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Ab Initio Torsion-Wag Surface for the Ethyl Radical[1] RAM S. BHATTA, DAVID S. PERRY, Department of Chemistry, The University of Akron — The torsion-wag potential of the ethyl radical has a 6-fold barrier to internal rotation and the minimum energy path involves deviations of the CH_2 wag angle of 6 to 11 degrees on either side of planar. Partially optimized 2-dimensional surfaces were calculated at the B3LYP, MP2, and CCSD(T) levels with 6-311++G(d,p) and 6-311++G(3df, 2p) basis sets and they were fit to a function containing a polynomial in the wag angle τ and trigonometric functions of the torsional angle α. Comparison is made with the corresponding surfaces for CH_3NH_2 and $CH_3OH_2^+$. Unlike $CH_3CH_2^\bullet$, both have a substantial barrier to inversion. The dominant torsion-wag coupling term in all three cases has the form $\tau\cos 3\alpha$.

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