Solvatomorphism: the inclusion of unexpected guests. An interesting case of study of different solvates in the tecton [Pd(1,10-phen)(2,3,5,6-S-C₆F₄H₂)]

Juan Manuel Germán-Acacio, Hugo Juárez Garrido, Reyna Reyes, Martínez, and David Morales-Morales

Red de Apoyo a la Investigación, Instituto Nacional de Ciencias Médicas y Nutrición SZ-Universidad Nacional Autónoma de México (CIC-UNAM), CDMX C.P. 14000, México.

Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, México, CDMX. 04510, México.

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In this work is described the crystalline structures of a non-solvated tecton [Pd(1,10-phen)(2,3,5,6-S-C₆F₄H₂)] (1) (phen = 1,10-phenanthroline) and three different solvatomorphs [Pd(1,10-phen)(2,3,5,6-S-C₆F₄H₂)]·S, S = C₆H₆ (2), S = C₆H₆·Cl (3) and S = C₆H₆·Br (4). In addition is described the formation of the crystalline solvate [Pd(1,10-phen)(2,3,4,5,6-S-C₆F₅)·C₆H₆·Br (5) for comparison purposes with the former compounds. In this case we are interested in getting deeper in the knowledge of the fascinating phenomena of solvatomorphism. Thus, we performed computational studies in order to elucidate the energetics involved of the non-solvated tecton and their solvatomorphs in attempt to establish how these unexpected guests are encrusted within the unit cell.

Tectons

1. SR₉ = 2,3,5,6-(C₆F₄H)
2. SR₉ = 2,3,5,6-(C₆F₄H)·C₆H₆
3. SR₉ = 2,3,5,6-(C₆F₄H)·C₆H₆·Cl
4. SR₉ = 2,3,5,6-(C₆F₄H)·C₆H₆·Br
5. SR₉ = 2,3,4,5,6-(C₆F₅)·C₆H₆·Br