

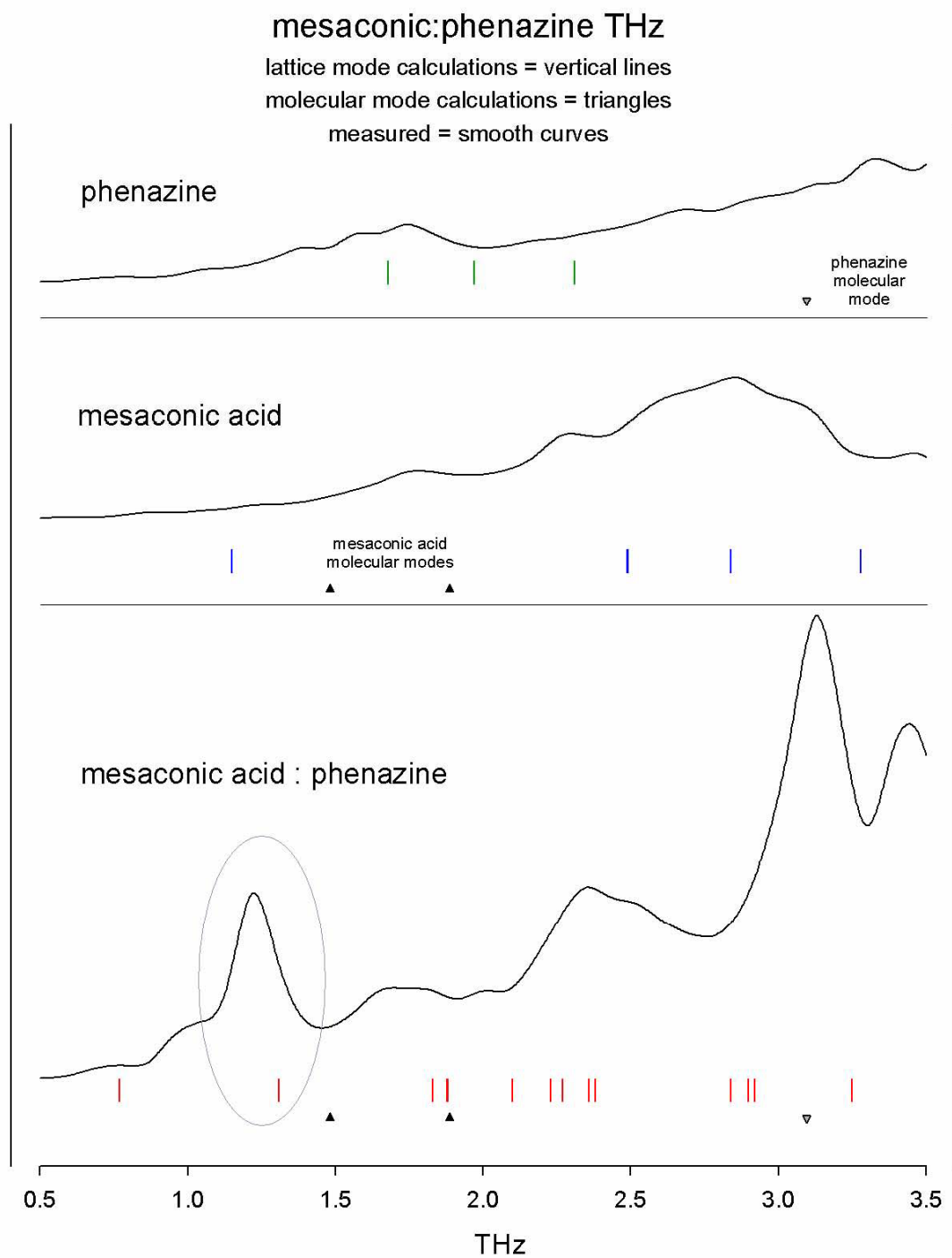
