

Fig. 1 Fingerprints of 3 different randomly chosen computational crystals of TNT (denoted with different colors).

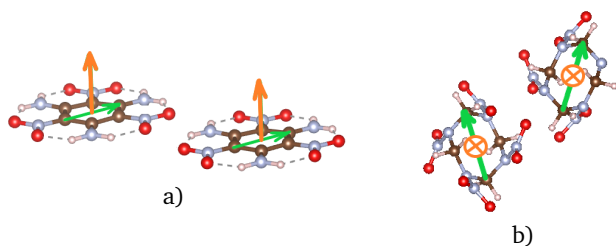


Fig. 2 Angles between vectors of identical colors are set as fingerprints for creating the energy surfaces for TATB (a) and HMX (b)

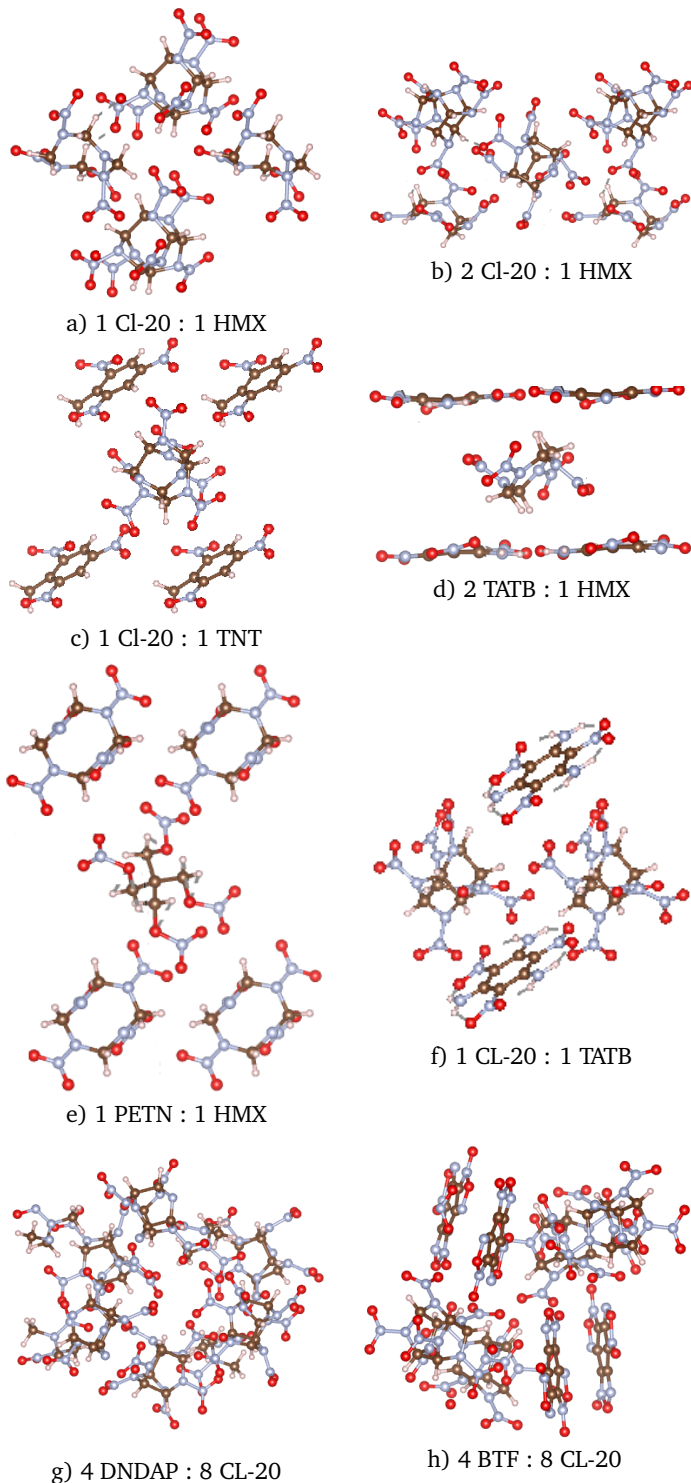


Fig. 3 Crystal structures of cocrystals of energetic materials predicted by USPEX.