

Electronic Supplementary Data

Remarks on the modelling of molecular binding forces in the Glue-DNT interaction

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Fig. S1. Low resolution absorption spectra of p-nitrotoluene in absolute ethanol (0.05 mole%) without glue curve 1, and with glue curve 2.

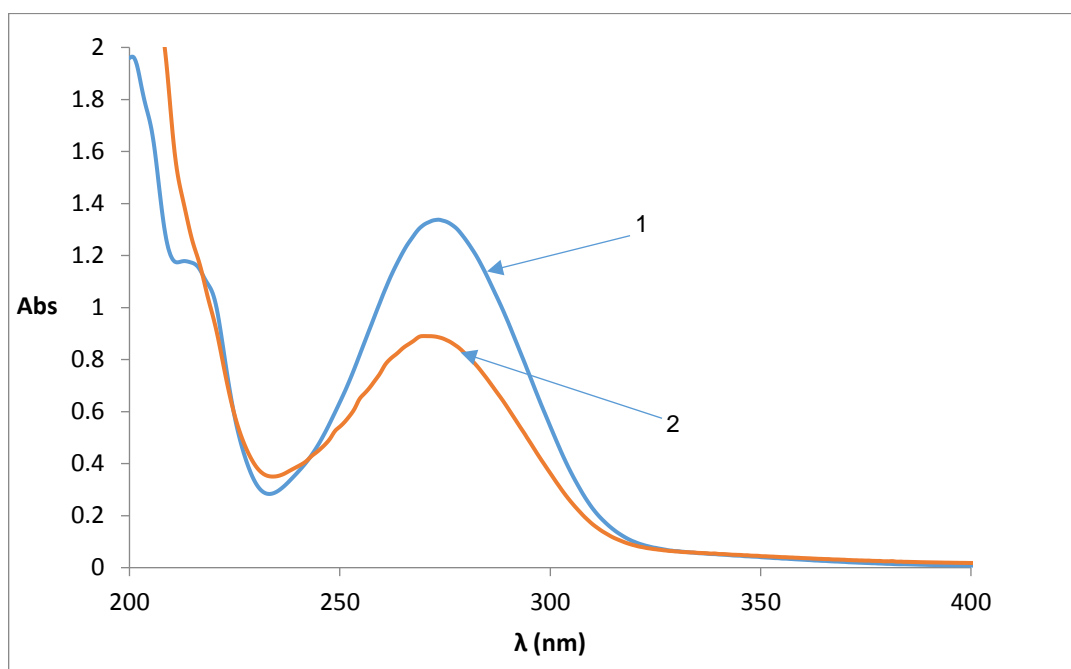


Figure S2. Low resolution absorption spectra of toluene in absolute ethanol (0.05 mole %), without glue curve 1, with glue curve 2.

