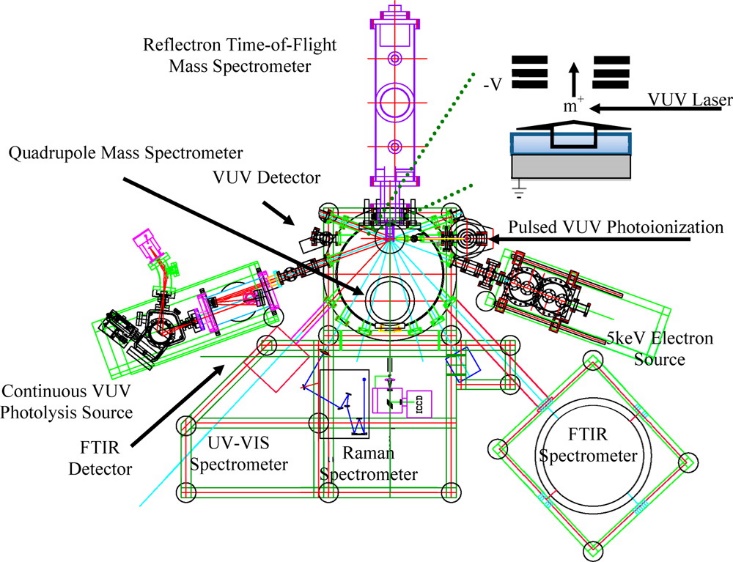
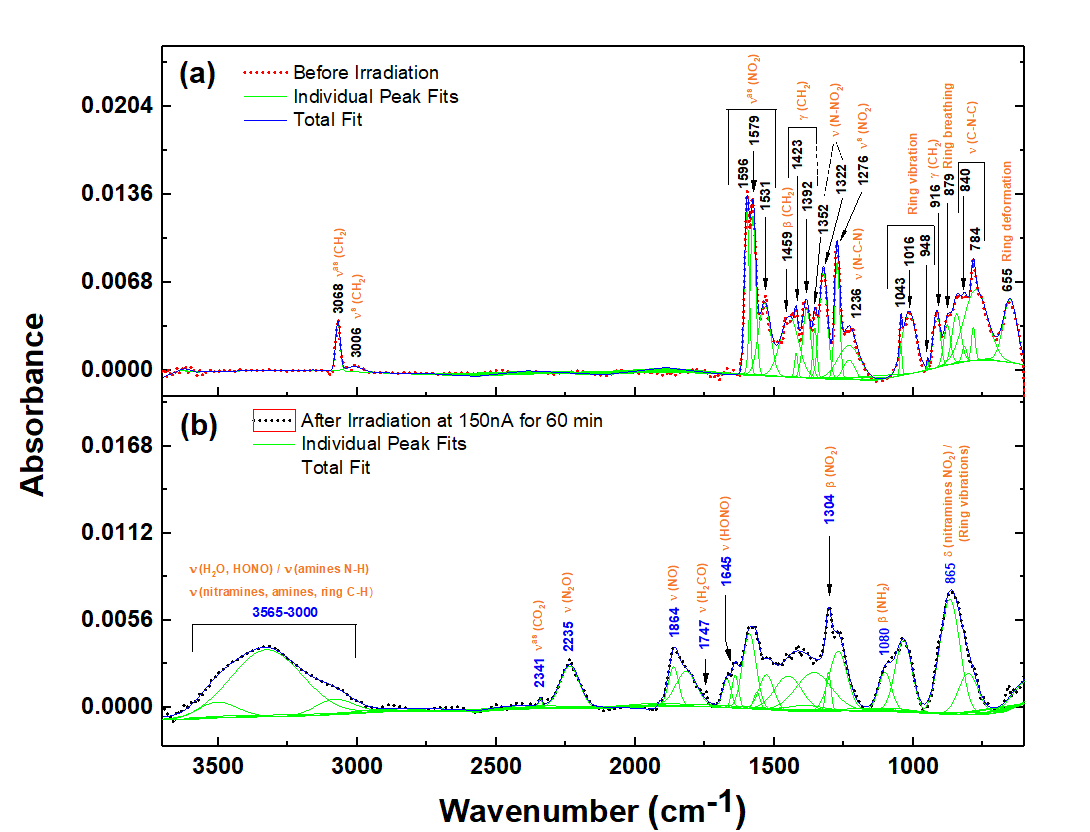


