Supporting Information

On the Formation of Hydroxylamine in Low-Temperature Interstellar Model Ices

Yetsedaw A. Tsegaw,[1] Sándor Góbi,[2,3] Marko Förstel,[2,3,4] Pavlo Maksyutenko,[2,3,5] Wolfram Sander*,[1] and Ralf I. Kaiser*,[2,3]

[1] *Lehrstuhl für Organische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany*

[2] *Department of Chemistry, University of Hawaii at Manoa, 2545 McCarthy Mall, 96822 HI, USA*

[3] *W. M. Keck Research Laboratory in Astrochemistry, University of Hawaii at Manoa, 2545 McCarthy Mall, 96822 HI, USA*

[4] *Present address: Berlin Institute of Technology, IOAP Hardenbergstrasse 36, 10623 Berlin, Germany*

[5] *Present address: Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge MA, USA*

Table S1. Infrared Absorption Features Recorded Before and After the Electron Irradiation of Ammonia−Oxygen (NH_3−O_2) 1:10 Ices at 5.5 K

This Work (cm^{-1})		Literature Value (cm^{-1})	Ref. [b]	Assignment [b]		
Before Irradiation [a]	After Irradiation [a]			Species	Vibration	Characterization
3426m, 3379vs	3418sh, 3378s	3372	1	NH_3	ν_3	Antisymmetric Stretch
3324sh, 3308vs	3308m	3290	1	NH_3	$2\nu_4$	Overtone
3269sh, 3236vs, 3203vs	3236m, 3204m	3212	1	NH_3	ν_1	Symmetric Stretch
…	3135–2976w,b	3209–3074	2, 3	NH_2OH	ν_2	N−H Stretch (Symmetric)
…	2903vw	2848	4	H_2O_2	$\nu_2 + \nu_6$	Combination
…	2936–2656w,vb	2943–2507	2, 3	NH_2OH	$\nu_3 + \nu_4$, $2\nu_4$, $\nu_3 + \nu_5$, $\nu_4 + \nu_8$	Combinations / Overtone
…	2232w	2235	2, 5, 6	N_2O	ν_3	N≡N Stretch
…	2104w	2105	7	O_3	$\nu_1 + \nu_3$	Combination
…	1875w	1875	2, 6, 8, 9	NO	ν_1	Fundamental
…	1836vw	1833–1851	2, 6, 9	N_2O_3	ν_1	N=O Stretch
…	1727vw	1737	2, 6, 9	$(NO)_2$	ν_1	N=O Stretch (Antisymmetric)
1646m, 1624m	1643w, 1624w	1628	1	NH_3	ν_4	Degenerated Deformation
…	1610m	1614	5	NO_2	ν_3	N=O Stretch (Antisymmetric)
1560w	1560vw	1549	7	O_2	ν_1	Fundamental
…	1507w	1507	2, 10, 11	HNO	ν_2	HNO Bend
…	1494w,b	1486	2-3	NH_2OH	ν_4	NOH Bend
…	1386w,b	1389	4	H_2O_2	ν_6	Antisymmetric Bend
…	1303w,b	1303	2, 6, 9	N_2O_3	ν_3	NO_2 Stretch (Symmetric)
…	1230vw	1240	12	N_2O_2	ν_1	NO_2 Stretch (Symmetric)
…	1100m,b	1144	2, 3	NH_2OH	ν_5	NH_2 Wag
1053m, 1025m, 981sh	1031m,b	1097	1	NH_3	ν_2	Symmetric Deformation
…	1036s	1037	7	O_3	ν_3	Antisymmetric Stretch
…	798vw	880	12	N_2O_2	ν_2	N−N Stretch
…	703vw	702	7	O_3	ν_2	Bend

[a] Band intensities, vs: very strong, s: strong, m: medium, w: weak, vw: very weak, sh: shoulder, b: broad, vb: very broad. [b] Assignment based on references.

