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Slip asymmetries and rotational defects in Cyclotrimethylene trinitramine (RDX)[1] CATALIN PICU, ANIRBAN PAL, NITHIN MATHEW, Rensselaer Polytechnic Institute — In this work we study the motion of dislocations and formation of point defects in the molecular crystal Cyclomethylene trinitramine (RDX) by means of atomistic simulations. We show that slip asymmetries exist in this crystal, i.e. dislocations in given slip system can move easier in one direction than in the other, and this effect is due to the steric hindrance of molecules. The effect can be correlated with the presence of a new type of point defects which are molecules placed in a rotated position relative to the perfect crystal configuration. The stability of these rotational point defects is discussed.

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