**Scheme 1.** Molecular structure of 1,3,5-trinitro-1,3,5-triazine (RDX).



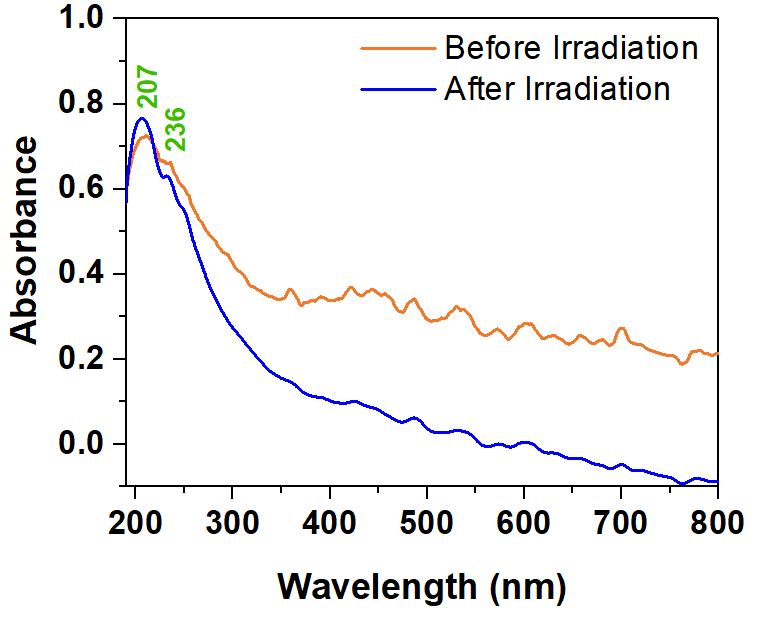
**Figure 1.** Schematic top view of the ultra-high vacuum chamber including the radiation sources (electron source), analytical instruments (FTIR, UV-VIS, ReTOF), and cryogenic target (point of convergence lines).46-48



**Figure 2.** Infrared spectra of RDX collected at 5 K (a) before and (b) after the irradiation of the high dose experiment.

**C:\Users\Ralf I. Kaiser\Desktop\Figure_3.tif**

**Figure 3.** Structures of the decomposition products detected through FTIR spectroscopy.



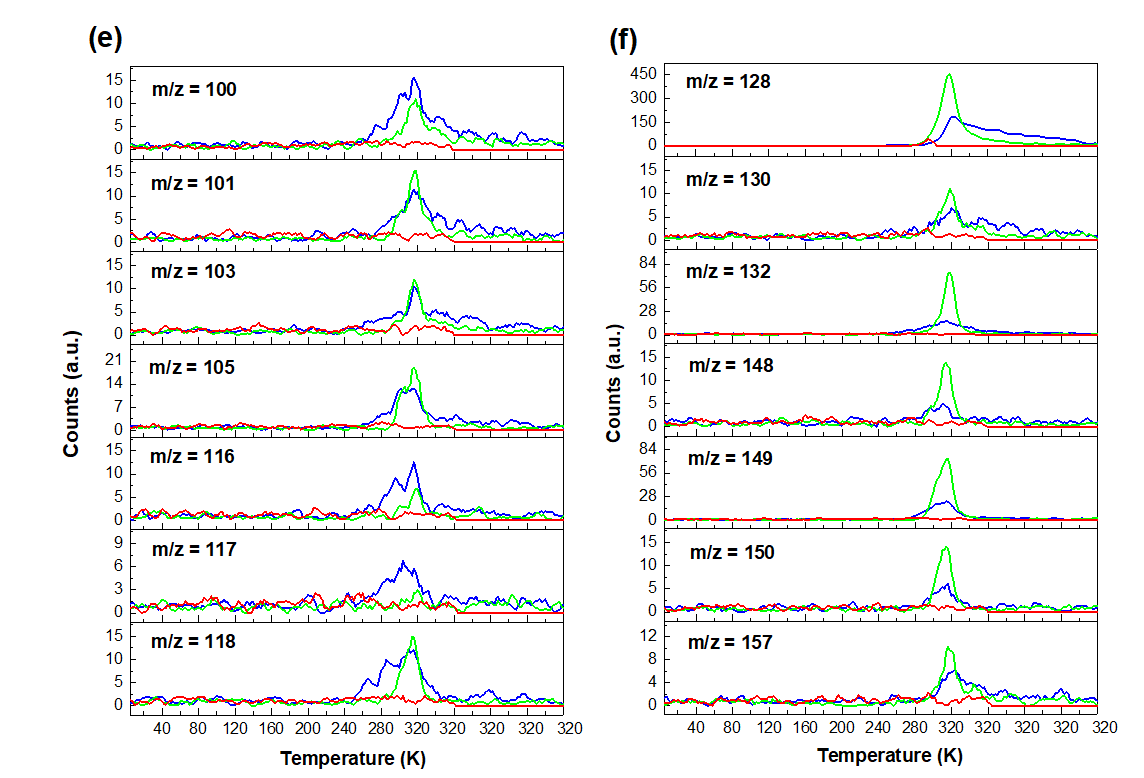
**Figure 4.** UV-VIS spectra of RDX collected at 5 K before and after the high dose.



