

Electronic excitation cross sections of H₂S by electron impact

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Abstract. We report calculated differential and integral cross sections for excitations leading to the three lowest triplet excited states from the ground state of H₂S by electron impact for incident energies ranging from near-threshold to 50 eV. A distorted-wave approximation is used in the present study. Some resonance-like structures are seen in our calculated integral cross sections and their probable physical origins are discussed. Unfortunately, the lack of reported experimental and other theoretical results seriously limits the discussion.

1. Introduction

Electronic excitation cross sections for electron scattering by atoms and molecules are of fundamental importance in a great variety of physical and chemical processes and thus their determination has been a subject of continuously increasing experimental and theoretical interest (Trajmar *et al* 1983). Hydrogen sulphide (H₂S) is a particularly interesting molecule and has attracted attention due to its participation in a great number of processes. For example, the presence of H₂S was recently found (Bockelee-Morvan *et al* 1991) in the comet Austin (1989C1) as well as in interstellar molecular clouds (Gulley *et al* 1993). Also, H₂S is known as one of the major pollutants of the Earth's atmosphere which gives the origin of corrosive processes in metals (Rolle *et al* 1993). So e[−]–H₂S collisions may be important for some astrophysical and environmental applications. Moreover, an atmosphere of H₂S is used (Tenne *et al* 1992) in the synthesis of a semiconductor, tungsten sulphide (WS₂), whose molecular structure is identical to fullerene (C₆₀). Also, mixtures of N₂, H₂ and H₂S is used in plasma nitrocarburizing processes (Ruset *et al* 1995). Since H₂S is a very strong polar molecule, its presence in a gas, even as a minor impurity, can have significant effects on the physical properties of the gas, such as the electrical conductivity.

Although measurements of vibrationally resolved and unresolved elastic differential cross sections (DCS) (Rohr 1978, Gulley *et al* 1993) and total cross sections (Sokolov and Sokolova 1981, Szmytkowski and Maciag 1986) as well as calculated elastic DCS and integral cross sections (ICS) (Jain and Thompson 1983, Jain *et al* 1990, Gianturco 1991, Lengsfeld *et al* 1992, Greer and Thompson 1994, Machado *et al* 1995) for electron–H₂S collisions have been reported over the past years, there are no available experimental and theoretical results for electronic excitation of H₂S by electron impact in the literature.

In this work we present a theoretical study of inelastic electron scattering by H_2S molecules. More specifically, we report the DCS and ICS for the lowest $X^1\text{A}_1 \rightarrow {}^3\text{A}_2(2\text{b}_1 \rightarrow 3\text{b}_2)$, $X^1\text{A}_1 \rightarrow {}^3\text{B}_1(2\text{b}_1 \rightarrow 6\text{a}_1)$ and $X^1\text{A}_1 \rightarrow {}^3\text{A}_1(5\text{a}_1 \rightarrow 6\text{a}_1)$ transitions in the H_2S molecule, within the Franck–Condon approximation framework, for incident energies ranging from near-threshold to 50 eV. The 3b_2 and 6a_1 orbitals represent the only two low-lying excited valence-shell orbitals of H_2S . The near ultraviolet spectra of the corresponding singlet excited states in H_2S have been widely studied from both experimental and theoretical viewpoints. The UV spectroscopy of this molecule has revealed a diffuse band lying in the frequency range 37 000 and 62 500 cm^{-1} . This band is attributed to two nearly degenerated valence-shell transitions $X^1\text{A}_1 \rightarrow {}^1\text{A}_2(2\text{b}_1 \rightarrow 3\text{b}_2)$ and $X^1\text{A}_1 \rightarrow {}^1\text{B}_1(2\text{b}_1 \rightarrow 6\text{a}_1)$. Although the former transition is dipole-forbidden in the C_{2v} symmetry, when the symmetry is lowered to C_s , it becomes dipole-allowed and also the potential curve of the excited state in C_s symmetry ($1^1\text{A}''$) becomes dissociative. In consequence of this, the absorptive band is completely structureless below 50 000 cm^{-1} . Above this frequency there is a nearly regular structure due to the bound character of ($2^1\text{A}''$) excited state (${}^1\text{B}_1$ in C_{2v}). To our knowledge however, there is no reported study for the corresponding triplet excited states of these valence orbitals. The lowest triplet excited state ${}^3\text{A}_2$ (in the C_{2v} symmetry) is metastable. This state can be generated either directly by electron impact from the ground state of the molecule or via cascading from higher-lying triplet states. The presence of excited molecules in this triplet state in plasmas, whether they are dissociative or not, can significantly influence the plasma properties. Also, from the theoretical point of view, the calculation of excitation cross sections for triplet excited states is easier than for singlet states since only short-range exchange interactions are involved.

