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Addition/Correction

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Correction to Accuracy of Calculations of Heats of Reduction/Hydrogenation: Application to Some Small Ring Systems

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Page 10369. As a result of an error in recording the CBS-QB3 enthalpy of H_2, the QB3 column of Table 7 in this paper was in error. The revised enthalpies are recorded in the new Table 7 and show that, for hydrogenolysis of C−C bonds, this level of theory is nearly as satisfactory as the other methods that have much higher computational requirements.

Table 7. Calculated Enthalpies of Hydrogenolysis, kcal/mol

reaction	QB3	G4	APNO	W1BD	obs
ethane + H_2 → 2 methane	−14.7	−15.4	−15.5	−15.3	−15.6 ± 0.2
propane + H_2 → ethane + methane	−12.0	−12.7	−12.8	−12.8	−12.8 ± 0.2
butane + H_2 → 2 ethane	−9.2	−9.7	−10.0	−10.2	−10.0 ± 0.2
2,3-dimethylbutane + H_2 → 2 propane	−6.9	−7.2	−7.9		−7.4 ± 0.3
hexamethylethane + H_2 → 2 isobutane	−8.4	−8.5	−9.4		−10.2 ± 0.4
cyclopropane + H_2 → propane	−37.4	−37.5	−38.4	−38.3	−37.7 ± 0.1
cyclobutane + H_2 → butane	−35.9	−36.4	−37.0	−36.9	−36.6 ± 0.3
cyclopentane + H_2 → n-pentane	−16.4	−17.0	−15.5		−16.8 ± 0.3
cyclohexane + H_2 → n-hexane	−10.0	−10.7	−11.1		−10.4 ± 0.3
bicyclo[1.1.0]butane + H_2 → cyclobutane	−46.0	−46.2	−44.1	−47.6	−45.3 ± 0.4
bicyclo[2.1.0]pentane + H_2 → cyclopentane	−54.3	−54.3	−57.5		na
bicyclo[2.2.0]hexane + H_2 → cyclohexane	−59.4	−59.6	−60.6		na
[1.1.1]propellane + H_2→ bc[1.1.1]pentane	−38.0	−37.6	−37.9	−39.1	na
[2.2.2]propellane + H_2→ bc[2.2.2]octane	−88.3	−88.0	−91.1		na
biphenyl + H_2 → 2 benzene	−0.9	−1.4			−4.0 ± 0.6
bibenzyl + H_2 → 2 toluene	−7.9	−8.2			−10.0 ± 0.4
rms error	1.5	1.1	0.7	1.0	

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