**Figure 5.** Temperature dependent ReTOF data of the decomposition products of RDX for the high dose (a), low dose (b), and blank (c) experiments.



**Figure 6.** TPD profiles of the ion counts recorded at mass-to-charge ratios of (a) 30, 31, 42, 43, 45, 46, (b) 56, 58, 60, 70, 71, 72, (c) 73, 74, 75, 81, 82, 83, and (d) 85, 87, 89, 91, 97 and 98 at a photoionization energy of 10.49 eV. Blue: high does; green: low dose; red: blank.



**Figure 6.** TPD profiles of the ion counts recorded at mass-to-charge ratios of (e) 100, 101, 103, 105, 116, 117, 118, (f) 128, 130, 132, 148, 149, 150 and 157 at a photoionization energy of 10.49 eV. Blue: high does; green: low dose; red: blank.

.

**Figure 7a.** Proposed decomposition mechanism of RDX into products at 157, 150, 149, 148, 132, 130, 128, 117, 97, 87, 85, 83 and 74 amu. Reactions mechanisms predicted by theoretical calculations are color coded in pink. 14, 16, 18, 22



**Figure 7b.** Proposed decomposition mechanism of RDX into products at 118, 116, 105, 103, 101, 100, 98, 91, 89, 75, 73, 72, 71, 70, 60, 58, 56, 46, 45, 43, 42, 31, and 30 amu. Reactions mechanisms predicted by theoretical calculations are color coded in pink.14, 16, 18

