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

Supporting Information

Direct observation of the intermediate radical in the photodissociation of 1,3-cyclohexane dinitrite

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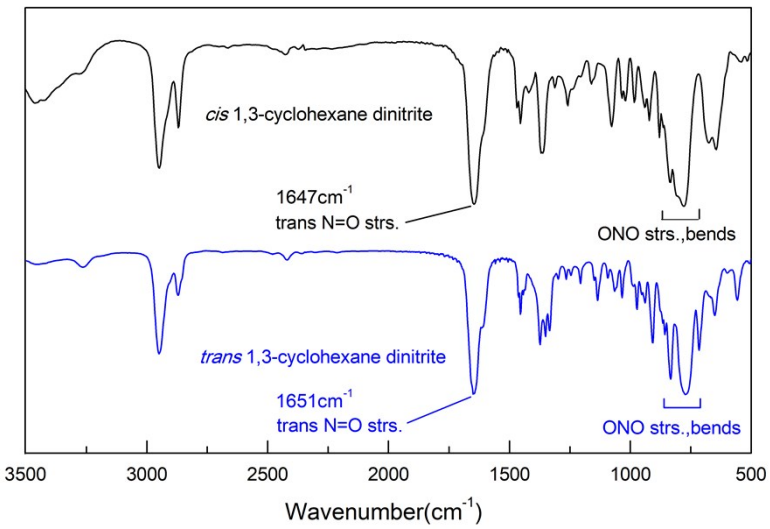


Fig. S1 IR spectra of *cis* 1,3-cyclohexane dinitrite and *trans* 1,3-cyclohexane dinitrite.

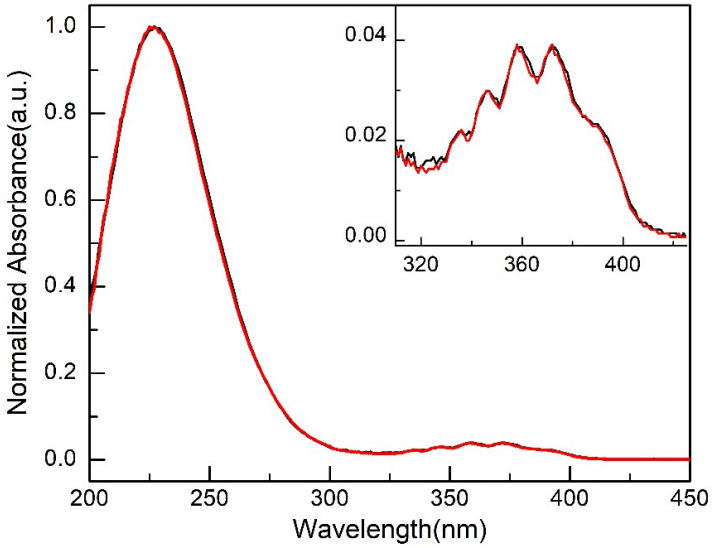


Fig. S2 UV absorption spectra of *cis* 1,3-cyclohexane dinitrite (black) and *trans* 1,3-cyclohexane dinitrite (red).

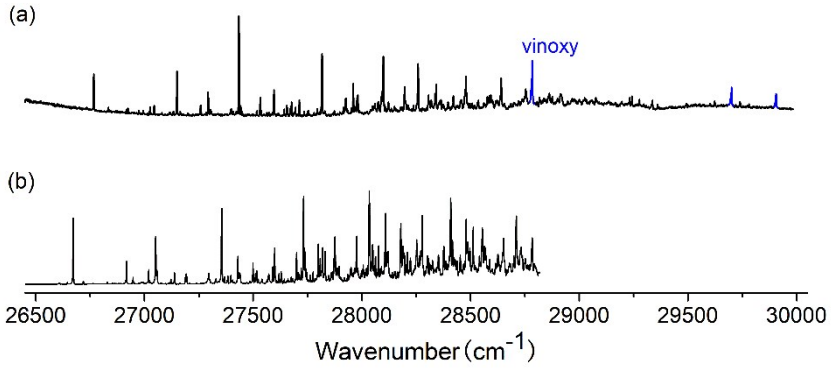
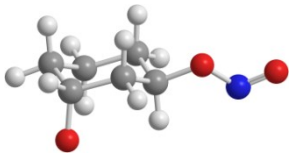


Fig. S3 (a) LIF spectra obtained by 355 nm laser photolysis of 1,3-cyclohexane dinitrite (*cis-trans* mixture), and (b) LIF spectra of 3-methyl substituted cyclohexoxy radical.

Table S1 Assignment of the LIF spectrum obtained by photodissociation of *trans* 1,3-cyclohexane dinitrite.

trans 3-nitrosooxy cyclohexoxy radical
chair (e,a) conformer



Band	Experimental[a]	Predicted[b]	Assignment
a	0		ν_{00}^{D-X}
b	139	115	ν_{53}
c	613	544	ν_{42}
d	752	746	ν_{40}
e	819	809	ν_{39}
f	959	948	ν_{34}

[a] Observed band maxima (cm^{-1}) relative to ν_{00}^{D-X} at 26838 cm^{-1}.

[b] Scaled CASSCF(9,7)/6-311++G(d,p) frequencies (scale factor 0.95) for the fundamentals, and sum of the fundamental frequencies (cm^{-1}) for combination and overtone bands.