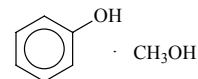
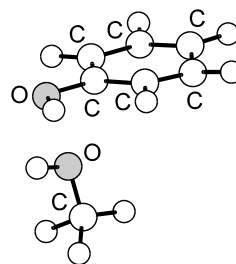


808
LIF $C_7H_{10}O_2$ **Phenol – methanol (1/1)**
(weakly bound complex) C_s
(effective symmetry class)
(large-amplitude motion)

State	S_0	S_1
Energy [eV]	0.00	4.455
$r_0(H...O)$ [Å]	2.909	



Mixtures of phenol and methanol alcohol diluted with a large excess of helium were expanded through a supersonic nozzle into a molecular beam machine. The latter consisted of three differentially pumped vacuum chambers that were 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 of the complex in the ground and excited states was derived. The structures of the phenol and methanol moieties were assumed to be the same as in the separated molecules. Four possible values are given for the hydrogen bond length in the S_0 state; the preferred value is given in the table. Due to the internal rotation of the methyl group in the methanol moiety, the spectrum of the 0-0 band is split into A and E subbands. The barrier to internal rotation is found to be 170 cm^{-1} in the S_0 state and 150 cm^{-1} in the S_1 state.



Schmitt, M., Küpper, J., Spangenberg, D., Westphal, A.: Chem. Phys. **254** (2000) 349.