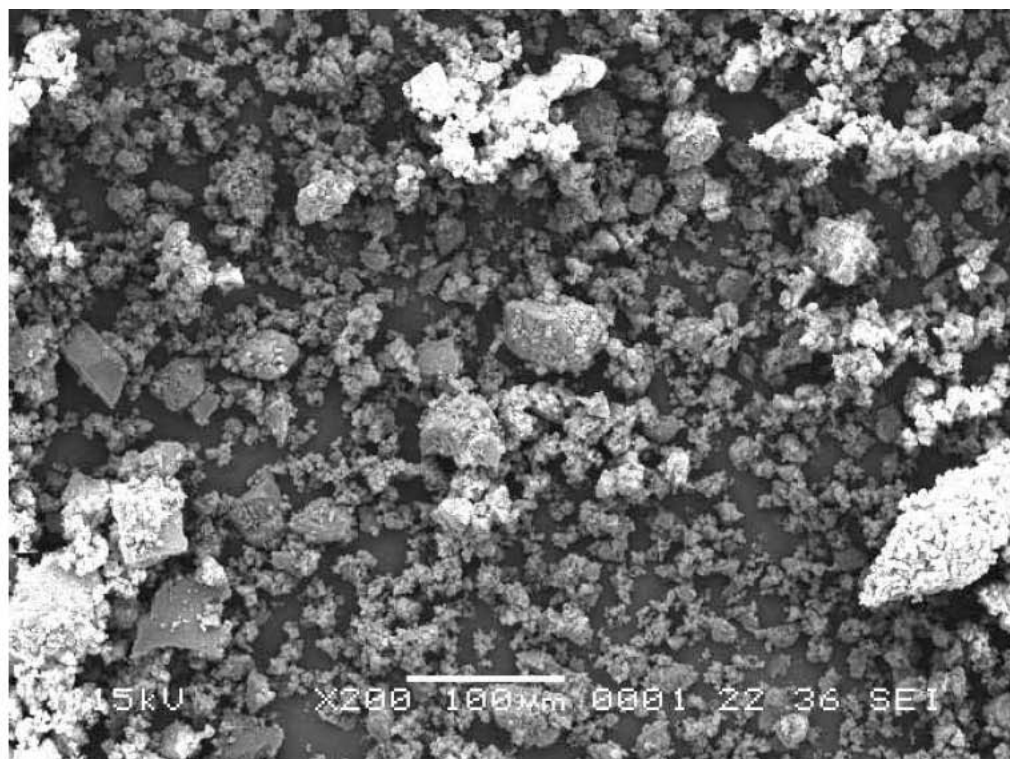