In the present work, the distorted-wave approximation (DWA) (Rescigno *et al* 1974, Fliflet and McKoy 1980, Lee and McKoy 1983, Lee *et al* 1990) is applied for these studies. Despite the development of several solid-based *ab initio* multichannel methods over the past decade (Lima *et al* 1988, Parker *et al* 1991, Branchett *et al* 1990, 1991), their applications to the inelastic e^- -molecule scattering have been restricted to a few molecular targets (Pritchard *et al* 1990, Rescigno and Schneider 1992, Sun *et al* 1992a). In addition, even for a small target such as H_2 , the calculated results of differential and integral excitation cross sections using different multichannel methods show significant discrepancies (Parker *et al* 1991, Branchett *et al* 1990, 1991, Sartori and Lima 1995). For larger molecules, such as C_2H_4 , discrepancies were seen in the calculated excitation cross sections even at the two-state coupling level of approximation (Rescigno and Schneider 1992, Sun *et al* 1992b). On the other hand, some earlier works (Lee *et al* 1990, 1996) have shown that the DWA can in general agree quite well with the calculated results using the multichannel methods at few-channel close-coupling levels (Lima *et al* 1988, Sun *et al* 1992a) for incident energies a few eV above threshold. Also, it is known that the DWA can in general reproduce the angular distribution of DCS although it usually overestimates the magnitude of the cross sections by a factor of 2 to 3. The reliability of the calculated cross sections increases with increasing incident energies. Thus, we hope the present results would help with the qualitative behaviour and quantitative magnitudes that can be expected for these physical quantities.

The organization of this paper is as follows. In section 2, the theory is briefly described and some details of the calculations are presented. Our calculated results and discussion are shown in section 3.

2. Theory and calculation

The details of the basic theory used in this work have already been presented elsewhere (Fliflet and McKoy 1980, Lee *et al* 1990) and will be only briefly described here. Excitation DCS for electron–molecule scattering averaged over the molecular orientations are given by:

$$\frac{d\sigma}{d\Omega} = SM_f \frac{k_f}{k_i} \frac{1}{8\pi^2} \int d\alpha \sin \beta d\beta d\gamma |f(\hat{k}_f')|^2 \quad (1)$$

where the S factor results from summing over the final and averaging over the initial spin sublevels, M_f is the degeneracy factor (except spin) of the final target state, \vec{k}_f' (\vec{k}_i') is the scattered (incident) electron linear momentum in the laboratory-frame (LF) and $f(\hat{k}_f')$ is the LF scattering amplitude. In our study, the direction of the incident electron linear momentum is taken as the LF z -axis and (α, β, γ) are the Euler angles which define the direction of the molecular principal axis. The body-frame (BF) scattering amplitude $f(\hat{k}_f, \hat{k}_i)$ is related to the transition T -matrix elements by the formula:

$$f(\hat{k}_f, \hat{k}_i) = -2\pi^2 T_{fi}. \quad (2)$$

In this calculation the DWA is used to obtain these T -matrix elements. Our DWA is derived using the two-potential formalism, where the projectile–target interaction potential, U , can be split into

