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Construction and analysis of dimensionally reduced potential energy surface of S_4 and its vibrational states[1] IGOR GAYDAY, DMITRI BABIKOV, Marquette University — Electronic structure calculations are carried out for S_4 molecule at the CCSD(T)-F12a/VTZ-F12 level of theory to map out its potential energy surface that possesses a double-well shape with low-energy barrier. Two degrees of freedom are considered, the distance R and the angle α between two weakly-perturbed S_2 dimers that form S_4. The resultant PES was computed near the bottom of the covalent well exposing transition state barrier energy of about 690 cm^{-1}. Vibrational states are computed on this 2D-surface and assigned quantum numbers based on their energies and shapes of wavefunctions. Two progressions of vibrational states are identified: a long progression that develop nodes along the "channels" on the surface, and a shorter progression of states that develop nodes across the "channels". Normal mode analysis indicates that these two modes in S_4 represent a significant mixture of conventional bending and stretching motions. Frequencies of the modes, approximately 180 cm^{-1} and 420 cm^{-1}, are in qualitative agreement with earlier *ab initio* studies of S_4, and with sparse experimental data.

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