

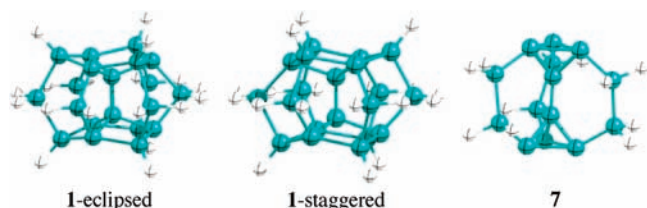
Additions and Corrections

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Shorter Still: Compressing C–C Single Bonds.

Page 4059. Structure **1** in our article (with a bond distance of 1.350 Å) is the *eclipsed* version of the *staggered* isomer examined by Huntley et al. (structure 15a in ref 5). The latter (*staggered*) structure, inadvertently excluded from the set of molecules we considered, has a particularly short C–C bond (reported to be 1.32 Å). Reference 6 in our paper is, therefore, a comparison of the two different isomers. Our results for the staggered isomer of **1**, which we present in this addition, are in good agreement with ref 5.



The computed (B3LYP and MP2) bond distances of the compressed central C–C bonds of the two isomers of **1** and structure **7** from our paper are listed in Table A.1. Remarkably, the C–C bonds in **1-staggered** and **7** are identical (to within 0.001 Å) at the B3LYP computational level for all

three basis sets. At the MP2 level, the compressed C–C bond in **7** is shorter than that in **1-staggered** by at least ~0.013 Å. The MP2/cc-pVTZ model chemistry returns, for instance, a bond distance of 1.302 Å for the **1-staggered** and 1.286 Å for **7**.

Table A.1. Computed Bond Lengths (in Å) Obtained at the B3LYP and MP2(full) Levels for the Short C–C Bonds in Structures **1-eclipsed**, **1-staggered**, and **7**

	6-311G**	6-311++G**	cc-pVTZ
B3LYP			
(1) C ₂₀ H ₁₈ (eclipsed)	1.350	1.351	1.345
(1) C ₂₀ H ₁₈ (staggered)	1.313	1.313	1.310
(7) C ₁₄ H ₁₂	1.313	1.314	1.310
MP2(full)			
(1) C ₂₀ H ₁₈ (eclipsed)	1.346	1.347	1.338
(1) C ₂₀ H ₁₈ (staggered)	1.311	1.311	1.302
(7) C ₁₄ H ₁₂	1.297	1.298	1.286

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