1	-1.0
74	N_2 ($^2\Sigma$ cation)	359.2	5.9	4.9	-3.2	1.3	-1.0
75	O_2	278.3	-4.8	-4.5	-8.7	-3.2	-4.6
76	P_2	242.8	1.4	-2.0	-2.8	-3.2	-3.8
77	S_2	215.9	2.4	-2.2	-2.0	0.0	-1.0
78	Cl_2	265.2	10.7	7.7	5.5	4.1	3.2
79	ClF	291.9	8.3	6.9	4.0	3.2	2.6
80	CS	261.3	3.2	2.6	0.5	-0.9	-1.0
81	SH_2 ($^2A_1$)	294.7	7.7	5.3	5.4	12.4	11.6
82	N_2 ($^2\Pi$ cation)	385.1	6.1	6.2	3.7	0.4	0.4
83	CN ($^3\Sigma^+$ cation)	313.6	-12.6	-11.4	-11.3	-14.6	-13.7
84	CHO	187.7	-4.4	-6.0	-5.7	-1.9	-2.5
85	H_2COH	174.2	0.7	-0.9	-1.1	0.4	0.0
86	CH_3O	247.4	10.1	8.7	5.7	3.5	2.9
87	CH_3OH	250.2	12.7	11.7	8.3	4.2	3.8
88	Si_2H_4	189.1	6.6	5.1	6.5	5.2	5.4
89	K	100.1	2.0	2.0	-2.0	-0.5	-0.9
90	Ca	140.9	3.0	3.0	1.1	1.4	1.0
91	Ga	138.3	-0.3	-0.3	1.2	2.0	1.8
92	Ge	182.2	-0.8	-0.8	2.0	2.0	1.8
93	As	225.7	-3.5	-3.5	0.4	-0.9	-1.1

94	Se	224.9	1.6	1.6	0.2	2.8	2.4
95	Br	272.4	-0.7	-0.7	-0.9	1.6	1.2
96	Kr	322.8	-1.9	-1.9	-1.5	-1.9	-2.2
97	AsH	222.3	-2.1	-2.1	0.9	0.2	-0.1
98	AsH_2	217.8	-1.2	-1.2	0.8	0.7	0.3
99	SeH	227.0	2.8	2.8	2.2	3.0	2.8
100	SeH_2	228.0	2.5	2.5	2.9	2.2	2.1
101	HBr	268.9	-1.1	-1.1	-0.4	-2.6	-2.7
102	Br_2	242.6	3.9	3.9	2.2	-2.5	-3.2
103	HOBr	245.3	7.4	7.4	4.7	4.0	3.2
104	BrF	271.7	3.5	3.5	1.1	-1.0	-1.6

[a] Except where noted otherwise taken from J. Chem. Phys. 110, 4703 (1999) for molecules 1 - 88, and from J. Chem. Phys. 123, 124107 (2005) for molecules 89 - 104

[b] Taken from J. Chem. Phys. 112, 7374 (2000)

See also references in a) and b).

Table 3: Perfomance of tested density functionals for electron affinities in the test set G3/05. Given are the experimental values as well as the deviations (exp. - theo.) in kcal mol^{-1}.

			deviation				
	molecule	Exp.	B-LYP	TPSS	B3-LYP	B2-PLYP	mPW2-PLYP
1	C	29.1	-2.0	-4.1	-0.6	1.4	1.7
2	O	33.7	-8.1	-0.5	-2.7	-0.6	0.4
3	F	78.4	-6.2	0.0	-0.6	-0.8	0.5
4	Si	32.0	3.8	-0.9	2.9	3.0	3.1
5	P	16.0	-4.5	-3.5	-3.9	-1.0	-1.0
6	S	47.9	-1.1	-0.3	-0.8	0.7	0.8
7	Cl	83.4	1.0	0.8	0.8	0.8	0.9
8	CH	28.6	-2.1	-3.5	-1.0	0.4	0.6
9	CH_2	15.0	-4.0	2.2	-1.1	0.2	0.6
10	CH_3	1.8	-0.8	2.7	1.8	1.8	2.3
11	NH	8.7	-4.8	2.2	-0.6	0.5	1.2
12	NH_2	17.7	-1.2	3.3	2.3	0.8	1.8
13	OH	42.2	-2.7	2.6	2.0	0.1	1.4
14	SiH	29.5	3.0	-1.3	2.1	2.6	2.5
15	SiH_2	26.0	1.6	-2.3	0.7	1.6	1.5
16	SiH_3	32.5	1.6	2.5	1.8	2.5	2.5
17	PH	23.8	0.0	1.0	0.3	1.5	1.6
18	PH_2	29.3	2.3	2.4	2.3	2.2	2.3
19	SH	54.4	2.7	2.5	2.7	2.4	2.5
20	O_2	10.1	-2.3	0.5	-0.1	1.1	1.3
21	NO	0.4	-6.0	-5.0	-5.5	-2.1	-2.5
22	CN	89.0	2.3	3.3	-2.1	-1.8	-2.7
23	PO	25.1	-0.1	-2.7	-1.6	0.3	-0.1
24	S_2	38.3	3.6	2.5	2.0	2.5	2.2
25	Cl_2	55.1	-7.6	-5.9	-7.6	-4.1	-4.4
26	Li	14.2	8.5	1.9	4.5	5.0	4.8
27	B	6.4	-3.7	-3.9	-2.5	0.4	0.6
28	Na	12.8	10.7	-0.1	1.5	2.4	2.0
29	Al	10.2	1.7	-1.4	1.4	2.6	2.6
30	CC ($^3\Pi_u$)	75.5	-3.5	-2.9	-2.4	-5.3	-4.7
31	C_2O	53.1	6.9	9.2	5.9	5.2	5.1
32	CF_2	4.1	-5.9	-5.8	-4.7	-2.2	-2.3
33	NCO	83.2	5.8	6.4	4.2	0.7	0.9
34	NO_2	52.4	4.7	6.9	3.1	3.2	2.6
35	O_3	48.5	-6.4	-5.0	-10.6	-2.7	-4.8
36	OF	52.4	0.1	4.6	1.6	0.7	1.2
37	SO_2	25.5	-2.1	-3.0	-4.1	-1.0	-1.8
38	S_2O	43.3	0.5	-1.3	-3.0	0.3	-0.9
39	C_2H	68.5	0.1	1.9	0.2	-0.3	-0.2
40	C_2H_3	14.4	-0.5	1.4	0.6	-0.2	0.1
41	$H_2C{=}C{=}C$	41.4	0.7	-1.5	-1.3	-1.0	-1.4
42	$H_2C{=}C{=}CH$	20.6	-0.1	0.9	1.0	-0.1	0.3
43	CH_2CHCH_2	10.9	-0.9	1.2	0.6	-0.9	-0.3

