Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Photodissociation dynamics of dinitrite at 355nm: initiation of a reactive pathway

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Table S1. The vapor pressures[a] (VP, in Torr) of dinitrites and the precursor diols at 25°C

Dinitrites	VP[a]	Diols	VP[a]
1,2-propyl dinitrite	21.4	1,2-propanediol	0.204
1,3-propyl dinitrite	14.8	1,3-propanediol	0.0343
1,2-butyl dinitrite	-	1,2-butanediol	0.148
1,3-butyl dinitrite	7.02	1,3-butanediol	0.0541
2,3-butyl dinitrite	9.87	2,3-butanediol	0.260

[a]Data taken from ACD/Labs, version 11.02, Advanced Chemistry Development, Inc., Toronto, ON, Canada, www.acdlabs.com, 2015.

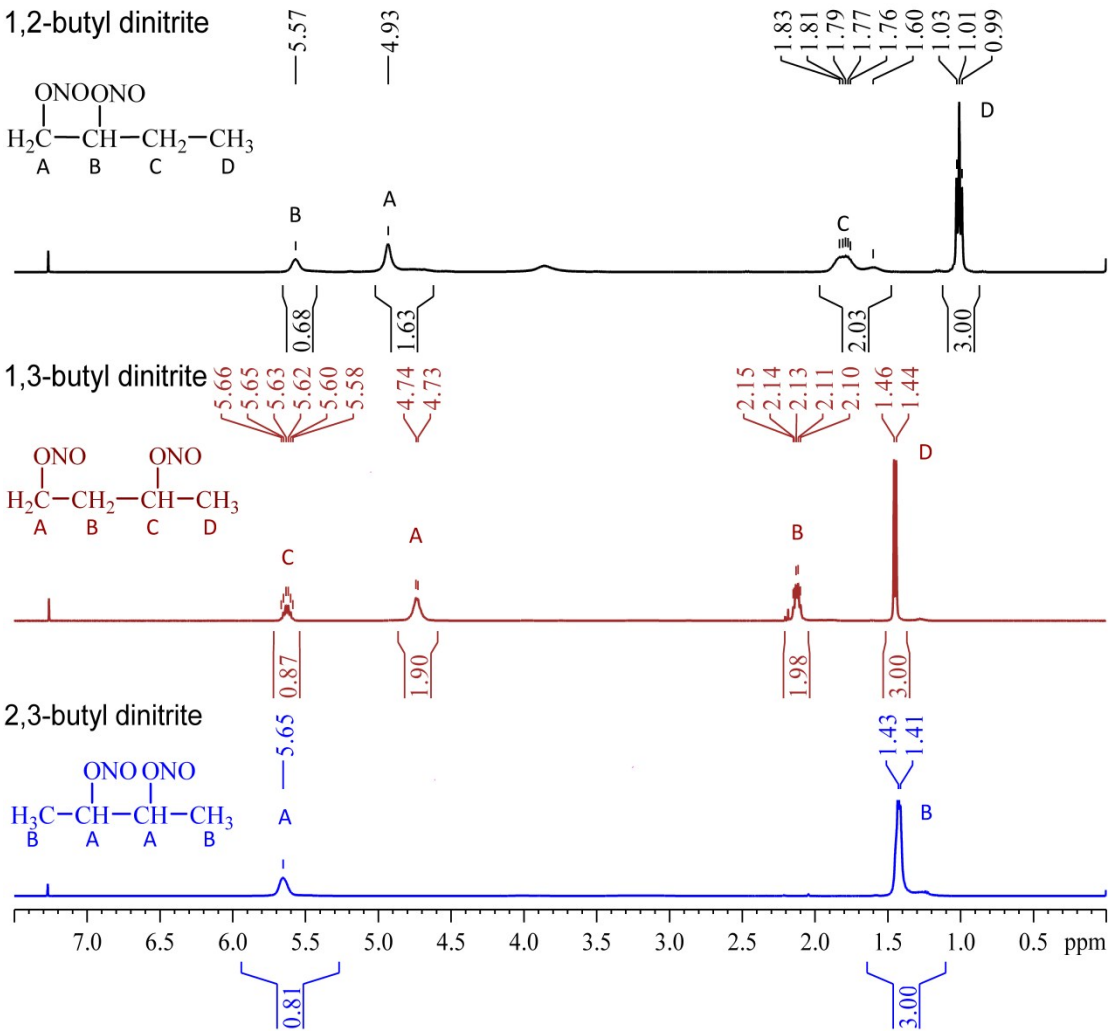

Fig. S1 NMR spectra of 1,2-butyl dinitrite ,1,3-butyl dinitrite and 2,3-butyl dinitrite.

