

MICROWAVE SPECTROSCOPY AND POTENTIAL ENERGY SURFACES OF Ne-OH and Kr-OH

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Three-dimensional potential energy surfaces for Ne-OH/OD and Kr-OH/OD have been determined from the data by Fourier-transform microwave spectroscopy with fine and hyperfine structures. For Ne-OH, data of rovibrational transitions between the levels with $P = 0.5$ and 1.5 have been utilized as well as those of the pure rotational transitions. Simultaneous least-squares analyses utilizing the data of the two isotopologues were performed, where all the freedom of motions for an atom-diatom system in the Jacobi coordinate, R , θ , and r , were considered. The initial values for the least-squares analyses were obtained by high-level *ab initio* calculations at the UCCSD(T)-F12 theory with the basis set of aug-cc-pV5Z for Ne-OH and aug-cc-pVQZ for Kr-OH. Dependences of the intermolecular interaction energy on the bond length of the OH monomer of the two complexes are compared with that of Ar-OH^b, where the interaction potential of Ar-OH has been redetermined using the new initial potential parameters by UCCSD(T)-F12/aug-cc-pV5Z.

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