**Table 1.** Molecular formula, mass, and ionization energies of decomposition products of RDX previously reported in gas-phase and condensed-phase studies.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Method** | **Products observed** | | | | **References** |
|  | **Formula** | **Name** | **Mass (amu)** | **IE (eV)** |  |
| Photodissociation of RDX at 225 nm in supersonic jet | NO | Nitrogen monoxide | 30 | 9.26 | Im, H.-S. *et al.*8 |
| Photodissociation at 226 nm in supersonic jet | NO | Nitrogen monoxide | 30 | 9.26 | Guo, Y. Q. *et al.* 7 |
| Photodissociation at 226 nm in supersonic jet | NO | Nitrogen monoxide | 30 | 9.26 | Lemire, G. W. et al. 10 |
| NO2 | Nitrogen dioxide | 46 | 8.80 |
| IR multiphoton dissociation in molecular beam | HCN | Hydrogen cyanide | 27 | 13.59 | Zhao, X. *et al.* 9 |
| CO | Carbon monoxide | 28 | 14.01 |
| NO | Nitrogen monoxide | 30 | 9.26 |
| H2CO | Formaldehyde | 30 | 10.88 |
| CH2NN | Diazomethane | 42 | 8.99 |
| N2O | Nitrous oxide | 44 | 12.77 |
| CO2 | Carbon dioxide | 44 | 13.77 |
| NO2 | Nitrogen dioxide | 46 | 8.80 |
| HONO | Nitrous acid | 47 | - |
| C2H4N2 | - | 56 | - |
| C3H3N3 | - | 74 | - |
| CH2N2O2 | s-triazene | 81 | 10.00 |
| C3H4N3 | - | 82 |  |
| C3H5N3 | - | 83 |  |
| C2H4N3O2 | - | 102 |  |
| CH2N3O4 | - | 120 |  |
| C2H4N4O3 | - | 132 |  |
| C2H3N4O4 | - | 148 |  |
| Shockwave Decomposition | NO2 | Nitrogen dioxide | 46 | 8.80 | Miao, M. *et al.* 25 |
| HONO | Nitrous acid | 47 |  |
| Thermal Decomposition | H2O | Water | 18 | 12.80 | Behrens, R. *et al.* 4 |
| NO | Nitrogen monoxide | 30 | 9.26 |
| CH2O | Formaldehyde | 30 | 10.88 |
| N2O | Nitrous oxide | 44 | 12.77 |
| NO2 | Nitrogen dioxide | 46 | 8.80 |
| (CH3)NHCHO | N-Methylformamide | 59 | 9.50 |
| C3H3N3OH | Hydroxytriazine | 98 | - |
| Thermal decomposition | H2O | Water | 18 | 12.80 | Maharrey, S. *et al.* 24 |
| HCN | Hydrogen cyanide | 27 | 13.59 |
| CO | Carbon monoxide | 28 | 14.01 |
| CH2O | Formaldehyde | 30 | 10.88 |
| NO | Nitrogen monoxide | 30 | 9.26 |
| N2O | Nitrous oxide | 44 | 12.77 |
| H2NCHO | N-Formamide | 45 | 10.20 |
| NO2 | Nitrogen dioxide | 46 | 8.80 |
| HONO | Nitrous acid | 47 | - |
| (CH3)3N | Trimethyl amine | 58 | 7.80 |
| (CH3)NHCHO | N-methyl formamide | 59 | 9.05 |
| C2H2N2O | - | 70 |  |
| (CH3)2NCHO | N,N-dimethyl formamide | 73 | 9.55 |
| (CH3)2NNO | N-nitroso dimethylamine, | 74 | 8.69 |
| C3H3N3 | s-triazene | 81 | 10.00 |
| C3H3N3O | oxo-s-triazine | 97 |  |
| C3H4N4O2 | **-** | 128 |  |
| C3H6N6O5 | ONDATA | 206 |  |
| CO2 Laser Pyrolysis | HCN | Hydrogen cyanide | 27 | 13.59 | Botcher, T. R. *et al.* 27 |
| NO | Nitrogen monoxide | 30 | 8.80 |
| N2O | Nitrous oxide | 44 | 12.77 |
| CO2 | Carbon dioxide | 44 | 13.77 |
| N2O4 | Nitrogen dioxide dimer | 92 |  |
| CO2 laser pyrolysis and combustion | H2 | Hydrogen molecule | 2 | 15.44 | Lee, Y. *et al.* 28 |
| H2O | Water | 18 | 12.80 |
| HCN | Hydrogen cyanide | 27 | 13.59 |
| CO | Carbon monoxide | 28 | 14.01 |
| H2CNH | Methyleneimine | 29 | 9.90 |
| NO | Nitrogen monoxide | 30 | 9.26 |
| H2CO | Formaldehyde | 30 | 10.88 |
| HNCO | Isocyanic acid | 43 | - |
| N2O | Nitrous oxide | 44 | 12.77 |
| NO2 | Nitrogen dioxide | 46 | 8.80 |
| C2H4N2 | Diazaethane | 46 |  |
| HONO | Nitrous acid, | 47 | - |
| C2H2N2 | Iminoacetonitrile | 54 | 11.60 |
| C2H2N2O | - | 70 | **-** |
| C3H3N3 | s-triazene | 81 | 10.00 |
| C3H3N3O | oxo-triazine | 97 |  |
| Thermal decomposition: Flash –heating | HNCO | Isocyanic acid | 43 | 11.60 | Gongwer, P. E. *et al.* 29 |
| HONO | Nitrous acid | 47 | - |
| C3H7NO2 | C-hydroxy-N-methylformamide, | 58 |  |
| C3H3N3 | s-triazene | 81 | 10.0 |
| Photodissociation at 248 nm | OH | Hydroxyl radical | 17 | OH | Capellos, C. *et al.* 30 |
| NO | Nitrogen monoxide | 30 | 9.26 |
| NO2 | Nitrogen dioxide | 46 | 8.80 |
| Photodissociation at 248 nm | H2 | Hydrogen | 2 | 15.44 | Dickinson, J. T. *et al.* 34 |
| OH | Hydroxyl radical | 17 | 13.6 |
| H2O | Water | 18 | 12.80 |
| HCN | Hydrogen cyanide | 27 | 13.59 |
| H2CO | Formaldehyde | 30 | 10.88 |
| NO | Nitrogen monoxide | 30 | 9.26 |
| CH2NN | Diazomethane | 42 | 9.00 |
| C2H4N | Ethanenitrilium | 42 |  |
| N2O | Nitrous oxide | 44 | 12.77 |
| C2H4N | Ethanenitrilium | 45 |  |
| NO2 | Nitrogen dioxide | 46 | 8.80 |
| CH2CH2N2 | Diazaoethane | 46 |  |
| CH2NNO2 | Methylene nitramine | 74 |  |
| C3H3N3 | s-triazene | 81 | 10.0 |
| Photolysis at 266 nm | O | Nascent Oxygen | 16 |  | Tang, T. B. *et al.* 31 |
| OH | Hydroxyl radical | 17 | 13.6 |
| CN | Cyanide radical | 26 |  |
| HCN | Hydrogen cyanide | 27 | 13.59 |
| NCN | Cyanonitrene | 40 | - |
| CHNN | Diazomethane radical | 41 | - |
| CH2NN | Diazomethane | 42 | 9.00 |
| NO2 | Nitrogen dioxide | 46 | 8.80 |
| Photolysis at 229 nm | NO2 | Nitrogen dioxide | 46 | 8.80 | Gares, K. L. *et al.* 33 |
| Thermal decomposition at high temperature and pressure | CO2 | Carbondioxide | 44 | - | Connor, L. E. *et al.* 38 |
| N2O | Nitrous oxide | 44 | 12.77 |
| Radiation-induced decomposition in solution | NO2 | Nitrogen dioxide | 46 | 8.80 | Markarov, I. E. *et al.* 26 |
| H2O2 | Hydrogen peroxide | 34 | 12.10 |
| Catalytic thermal decomposition | CO | Carbon monoxide | 28 | 14.01 | Song, N. –M. *et al.* 39 |
| N2 | Nitrogen | 28 |  |
| N2O | Nitrous oxide | 44 | 12.77 |
| NO2 | Nitrogen dioxide | 46 | 8.80 |
| Photodissociation at 236 nm | NO fragments | Nitrogen monoxide | 30 | 9.26 | Wynn, C. M. *et al.* 40 |