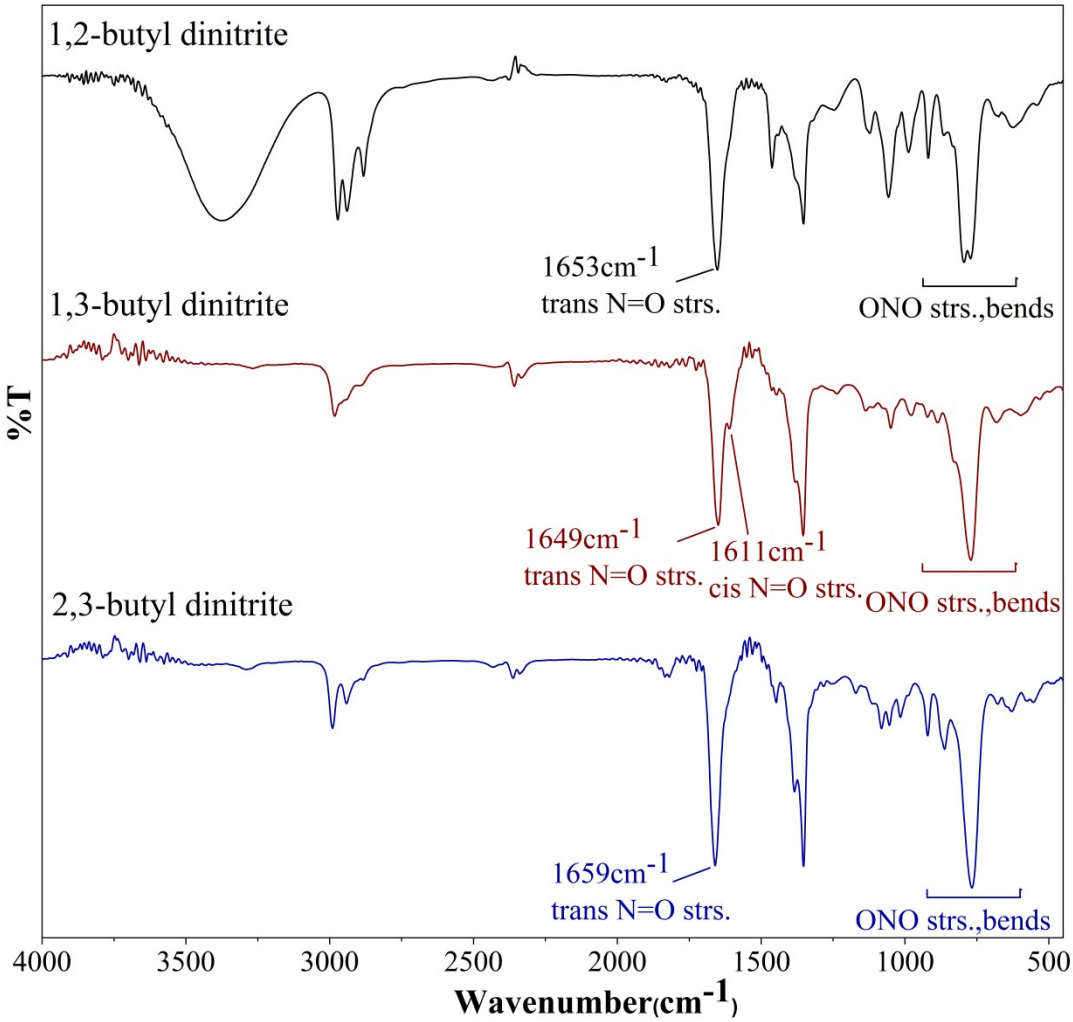

Fig. S2 IR spectra of 1,2-butyl dinitrite ,1,3-butyl dinitrite and 2,3-butyl dinitrite.