Figure S1. From top to bottom: comparison of simulated and measured THz spectra for phenazine, mesaconic acid and the phenazine-mesaconic acid cocrystal.

a)



b)

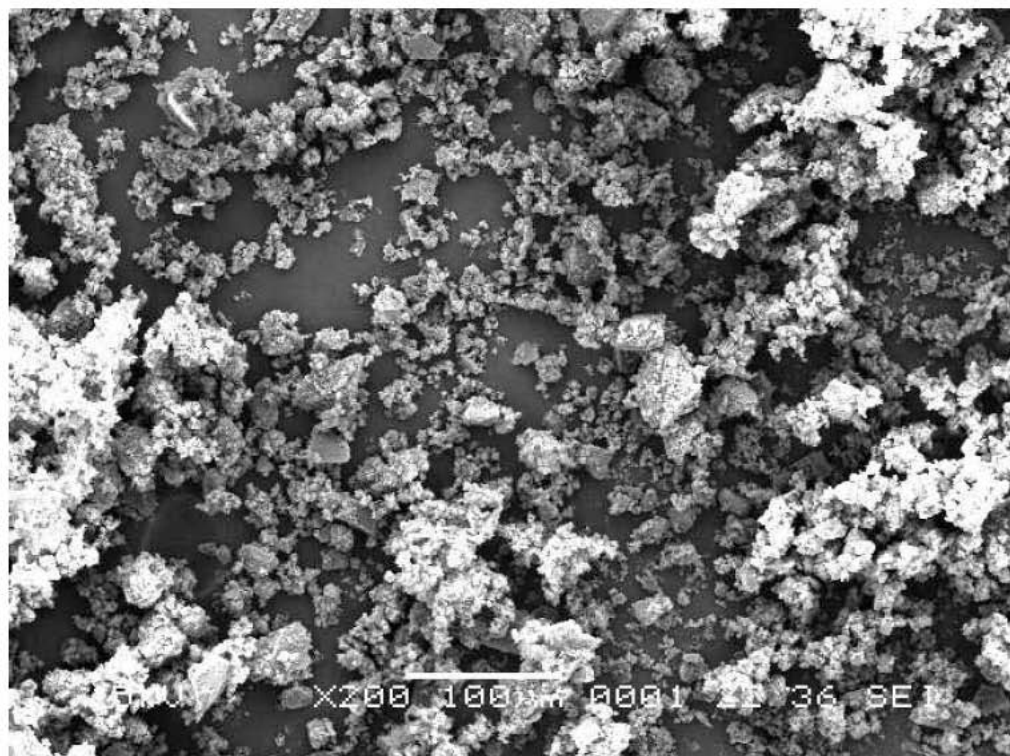
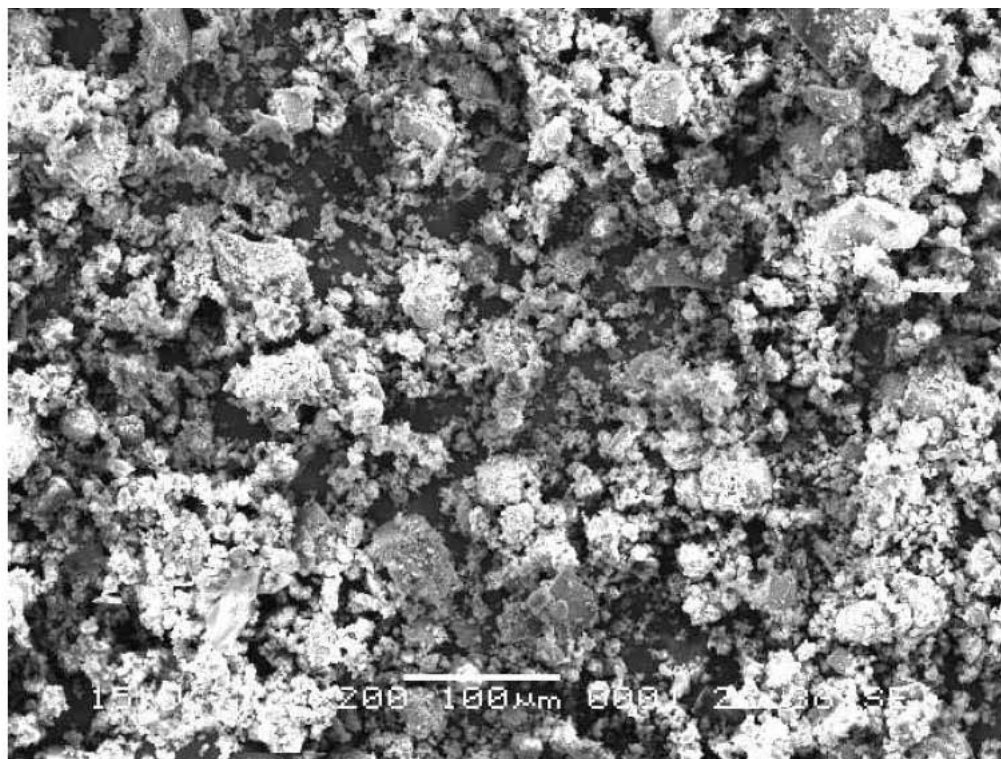


Figure S2. SEM images of the 1:1 mixture of phenazine and mesaconic acid ground for 60 minute: a) freshly prepared sample and b) sample after standing over a period of 4 days.

a)



b)

