Supplementary Material (ESI) for CrystEngComm

Solvates and polymorphic phase transformations of 2-chloro-4-nitrobenzoic acid

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Electronic Supplementary Information

(10 Pages)

Contents

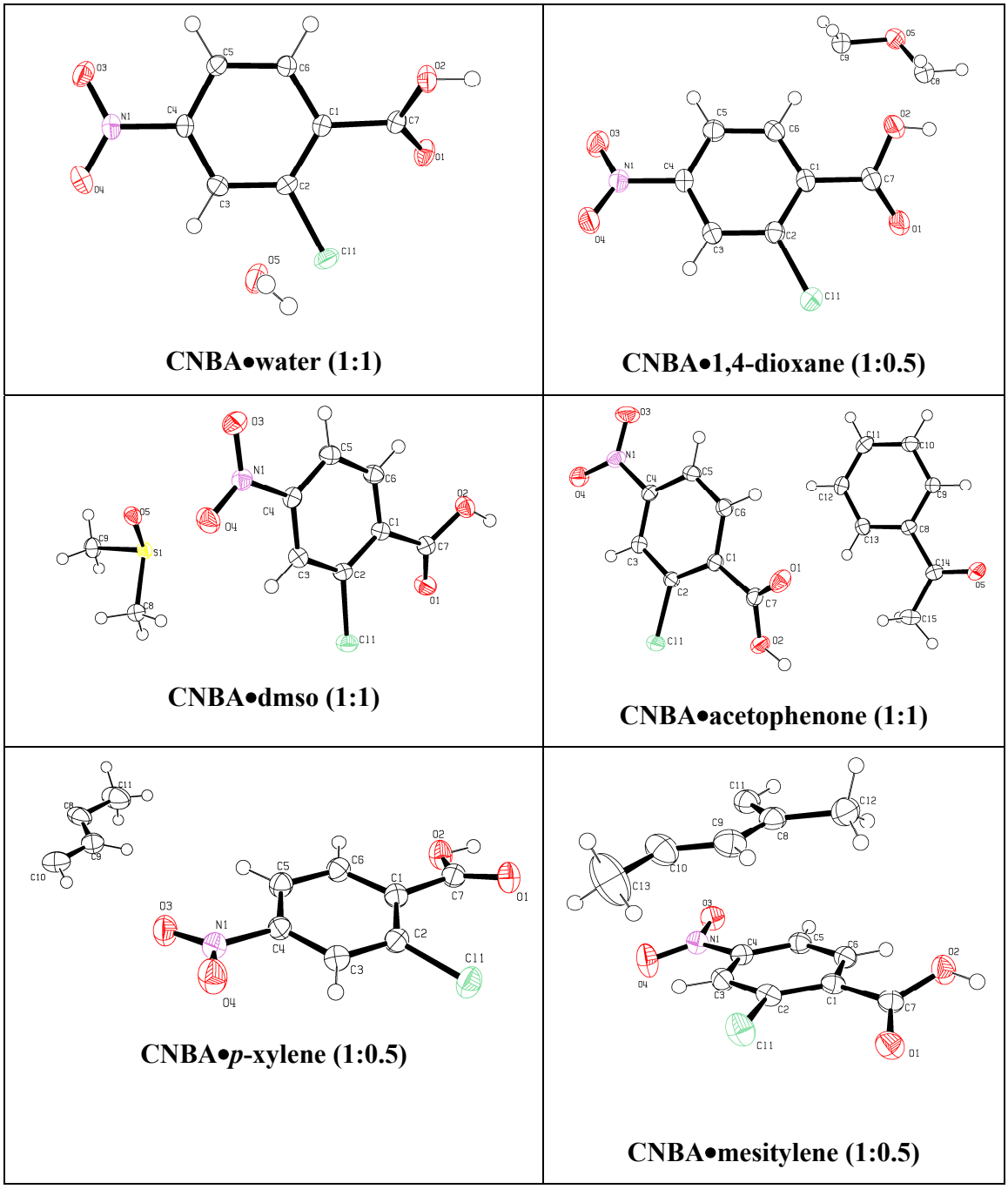

Figure S1. ORTEP diagrams for the hydrate and solvates of CNBA showing the atom numbering. Thermal ellipsoids were drawn at 50 % probability.