Table S2 Vertical excitation energies (VEE, eV) and oscillator strengths (OS) for 1,2-butyl dinitrite, 1,3-butyl dinitrite and 2,3-butyl dinitrite of the singlet-singlet transitions by TDDFT method

	1,2-butyl dinitrite			2,3-butyl dinitrite		
	Excitation(no. of initial orbital-the no. of final orbital)	VEE	OS	Excitation(no. of initial orbital-the no. of final orbital)	VEE	OS
1	39(HOMO)-40(LUMO)	3.43	0.0004	39(HOMO)-40(LUMO)	3.42	0.0003
2	38(HOMO-1)-40(LUMO)	3.45	0.0012	38(HOMO-1)-40(LUMO)	3.45	0.0012
3	39(HOMO)-41(LUMO+1)	4.58	0.0013	39(HOMO)-41(LUMO)	4.59	0.0021
4	38(HOMO-1)-41(LUMO+1)	4.64	0.0008	38(HOMO-1)-41(LUMO+1)	4.60	0.0004
5	37(HOMO-2)-40(LUMO)	5.10	0.0415	37(HOMO-2)-40(LUMO)	5.21	0.0373
6	37(HOMO-2)-41(LUMO+1)	5.32	0.0500	37(HOMO-2)-41(LUMO+1)	5.41	0.0457
7	36(HOMO-3)-40(LUMO)	5.92	0.0356	36(HOMO-3)-40(LUMO)	5.79	0.0503
8	36(HOMO-3)-41(LUMO+1)	6.11	0.0034	36(HOMO-3)-41(LUMO+1)	5.97	0.0069

	1,3-butyl dinitrite		
	Excitation(no. of initial orbital-the no. of final orbital)	VEE	OS
1	39(HOMO)-40(LUMO)	3.39	0.0008
2	38(HOMO-1)-40(LUMO)	3.42	0.0013
3	39(HOMO)-40(LUMO)	4.57	0.0001
4	38(HOMO-1)-41(LUMO+1)	4.67	0.0000
5	37(HOMO-2)-40(LUMO)	5.42	0.1315
6	37(HOMO-2)-41(LUMO+1)	5.51	0.0031
7	36(HOMO-3)-40(LUMO)	5.69	0.0226
8	36(HOMO-3)-41(LUMO+1)	5.73	0.0011

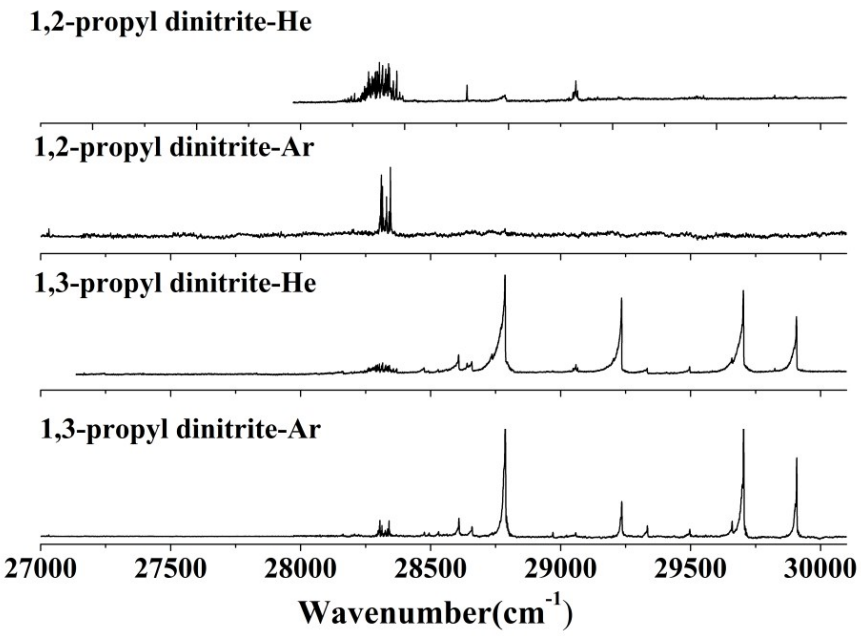

Fig.S3 The LIF spectra obtained via 355 nm photolyzation of 1,2-propyl dinitrite and 1,3-propyl dinitrite in the supersonic jet with He or Ar as carrier gas.