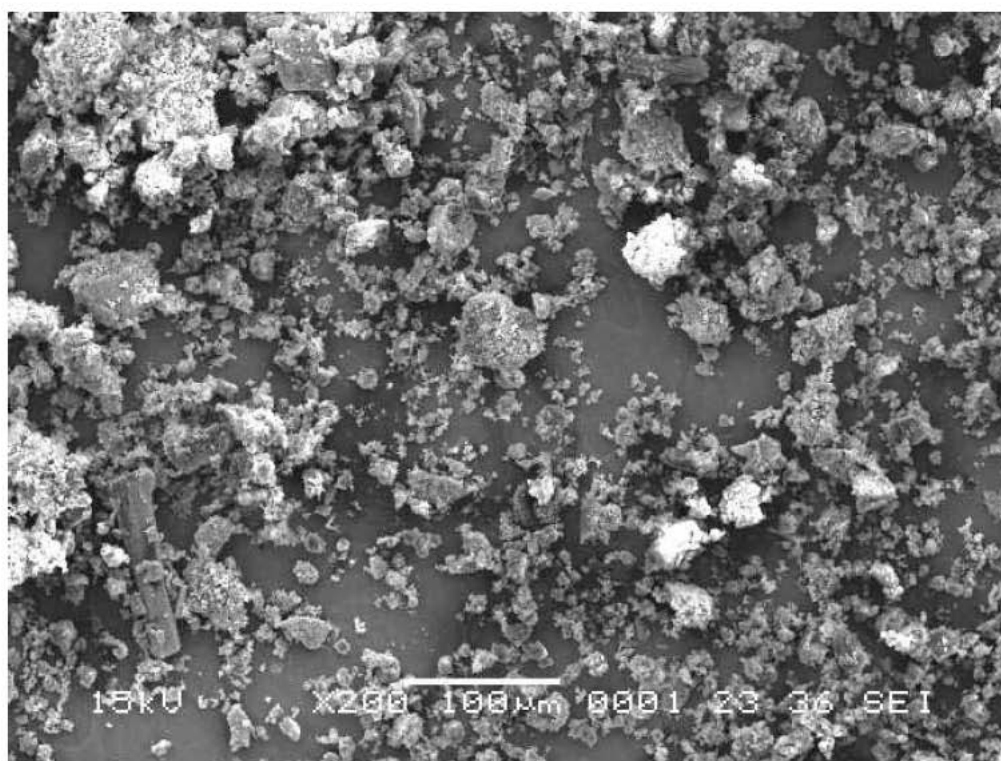
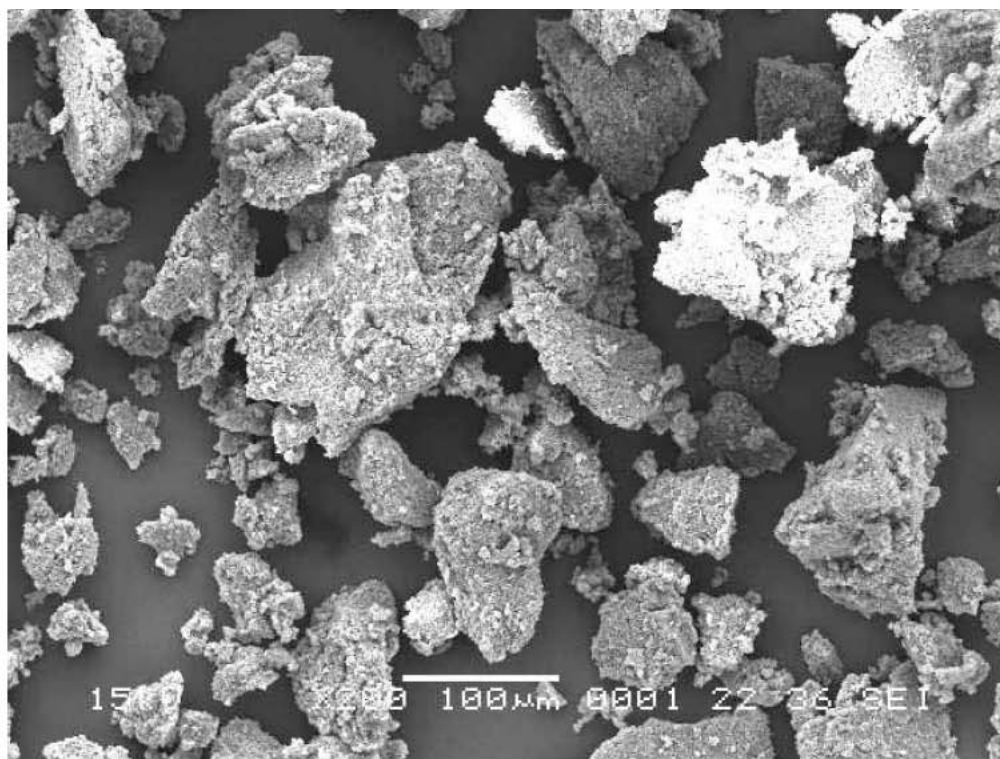