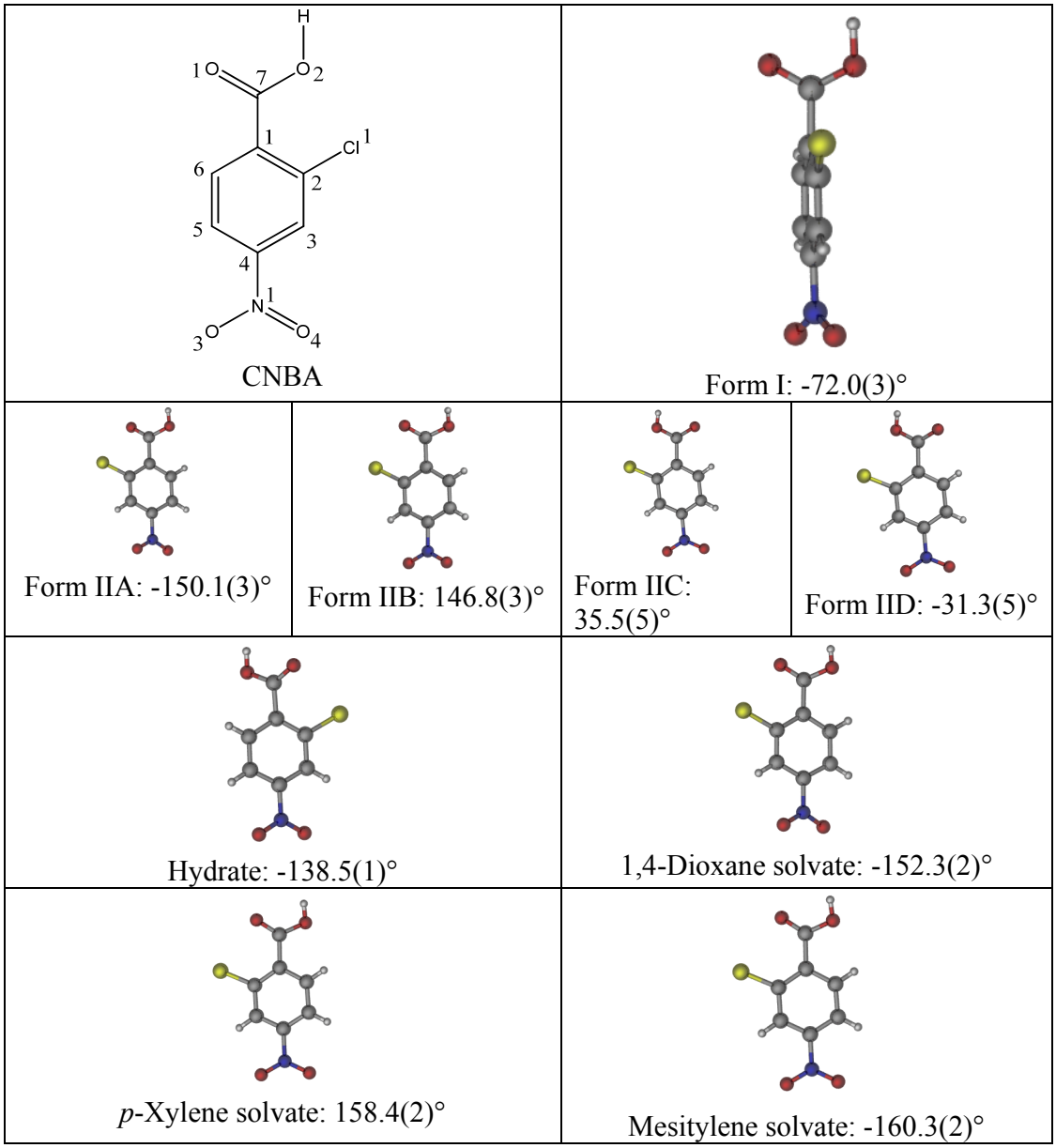

Figure S2. Summary of the different conformations and their corresponding torsion angles (C2–C1–C7–O2) of CNBA as observed in its two polymorphs and hydrate/solvates. All 4 symmetry independent molecules of Form II were shown. Notice that conformations of the CNBA in hydrate/solvates are similar and they are also similar to two of the conformations found in Form II (IIA and IIB) (all these conformations have the OH group *anti* to the Cl atom), but they are significantly different from others in Form II and Form I.