$$U = U_1 + U_2 \quad (3)$$

where U_1 describes a part of the interaction potential that can be treated exactly and U_2 is a perturbation. The DWA transition matrix is given by:

$$T_{fi}^{\text{DWA}} = \langle \varphi_1 \chi_{\vec{k}_f}^- | U_2 | \varphi_0 \chi_{\vec{k}_i}^+ \rangle \quad (4)$$

where φ_0 and φ_1 are the initial and the final target wavefunctions, respectively, and $\chi_{\vec{k}_i}^+$ and $\chi_{\vec{k}_f}^-$ are the initial and the final one-electron distorted continuum wavefunctions. These distorted wavefunctions are solutions of the Lippmann–Schwinger equation:

$$\chi_{\vec{k}}^\pm = \Phi_{\vec{k}} + G_0^\pm U_1 \chi_{\vec{k}}^\pm \quad (5)$$

with G_0^\pm being the free-particle Green's operator with outgoing- (G_0^+) or incoming-wave (G_0^-) boundary conditions, and $\Phi_{\vec{k}}$ the plane wavefunction, with linear momentum \vec{k} . As in our previous works (Lee and McKoy 1983, Lee *et al* 1990, 1995), U_1 is taken to be the static-exchange (SE) potential of the initial (ground) state of the target.

Equation (5) is solved using the Schwinger variational iterative method (SVIM) (Lucchese *et al* 1982, Brescansin *et al* 1992). In order to take advantage of the C_{2v} symmetry of the target, symmetry adapted functions $X_{lh}^{p\mu}(\hat{r})$ (Burke *et al* 1972) are used. In these functions, p is an irreducible representation (IR) of the molecular point group, μ is a component of this representation and h distinguishes between different bases of the same IR corresponding to the same value of l . In the C_{2v} symmetry, h corresponds to the magnitude of projections of the angular momentum \vec{l} on the principal molecular axis. Further, the LF scattering amplitude given in equation (1) can be expanded in a j_t basis (Fano and Dill 1972) as

$$f(\hat{k}_f') = \sum_{j_t m_t m_t'} B_{m_t m_t'}^{j_t}(\hat{k}_f') D_{m_t m_t'}^{j_t}(\alpha, \beta, \gamma) \quad (6)$$

where $D_{m_i m_t}^{j_i}(\alpha, \beta, \gamma)$ are the usual rotation matrices (Edmonds 1974), $\vec{j}_i = \vec{l}' - \vec{l}$ is the angular momentum transferred during the collision, and m'_i, m_t are the projections of \vec{j}_i along the laboratory and molecular axes, respectively. The expansion coefficient $B_{m_i m_t}^{j_i}(\hat{k}_f')$ can be expressed as

$$B_{m_i m_t}^{j_i}(\hat{k}_f') = \sum_{l' l m' m} (-1)^m a_{l' m m'}(l' 0 m_t | j_i m_t)(l' m m' | j_i m'_t) Y_{l m_l}(\hat{k}_f') \quad (7)$$

where the dynamical coefficients $a_{l' m m'}$ for the transition from an initial to a final target state can be written in terms of fixed-nuclei partial-wave components of the electronic portion of the DWA T -matrix elements as

$$a_{l' m m'}(f \leftarrow i) = -\left(\frac{\pi}{2}\right) [4\pi(2l' + 1)]^{(1/2)} i^{l' - l} T_{l m l' m'}^{\text{DWA}}. \quad (8)$$

After substituting equation (6) into equation (1) and performing the angular integrations, the LF DCS can be written as

$$\frac{d\sigma}{d\Omega}(f \leftarrow i) = S M_f \frac{k_f}{k_i} \sum_{j_i m_i m'_i} \frac{1}{(2j_i + 1)} |B_{m_i m'_i}^{j_i}(f \leftarrow i, k_i, k_f, \hat{r}')|^2. \quad (9)$$

