Temperature dependence of rotational disorder in a nor crystallography and molecular dynamics simulation

Physical Chemistry Chemical Physics

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Citation Report

#	Article	IF	Citations
1	Towards extracting the charge density from normal-resolution data. Journal of Applied Crystallography, 2009, 42, 1110-1121.	1.9	50
2	Molecular dynamics simulations of structure and dynamics of organic molecular crystals. Physical Chemistry Chemical Physics, 2010, 12, 14916.	1.3	51
3	Validation of experimental charge densities: refinement of the macrolide antibiotic roxithromycin. Acta Crystallographica Section B: Structural Science, 2010, 66, 568-577.	1.8	33
4	Experimental and Theoretical Charge Density Analysis of Polymorphic Structures: The Case of Coumarin 314 Dye. Crystal Growth and Design, 2010, 10, 1516-1526.	1.4	35
5	Verification of structural and electrostatic properties obtained by the use of different pseudoatom databases. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, 141-153.	0.3	66
6	Electrostatic properties of nine fluoroquinoloneantibiotics derived directly from their crystal structure refinements. CrystEngComm, 2012, 14, 2520-2531.	1.3	39
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8	Contributions of charge-density research to medicinal chemistry. IUCrJ, 2014, 1, 457-469.	1.0	28
9	On the use of molecular dynamics simulation to calculate X-ray thermal diffuse scattering from molecular crystals. Journal of Applied Crystallography, 2015, 48, 1420-1428.	1.9	7
10	Aspherical‐Atom Modeling of Coordination Compounds by Single‐Crystal X‐ray Diffraction Allows the Correct Metal Atom To Be Identified. ChemPhysChem, 2015, 16, 412-419.	1.0	33
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15	Fast energy minimization of the CCDC drug-subset structures by molecule-in-cluster computations allows independent structure validation and model completion. CrystEngComm, 2020, 22, 7420-7431.	1.3	5
16	Solid-state NMR spectroscopy for the analysis of element-based non-covalent interactions. Coordination Chemistry Reviews, 2020, 411, 213237.	9.5	32
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