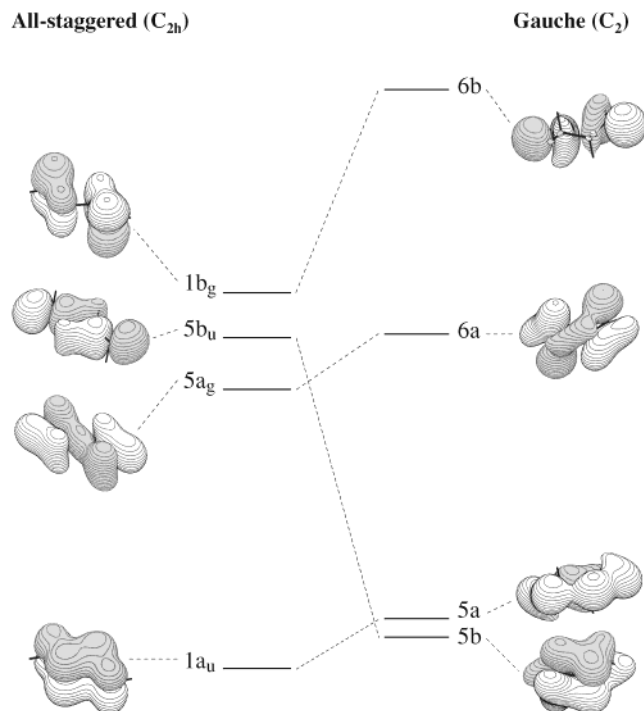


Probing Molecular Conformations with Electron Momentum Spectroscopy: The Case of *n*-Butane [*J. Am. Chem. Soc.* **2001**, *123*, 4049–4061]. M. S. Deleuze,* W. N. Pang, A. Salam, and R. C. Shang

Page 4054, Figure 3. The correlations displayed between the lowest four outer-valence orbitals of *n*-butane in its all-staggered (C_{2h}) and gauche (C_2) forms are erroneous. Orbitals $1a_u$, $5a_g$, $5b_u$, and $1b_g$ correctly relate to orbitals 5a, 6a, 5b, and 6b, respectively. These correlations are shown in the figure below which should replace that given in the paper.



The strongest energy variations induced by torsion of the carbon backbone arise therefore with the $5b_u$ and $1b_g$ orbitals of the all-staggered form (-1.30 and $+0.91$ eV, respectively). Correspondingly, opposite variations in the topology of the related momentum densities are seen (Figures 5b and 5c) upon conversion of these orbitals into the 5b and 6a ones. The $1a_u$ orbital gets destabilized by 0.28 eV upon conversion into the 5a orbital. Both the $1a_u$ and 5a electron densities display a p-type profile in momentum space.

Page 4057, right column, lines 13–33. The discussion of the electron momentum profiles provided in Figure 4c pertains to orbitals $4a_g$ and 4a, rather than orbitals $3a_g$ and 3a. Thus, in this paragraph, the $3a_g$ and 3a labels should be systematically replaced by the $4a_g$ and 4a labels, respectively.

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