Supplementary Material for Organic & Biomolecular Chemistry

Supplementary data

Table S1. Absolute Energies ($-E_{tot}$), Energies Corrected to 0K ($-E_0$), and Enthalpies at 298K ($-E_{298}$) for Stationary Points in the Reaction of 3-Chlorobut-2-yl Radical (**1**) [in Hartree].

	1a	**5**	**6**	**7**	**1b**	**8**
$-E_{tot}$						
B3LYP/aug-cc-pVDZ	617.435437	617.431247	617.4269386	617.427866	617.433885	617.429474
B3LYP/aug-cc-PVTZ//SP[a]	617.495067	617.491120	617.4866088	617.487425	617.493326	617.489663
G3(MP2)B3[a]	616.8360684	616.8247654	616.8305974	616.8313175	616.8349003	616.8231974
BHLYP/aug-cc-pVDZ	617.3139921	617.3037294	617.3069024	617.3080119	617.3125022	617.3018708
BHLYP/aug-cc-PVTZ//SP[b]	617.369951	617.359681	617.362956	617.363965	617.368281	617.359681
$-E_0$						
B3LYP/aug-cc-pVDZ	617.327919	617.323528	617.320051	617.321048	617.326165	617.321836
G3(MP2)B3	616.7285504	616.7170464	617.7237098	616.7244995	616.7271803	616.7155594
BHLYP/aug-cc-pVDZ	617.202645	617.192211	617.196167	617.197413	617.200948	617.190357
$-H_{298}$						
B3LYP/aug-cc-pVDZ	617.319799	617.315795	617.312702	617.313617	617.318068	617.313980
G3(MP2)B3	616.7204304	616.7093134	616.7163608	616.7170685	616.7190833	616.7077034
BHLYP/aug-cc-pVDZ	617.194737	617.184641	617.188971	617.190099	617.193079	617.182695

[a] B3LYP/aug-cc-pVDZ geometries. [b] BHLYP/aug-cc-pVDZ geometries.