Figure S3. SEM images of the 1:1 mixture of phenazine and mesaconic acid ground for 90 minute: a) freshly prepared sample and b) sample after standing over a period of 4 days.

a)



b)

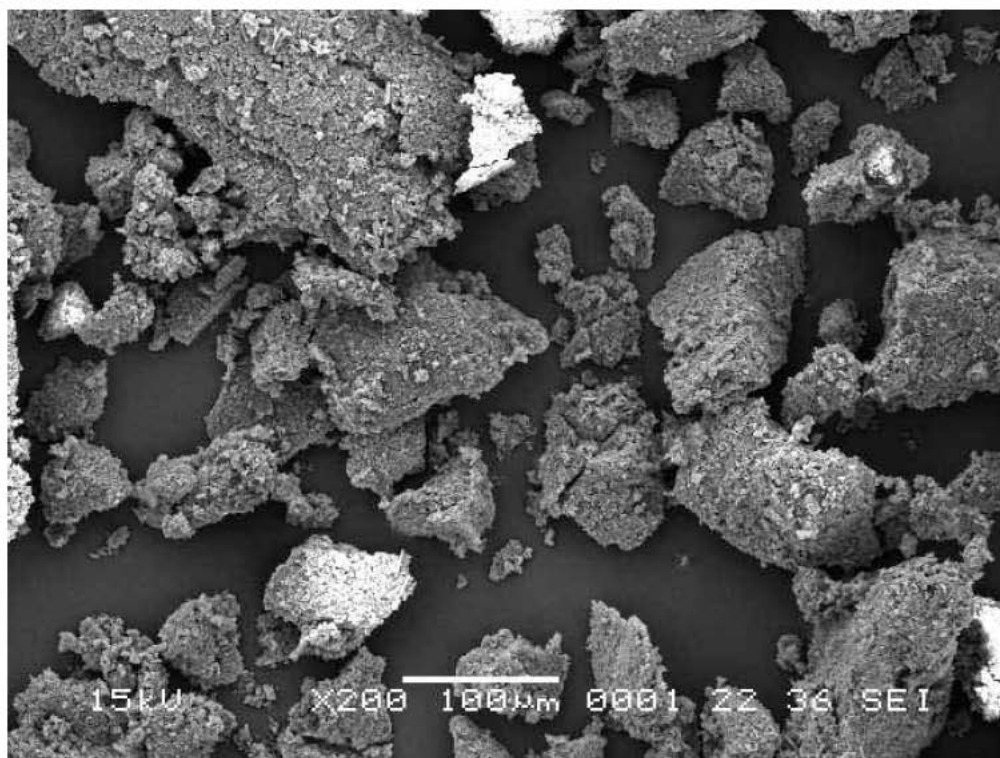


Figure S4. SEM images of the 1:1 mixture of phenazine and mesaconic acid ground for 15 minutes in the presence of ethanol: a) freshly prepared sample and b) sample after standing over a period of 4 days.

