Single crystal structure of energetic hypergolic ionic liquid salts, HMEDA-(DCA)₂

Single crystal structure of N^1, N^1, N^2, N^2, N^2 -hexamethylethane-1,2-diaminium dicyanamide(HMEDA-(DCA)₂) prepared using N^1, N^1, N^2, N^2 -tetramethylethane-1,2-diamine through the quaternization and subsequent ion exchange was determined readily with charge flipping method. The structure of HMEDA-(DCA)₂ was triclinic, *P*1 with lattice parameters of *a*=6.427 Å, *b*=8.725 Å, *c*=14.069 Å, a=88.658°, β=87.874° and y=71.712° in which the chemical composition was $C_{24}H_{44}N_{16}$ with R_1/wR_2 =9.18/15.20 over 1477 reflections for I>3 σ (I). The largest difference peak was 0.85 and the deepest hole was -0.53 eÅ³. The goodness-of-fitness index was 2.22. The final maximum (change/s.u.) was 0.0437.