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Additions and Corrections

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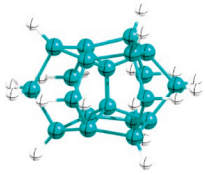
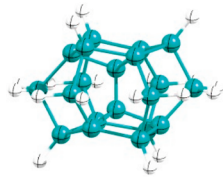
Gerardo Martínez-Guajardo, Kelling J. Donald,* Bernard K. Wittmaack, Miguel Angel Vazquez, and Gabriel Merino*

Shorter Still: Compressing C−C Single Bonds.

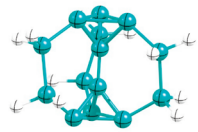
Page 4059. Structure **1** in our article (with a bond distance of 1.350 Å) is the *eclipsed* version of the *staggered* isomer examined by Huntley et al. (structure 15a in ref 5). The latter (*staggered*) structure, inadvertently excluded from the set of molecules we considered, has a particularly short 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.



1-eclipsed



1-staggered



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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

We thank Georgios Markopoulos for bringing the omission of the staggered isomer to our attention and for supplying the coordinates for that structure as well.

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