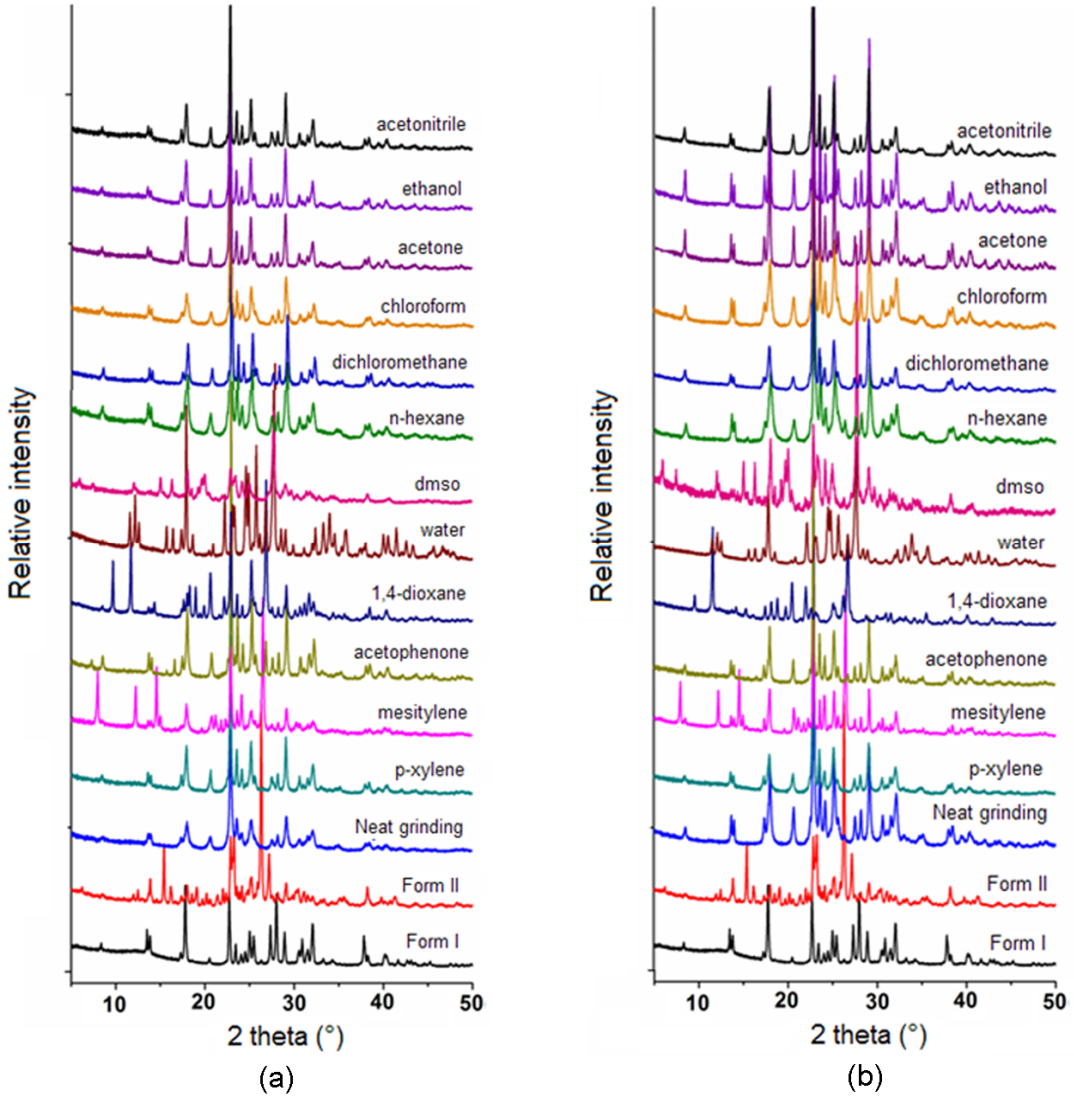

Figure S3. Comparison of the PXRD patterns of the samples obtained in the grinding experiments on Form I (a) and Form II (b) of the CNBA. The solvent used for the SDG is indicated on the right of both the figures.

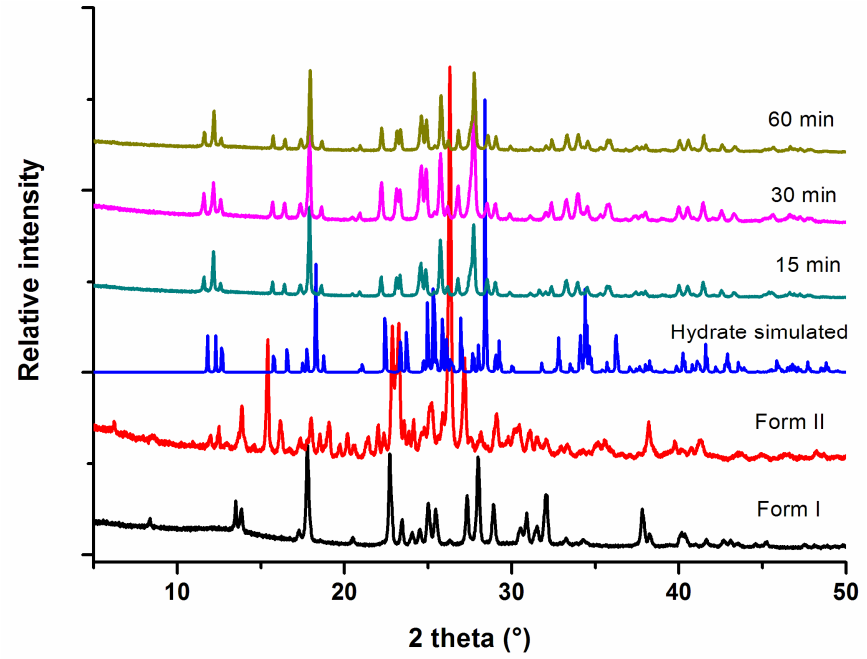

Figure S4. Comparison of the PXRD patterns of the samples obtained from grinding Form I with 2 drops of water. Notice that all the experiments resulted in the hydrate.

