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Absorption and resonance emission spectra of $\text{SO}_2(X\ 1A_1/C\ 1B_2)$ calculated from ab initio potential energy and transition dipole moment surfaces

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#	Paper	IF	Citations
26	Doubling of Chebyshev correlation function for calculating narrow resonances using low-storage filter diagonalization. <i>Chemical Physics Letters</i> , 2001 , 336, 143-148	2.5	17
25	CALCULATION OF TRANSITION AMPLITUDES WITH A SINGLE LANCZOS PROPAGATION. <i>Journal of Theoretical and Computational Chemistry</i> , 2002 , 01, 173-185	1.8	35
24	Single-Valued Double Many-Body Expansion Potential Energy Surface of Ground-State SO ₂ . <i>Journal of Physical Chemistry A</i> , 2002 , 106, 556-562	2.8	23
23	A realistic double many-body expansion potential energy surface for SO ₂ (X ¹ A ₁) from a multiproperty fit to accurate ab initio energies and vibrational levels. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002 , 58, 629-47	4.4	33
22	Probing highly excited vibrational eigenfunctions using a modified single Lanczos propagation method: Application to acetylene (HCCH). <i>Journal of Chemical Physics</i> , 2003 , 118, 7273	3.9	29
21	THEORETICAL STUDIES OF $\tilde{A}^1 A^{\prime}$ RESONANCE EMISSION SPECTRA OF HCN/DCN USING SINGLE LANCZOS PROPAGATION METHOD. <i>Journal of Theoretical and Computational Chemistry</i> , 2003 , 02, 639-648	1.8	4
20	O(3P _J) Alignment from the Photodissociation of SO ₂ at 193 nm. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 7965-7976	2.8	46
19	The asymptotic region of the potential energy surfaces relevant for the O(3P) + SO(X ³) reaction. <i>Chemical Physics Letters</i> , 2005 , 411, 457-462	2.5	3
18	Excited electronic states of the cyclic isomers of O ₂ and SO ₂ . <i>Journal of Physical Chemistry A</i> , 2005 , 109, 11304-11	2.8	17
17	Recursive Solutions to Large Eigenproblems in Molecular Spectroscopy and Reaction Dynamics. <i>Reviews in Computational Chemistry</i> , 2007 , 285-348		73
16	Rather exotic types of cyclic peroxides: heteroatom dioxiranes. <i>Chemical Reviews</i> , 2007 , 107, 3247-85	68.1	57
15	Theoretical studies of . <i>Chemical Physics Letters</i> , 2007 , 439, 280-283	2.5	36
14	Emission spectrum and relaxation kinetics of SO ₂ induced by 266 nm laser. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010 , 77, 141-5	4.4	4
13	Theoretical studies of absorption cross sections for the C (1)B(2)-X (1)A(1) system of sulfur dioxide and isotope effects. <i>Journal of Chemical Physics</i> , 2010 , 132, 024301	3.9	30
12	Mass-independent fractionation of sulfur isotopes during broadband SO ₂ photolysis: Comparison between ¹⁶ O- and ¹⁸ O-rich SO ₂ . <i>Chemical Geology</i> , 2013 , 362, 56-65	4.2	16
11	Non-adiabatic and intersystem crossing dynamics in SO ₂ . II. The role of triplet states in the bound state dynamics studied by surface-hopping simulations. <i>Journal of Chemical Physics</i> , 2014 , 140, 204302	3.9	58
10	Millimeter-wave optical double resonance schemes for rapid assignment of perturbed spectra, with applications to the C (1)B(2) state of SO ₂ . <i>Journal of Chemical Physics</i> , 2015 , 142, 144201	3.9	17

9	New ab initio adiabatic potential energy surfaces and bound state calculations for the singlet ground X (1)A1 and excited C (1)B2(2(1)A(0)) states of SO2. <i>Journal of Chemical Physics</i> , 2016 , 144, 174301	3.9	13
8	The origin of unequal bond lengths in the C (1)B2 state of SO2: Signatures of high-lying potential energy surface crossings in the low-lying vibrational structure. <i>Journal of Chemical Physics</i> , 2016 , 144, 144313	3.9	9
7	Observation of b2 symmetry vibrational levels of the SO2 C (1)B2 state: Vibrational level staggering, Coriolis interactions, and rotation-vibration constants. <i>Journal of Chemical Physics</i> , 2016 , 144, 144311	3.9	12
6	ExoMol molecular line lists LXIV. The rotation-vibration spectrum of hot SO2. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016 , 459, 3890-3899	4.3	47
5	Final State Resolved Quantum Predissociation Dynamics of SO(C B) and Its Isotopomers via a Crossing with a Singlet Repulsive State. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 4930-4938	2.8	6
4	First-principles C band absorption spectra of SO and its isotopologues. <i>Journal of Chemical Physics</i> , 2017 , 146, 154305	3.9	6
3	Ro-vibronic transition intensities for triatomic molecules from the exact kinetic energy operator; electronic spectrum for the C B \leftarrow X A transition in SO. <i>Journal of Chemical Physics</i> , 2017 , 147, 094305	3.9	5
2	Isotope shifts and band progressions in SO2 rovibrational energy levels: using quantum theory to extract rotational constants. <i>Molecular Physics</i> , 2019 , 117, 2456-2469	1.7	3
1	Accurate characterization of the lowest triplet potential energy surface of SO with a coupled cluster method. <i>Journal of Chemical Physics</i> , 2019 , 150, 144303	3.9	1