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LIF C_6H_6O

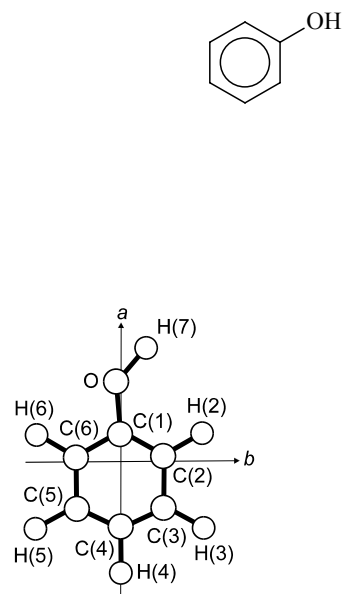
Phenol

 C_s

State	S_0	S_1
Energy [eV]	0.00	4.507
$r_0[C(1)-C(2)]$ [Å]	1.383(75)	1.442(25)
$r_0[C(2)-C(3)]$ [Å]	1.402(19)	1.453(9)
$r_0[C(3)-C(4)]$ [Å]	1.399(17)	1.422(5)
$r_0[C(1)-O]$ [Å]	1.369(33)	1.326(17)
$r_0(O-H)$ [Å]	0.962(26)	0.992(52)
$r_0(C-H)$ [Å]	1.079(6)	1.071(3)
$\theta_0[C(1)-O-H]$ [deg]	107.8(42)	107.5(31)
$\theta_0[C(2)-C(1)-O]$ [deg]	123.3(44)	119.79(145)
$\theta_0[C(1)-C(2)-C(3)]$ [deg]	120.2(12)	118.28(36)
$\theta_0[C(2)-C(3)-C(4)]$ [deg]	119.7(16)	117.99(38)
$\theta_0[C(1)-C(2)-H(2)]$ [deg]	120.1(13)	123.73(71)

Values for pseudo- r_s , $r_m^{(1)}$ and $r_m^{(2)}$ parameters are also given in the original paper.

High resolution laser-induced fluorescence experiments were carried out on phenol and 11 of its deuterated derivatives. The molecular beam machine used consisted of three differentially pumped vacuum chambers that are linearly connected by skimmers. Fluorescence was excited by a ring dye laser coupled to an external folded ring cavity for second harmonic generation. The fluorescence was collected and monitored as the dye laser was scanned. Rotational analyses of the spectra produced molecular constants from which information on molecular geometries in the ground and excited states was derived. It should be noted that there is a small increase in the C–C bond lengths in the excited state but no observable tendency towards a quinonoid structure.



Ratzer, C., Küpper, J., Spangenberg, D., Schmitt, M.: Chem. Phys. **283** (2002) 153.

Replaces [II/25D \(3, 2246\)](#), LIF