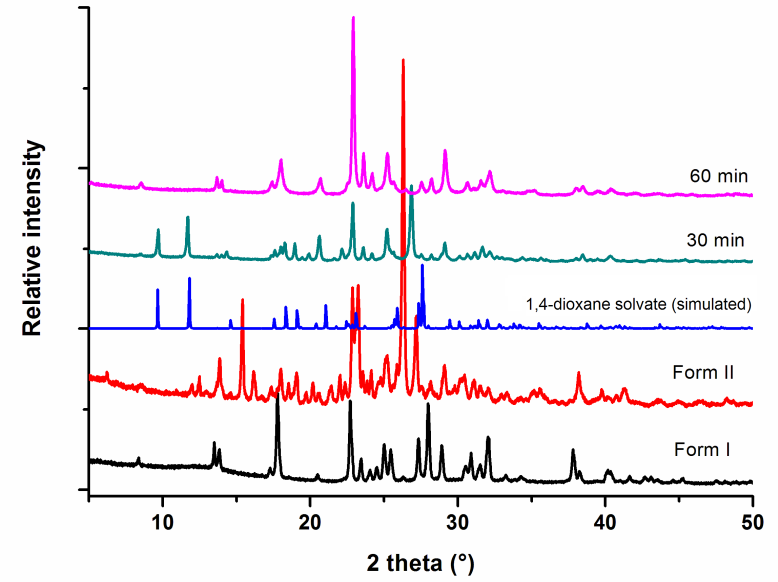

Figure S5. Comparison of the PXRD patterns of the samples obtained from the grinding experiments on Form I with 2 drops of 1,4-dioxane. Notice that 30-min grinding resulted in the solvate and 60-min grinding resulted in the phase transformation from solvate to Form I.

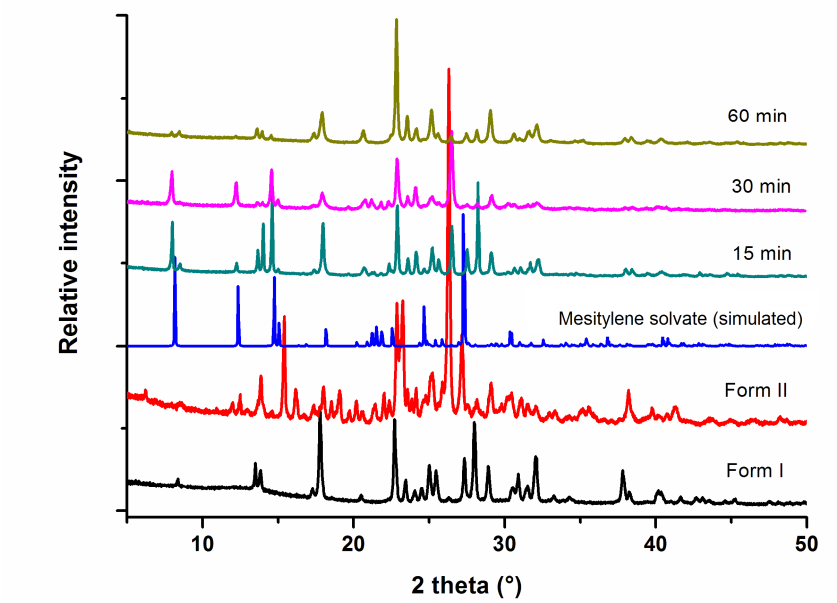

Figure S6. Comparison of the PXRD patterns of the samples obtained from the grinding experiments on Form I with 2 drops of mesitylene. Notice that 15- and 30-min grinding resulted in the solvate and 60-min grinding resulted in the phase transformation from solvate to Form I.

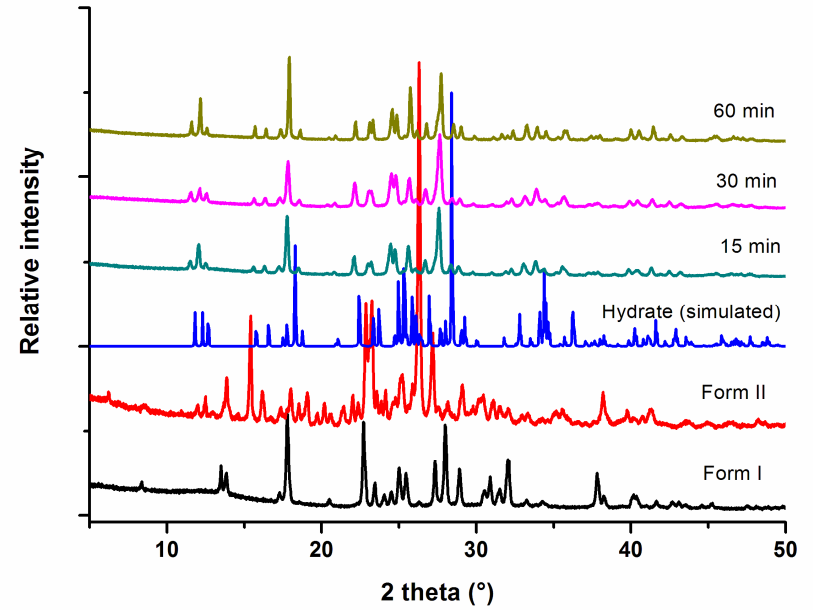

Figure S7. Comparison of the PXRD patterns of the samples obtained from grinding Form II with 2 drops of water. Notice that all the experiments resulted in the hydrate.

