Single crystal structure of HMEDA-$(DCA)_2$, energetic hypergolic ionic liquid salts

Sung June Cho[1,*], Hoi-Gu Jang[1], Jin Hee Park[1], Gyeong Cheol Jo[1], Eun Mee Goh[2]

[1]Department of Chemical Engineering, Chonnam National University, 77 Yongbong-ro, Buk-gu, Gwangju 500-757, Republic of Korea

[2]Agency for Defense Development, Yuseong P.O. box 35, Daejeon 305-600 Korea

*E-mail: sjcho@chonnam.ac.kr

Accurate altitude and attitude control of the satellite is critical technology. Chemical propulsion system using hydrazine as a monopropellant has been the state of art system.[1] However, anhydrous hydrazine (> 97%) is very toxic because of high vapor pressure. Therefore, large research effort has been directed to find non-toxic fuel for the same purpose, especially such as energetic *hypergolic* ionic liquid for non-catalytic chemical propulsion.

Previously, TMEDA was converted into N^1,N^1,N^1,N^2,N^2,N^2-hexamethylethane-1,2-diaminium dicyanamide (HMEDA-$(DCA)_2$) through the scheme shown in Figure 1. HMEDA-$(DCA)_2$ has been prepared using the simple quaternization and subsequent ion exchange of dicyanamide. The HMEDA-$(DCA)_2$ solution, 60 wt% had ID in the range of 100 msec with white fuming nitric acid as the oxidizer. Further, the ID of the HMEDA-$(DCA)_2$ solution was decreased to 20-30 msec upon introducing co-catalyst.[2]

In this work, the crystal structure of HMEDA-$(DCA)_2$ has been studied for better understanding of the decomposition mechanism. Single crystal data of HMEDA-$(DCA)_2$ was collected using synchrotron radiation. The charge flipping method was applied to obtain the structural solution using the *superflip* program implemented in JANA2006.

The structure of HMEDA-$(DCA)_2$ was found to be triclinic, *P-1* with lattice parameters of a=6.427 Å, b=8.726 Å, c=14.069 Å, α=88.658°, β=87.874° and γ=71.712° in which the chemical composition was $C_8H_{22}N_2$-$2(C_2N_3)$ with R_1/wR_2 = 0.0867/0.2157 over 1472 reflections for $I > 3\sigma(I)$. The largest difference peak was 1.06 and the deepest hole was -0.50 eÅ^3. The goodness-of-fitness index was 2.11. The final maximum (change/s.u.) was 0.0437.

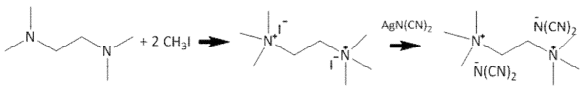

Fig.1 Schematic diagram for the synthesis of HMEDA-$(DCA)_2$ from TMEDA.

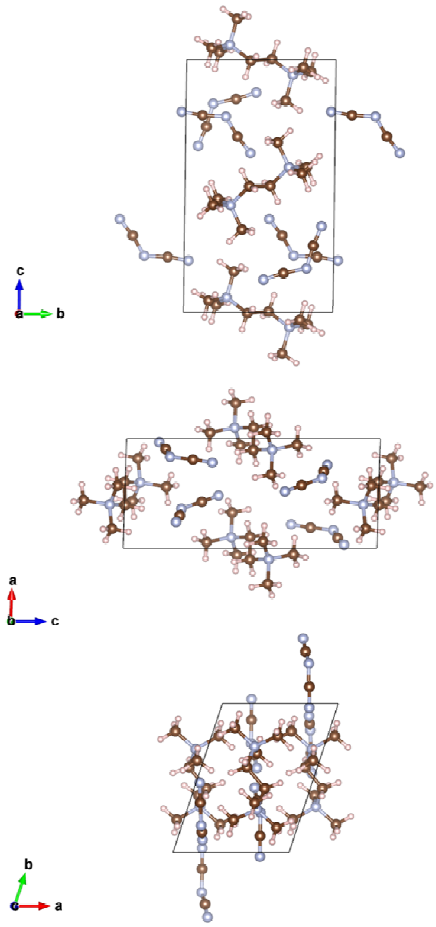

Fig.2 Crystal structure of HMEDA-$(DCA)_2$.

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