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Journal Name:	Asian Journal of Chemical Sciences
Manuscript Number:	Ms_AJOCS_32615
Title of the Manuscript:	XRD Studies, Spectral Characteristics, TGA and DFT of 2,4-Diamino-6-phenyl-1,3,5-triazine:Phenylthioacetic acid Cocrystal
Type of the Article	Original Research Article

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PART 1: Review Comments

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
Compulsory REVISION comments	In this article, details of crystal and molecular structure of DAPT:PTAA are presented together with a characterization by means of FTIR, TGA and LC-MS. Some physical and chemical properties of the cocrystal are predicted using DFT theoretical calculations. Methods were used appropriately but results were not described in details. Therefore serious major corrections of the paper would be necessary before it can be considered for a publication. The authors should consider the following remarks in their revisions. <u>Major remarks</u> 1. First of all, Authors listed 15 references describing properties of DAPT and PTAA but in The Cambridge Structural Database (CSD) Authors can find and used for the comparison purposes many structures of cocrystals with DAPT. None of these references are cited. This article describes results for one cocrystal (DAPT:PTAA, CDA refcode: UHUFUA) but I suppose that also structures UHUFOU (cocrystal with DAPT) and UHUZII (cocrystal with PTAA) belong to Authors. In my opinion these structures should be described and compared together. But it is only a suggestion. 2. The chapter 3.1 needs a substantial rewrite to be more readable. The figure with the comparison of IR spectra of DAPT, PTAA and the cocrystal should be included in the supplementary information. Without these spectra I cannot verify the text. Authors mention about OH stretching vibrations but they are	



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	almost in the same wavenumbers range as N-H stretching vibrations. 3. Mass spectra should be included in the supplementary information. I cannot verify the text. Lines 88-92: The LC-MS mass spectrum of DAPT:PTAA in negative ion mode shows the base (?) (base is DAPT, 187.20) peak at 167.04 (M+• should be M-• of PTAA is 168.04). This indicates the loss of an amu by the acid. The mass spectrum of DAPT:PTAA cocrystal in positive ion mode shows the base peak at 188.08 (M+• of DAPT is 187.08). This is due to the acceptance of a proton by DAPT from PTAA. (?) – this is a wrong conclusion. LC-MS spectra of individual DAPT, PTAA and DAPT:PTAA should be compared. The following conclusion in the abstract " LC-MS indicates the transfer of a proton from the acid to the base" cannot be formed from the description in 3.2 chapter. 4. TGA curves with their derivatives should be included in the supplementary information. I cannot verify the text. The authors should provide melting points of individual DAPT, PTAA and DAPT:PTAA. The cocrystal cannot be intact until 150°C if in the temperature range of 125.8-141.3 °C there is a mass loss due to a partial decomposition. 5. The chapter 3.4 needs a substantial rewrite to more readable. Line 137 "normal bond length of –O-H is 0.835 Å" Such precise value needs reference. 6. The comparison of simulated powder diffractogram, obtained on the basis of rentgenostructural analysis, with the experimental diffractogram should be provided. The SCXRD analysis was performed at about 100K but at the room temperature the cocrystal can have a different crystal structure. Between 100 K and room temperature the phase transition is possible. For	
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	this reason diffractograms comparison is needed. 7. Line 212, ΔE of cocrystal is <u>higher</u> than ΔE of PTAA.	
Minor REVISION comments	Minor remarks 1. The Authors should check and correct numbering of references in the article. 2. English language corrections are strongly recommended. 3. Line 17, correct XRP into SCXRD. 4. Line 83, ref 23 and 24 do not describe IR data. 5. Line 89, correct "M+•" into "M-•". 6. Lines from 100 to 106 should be in the experimental part. 7. In line 101, there is 90 K (measurement temperature?) but in the table 1 there is 110.15 K. It is misleading. 8. It table 1, A0 should be corrected into Å. 9. The chemical structure of the cocrystal DAPT:PTAA presented in Fig 1 is wrong. 10. Line 146, correct into "the COOH" – carboxyl. 11. Line 149, correct into "ÅO2-H" 12. The description of Table 3 in lines 181-183 does not agree with the content of table 3 (p. 10).	
Optional/General comments		

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