American Mineralogist, Volume 84, pages 1461–1463, 1999

Structural environment of krypton dissolved in vitreous silica

REINHARD WULF,^{1,*} GEORGE CALAS,¹ ALINE RAMOS,¹ HEINZ BÜTTNER,² KNUT ROSELIEB,² AND MATTHIAS ROSENHAUER^{2,}[†]

¹Laboratoire de Minéralogie-Cristallographie, UMR CNRS 7590, Universités de Paris 6 et 7 and Institut de Physique du Globe de Paris, 4 place Jussieu, 75252 Paris, France

²Mineralogisch-Petrologisches Institut der Universität Göttingen, V.M. Goldschmidt Strasse 1, 37077 Göttingen, Germany

ABSTRACT

X-ray absorption measurements on Kr dissolved homogeneously in vitreous silica (1.97 wt% Kr) have been carried out at the Kr K-edge at 4.5 K, representing the first direct determination of the sites occupied by a noble gas. The presence of EXAFS oscillations shows that the Kr atoms are surrounded by a well-defined shell of nearest neighbors, identified as oxygen atoms. The mean Kr-O distances are 3.45 ± 0.1 Å, based on a simple model of Gaussian disorder, with a Debye-Waller factor of $\sigma^2 = 0.06$ Å². The large Kr-O distance, which is at the upper limit of the size of the holes existing in vitreous silica, together with the existence of well-defined sites suggests a forced, densely packed environment of oxygen around Kr atoms characteristic of clathrasil surroundings.