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Theoretical Research on Packing Structures of Energetic Cocrystals

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Abstract: Packing structures of the reported CL-20, HMX, BTF and TNT cocrystals were studied by Hirshfeld surface and fingerprint plot from densities, packing coefficients and molecular interaction contributions. Results show that the packing coefficients of most energetic cocrystals are between their conformers. Energetic molecules in different energetic cocrystals possess different intermolecular interactions with neighboring molecules. The total percentage of O…H and O…O in CL-20 cocrystals are more than 70%, indicating the two interactions making cocrystals stable. O…H in HMX cocrystals plays an dominant role with the amount of more than 50%. C…O and C…C in BTF cocrystals and TNT cocrystals are more than that in CL-20 cocrystals and HMX cocrystals, which proves π packing is obvious in BTF cocrystals and TNT cocrystals.

Key words: energetic cocrystal; packing coefficient; Hirshfeld surface; fingerprint plot
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《含能材料》固体推进剂专栏征稿

高能量、低特征信号、低易损、低成本、低污染、灵活能量管理和高可靠性成为当前固体推进剂面临的紧迫课题，为促进其研究，本刊将于2015年开设推进剂研究专栏，以专题报道固体推进剂研究的最新研究进展。欢迎广大学者投稿，来稿时请选择对应的专栏。

《含能材料》编辑部

更正

因本人疏忽，发表在《含能材料》2015年第8期《含5-氨基四唑硝酸盐推进剂的能量特性》一文中，误将第一作者杜旭杰所属单位写成“湖北航天飞行器研究所”，第一作者杜旭杰所属单位名称应为"湖北航天技术研究院总体设计所"。

特此更正，对读者带来的不便深表歉意！

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