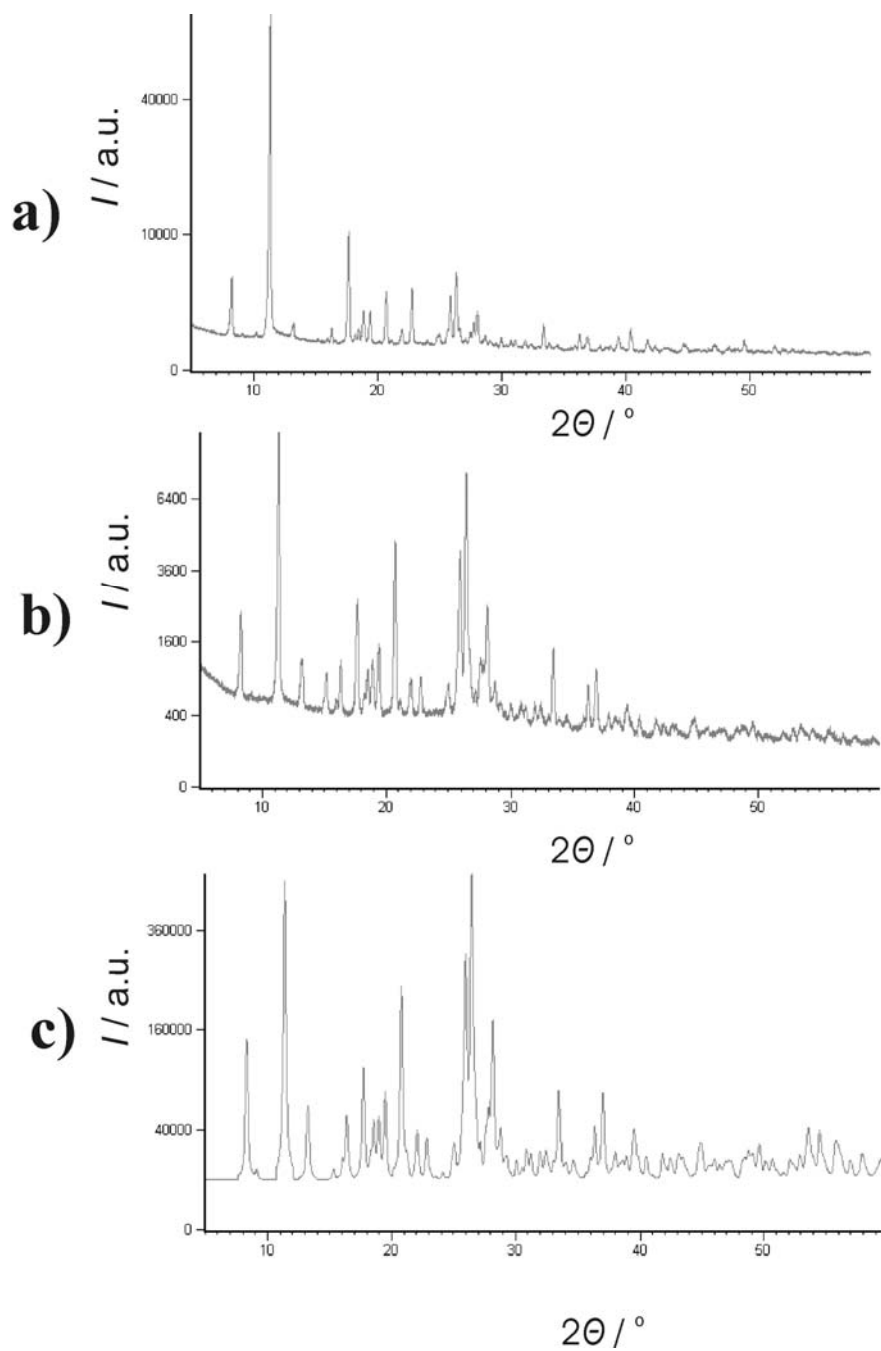


Figure S5. Powder X-ray diffraction patterns of: **a** **(phen)(mes)** cocrystal; **b** an equimolar mixture of **phen** and **mes**, ground for 15 minutes with a single drop of ethanol and **c** simulated pattern of **(phen)(mes)**.

