STRUCTURE DETERMINATION OF RESORCINOL ROTAMERS BY HIGH RESOLUTION UV SPECTROSCOPY

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Several rotationally resolved $S_1 \leftarrow S_0$ electronic origins of deuterated resorcinol rotamers cooled in a molecular beam were recorded. An automated assignment of the observed spectra was performed using a genetic algorithm approach with an asymmetric rotor Hamiltonian. The structure of resorcinol A and resorcinol B was derived from the rotational constants of several deuterated species for both electronic states. The lifetimes of different resorcinol isotopomers in the S_1 state are also reported. Like in phenol these lifetimes mainly depend on the position of deuteration. A nearly perfect additivity of the zero-point energies after successive deuterations in resorcinol rotamers was discovered and subsequently used in the full assignment of the previously reported low resolution spectra of deuterated resorcinol A[a]. The analogous spectrum was also predicted for the resorcinol B rotamer.

[a]M. Gerhards, C. Unterberg, and S. Schumm, *J. Chem. Phys.*, 1999, **111**, 7966–7975.