The electronic configuration of the ground-state H_2S is $1a_1^2 2a_1^2 3a_1^2 1b_1^2 1b_2^2 4a_1^2 2b_2^2 5a_1^2 2b_1^2$, X^1A_1 . The SCF wavefunction is calculated from a standard [2s/6s4p] contracted basis set (Huzinaga 1965) augmented by one s ($\alpha = 0.0335$), three p ($\alpha = 1.120, 0.271$ and 0.0697) uncontracted functions on the hydrogen centres and three s ($\alpha = 0.0507, 0.0171$ and 0.0057), four p ($\alpha = 0.0503, 0.0167, 0.0053$ and 0.0027) and two d ($\alpha = 1.4137$ and 0.3043) uncontracted functions on the sulphur centre. At the experimental equilibrium geometry ($R_{\text{H-S}} = 2.52 a_0$ and $\theta_{\text{H-S-H}} = 92.2^\circ$) (Snyder and Basch 1972), this basis set gives an SCF energy of -398.68 au which compares well with the calculated value of -398.61 au (Cacelli *et al* 1995) and an electric dipole moment of 0.43 au, exactly the same calculated value of Greer and Thompson (1994). The experimental dipole moment is 0.38 au (Gianturco 1991). The same basis set is also used to calculate the $3b_2$ and $6a_1$ excited orbitals using the improved virtual orbital (IVO) approximation (Hunt and Goddard 1974). The calculated vertical excitation energies for the $2b_1 \rightarrow 3b_2$, $2b_1 \rightarrow 6a_1$ and $5a_1 \rightarrow 6a_1$ transitions at the equilibrium geometry of the ground state are $5.69, 6.07$ and 9.27 eV, respectively. The first two vertical excitation energies lie within the diffuse band of $37\,000$ – $62\,500$ cm^{-1} in the UV spectra.

In the SVIM calculations we have limited the partial-wave expansions for both distorted wavefunctions and T -matrix elements up to $l_c = 11$ for each symmetry. All the possible values of $h \leq l$ were retained. In addition, all matrix elements appearing in the calculations were computed using the single-centre technique with radial integrals evaluated using a Simpson quadrature. The basis set of Cartesian Gaussian functions used as an initial guess for the distorted wavefunctions is listed in table 1. Four iterations were needed to yield converged solutions of equation (5).

3. Results and discussion

In figures 1–3 we show the calculated DCS at some selected incident energies for the $2b_1 \rightarrow 3b_2$, $2b_1 \rightarrow 6a_1$ and $5a_1 \rightarrow 6a_1$ transitions in H_2S , respectively. Unfortunately, there is no available experimental or other calculated results in literature for comparison. However, some comments on the calculated results themselves can be made. At incident energies near threshold the angular distributions of DCS are quite isotropic for all studied transitions. The number of oscillations in the DCS curves increases with increasing incident

Table 1. Basis sets used in separable potential.

Scattering symmetry	Centre	Cartesian Gaussian function ^a	Exponents
ka_1	S	s	8.0, 4.0, 2.0, 0.5, 0.1, 0.025
		z	4.0, 2.0, 0.5, 0.05
		x^2, y^2, z^2	1.5, 0.5, 0.1
	H	s	3.2, 1.6, 0.8, 0.2, 0.05
		x, z	0.5, 0.1
ka_2	S	xy	8.0, 4.0, 2.0, 1.0, 0.5, 0.1, 0.025
	H	y	4.8, 1.2, 0.4, 0.1
kb_1	S	y	8.0, 4.0, 2.0, 1.0, 0.5, 0.1, 0.025
		yz	4.0, 2.0, 1.0, 0.5, 0.1, 0.025
	H	y	2.0, 1.0, 0.5, 0.01
kb_2	S	x	8.0, 4.0, 2.0, 1.0, 0.5, 0.1
		xz	4.0, 2.0, 1.0, 0.5, 0.1
	H	s	4.0, 2.0, 1.0, 0.5, 0.1

^a Cartesian Gaussian basis functions are defined as

$$\phi^{\alpha,\ell,m,n,A}(\mathbf{r}) = N(x - A_x)^\ell(y - A_y)^m(z - A_z)^n \exp(-\alpha|\mathbf{r} - \mathbf{A}|^2)$$

with N a normalization constant.

