

Production of Oxygen in Ice

Introduction

Although the radiolysis and photolysis of ice is an old subject, in 1982 we first suggested that it was important in the production of oxygen atmospheres on the icy Galilean satellites. Such atmospheres were confirmed to be present in 1998 and oxygen and ozone were observed to be present as trapped species in ice around the same time.

In 2003 we developed the first chemical model that is consistent with laboratory data for production of O₂ in ice due to incident UV photons, low energy electrons and energetic ions. Since the production rates depend on sample formation, radiation history, sample temperature, and radiation type and energy, listing all of the data would be inappropriate. Therefore, below we described an approximate quantitative model that roughly fits the data. We also give parameters for a number of radiation types and the physical basis for these parameters.

Model

At low radiation doses, the production and trapping of O appears to be the precursor step needed for forming molecular oxygen in ice. O₂ is formed by the production of a subsequent O (or OH) that interacts with the trapped O. The initially trapped O is called the precursor. Its formation depends on the defect density and density of competing reaction sites (e.g. trapped sulfur, carbon or nitrogen species). Since trapped O can be converted to peroxide and peroxide converted to trapped O, after high dose, O₂ can also be formed efficiently from excitation of peroxide dimers in peroxide inclusions.

The yield, Y, is defined as the number of O₂ molecules per incident particle (ion, electron or photon). Since O₂ production from ice requires the formation of a precursor, the yield at low radiation doses can be written roughly as

$$Y \approx Y_{\max} \exp[-\sigma \Phi] \quad (1)$$

Here σ is the damage cross section for the precursor and Φ is the irradiation time given as a fluence (particles incident per unit area per unit time onto the sample). $[\sigma_p \Phi]$ can also be written as $[D/D_0]$, where D is the radiation dose (energy / volume) and D₀ a parameter. The quantities σ_p and D₀ are roughly independent of T below ~ 140 K. The simple form in Eq. 1 gives a rough fit to the yield vs. fluence at low doses (Table I).

The steady state value of the yield is

$$Y_{\max} \approx N \sigma_p \sigma_{O_2} / \sigma \quad (2)$$

Here N is the larger of the escape depth for O₂ formed, the thickness of the sample, and the penetration depth of the radiation. It is given as the number of water molecules per unit area from which O is formed and escapes. σ_p is the cross section for production of the precursor (e.g. trapped O) and σ_{O_2} is the production of O₂ from the precursor. Using chemical rate equations, Y_{max} can be written as

$$Y_{\max} \approx N [\sigma_O^2 / \sigma_H] \times \zeta \\ \zeta \approx [\sigma_{O,O_t} / \sigma_{H,O_t}] [L_t / L_R]$$

Here σ_O is the cross section for H₂O → O + H₂; σ_H is the cross section for H₂O → O + OH; σ_{O,O_t} and σ_{H,O_t} are the cross sections for mobile O and H interacting with trapped O_t; L_t is the mean distance for a mobile O to trap at a defect in ice, and L_R is the mean distance for a mobile H to react with an impurity or a dissociation product. ζ depends primarily on the trap density via L_t and the first set of brackets in ζ is of the order of unity. The trap density in turn depends on the sample formation temperature, T_s, and on the amount of radiation damage. Therefore, laboratory data show that

$$\zeta \approx \zeta_0 \exp[-E_a / kT_s]$$

Here E_a is the defect formation energy: $\sim 0.02 - 0.03$ eV for lightly damaging radiations, with E_a increasing to ~ 0.07 eV for highly damaging radiation.

FITS TO DATA

Radiation	E(eV)	T(K)	σ^*	σ_H	Y_∞	E_a (eV)
e	30 – 100	110	0.8 – 3	1		0.02 – 0.03
h ν	~ 10	~ 10	> 0.1	0.09		0.03
H $_e^+$	10^6					0.03
N $_e^+$	1.5×10^6	10	62	$< \sim 35$		0.02 – 0.07
Av $^+$	10^4					