**Table 2.** (a) Infrared features of RDX before the irradiation along with (b) new bands observed in the spectrum in the high dose experiment at 5 K.

|  |  |  |  |
| --- | --- | --- | --- |
| (a) Before Irradiation | | | |
| Wavenumber  Observed (cm-1) | Wavenumber  Literature (cm-1)55 | Vibrational  Assignments | Vibrational Modes |
| 3068 | 3068 | νas (CH2) | C-H asymm. stretch |
| 3006 | 3004 | νs (CH2) | C-H symm. stretch |
| 1596 | 1593 | νas (NO2) | NO2 asymm. stretch |
| 1579 | 1576 | νas (NO2) | NO2 asymm. stretch |
| 1531 | 1535 | νas (NO2) | NO2 asymm. stretch |
| 1459 | 1460 | β(CH2) | CH2 Bending in plane |
| 1435 | 1435 | β(CH2) | CH2 Bending in plane |
| 1423 | 1424 | γ(CH2) | CH2 Bending out of plane |
| 1392 | 1391 | γ(CH2) | CH2 Bending out of plane |
| 1352 | 1352 | νs (N-NO2) | N-N symm. stretch |
| 1322 | 1322 | νs (N-NO2) | N-N symm. stretch |
| 1276 | 1275 | νs (NO2) | NO2 symm. stretch |
| 1236 | 1232 | ν(N-C-N) | Ring skeletal vibrations |
| 1218 | 1219 | ν(N-C-N) | Ring skeletal vibrations |
| 1043 | 1040 | νas (Ring) | Ring symm. vibrations |
| 1016 | 1020 | νas (Ring) | Ring symm. vibrations |
| 948 | 947 | νas (Ring) | Ring symm. vibrations |
| 916 | 917 | γ(CH2) | CH2 Bending out of plane |
| 879 | 882 | νs (Ring) | Ring symm. vibration |
| 840 | 844 | ν(C-N-C) | Ring skeletal vibrations |
| 784 | 790 | ν(C-N-C) | Ring skeletal vibrations |
| 655 | 670 | δ(Ring) | Ring deformation |
| (b) After Irradiation | | | |
| 3565-3000 |  | ν(H2O)  ν(HONO)  ν(NH2)  ν(CH2NNO2)  ν(NH2)  ring | O-H stretch of H2O  O-H stretch of HONO  N-H stretch of amines  C-H stretch of nitramines  C-H stretch of amines  C-H stretch of ring |
| 2341 | 234227 | ν(CO2) | C=O stretch of CO2 |
| 2235 | 223727 | ν(N2O) | N=N stretch of N2O |
| 1864 | 186427 | ν(NO) | Free NO stretch |
| 1747 | 174256 | ν(H2CO) | C=O stretch of formaldehyde |
| 1670 |  | ν(Aryl CO) | C=O stretch of aromatic ring |
| 1645 | 164057 | ν(HONO) | N=O stretch of HONO |
| 1304 | 130458 | β(NO2) | NO2 deformation |
| 1080 |  | β (NH2) | NH2 bending modes of amine |
| 865 | 87127 | δ(NNO2) | Deformation modes of nitramines  / ring vibrations |