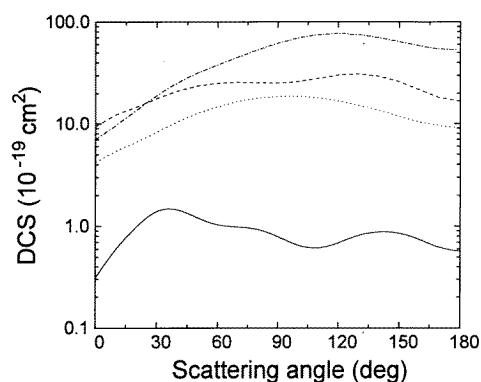


Figure 1. Calculated differential cross sections for the $X^1A_1 \rightarrow ^3A_2(2b_1 \rightarrow 3b_2)$ transition in H₂S by electron impact at 6 eV (dotted curve), 10 eV (chain curve), 20 eV (broken curve) and 50 eV (full curve).

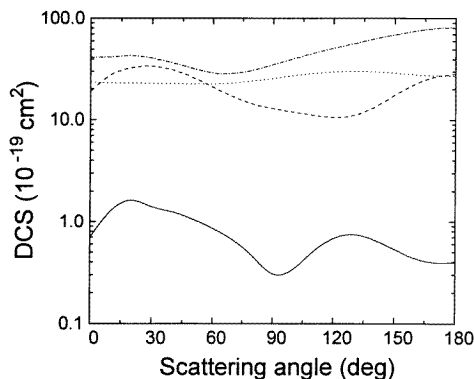


Figure 2. Calculated differential cross sections for the $X^1A_1 \rightarrow ^3B_1(2b_1 \rightarrow 6a_1)$ transition in H₂S by electron impact at 7 eV (dotted curve), 10 eV (chain curve), 20 eV (broken curve) and 50 eV (full curve).

energies. This behaviour is in accordance with the one generally expected for singlet to triplet types of transitions and has also been observed in diatomic (Lee *et al* 1996) and other polyatomic (Lee *et al* 1995) molecules.

Since H₂S is isoelectronic in valence shell with H₂O, figures 4(a) and (b) compare the DCS for the $5a_1 \rightarrow 6a_1$ transition in H₂S with the corresponding ($3a_1 \rightarrow 3sa_1$) transition in H₂O (Lee *et al* 1995) at 20 and 30 eV incident energies, respectively. At both energies, the calculated DCS for the H₂O target show a minimum at scattering angles around 90°, which can be attributed to the dominance of the p-wave contributions whereas the DCS for H₂S show a characteristic d-wave dominant double-well structure. Moreover, the DCS for H₂S lie systematically above those for H₂O at 20 eV whereas, at 30 eV, the DCS for H₂S

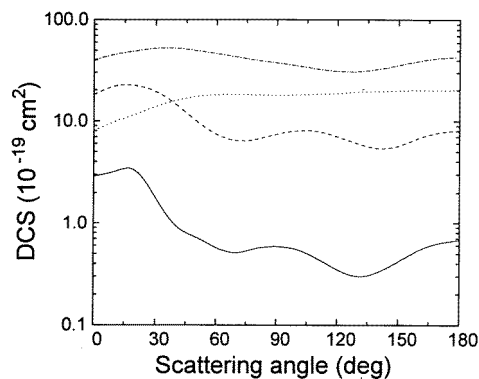


Figure 3. Calculated differential cross sections for the $X^1A_1 \rightarrow {}^3A_1(5a_1 \rightarrow 6a_1)$ transition in H_2S by electron impact at 11 eV (dotted curve), 15 eV (chain curve), 25 eV (broken curve) and 50 eV (full curve).