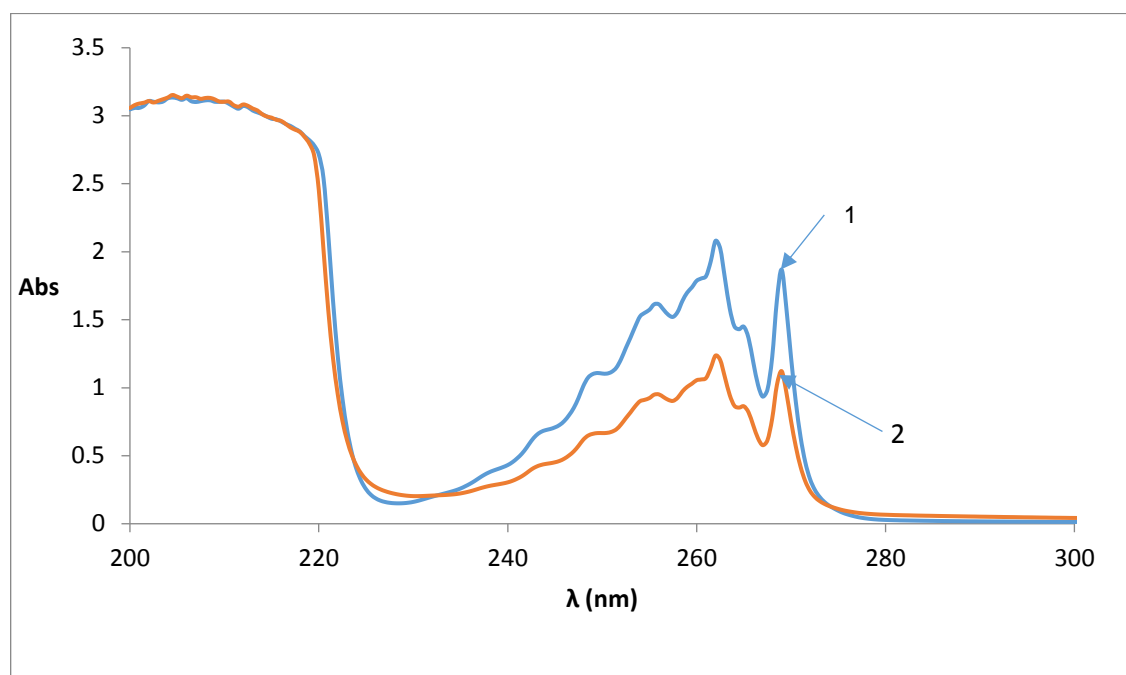


Figure S3. Low resolution absorption spectra of 2,4-DNT in absolute ethanol (0.05 mole%) without glue curve 1, and with glue curve 2.

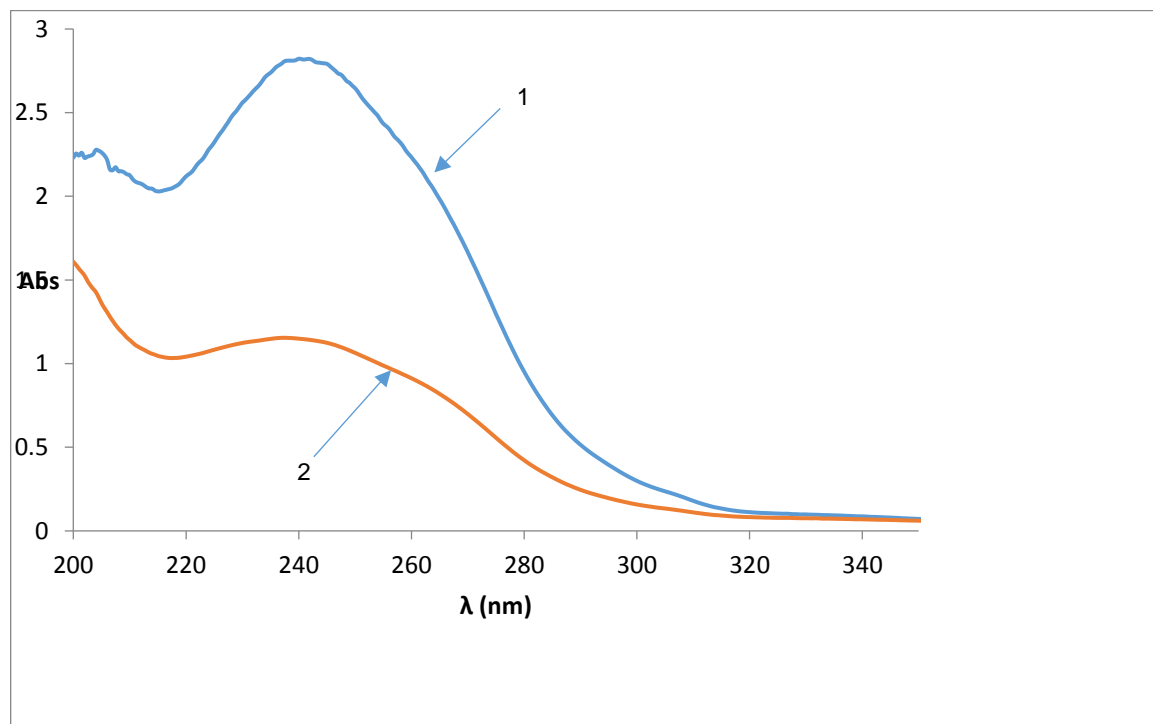


Figure S4. Plot of relative infrared and nmr shifts for 2,4-DNT in glue matrix. Insert shows the function corresponding to lower coordinates (ppm vs pph).