**Table 3.** Data applied to calculate the average dose per RDX molecule for the low and high dose experiments.

|  |  |  |
| --- | --- | --- |
|  | **(a)** | **(b)** |
| Initial Kinetic energy of the electrons | 5keV | 5keV |
| Irradiation current (I) | 20±2 nA | 150±2 nA |
| Irradiation time (t) | 1800 s | 3600 s |
| Average penetration depth, l | 267±80 nm | 267±80 nm |
| Average kinetic energy of backscattered electrons, Ebsa | 3.6±0.3 keV | 3.6±0.3 keV |
| Fraction of backscattered electrons, fbsa | 0.6±0.1 | 0.6±0.1 |
| Average kinetic energy of transmitted electrons, Etransa, | 0.0 keV | 0.0 keV |
| Fraction of transmitted electrons, ftransa | 0 | 0 |
| Density of the ice, ρ | 1.82 gcm-3 | 1.82 gcm-3 |
| Irradiated area, A | 1.0±0.1 cm2 | 1.0±0.1 cm2 |
| total number of molecules processed | (1.1±0.2)×1018 | (1.6±0.2)×1019 |
| dose per molecule, D | 8.1 ± 1.0 eV | 100 ± 16 eV |
| Total number of electrons | (2.3±1.0)×1014 | (3.4±1.0)×1015 |

a Values from CASINO simulations.

**Table 4.** Molecular formula, structure and ionization energies of the masses observed in ReTOF mass spectrometer via photoionization at 10.49 eV. Masses marked with green color are reported previously by both experiment and theoretical calculations, while the masses marked with blue color are observed only in previous experimental studies and masses marked with red color are supported only through theoretical calculations reported in the literature

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **m/z** | **Molecular formula** | **Structure** | **I.E.**  **(eV)** | **Low Dose** | **High Dose** |
| 30 | NO |  | 9.26 | + | + |
| 31 | HNO |  | 10.1 |  | + |
| CH3NH2 |  | 8.90 |
| 42 | CH2N2 |  | 8.99 |  | + |
| 43 | C2H5N |  | 9.30 |  | + |
|  | 9.20 |
| 45 | CH3NO |  | 10.16 |  | + |
|  | 9.30 |
|  | 10.11 |
| 46 | NO2 |  | 9.58 | + | + |
| 56 | C2H4N2 |  | 8.95 | + | + |
| 58 | CH2N2O |  | - | + | + |
| C2H6N2 |  |  |
| 60 | CH4N2O |  | - |  | + |
| 70 | C3H6N2 |  | - |  | + |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **m/z** | **Molecular formula** | **Structure** | **I.E.**  **(eV)** | **Low Dose** | **High Dose** |
| 71 | C2H5N3 |  |  | + | + |
| 72 | C3H8N2 |  | - | + | + |
| 73 | C2H7N3 |  | - | + | + |
| 74 | CH2N2O2 |  |  | + | + |
| 75 | C2H9N3 |  |  | + | + |
| 81 | C3H3N3 |  | 9.80 | + | + |
| 82 | C3H4N3 |  |  | + | + |
| 83 | C3H5N3 |  |  | + | + |
| 85 | C3H7N3 |  |  | + | + |
| 87 | C3H9N3 |  |  | + | + |
| 89 | CH3N3O2 |  |  | + | + |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **m/z** | **Molecular formula** | **Structure** | **I.E.**  **(eV)** | **Low Dose** | **High Dose** |
| 91 | CH5N3O2 |  |  | + | + |
| 97 | C3H3N3O |  |  | + | + |
| 98 | C2H2N4O |  |  | + | + |
| 100 | C2H4N4O |  |  | + | + |
| 101 | C2H3N3O2 |  |  | + | + |
| 103 | C2H5N3O2 |  |  | + | + |
| 105 | C2H7N3O2 |  |  | + | + |
| 116 | C2H4N4O2 |  |  | + | + |
| 117 | C3H7N3O2 |  |  |  | + |
| 118 | C2H6N4O2 |  |  | + | + |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **m/z** | **Molecular formula** | **Structure** | **I.E.**  **(eV)** | **Low Dose** | **High Dose** |
| 128 | C3H4N4O2 |  |  | + | + |
| 130 | C3H6N4O2 |  |  | + | + |
| C3H6N4O2 |  |  |
| 132 | C3H8N4O2 |  |  | + | + |
|  |  |
| 148 | C2H4N4O4 |  |  | + | + |
| 149 | C2H7N5O3 |  |  | + | + |
| 150 | C2H6N4O4 |  |  | + | + |
| 157 | C3H3N5O3 |  |  | + | + |

