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Crystal Structure and Thermal Properties of *N,N'*-Bis(2-fluoro-2,2'-dinitroethyl)-3,4-diaminofurazan

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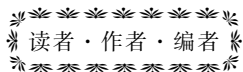
Abstract: The single crystal of *N,N'*-bis(2-fluoro-2,2'-dinitroethyl)-3,4-diaminofurazan (LLM-208) was cultivated by solvent evaporation using anhydrous methanol as solvent at the temperature of 10–15 °C. Its crystal structure was determined by a X-ray single-crystal diffractometer. Results show that the crystal density of LLM-208 is 1.895 g · cm⁻³ at 130 K and 1.848 g · cm⁻³ at 298 K, which belongs to monoclinic system, space group *C*2, *a*=19.225(5) Å, *b*=5.5779(15) Å, *c*=6.4176(17) Å, β =108.551(5)°, *V*=909.4(6) Å³, *Z*=2, μ =0.192 mm⁻¹, *F*(000)=376. Hirshfeld-surface analysis suggests that the dominant contacts and distributions of LLM-208 crystal are shown as follows (*R* represents ratio): $R_{O\dots H/H\dots O}$ = 35.0%, $R_{O\dots O}$ = 22.3%, $R_{F\dots O/C\dots F/F\dots F}$ = 12.5%. The activation energies calculated by using Kissinger, Flynn-Wall-Ozawa and Starink methods are 112.28, 114.49, 112.49 kJ · mol⁻¹, respectively. The pre-exponential factor by Kissinger method is 10^{21.30} s⁻¹.

Key words: energetic materials; *N,N'*-bis(2-fluoro-2,2'-dinitroethyl)-3,4-diaminofurazan (LLM-208); crystal structure; thermal properties

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