Table S2. Mass Balance of the Ammonia−Oxygen (NH_3−O_2) 1:10 Ice Sample as well as that of the Irradiation Products Determined from their Experimental IR Decay/Growth Curves at 5.5 K

Process	Decay Product	Number of Molecules Produced/Decomposed During Irradiation
$NH_3 \rightarrow X$		$(6.9 \pm 0.7) \times 10^{16}$
Fraction of NH_3 degraded		95 ± 20%
$O_2 \rightarrow O$	O	$(5.0 \pm 0.5) \times 10^{17}$
Fraction of O_2 degraded		88 ± 19%
Number of molecules in sample after irradiation	NH_2OH	$(3.6 \pm 0.2) \times 10^{16}$
	O_3	$(1.2 \pm 0.5) \times 10^{16}$
	NO	$(7.3 \pm 0.1) \times 10^{15}$
	$(NO)_2$	$(5.0 \pm 0.5) \times 10^{14}$
	N_2O_2	$(1.2 \pm 0.6) \times 10^{14}$
	NO_2	$(9.6 \pm 0.4) \times 10^{14}$
	H_2O_2	$(4.2 \pm 0.6) \times 10^{14}$
	N_2O	$(3.8 \pm 0.1) \times 10^{14}$
	N_2O_3	$(1.2 \pm 0.1) \times 10^{14}$
	HNO	$(< 6.0 \pm 4.1) \times 10^{13}$
	H_2O	$(< 3.1 \pm 0.2) \times 10^{13}$
Nitrogen balance [a]		66 ± 7%
Oxygen balance [b]		6 ± 1%

[a] Fraction of nitrogen atoms originating from ammonia destruction that are needed for the formation of the irradiation products. [b] Fraction of oxygen atoms originating from molecular oxygen destruction that are needed for the formation of the irradiation products.

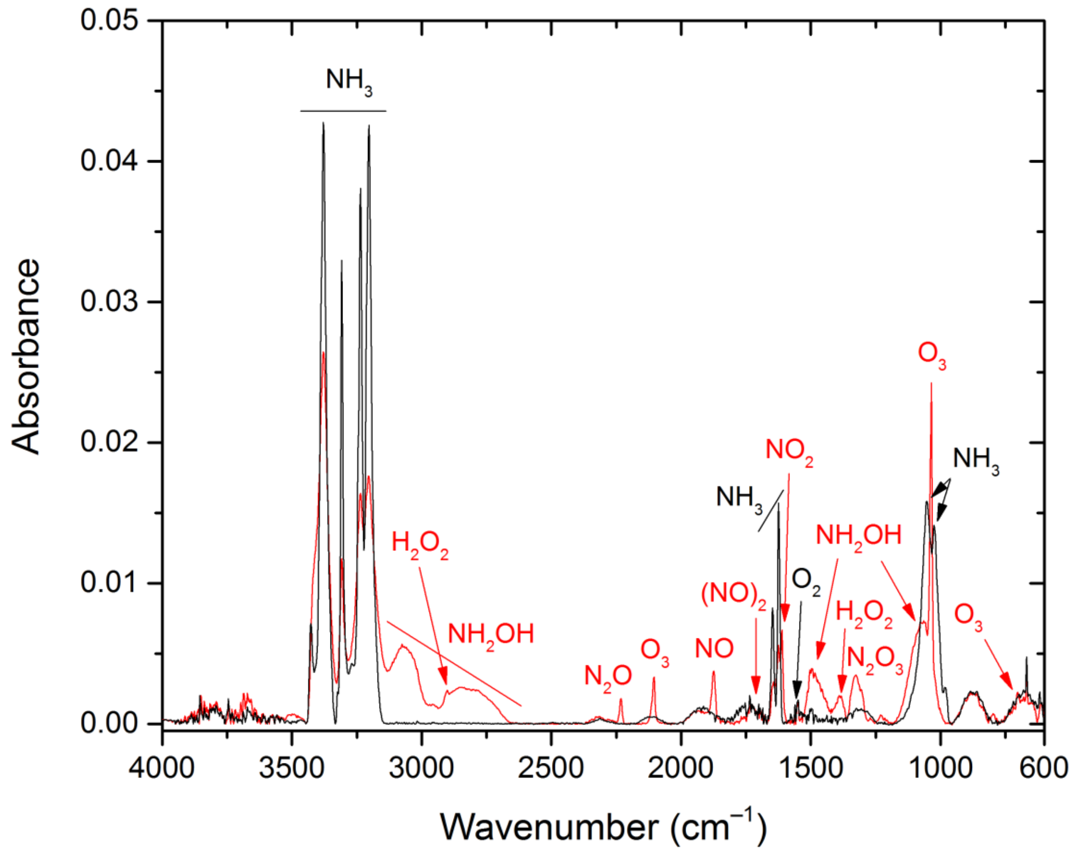

Figure S1. Infrared spectrum of the ammonia−oxygen (NH_3−O_2) 1:10 ice at 5.5 K before (black line) and after (red line) 5 keV electron irradiation with the most important radiolysis products marked. The infrared assignments before and after the irradiation are compiled in Table S1.

