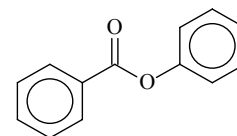


918 **C₁₃H₁₀O₂**ED, *ab initio* and
DFT calculations**Benzoic acid phenyl ester**

Phenyl benzoate

C₁

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(1'')=O(2)	1.208(4)	O(2)=C-O(1)	124.2(13)
C(1'')-O(1) ^{b)}	1.362(6)	O(2)=C-C	127.3(12)
O(1)-C(1) ^{b)}	1.405(6)	C-O(1)-C	121.4(22)
C(1'')-C(1')	1.478(10)	tilt[C(1)] ^{c)}	3.0(15)
C-C (ring) ^{d)}	1.396(1)	tilt[(C1')] ^{c)}	4.8(17)
		τ_1 ^{f)}	64(⁺²⁶ ₋₁₂)
		τ_2 ^{g)}	0 ^{h)}

It was assumed that the C(1')C(1'')O(2)O(1)C(1) moiety is planar and C(1'')=O(2) is *syn* to O(1)-C(1). The C-C-C angles of the rings were assumed at the values from RHF/6-31G** calculations. The phenyl torsions were treated as large-amplitude motions using the potential function $V(\tau_1, \tau_2) = V_{12}(1 - \cos 2\tau_1)/2 + V_{14}(1 - \cos 4\tau_1)/2 + V_{22}(1 - \cos 2\tau_2)/2$ with the potential constants (in kcal mol⁻¹) $V_{12} = -1.3$ (assumed), $V_{14} = -0.5(9)$ and $V_{22} = 3.5(15)$.

The nozzle temperature was *ca.* 409 K.

^{a)} Three times the estimated standard errors.

^{b)} Differences in the C-C bond lengths of the rings and between the C(1'')-O(1) and O(1)-C(1) bond lengths were constrained to the values from RHF/6-31G** calculations.

^{c)} Defined as tilt [C(1)] = {[O(1)-C(1)-C(6)] - [O(1)-C(1)-C(2)]}/2.

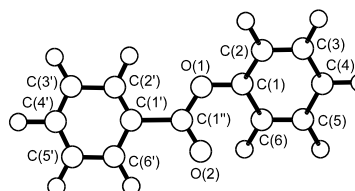
^{d)} Average value.

^{e)} Defined as tilt [C(1')] = {[C(1'')-C(1')-C(2')] - [C(1'')-C(1')-C(6')]} / 2.

^{f)} Torsional angle C(1'')-O(1)-C(1)-C(6).

^{g)} Torsional angle O(1)-C(1'')-C(1')-C(2').

^{h)} Assumed.



Tsuji, T., Takeuchi, H., Egawa, T., Konaka, S.: J. Am. Chem. Soc. **123** (2001) 6381.