44	HCO	7.2	-1.3	0.6	0.2	1.7	1.9
45	HCF	12.5	-5.0	-5.4	-3.9	-2.0	-2.0
46	CH_3O	36.2	0.0	2.8	2.7	0.7	1.7
47	CH_3S	43.1	3.2	2.8	3.1	2.3	2.4
48	CH_2S	10.7	-1.8	-3.5	-3.3	-1.5	-2.1
49	CH_2CN	35.6	1.7	3.0	1.7	0.1	0.4
50	CH_2NC	24.4	-0.9	0.6	0.7	-1.1	-0.4
51	CHCO	54.2	1.1	2.0	2.1	-0.7	-0.2
52	CH_2CHO	42.1	0.3	-4.8	1.5	-0.4	0.1
53	CH_3CO	9.8	-1.9	0.8	1.1	1.7	1.9
54	CH_3CH_2O	38.0	-3.1	0.2	0.2	-2.0	-1.1
55	CH_3CH_2S	44.0	2.0	1.6	2.2	1.1	1.2
56	LiH	7.8	6.6	-0.6	0.2	1.1	1.0
57	HNO	7.8	-6.4	-5.4	-5.8	-3.3	-3.6
58	HO_2	24.8	1.4	5.3	3.5	1.7	2.3
59	K	11.5	3.3	0.2	2.5	2.8	2.5
60	Ge	28.4	0.5	-3.5	-0.4	-0.3	-0.4
61	Br	77.6	-1.2	-2.5	-2.1	-2.2	-2.2
62	BrO	54.4	3.8	4.4	2.4	-0.6	-0.3
63	SeH	51.0	-0.6	-1.5	-1.0	-1.3	-1.3

[a] Taken from J. Chem. Phys. 110, 4703 (1999) for molecules 1 - 58, and from J. Chem. Phys. 123, 124107 (2005) for molecules 59 - 63 See also references therein.

Table 4: Perfomance of tested density functionals for proton affinities in the test set G3/05. Given are the experimental values as well as the deviations (exp. - theo.) in kcal mol^{-1}.

	molecule	Exp.[a]	deviation				
			B-LYP	TPSS	B3-LYP	B2-PLYP	mPW2-PLYP
1	NH_3	202.5	2.0	-1.9	0.3	0.5	0.5
2	OH_2	165.1	3.2	-0.2	-1.6	1.9	1.9
3	C_2H_3	152.3	-1.5	-5.3	-2.6	0.0	-1.2
4	SiH_4	154.0	-0.5	-1.8	0.5	1.3	1.8
5	PH_3	157.1	2.2	-2.3	0.6	0.4	0.4
6	SH_2	168.8	0.2	-2.3	0.1	0.7	1.0
7	ClH	132.9	-0.3	-2.3	0.1	0.6	1.0
8	H_2	100.8	2.1	-2.0	1.7	1.8	2.2
9	Br^-	322.6	-1.7	-4.3	-1.3	-1.2	-0.9
10	CH_3Br	157.3	-2.4	-4.2	-1.4	-1.6	-1.0

[a] Taken from J. Chem. Phys. 110, 4703 (1999) for molecules 1 - 8, and from J. Chem. Phys. 123, 124107 (2005) for molecules 9 - 10 See also references therein.

Table 5: Perfomance of tested density functionals for hydrogen bridged complex binding energies in the test set G3/05. Given are the experimental values as well as the deviations (exp. - theo.) in kcal mol^{-1}.

	complex	Exp.[a]	deviation				
			B-LYP	TPSS	B3-LYP	B2-PLYP	mPW2-PLYP
1	$(H_2O)_2$	-3.6	-1.2	-0.9	-1.0	-0.8	-0.3
2	$(CH_3OH)_2$	-3.5	-0.4	-0.1	0.0	0.5	1.0
3	$(CH_3COCH_3)_2$	-3.2	-2.0	-1.6	-1.6	-1.0	-0.5
4	$(HCl)_2$	-1.2	-0.8	-0.3	-0.6	-0.3	0.0
5	$(CH3COOH)_2$	-14.9	-1.9	-0.1	-0.8	-0.2	0.7
6	$(HF)_2$	-3.0	0.0	0.2	0.2	0.3	0.8

[a] Taken from J. Chem. Phys. 123, 124107 (2005)
See also references therein.