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Supporting information for article:

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SUPPLEMENTARY MATERIAL

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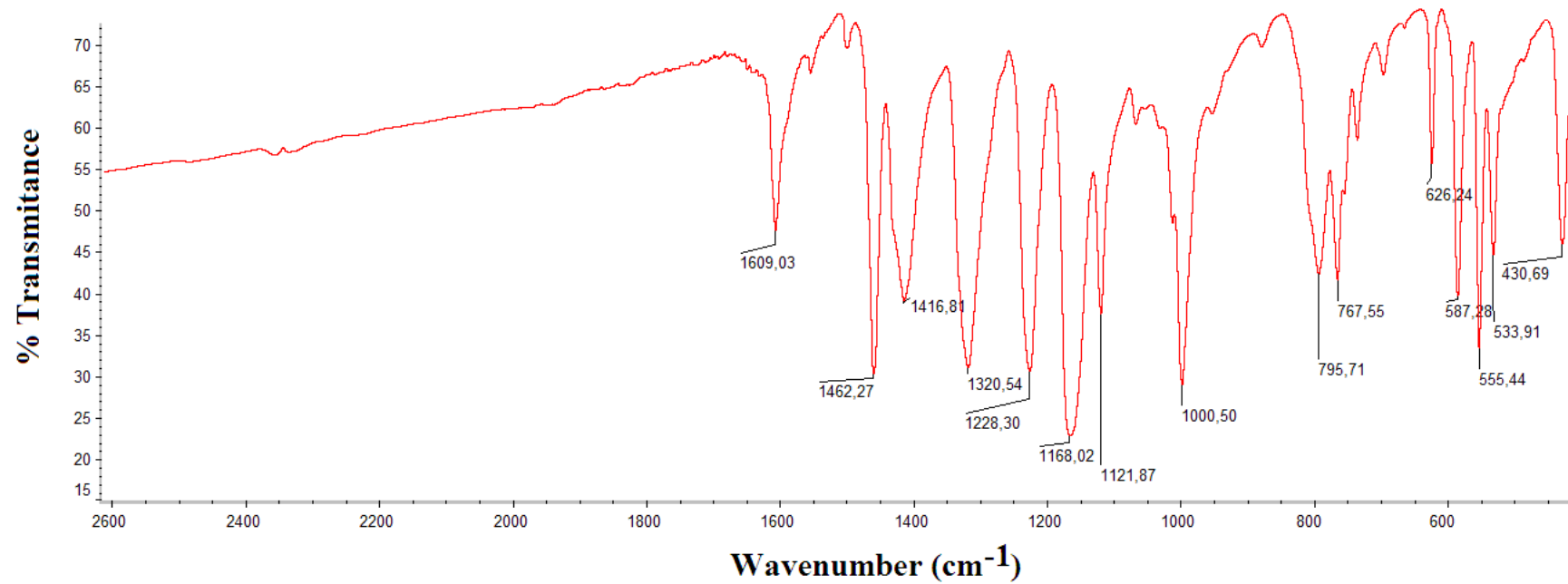


Figure S1. IR spectrum of (I).