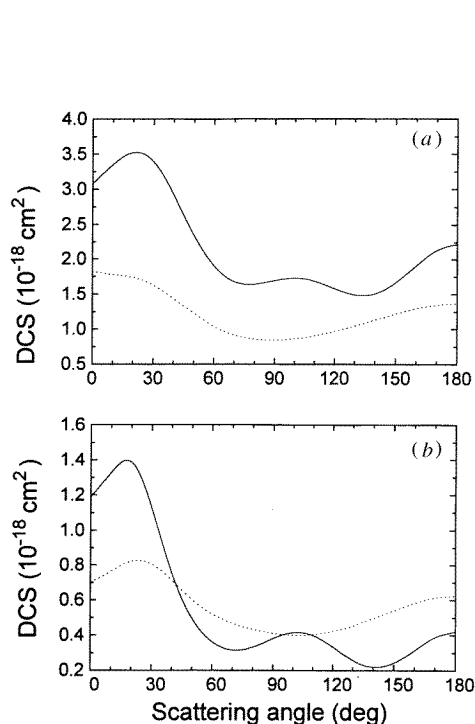


Figure 4. Comparison of the calculated differential cross sections for the $X^1A_1 \rightarrow {}^3A_1(5a_1 \rightarrow 6a_1)$ transition in H_2S with the $X^1A_1 \rightarrow {}^3A_1(3a_1 \rightarrow 3sa_1)$ transition in H_2O by electron impact at (a) 20 eV and (b) 30 eV. Full curve, results for H_2S ; dotted curve, results for H_2O (Lee *et al* 1995).

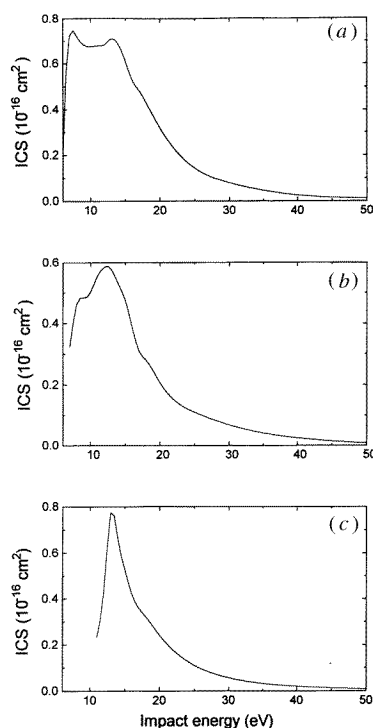


Figure 5. Calculated ICS for the (a) $X^1A_1 \rightarrow {}^3A_2(2b_1 \rightarrow 3b_2)$, (b) $X^1A_1 \rightarrow {}^3B_1(2b_1 \rightarrow 6a_1)$ and (c) $X^1A_1 \rightarrow {}^3A_1(5a_1 \rightarrow 6a_1)$ transitions in H_2S by electron impact.

is larger at small scattering angles.

In figures 5(a)–(c) we show the calculated ICS for the $2b_1 \rightarrow 3b_2$, $2b_1 \rightarrow 6a_1$ and $5a_1 \rightarrow 6a_1$ transitions in H_2S by electron impact in the energy range from near-threshold to 50 eV, respectively. The ICS for the $2b_1 \rightarrow 3b_2$ transition (figure 5(a)) show two resonance-like structures at incident energies of 7.5 and 13 eV. Resonance structures are also seen for the $2b_1 \rightarrow 6a_1$ transition (figure 5(b)) at 8 and 12 eV. For the $5a_1 \rightarrow 6a_1$

transition (figure 5(c)) only one strong resonance lying at incident energy around 13 eV is seen. The similarity of the positions of resonances for the transitions from $2b_1$ bound orbital suggests that they probably have the same physical origin.

