

## INTERMOLECULAR INTERACTIONS OF TOLUNITRILES ( $\text{CH}_3\text{C}_6\text{H}_4\text{CN}$ )

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Aromatic rings have taken a lot of attention of the scientific community during the last years due, in part, to their detection in the interstellar medium (ISM). Benzonitrile, cyanonaphthalene, and cyanoindene are examples of the first and the few individual aromatic species detected, all of them in TMC-1 molecular cloud.<sup>a</sup> Their presence is certain but their formation under the ISM conditions remains unclear. In the present work, we have analyzed the intermolecular interactions in small gas-phase clusters of a family of aromatic species: tolunitriles, also known as methylbenzonitriles ( $\text{CH}_3\text{C}_6\text{H}_4\text{CN}$ ). Our aim is to understand the very first steps of the reactivity of small aromatic molecules by unveiling the principal binding sites for polar molecules, where the reactions might be initiated. Likewise, we have analyzed the influence of the relative position of the ring substituents (methyl and cyano groups). The rotational spectra of the complexes of *ortho*, *meta* and *para* tolunitriles were studied using a broadband chirped pulsed Fourier transform microwave spectrometer with an operating frequency range of 2-8GHz. We have employed water as polar probing molecule. A comparative analysis of the hydration sites of the three tolunitriles together with that of benzonitrile<sup>b</sup> has unveiled the influence of the methyl group in the water anchoring site.

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<sup>a</sup>McGuire B. *et al.*, *Science*, 359, 202-205, **2018**; McGuire B. *et al.*, *Science*, 371, 1265-1269, **2021**; Sita M.L. *et al.*, *ApJL*, 938, L12, **2022**

<sup>b</sup>Melandri, S. *et al.*, *J.Chem.Phys.* 111, 3874 **1999**