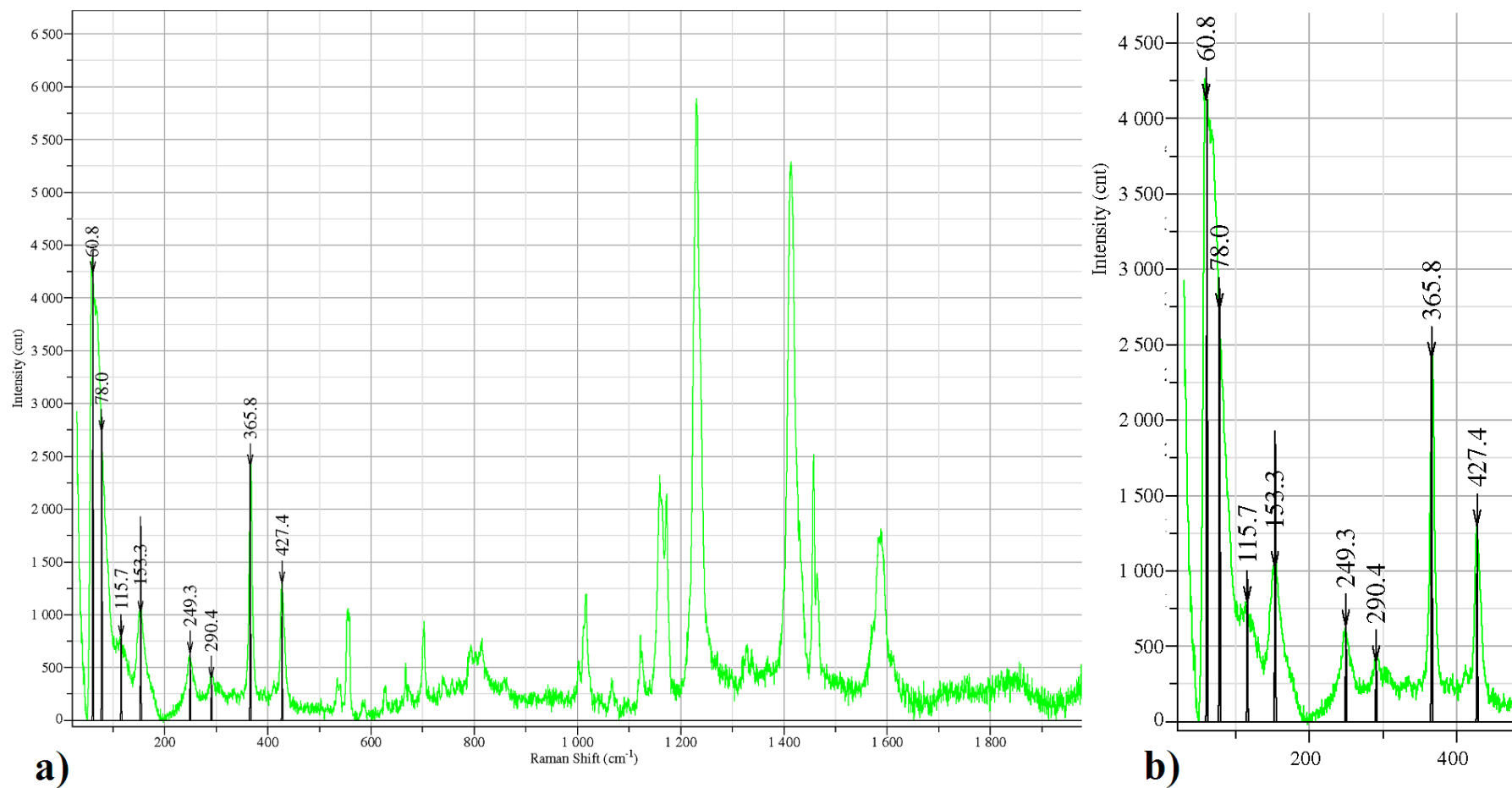


Figure S2. a) Full Raman spectrum of (I).. b) An enlarged view of the low frequency region.

AIM: brief theoretical background.

The quantum theory of "atoms-in-molecules" (AIM; Bader, 1990) provides an approach to the analysis of the electron density distribution of a molecule, an experimental observable, based on its topology. Each point in space is characterized by a charge density $\rho(r)$, and further quantities such as: the gradient of $\rho(r)$, the Laplacian functions of $\rho(r)$, and the matrix of the second derivatives of $\rho(r)$ (Hessian matrix). The magnitudes of the density at the critical points gives a measure of bond order and interaction strength and can be used to assess, at least in comparative terms, the real significance of some non-covalent interactions, usually evaluated only on geometrical grounds (Bader, 2009). Some critical viewpoints concerning the application of this method when *absolute* AIM values are analyzed have recently been raised (Spackman, 2015); nevertheless, its use for *relative comparisons* is still growing (Wang *et. al.*, 2016).

References

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