

A

氢-水同位素交换分离因子理论计算

@钟正坤\$中国工程物理研究院核物理与化学研究所!四川绵阳621900 @张莉\$四川大学原子分子物理研究所!四川成都610065 @孙颖\$中国工程物理研究院核物理与化学研究所!四川绵阳621900 @陈银亮\$中国工程物理研究院核物理与化学研究所!四川绵阳621900 @朱正和\$四川大学原子分子物理研究所!四川成都610065

收稿日期 2003-5-27 修回日期 网络版发布日期:

摘要 采用量子化学从头计算法计算得到氢-水同位素交换体系 $\text{HDg}/\text{H}_2\text{O}$ 和 $\text{DTg}/\text{D}_2\text{O}$ 在 0.1MPa、283.2~373.2K下的气相反应平衡常数,并根据相应同位素水的饱和蒸气压求得气-液交换过程的分离因子,得出了两种氢-水同位素交换体系总反应分离因子。

关键词 [氢同位素交换](#) [分离因子](#) [理论计算](#)

分类号 [TL278](#) [TQ131.11](#)

Calculation of the Separation Factors for Hydrogen and Water Isotopic Exchange Reaction

ZHONG Zheng-kun¹, ZHANG Li², SUN Ying¹, CHEN Yin-liang¹, ZHU Zheng-he²
(1. Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, P.O.Box 919-214, Mianyang 621900, China; 2. Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China)

Abstract The equilibrium constants K_g for the isotopic exchange reactions between hydrogen and water vapor are calculated using the ratios of partition functions of the molecules of reactants and products. Saturation vapor pressures of the isotopic waters are adopted to evaluate the separation factors α_{g-l} for the isotopic exchange reactions between water vapor and liquid water. Eventually, the K_g and the α_{g-l} give the total separation factors α_{tol} for the isotopic exchange reactions between hydrogen and liquid water. Here we present the calculation results of the HD-H₂O and DT-D₂O isotopic exchange reactions in the temperature range of 283.2~373.2 K at the pressure 0.1 MPa.

Key words [hydrogen isotopic exchange](#) [separation factor](#) [theoretical calculation](#)

DOI

通讯作者

扩展功能

本文信息

▶ [Supporting info](#)

▶ [\[PDF全文\]\(236KB\)](#)

▶ [\[HTML全文\]\(0KB\)](#)

▶ [参考文献](#)

服务与反馈

▶ [把本文推荐给朋友](#)

▶ [文章反馈](#)

▶ [浏览反馈信息](#)

相关信息

▶ [本刊中 包含“氢同位素交换”的相关文章](#)

▶ [本文作者相关文章](#)