In our DWA, both the incoming and outgoing waves are determined in the SE potential field of the initial target state and thus resonance behaviour in the elastic channel would be reflected in the calculated excitation cross sections. In fact, an eigenphase analysis shows one p-wave ($l = 1$) shape resonance in the ka_1 scattering channel located at about 8.5 eV and one d-wave ($l = 2$) in the kb_2 channel at about 4 eV incident energies. These resonances were already seen in our previous study for the low-energy elastic electron- H_2S scattering (Machado *et al* 1995). A d-wave resonance associated with the ${}^2B_2(kb_2)$ scattering channel was also observed in the calculations of Lengsfeld *et al* (1992) and Jain and Thompson (1983), though slightly shifted to lower energies. However, our analysis does not reveal evidences of shape resonances at around 13 eV incident energies.

Therefore, the structures seen at 7.5 eV in the $2b_1 \rightarrow 3b_2$ transition and at 8 eV in $2b_1 \rightarrow 6a_1$ transition can probably be attributed to the ka_1 shape resonance in the initial scattering channel. On the other hand, the structures seen at around 13 eV are not due to the resonances occurring in the initial scattering channel. However, if one subtracts the vertical excitation energies of these transitions from their corresponding resonance positions, the resulting kinetic energies of the scattered electrons are 7.4 eV for the $2b_1 \rightarrow 3b_2$ and $2b_1 \rightarrow 6a_1$ transitions and 3.7 eV for the $5a_1 \rightarrow 6a_1$ transition. Thus, for the transitions from $2b_1$ bound orbital the structures can be attributed to the shape resonance in the ka_1 final scattering channel whereas the structure in the $5a_1 \rightarrow 6a_1$ is possibly due to the kb_2 shape resonance in the final scattering channel. Nevertheless, as discussed by Lee and McKoy (1983), the resonance structures in excitation ICS calculated by DWA can eventually be unphysical. Unfortunately, there is no way to determine whether the resonances in our

Table 2. DCS and ICS (in 10^{-18} cm^2) for the $X^1A_1 \rightarrow {}^3A_2(2b_1 \rightarrow 3b_2)$ transition in H_2S .

Angle (deg)	E_0 (eV)							
	8	12	15	18	20	30	40	50
10	1.55	1.26	1.95	1.62	1.22	0.40	0.11	0.060
20	2.02	1.56	2.30	1.94	1.55	0.48	0.16	0.098
30	2.73	1.94	2.75	2.35	1.96	0.61	0.22	0.139
40	3.59	2.27	3.08	2.75	2.34	0.74	0.26	0.144
50	4.50	2.55	3.21	3.01	2.57	0.84	0.27	0.121
60	5.36	2.84	3.21	3.08	2.64	0.89	0.27	0.103
70	6.13	3.31	3.26	3.04	2.61	0.87	0.28	0.098
80	6.74	4.11	3.60	3.04	2.58	0.78	0.26	0.093
90	7.16	5.30	4.39	3.22	2.64	0.64	0.23	0.079
100	7.35	6.70	5.59	3.65	2.82	0.50	0.18	0.066
110	7.28	8.04	6.93	4.26	3.09	0.43	0.15	0.062
120	6.97	8.99	8.03	4.83	3.36	0.41	0.14	0.069
130	6.44	9.30	8.51	5.13	3.47	0.44	0.15	0.081
140	5.76	8.92	8.23	4.96	3.28	0.44	0.16	0.088
150	5.04	8.01	7.28	4.37	2.79	0.39	0.15	0.085
160	4.42	6.93	6.06	3.55	2.13	0.30	0.12	0.074
170	3.98	6.06	5.05	2.86	1.58	0.21	0.096	0.062
180	3.83	5.73	4.66	2.59	1.36	0.18	0.085	0.057
ICS	72.19	68.37	61.32	44.73	31.79	8.00	2.57	1.16

Table 3. DCS and ICS (in 10^{-18} cm²) for the $X^1A_1 \rightarrow {}^3B_1(2b_1 \rightarrow 6a_1)$ transition in H₂S.

