ELECTRONIC SUPPORTING INFORMATION

Potential energy barrier for proton transfer in compressed benzoic acid

Dominik Kurzydłowski[1*]

[1] *Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University in Warsaw, 01-038 Warsaw, Poland;*

Table S 1 Comparison of the calculated and experimental geometry of BA crystals. Bond distances and cell vector lengths are given in Å, volume in Å^3. Percentage difference between experimental data and r^{2}SCAN calculations is given in parenthesis. Theoretical values are reported for the A tautomeric form.

p = 0 GPa	**Exp (ref. 1)**	**Theory**	**p = 0.3 GPa**	**Exp (ref. 2)**	**Theory**
a	5.401	5.483 (+1.5)	a	5.315	5.405 (+1.7)
b	5.004	5.037 (+0.7)	b	4.987	4.979 (–0.2)
c	21.879	21.945 (+0.3)	c	21.630	21.631 (0.0)
V	584.8	602.92 (+3.1)	V	566.3	575.4 (+1.6)
$R_{O\cdots O}$	2.623	2.564 (–2.2)			
R_{O-H}	1.019	1.021 (+0.2)			
R_{C-O}	1.320	1.316 (–0.3)			
$R_{C=O}$	1.233	1.242 (+0.7)			
p = 2.2 GPa	**Exp (ref. 3)**	**Theory**	**p = 15 GPa**	**Exp (ref. 4)**	**Theory**
a	5.077	5.094 (+0.3)	a	4.768	4.608 (–3.4)
b	4.893	4.852 (–0.8)	b	4.692	4.597 (–2.0)
c	21.1	20.998 (–0.5)	c	19.983	19.431 (–2.8)
V	515.0	509.4 (–1.1)	V	428.2	396.6 (–7.4)

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