22nd International Conference on
Diffusion in Solids and Liquids
22 TO 26 JUNE 2026 | RHODES, GREECE

ABSTRACT:

Infrared Spectroscopic Study of Nuclear Spin Conversion in a Solid Parahydrogen Matrix

K. Yamakawa,
Advanced Science Research Center, Japan Atomic Energy Agency, Japan

Hydrogen molecules exist as two kinds of nuclear spin isomers depending on the total spin (I) of their protons: ortho (I = 1) and para (I = 0). Dictated by the Pauli exclusion principle, the rotational quantum number (J) is restricted to odd integers for the ortho isomer and even integers for the para isomer. Under cryogenic conditions where H2 condenses, these isomers predominantly settle into their lowest rotational states, meaning para H2 occupies J = 0 while ortho H2 occupies J = 1. Solid para H2 is widely recognized as a quantum solid and is often referred to as an ideal matrix. Thanks to its substantial zero-point vibrational amplitude and the absence of a permanent multipole moment, it can encapsulate guest particles, such as molecules, radicals, ions, and clusters, with minimal interaction or perturbation. While the para H2 matrix isolation technique has been widely utilized to investigate the nuclear spin interconversion of CH3X species (where X = H [1], F [2], OH [3]), the conversion between the ortho and para isomers of methyl iodide (CH3I) has not yet been documented. CH3I is of great importance in astrochemistry because its photodissociation generates the CH3 radical, a critical precursor in the formation of hydrocarbons [4]. In this research, we utilized in situ infrared absorption spectroscopy to observe the nuclear spin conversion and photolysis of CH3I isolated within solid para H2 at 3.6 K. The upcoming presentation will detail the effects of thermal annealing, oxygen doping, and the diffusion of residual ortho H2 on the infrared spectrum.

[1] Y. Miyamoto, M. Fushitani, D. Ando, and T. Momose, J. Chem. Phys. 128, 114502 (2008).
[2] Y. P. Lee, Y. J. Wu, and J. T. Hougen, J. Chem. Phys. 129, 104502 (2008).
[3] Y. P. Lee, Y. J. Wu, R. M. Lees, L. H. Xu, and J. T. Hougen, Science 311, 365 (2006).
[4] M. Fushitani and T. Momose, J. Chem. Phys. 116, 10739 (2002).