

Unexpected formation of (trinitromethyl)pyrazines

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Table 1S Close intermolecular contacts (Å) and energies of pair interactions (kcal/mol) for compound **2a**.

Entry	Close contact	Symmetry code	Distance	Energy
1	O5...H6	-x,-1/2+y,1/2-z	2.528	-3.8
2	H6...O5	-x,1/2+y,1/2-z	2.528	-3.8
3	C5...O2	-1/2+x,y,1/2-z	3.048	-3.8
4	O2...C5	1/2+x,y,1/2-z	3.048	-3.8
5	O7...C5	1/2-x,2-y,-1/2+z	3.074	-3.3
6	C5...O7	1/2-x,2-y,1/2+z	3.074	-3.3
7	O7...O3	1/2-x,-1/2+y,z	2.824	-3.0
	O7...N5		3.165	
8	O3...O7	1/2-x,1/2+y,z	2.824	-3.0
	N5...O7		3.165	
9	No close contacts	-x,2-y,1-z		-1.5
10	O4...C8	x,1.5-y,-1/2+z	3.153	-1.5
11	C8...O4	x,1.5-y,1/2+z	3.153	-1.5

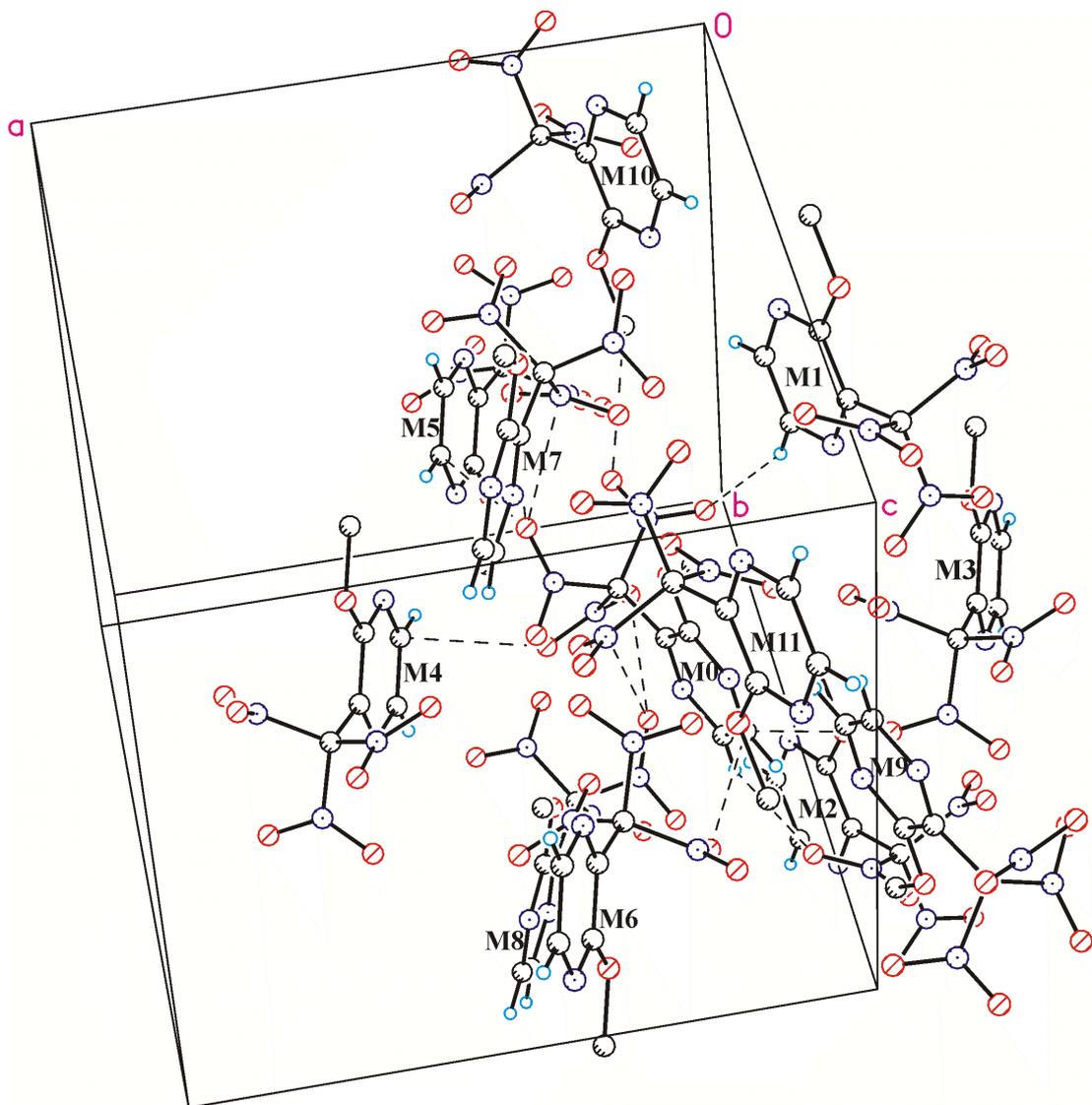


Figure 1S Crystal packing fragment showing closest environment of the central molecule (M0) in the crystal structure of compound **2a**. Numbers of neighbours correspond to those in Table 1S. The H atoms of the methyl group are omitted for clarity.