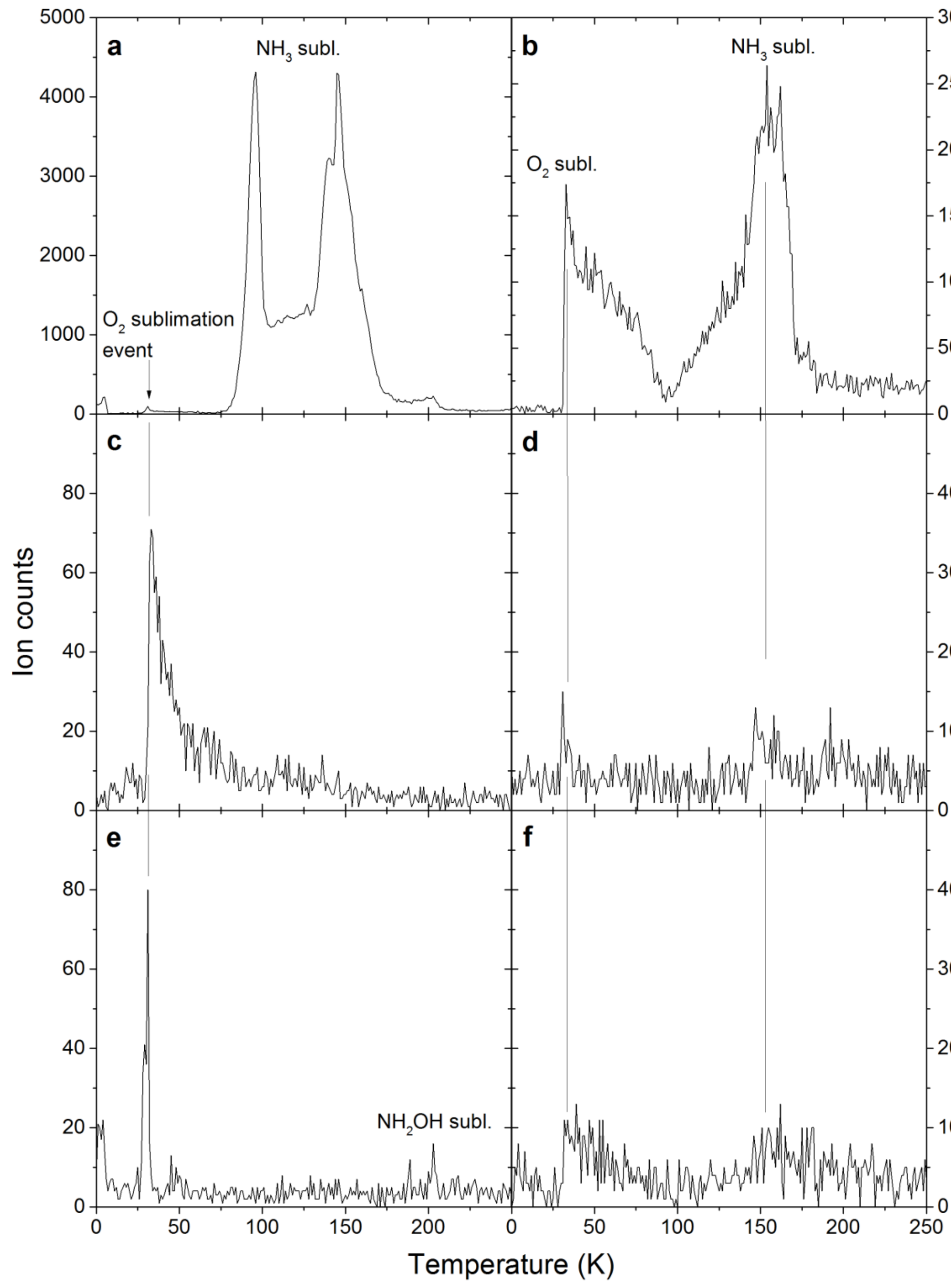

Figure S2. Selected TPD profiles of (a) *m/z* = 17 (NH_3^+), (b) *m/z* = 30 (NO^+), (c) *m/z* = 35 (NH_3–H_2O^+), (d) *m/z* = 31 (HNO^+), (e) *m/z* = 33 (NH_2OH^+), and (f) *m/z* = 46 (NO_2^+) subliming from the irradiated ammonia–oxygen (NH_3–O_2) 1 : 10 ice recorded at photoionization energies of 10.49 eV.

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