**References**

4. Behrens, R.; Bulusu, S., Thermal decomposition of energetic materials. 3. Temporal behaviors of the rates of formation of the gaseous pyrolysis products from condensed-phase decomposition of 1,3,5-trinitrohexahydro-s-triazine (RDX). *J. Phys. Chem.* **1992,** *96*, 8877-8891.

7. Guo, Y. Q.; Greenfield, M.; Bhattacharya, A.; Bernstein, E. R., On the excited electronic state dissociation of nitramine energetic materials and model systems. *J. Chem. Phys.* **2007,** *127*, 154301.

8. Im, H.-S.; Bernstein, E. R., On the initial steps in the decomposition of energetic materials from excited electronic states. *J. Chem. Phys.* **2000,** *113*, 7911-7918.

9. Zhao, X.; Hintsa, E. J.; Lee, Y. T., Infrared multiphoton dissociation of RDX in a molecular beam. *J. Chem. Phys.* **1988,** *88*, 801-810.

10. Lemire, G. W.; Simeonsson, J. B.; Sausa, R. C., Monitoring of vapor-phase nitro compounds using 226-nm radiation: fragmentation with subsequent NO resonance-enhanced multiphoton ionization detection. *Anal. Chem.* **1993,** *65*, 529-533.

14. Chakraborty, D.; Muller, R. P.; Dasgupta, S.; Goddard, W. A., The Mechanism for unimolecular decomposition of RDX (1,3,5-Trinitro-1,3,5-triazine), an ab initio study. *J. Phys. Chem. A* **2000,** *104*, 2261-2272.

16. Schweigert, I. V., Ab initio molecular dynamics of high-temperature unimolecular dissociation of gas-phase RDX and its dissociation products. *J. Phys. Chem. A* **2015,** *119*, 2747-2759.

18. Harris, N. J.; Lammertsma, K., Ab initio density functional computations of conformations and bond dissociation energies for hexahydro-1,3,5-trinitro-1,3,5-triazine. *J. Am. Chem. Soc.* **1997,** *119*, 6583-6589.

22. Irikura, K. K., Aminoxyl (Nitroxyl) radicals in the early decomposition of the nitramine RDX. *J. Phys. Chem. A* **2013,** *117*, 2233-2241.

24. Maharrey, S.; Behrens, R., Thermal decomposition of energetic materials. 5. Reaction processes of 1,3,5-trinitrohexahydro-s-triazine below its melting point. *J. Phys. Chem. A* **2005,** *109*, 11236-11249.

25. Miao, M.; Dreger, Z. A.; Patterson, J. E.; Gupta, Y. M., Shock wave induced decomposition of RDX: Quantum chemistry calculations. *J. Phys. Chem. A* **2008,** *112*, 7383-7390.

26. Makarov, I. E.; Zhestkova, T. P.; Zhukova, T. N., Radiation-induced decomposition of cyclotrimethylenetrinitramine in aqueous solutions. *High Energy Chem.* **2011,** *45*, 89-92.