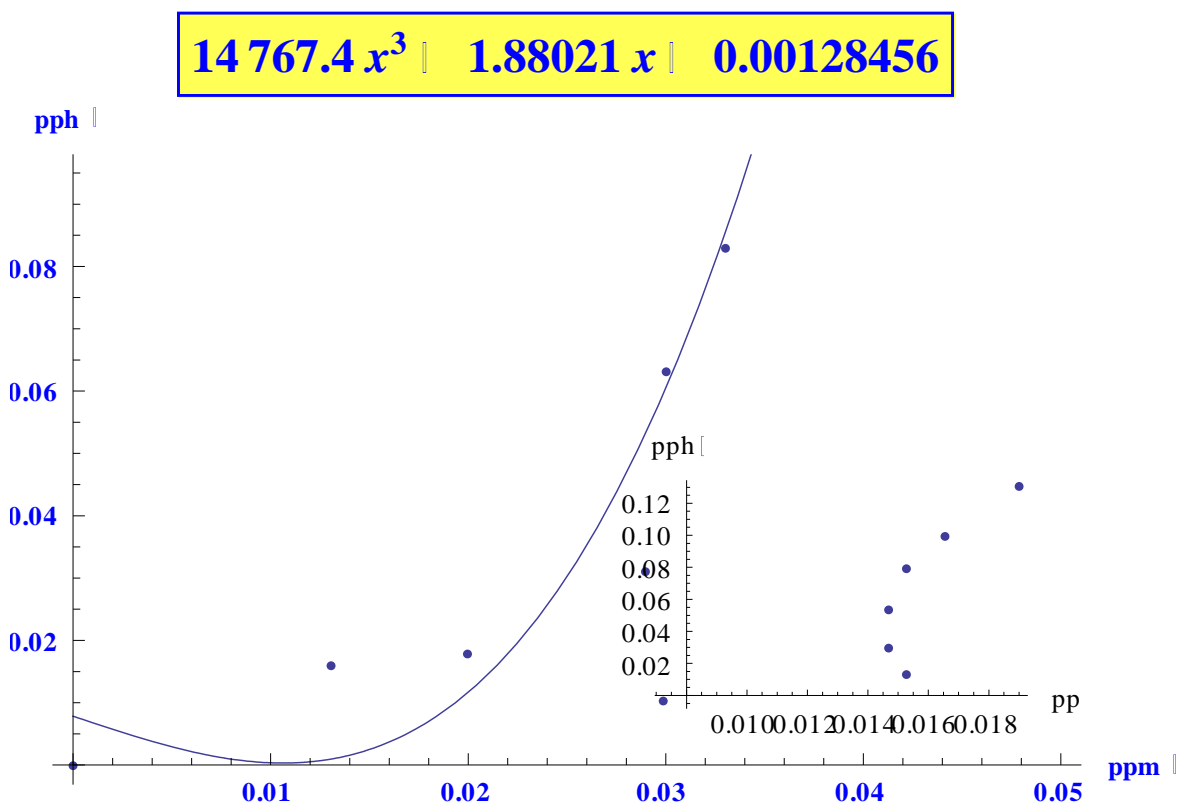


Fig. S4. Plot of relative infrared and nmr shifts for 2,4-DNT in glue matrix. Insert shows the function corresponding to lower coordinates (ppm vs pph). Regarding the boxed function the sign preceding the constant term is (+) and the sign preceding the x term is (-).