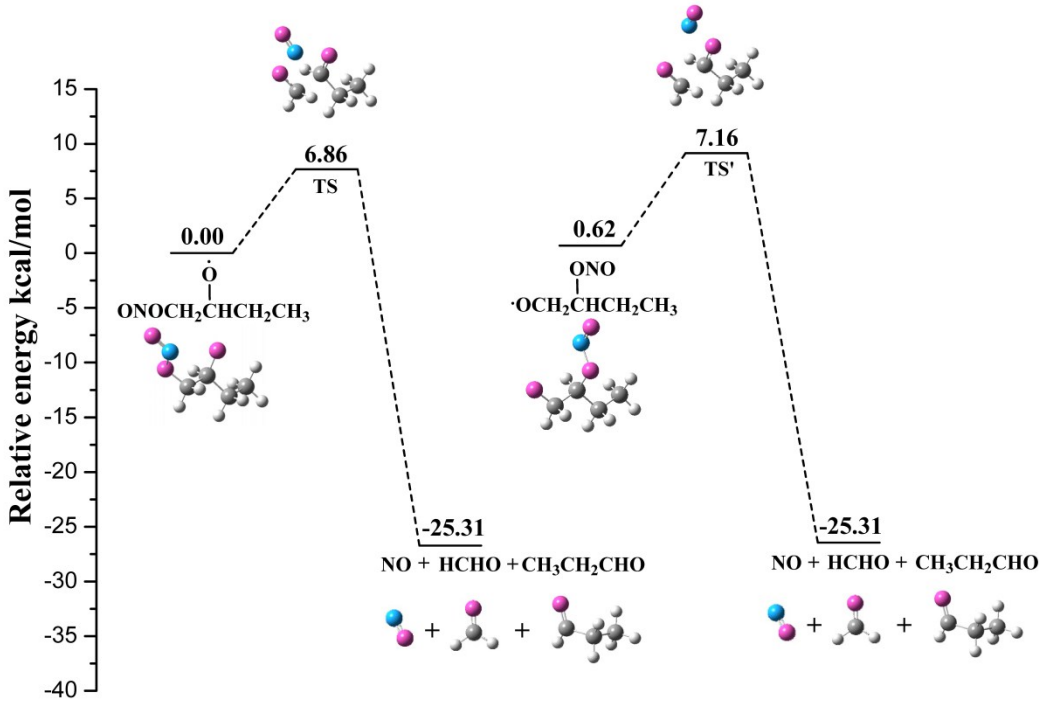

Fig. S4 Schematic energy diagram of the secondary dissociation of 1,2-butyl dinitrite in the ground state (energy is given in kcal/mol).

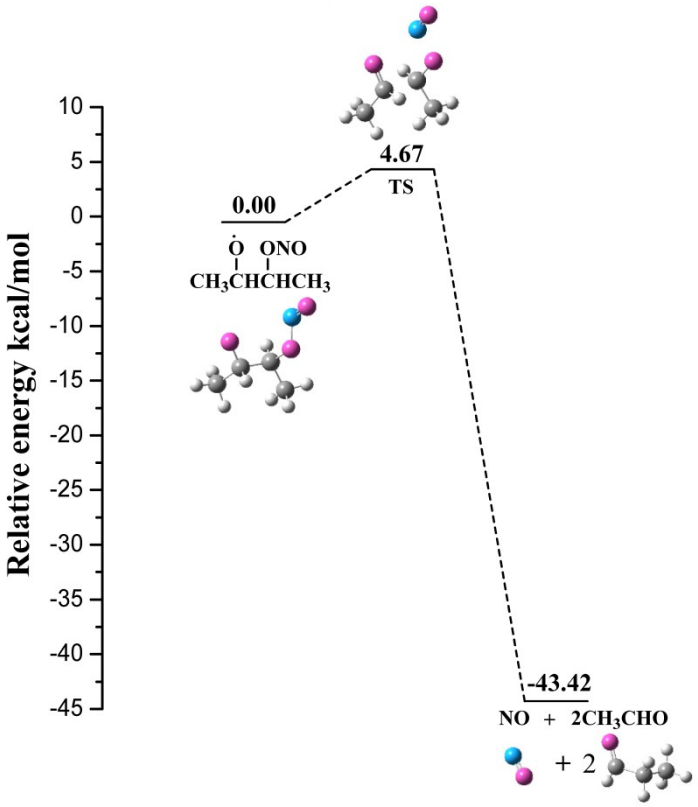

Fig. S5 Schematic energy diagram of the secondary dissociation of 2,3-butyl dinitrite in the ground state (energy is given in kcal/mol).