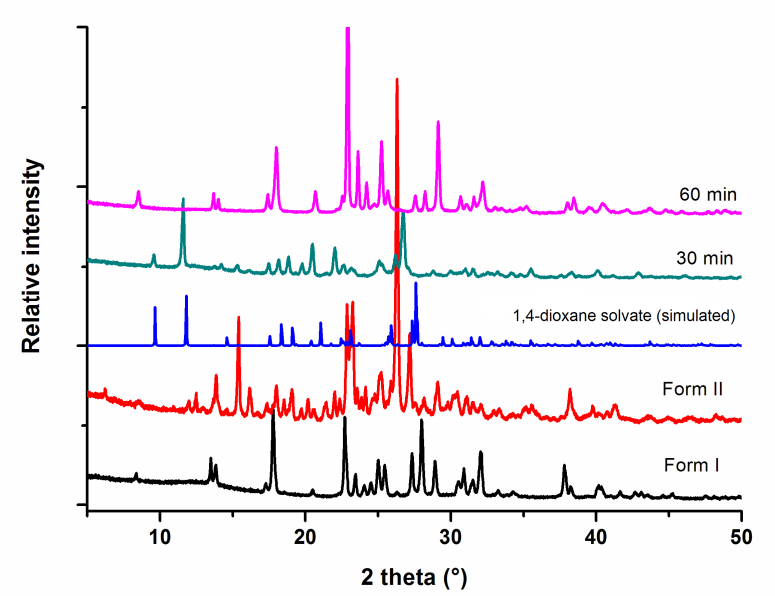

Figure S8. Comparison of the PXRD patterns of the samples obtained from the grinding experiments on Form II with 2 drops of 1,4-dioxane. Notice that 30-min grinding resulted in the solvate and 60-min grinding resulted in the phase transformation from solvate to Form I.

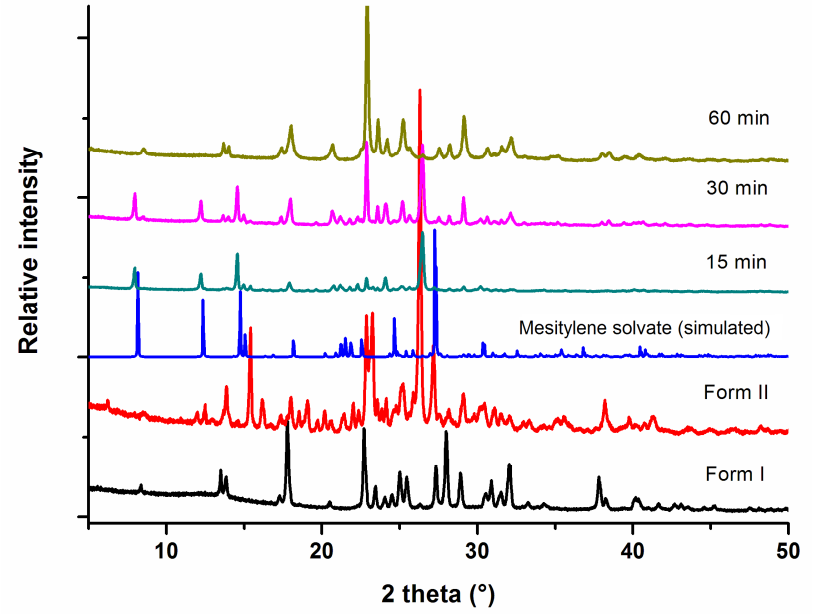

Figure S9. Comparison of the PXRD patterns of the samples obtained from the grinding experiments on Form II with 2 drops of mesitylene. Notice that 15- and 30-min grinding resulted in the solvate and 60-min grinding results in the phase transformation from solvate to Form I.

