Electronic Supplementary Information

Comment on 'Solution growth and thermal treatment of crystals lead to two new forms of 2-((2,6-dimethylphenyl)amino)benzoic acid' by R. Hu, Y. Zhoujin, M. Liu, M. Zhang, S. Parkin, P. Zhou, J. Wang, F. Yu and S. Long, RSC Adv., 2018, 8, 15459

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Refinement

In the new refinement, we first performed a check CIF analysis, which is a service of the International Union of Crystallography where it reports the consistency and integrity of crystal structure determinations using the CIF format archive. Three alerts in B caught our attention, as they suggested possible pseudo/new space group. From the .cif file, the .ins file was generated and refined from this. Then, we utilized the PLATON software[1] with the ADDSYM option. A cell transformation was suggested to reduce the unit cell, and data from the matrix to perform the transformation were provided. The transformation was carried out, leading to a unit cell with new cell parameters. From this, the structure was solved by the SIR92[2] and generated only one molecule in the asymmetric unit ($Z' = 1$), which is the same as the reported Form **II** by Long et al..[3]

The structure was solved and refined using the WinGX software package.[4] Anisotropic displacement parameters for non-hydrogen atoms were applied. The hydrogens were geometrically fixed except for hydrogen H1B, which was fixed by the Qpeak electronic density. The structures were refined based on the full-matrix least-squares method using the SHELXL program.[5] The ORTEP projection of the molecular structure of Form **I** with the new refinement was generated using the software ORTEP-3[6] (Fig. S1 of this comment article). Additionally, Long et al.[1] mentioned that "the previous Form **I** crystals were obtained as colorless plates". However, this piece of information is different from what is reported in the .cif file, in which the crystal form was defined as "prism".

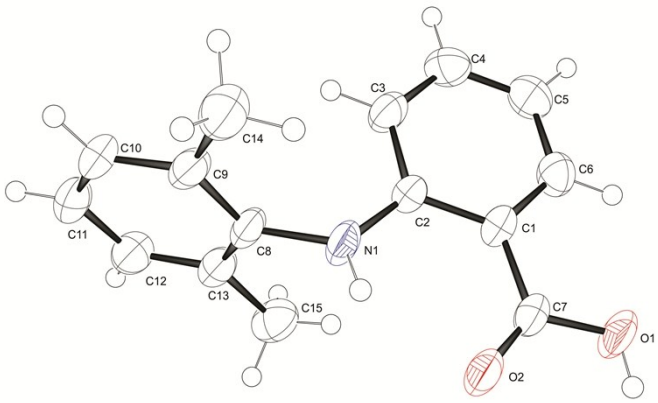

Fig. S1 ORTEP diagram of Form **I** re-refined based on the original data obtained by Kovala-Demertzi et al.[2] Displacement ellipsoids are drawn at 50% probability level, and H atoms are represented by circles with arbitrary radii.[13]

Table S1 Bond length of C1–N7 and N7–C8 in the molecules.

Molecule	C1–N7 (Å)	N7–C8(Å)
Form **II**[3]	1.375	1.441
Form **I** re-refined	1.373	1.441

Table S2 Torsion angle of the molecules.

Molecule	Torsion angle (C1–N7–C8–C9/C13) (°)
Form **II**[3]	79.63/-99.50
Form **I** re-refined	79.60/-98.62

Spectroscopic Characteristics

Long et al.[3] presented IR and Raman analyses of the supposed new forms of HDMPA. The IR peaks were already reported in Kovala-Demertzi et al.[7] study of Form **I**, and the values are almost the identical to the values of the supposed Form **II**. Therefore, the results in this section (Table 4 and Fig. 8 of the original study) were affected and are redundant. The Raman analysis was not reported previously, therefore, should be considered only as an additional characterization of Form **I** previously reported by Kovala-Demertzi et al.[7] (Data from Table 5 and Fig. 9 of the original study are affected). All comparisons should be observed not as Form **II** vs Form **III**, but Form **I** vs the supposed new form observed by DSC. Once again, only subtle differences are observed to assess the existence of Form **III**.

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