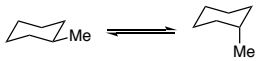
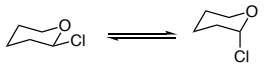
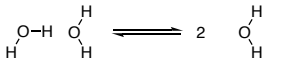
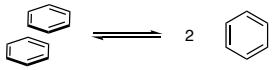
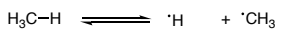
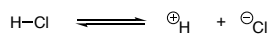
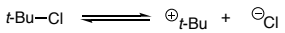
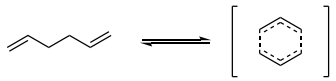
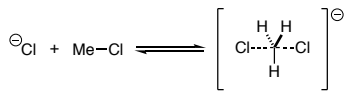
Comparing Computational Methods

all values in kcal/mol, in the gas phase, based on electronic energies only

Basis Set Abbreviations:
dz = cc-pVDZ
augtz = aug-cc-pVTZ
augqz = aug-cc-pVQZ

		B3LYP	B3LYP	B3LYP-D3	wB97X-D	M06-2X	Hartree–Fock			MP2	MP3	MP4	DLPNO-CCSD(T)	Exp.
		6-31G(d)	augtz	augtz	augtz	augtz	dz	augtz	augqz	augtz	augtz	augtz	augtz	
Methyl A-Value		2.23	2.32	1.74	1.58	1.73	2.49	2.53	2.54	1.69	1.85	1.65	1.72	1.74
Anomeric Effect		3.71	3.31	3.97	3.31	3.29	3.10	2.18	2.07	2.90	2.57	3.02	2.86	*2.86*
Water Dimer		7.11	4.54	5.16	5.00	5.17	5.87	3.81	3.80	5.17	5.16	5.19	5.09	5.02
Benzene Dimer		–1.52	–2.50	3.24	3.35	2.53	–2.81	–3.60	–3.76	5.83	2.72	4.66	3.66	2.82
Methane BDE		112.8	110.9	111.2	111.7	111.8	85.1	85.2	85.2	110.6	110.7	111.8	111.2	*111.2*
Cl- Proton Affinity		341.0	334.9	335.3	336.7	334.1	343.3	335.0	335.5	335.2	337.5	337.4	337.7	*337.7*
tBuCl Ionization		160.4	149.4	153.3	154.6	160.3	152.5	142.7	143.1	168.0	162.5	166.0	164.6	*164.6*
Cope Barrier		34.4	35.9	33.4	37.3	35.1	58.4	58.8	59.0	25.5	39.0	31.3	35.5	35.8
S_N2 Barrier		6.8	8.5	8.3	13.4	13.4	12.7	14.7	15.0	14.4	15.2	12.7	12.9	13.6
Formal Scaling		N^4	N^4	N^4	N^4	N^4	N^4	N^4	N^4	N^5	N^6	N^7		
Relative Time (benzene dimer)		1	74	78	104	91	0.7	73	771	230	5552	20401	2063	