

Values of the torsion angle τ_1 ($^\circ$) in the benzyl alcohol gauche-conformer obtained using various quantum chemical methods and basis sets.

	MP2	PBE0	B3LYP
6-31G(d)	37,0	31,3	34,2
cc-pVDZ	32,1	27,2	29,4
cc-pVTZ	39,8	32,5	38,0
6-31+G(d)	59,3	42,4	53,0
6-311++G(d,p)	58,0	41,2	49,6
aug-cc-pVDZ	60,4	40,1	52,0
aug-cc-pVTZ		39,5	54,3

Experimental data: ca. 54° (²⁸ M. Traetterberg, H. Ostensen and S. Raghild, *Acta Chem. Scand. A*, 1980, **34**, 449.)