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Keywords: graphite, grganometallic

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XRD characterization of bulk graphene-based material

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Graphene is a nanostructure with unique physical properties that can be used to prepare a number of novel functional materials [1]. Bulk-quantities of graphene can be produced by exfoliation of expanded graphite with ultrasounds [2]. The expanded graphite is a commercial material which is obtained by thermal reduction of graphite oxide at temperatures close to 1000°C (graphite oxide is usually prepared by chemical oxidation of natural graphite using a mixture of strong chemical oxidants like: nitric acid, sulfuric acid and potassium permanganate). The degree of exfoliation strictly depends on the graphite oxidation level and the thermal shock treatment undergone by the graphite oxide; such a parameter is of a fundamental importance for the resulting physical properties of the nanostructured material that are prepared by intercalation of graphene with polymers and/or other types of nanostructures (e.g., CNTs, fullerenes, ceramic or metal nanoparticles, etc.).

The graphite oxidation/reduction process can be accurately investigated by wide-angle X-ray powder diffraction (XRD) [3] looking at the shift of the (002) peak in the diffraction pattern [4]. The presence of defects in the graphite structure like oxygen-groups (-OH, -COOH, etc.) and/or intercalated molecules (e.g., H_2SO_4) has the effect to modify the interlayer spacing, thus shifting the position of the peaks.

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Polymorphs of some common drugs and bioactive agents

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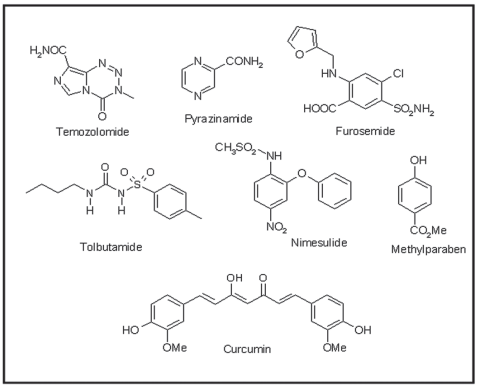
Novel polymorphs of important drugs such as Temozolomide, Pyrazinamide, Furosemide, Tolbutamide and Nimesulide, bioactive agents Methylparaben and Curcumin, and some model sulfonamides and hydroxybenzoic acids will be presented. We have found that screening against a large number of crystallization methods such as solvent-antisolvent, temperature variation and ramping, coformers and additives, solventless melt and sublimation techniques, and ionic liquids afforded novel crystalline forms of materials. Success seems to be more a factor of McCrone's famous dictum and the approach is still quite heuristic in terms of which methods work best for what kind of molecule. The success of our methodology will be presented through case studies involving different types of molecules taken up for polymorph search in our group.



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High throughput crystallization of orcinol with various N-acceptor coformers: An alternative approach for exploring the structural landscape

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An exhaustive search of the structural landscape of orcinol, 5-methyl-1,3-dihydroxybenzene, was carried out with high throughput crystallography. Polymorphs, pseudopolymorphs (solvates) and co-crystals are described. Several packing modes were identified for the orcinol co-crystals with various N-bases. In these several structural variations, the OH group conformations in the orcinol molecule (Figure 1) were found to depend on the choice of co-formers and the crystallization conditions employed. The study provides an alternative and more efficient approach to look into the various possibilities available for co-crystal formation.

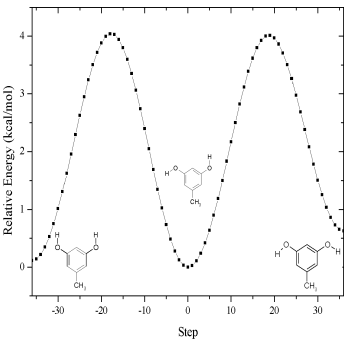

Figure 1 Relaxed potential energy surface scan performed for the OH group rotations in the orcinol molecule.