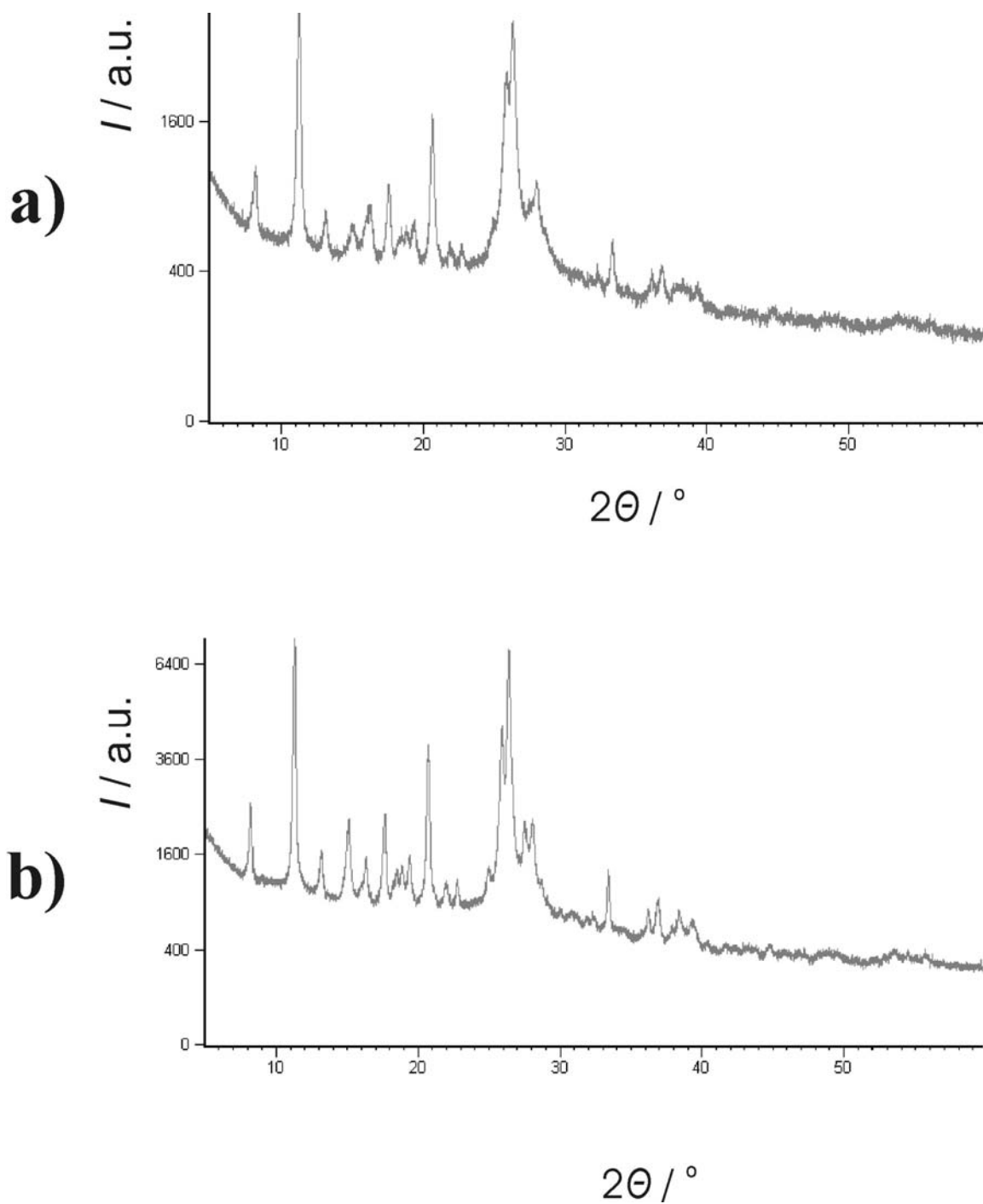


Figure S6. Powder X-ray diffraction patterns of an equimolar mixture of **phen** and **mes** ground for 20 minutes: **a** immediately after grinding and **b** after 4 days ageing.

Details of lattice dynamics calculations

THz spectra were calculated using rigid molecule lattice dynamics¹, in the same way as described before². Molecular geometries were taken from the experimentally determined crystal structures. Intermolecular interactions were evaluated using the W99 model potential³ and a distributed multipole analysis for electrostatic model, derived from a B3LYP/6-31G** wavefunction (calculated using the CADPAC program⁴). Phonon frequencies were calculated at the lattice energy minimum for each crystal structure using the program DMAREL⁵.

1. Walmsley, S. H. *J. Chem. Phys.* **48**, 1438-1444 (1968).
2. Day, G. M., Zeitler, J. A., Jones, W., Rades, T., Taday, P. F. *J. Phys. Chem. B* **110**, 447-456 (2006).
3. Williams, D. E. *J. Comput. Chem.* **22**, 1154-1166 (2001).
4. Amos, R. D.; with contributions from Alberts, I. L.; Colwell, S. M.; Andrews, J. S.; Handy, N. C.; Jayatilaka, D.; Knowles, P. J.; Kobayashi, R.; Koga, N.; Laidig, K. E.; Maslen, P. E.; Murray, C. W.; Rice, J. E.; Sanz, J.; Simandiras, E. D.; Stone, A. J.; Su, M.-D. *CADPAC*, version 6.5; Cambridge (2001).
5. Price, S. L.; Willock, D. J.; Leslie, M.; Day, G. M. *DMAREL*, version 3.1; (2001).