EXPERIMENTAL AND THEORETICAL INVESTIGATIONS OF HBr+He ROTATIONAL ENERGY TRANSFER

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Optically pumped HBr lasers are currently being investigated to evaluate their potential for high-energy laser applications. Vibrational cascade lasing from molecular HBr at wavelengths near 4-μm has been demonstrated when the 3-0 vibrational overtone was excited by a Nd:YAG laser (Kletecka et al. IEEE J. Quant. Electron. 40, 1471 (2004)). Lasing was observed on various rotational lines of the 3-2 and 2-1 bands. For computational modeling and optimization of the HBr laser, state-to-state rotational energy transfer rate constants are needed for HBr+HBr and HBr+He collisions. The present work is focused on the latter.

Rotational energy transfer in HBr+He collisions was investigated using an ionization-detected pump-probe double resonance technique at ambient temperature. Rotational state selective excitation of $v = 1$ for $J = 0 - 8$ was achieved using a pulsed infrared OPO/OPA system, and the time evolution of HBr ($v = 1$, J) was monitored using 2+1 resonantly enhanced multiphoton ionization (REMPI) spectroscopy via the $g^3\Sigma^-$-$X^1\Sigma^+$ (0-1) band. The experimental data was simulated by fitting to numerical solutions of a set of coupled differential equations describing the full relaxation processes. State-to-state rate constant matrices were generated using fitting and scaling laws. State-to-state rotational transfer rate constants were also calculated using a HBr+He potential energy surface (obtained using the CCSD(T) level of theory) and quantum scattering calculations. Comparisons of experimental and theoretical results will be presented.