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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 ℃. 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)Å^3, *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): $R_{O\cdots H/H\cdots O}$=35.0%, $R_{O\cdots O}$=22.3%, $R_{F\cdots O/C\cdots F/F\cdots F}$=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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