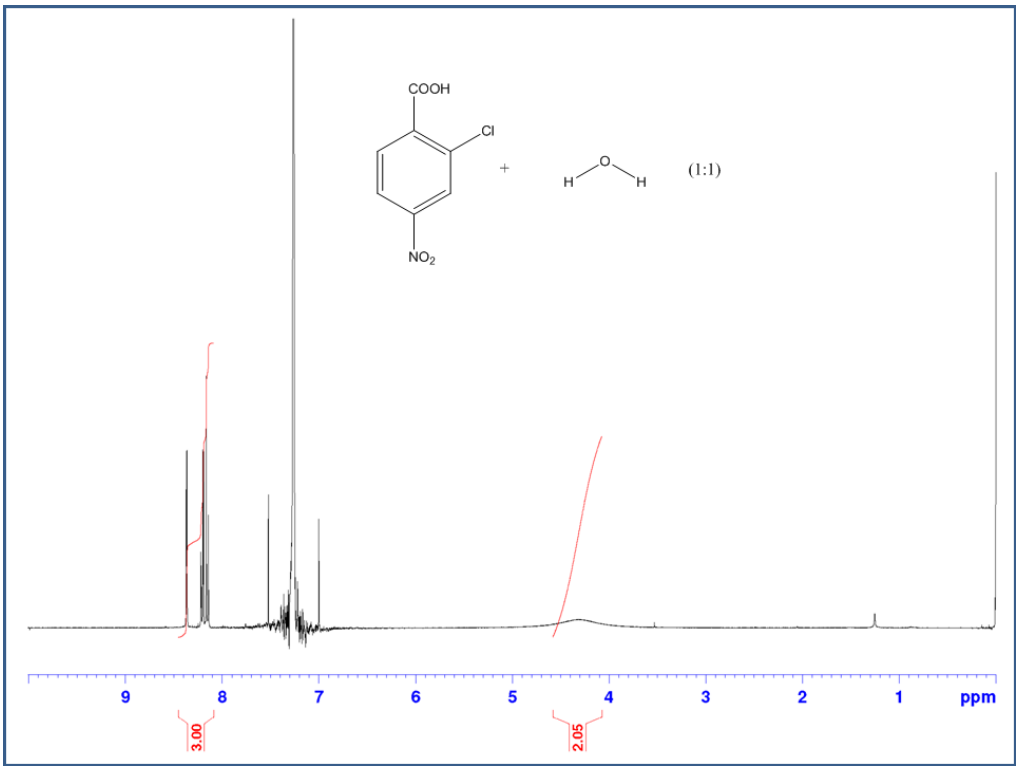

Figure S10. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of CNBA-water (1:1).

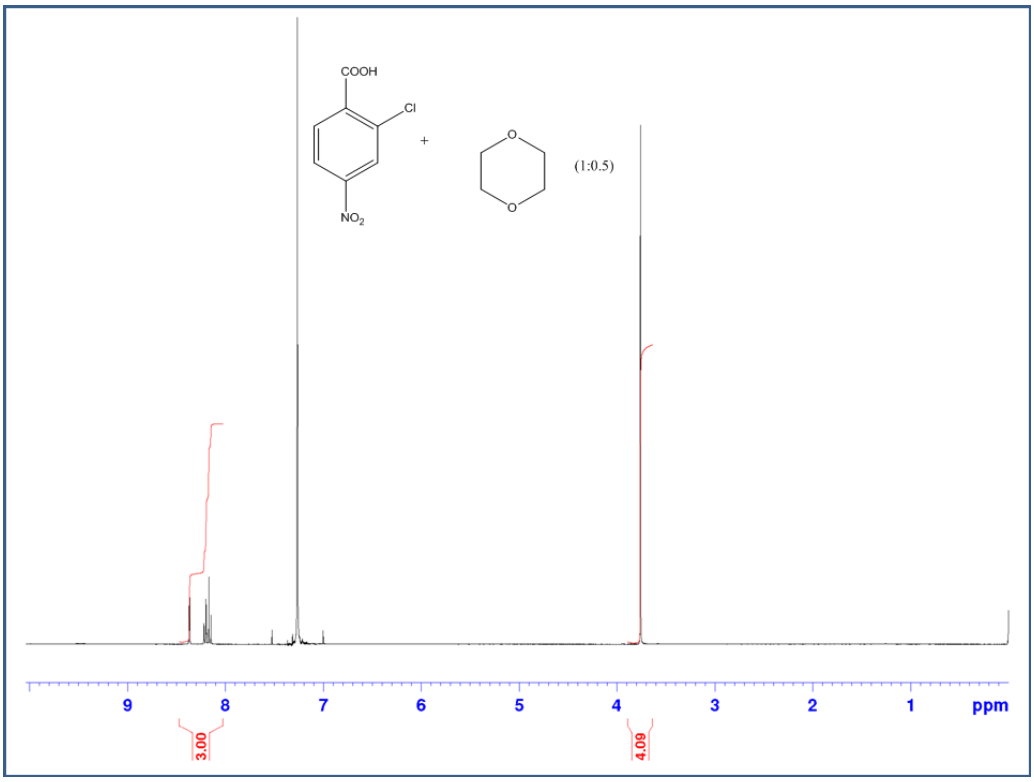

Figure S11. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of CNBA-1,4-dioxane (1:0.5).

