

ROTATIONAL SPECTROSCOPIC STUDY OF MICROSOLVATED CLUSTERS OF 1- AND 2-NITRONAPHTHALENE

SHEFALI SAXENA, M. EUGENIA SANZ, *Department of Chemistry, King's College London, London, United Kingdom.*

Polycyclic aromatic hydrocarbons containing the nitro group (nitro-PAHs) are pollutants found in the atmosphere as the result of direct release from exhaust or of radical reactions on naphthalene involving hydroxyl radical (daytime), nitrate radical (night time) and nitrogen dioxide. Among them, the nitro-PAHs 1-nitronaphthalene (1NN) and 2-nitronaphthalene (2NN) are relevant as they are highly toxic and major environmental contaminants in urban areas. We have investigated 1NN and 2NN and their complexes with water by broadband rotational spectroscopy and determined their structures. Water primarily interacts with the $-\text{NO}_2$ group forming an $\text{O}-\text{H} \cdots \text{O}$ hydrogen bond. Experimental observations are compared with predictions by theoretical methods to evaluate the performance of the latter. Our results contribute to understanding the microsolvation processes of atmospheric pollutants in the gas phase.