27. Botcher, T. R.; Wight, C. A., Transient thin film laser pyrolysis of RDX. *J. Phys. Chem.* **1993,** *97*, 9149-9153.

28. Lee, Y.; Tang, C.-J.; Litzinger, T. A., A study of the chemical and physical processes governing CO2 laser-induced pyrolysis and combustion of RDX. *Combust. Flame* **1999,** *117* (3), 600-628.

29. Gongwer, P. E.; Brill, T. B., Thermal decomposition of energetic materials 73: the identity and temperature dependence of “minor” products from flash-heated RDX. *Combust. Flame* **1998,** *115*, 417-423.

30. Capellos, C.; Papagiannakopoulos, P.; Liang, Y.-L., The 248 nm photodecomposition of hexahydro-1,3,5-trinitro-1,3,5-triazine. *Chem. Phys. Lett.* **1989,** *164*, 533-538.

31. Tang, T. B.; Chaudhri, M. M.; Rees, C. S.; Mullock, S. J., Decomposition of solid explosives by laser irradiation: A mass spectrometric study. *J. Mater. Sci.* **1987,** *22*, 1037-1044.

33. Gares, K. L.; Bykov, S. V.; Brinzer, T.; Asher, S. A., Solution and solid hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) ultraviolet (UV) 229 nm photochemistry. *Appl. Spectrosc.* **2015,** *69*, 545-554.

34. Dickinson, J. T.; Jensen, L. C.; Doering, D. L.; Yee, R., Mass spectroscopy study of products from exposure of cyclotrimethylene‐trinitramine single crystals to KrF excimer laser radiation. *J. Appl. Phys.* **1990,** *67*, 3641-3651.

38. Connor, L. E.; Morrison, C. A.; Oswald, I. D. H.; Pulham, C. R.; Warren, M. R., Carbon dioxide binary crystals via the thermal decomposition of RDX at high pressure. *Chem. Sci.* **2017,** *8*, 4872-4878.

39. Song, N.-M.; Yang, L.; Han, J.-M.; Liu, J.-C.; Zhang, G.-Y.; Gao, H.-X., Catalytic study on thermal decomposition of Cu-en/(AP, CL-20, RDX and HMX) composite microspheres prepared by spray drying. *New J. Chem.* **2018,** *42*, 19062-19069.

40. Wynn, C. M.; Palmacci, S.; Kunz, R. R.; Clow, K.; Rothschild, M., Detection of condensed-phase explosives via laser-induced vaporization, photodissociation, and resonant excitation. *Appl. Opt.* **2008,** *47*, 5767-5776.

46. Bennett, C. J.; Brotton, S. J.; Jones, B. M.; Misra, A. K.; Sharma, S. K.; Kaiser, R. I., High-sensitivity raman spectrometer to study pristine and irradiated Interstellar Ice Analogs. *Anal. Chem.* **2013,** *85*, 5659-5665.

47. Jones, B. M.; Kaiser, R. I., Application of reflectron time-of-flight mass spectroscopy in the analysis of astrophysically relevant ices exposed to ionization radiation: Methane (CH4) and D4-Methane (CD4) as a case Study. *J. Phys. Chem. Lett.* **2013,** *4*, 1965-1971.

48. Bergantini, A.; Abplanalp, M. J.; Pokhilko, P.; Krylov, A. I.; Shingledecker, C. N.; Herbst, E.; Kaiser, R. I., A combined experimental and theoretical study on the formation of interstellar propylene oxide (CH3CHCH2O)—A Chiral Molecule. *Astrophys. J* **2018,** *860* (2), 108.

55. Infante-Castillo, R.; Pacheco-Londoño, L.; Hernández-Rivera, S. P., Vibrational spectra and structure of RDX and its 13C- and 15N-labeled derivatives: A theoretical and experimental study. *Spectrochim. Acta A* **2010,** *76*, 137-141.

56. Alix, J.; Collins, S., The photochemistry of RDX in solid argon at 10 K. *Can. J. Chem.* **1991,** *69*, 1535-1538.

57. Kagann, R. H.; Maki, A. G., Infrared absorption intensities of nitrous acid (HONO) fundamental bands. *J. Quant. Spectrosc. Radiat. Transf.* **1983,** *30*, 37-44.