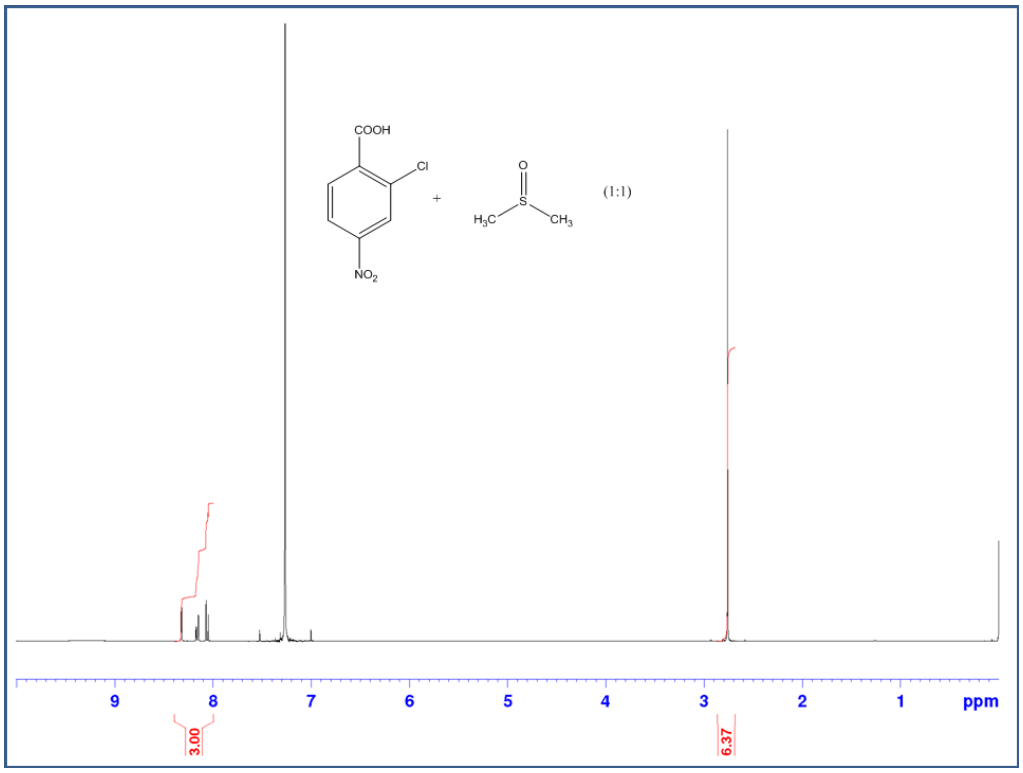

Figure S12. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of CNBA-dmso (1:1).

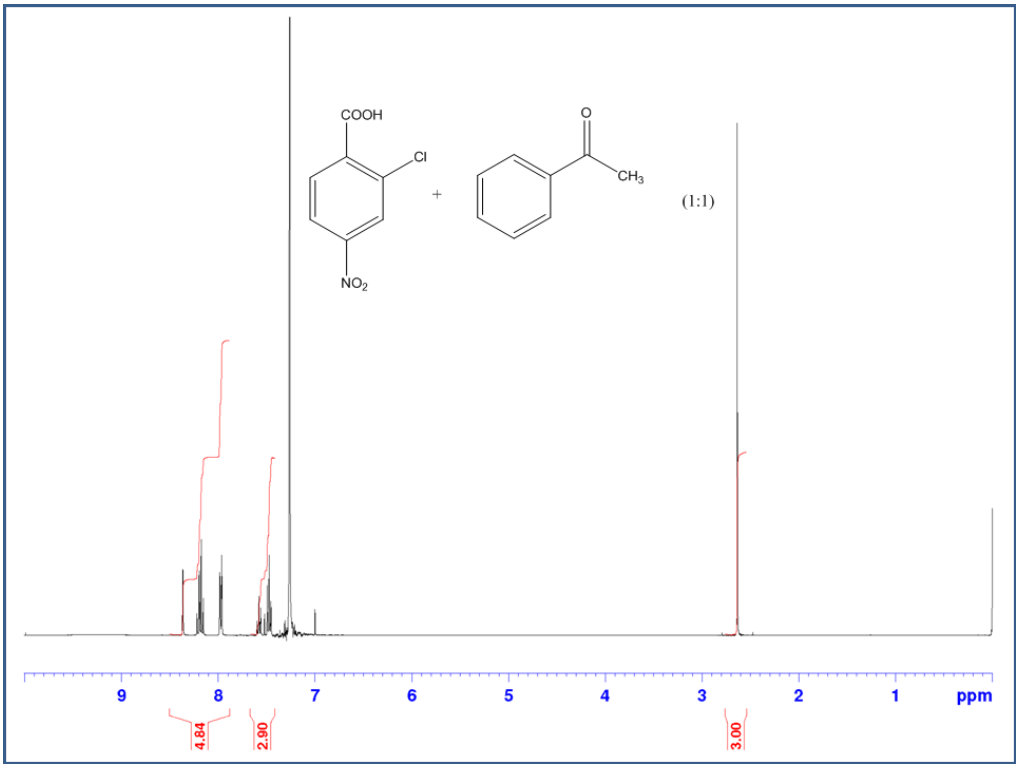

Figure S13. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of CNBA-acetophenone (1:1).