Angle (deg)	E_0 (eV)							
	8	12	15	18	20	30	40	50
10	2.33	7.04	6.37	4.00	2.78	0.72	0.27	0.13
20	2.39	6.80	6.53	4.42	3.25	1.02	0.36	0.16
30	2.45	6.19	6.29	4.48	3.39	1.16	0.33	0.14
40	2.48	5.22	5.54	4.06	3.11	1.17	0.28	0.13
50	2.50	4.16	4.51	3.38	2.61	1.08	0.24	0.11
60	2.58	3.28	3.54	2.68	2.09	0.90	0.20	0.086
70	2.78	2.79	2.82	2.14	1.68	0.67	0.16	0.066
80	3.12	2.71	2.41	1.79	1.42	0.47	0.12	0.045
90	3.58	2.95	2.26	1.60	1.28	0.32	0.086	0.031
100	4.07	3.39	2.28	1.50	1.19	0.24	0.070	0.034
110	4.53	3.94	2.41	1.44	1.11	0.20	0.076	0.050
120	4.85	4.63	2.71	1.46	1.05	0.20	0.095	0.068
130	4.98	5.52	3.28	1.64	1.10	0.22	0.11	0.075
140	4.94	6.64	4.18	2.08	1.32	0.27	0.12	0.066
150	4.77	7.92	5.37	2.78	1.74	0.34	0.13	0.053
160	4.55	9.15	6.60	3.58	2.24	0.42	0.15	0.043
170	4.38	10.06	7.54	4.22	2.67	0.48	0.16	0.040
180	4.31	10.39	7.90	4.47	2.83	0.51	0.17	0.040
ICS	46.40	58.03	47.60	30.15	20.75	6.78	1.94	0.80

Table 4. DCS and ICS (in 10^{-18} cm²) for the $X^1A_1 \rightarrow {}^3A_1(5a_1 \rightarrow 6a_1)$ transition in H₂S.

Angle (deg)	E_0 (eV)							
	12	14	16	18	20	30	40	50
10	1.76	5.84	4.02	3.69	3.35	1.33	0.61	0.32
20	2.24	6.29	4.37	3.93	3.52	1.39	0.66	0.33
30	2.81	6.68	4.58	3.93	3.39	1.13	0.44	0.18
40	3.24	6.77	4.48	3.60	2.92	0.75	0.25	0.094
50	3.45	6.53	4.17	3.12	2.34	0.49	0.17	0.072
60	3.45	6.11	3.82	2.71	1.90	0.36	0.13	0.057
70	3.33	5.64	3.54	2.48	1.67	0.32	0.12	0.051
80	3.22	5.22	3.35	2.40	1.64	0.33	0.12	0.056
90	3.18	4.86	3.17	2.35	1.69	0.38	0.14	0.059
100	3.26	4.54	2.97	2.26	1.73	0.41	0.12	0.055
110	3.46	4.31	2.75	2.12	1.68	0.40	0.089	0.045
120	3.74	4.21	2.59	1.98	1.58	0.33	0.066	0.035
130	4.07	4.30	2.57	1.93	1.49	0.26	0.063	0.030
140	4.39	4.61	2.77	2.06	1.51	0.22	0.085	0.033
150	4.68	5.08	3.13	2.35	1.66	0.24	0.12	0.042
160	4.90	5.60	3.56	2.72	1.91	0.31	0.14	0.054
170	5.04	6.00	3.91	3.03	2.13	0.39	0.15	0.063
180	5.09	6.14	4.04	3.15	2.22	0.42	0.16	0.068
ICS	44.20	66.40	42.48	32.35	24.53	5.68	2.03	0.88

calculated ICS are real and, as far as we know, there is no reported experimental data to confirm the existence of these structures.

For the sake of completeness, numerical values of DCS and ICS for the studied transitions are shown in tables 2–4.

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