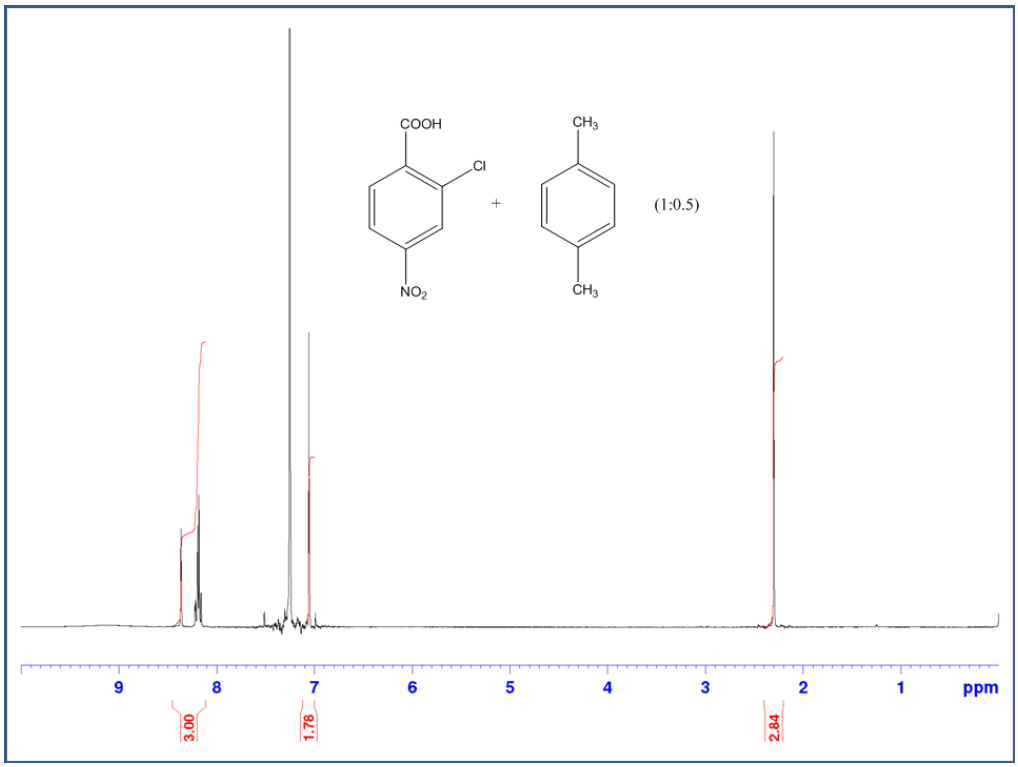

Figure S14. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of CNBA-*p*-xylene (1:0.5).

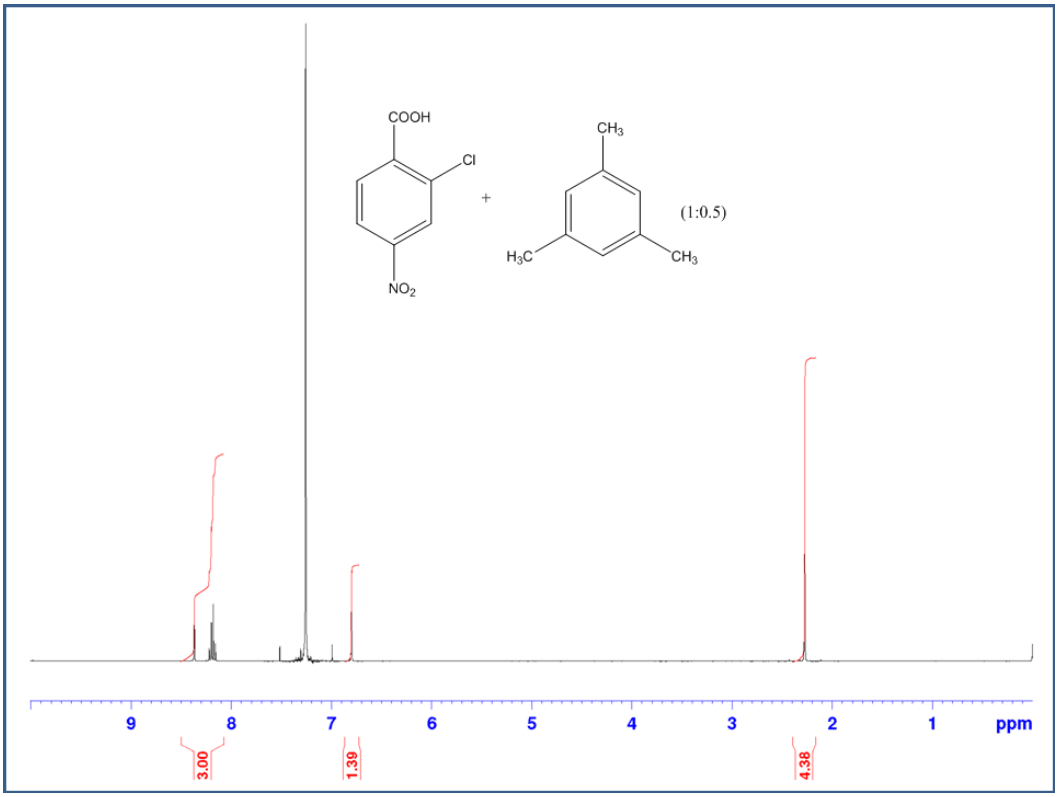

Figure S15. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of CNBA-mesitylene (1:0.5).