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EXCITATION OF THE FIRST FOUR VALENCE STATES OF H₂S BY LOW ENERGY ELECTRONS

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Utilizing the crossed electron-beam molecular-beam scattering technique, energy-loss spectra of H₂S molecule were obtained. The covered energy region was from 4.5 to 10.5 eV (first ionization limit is 10.47 eV [1]). Two distinct regions were observed, the first from 4.5 to 7.0 eV as a continuum and the second from 7.0 to 10.5 eV as discrete states excitation. Excitation of the first valence states ^{3,1}B₁ and ^{3,1}A₂ states was observed as a broad feature. The maximum of the feature moves to the smaller energy-losses when the impact energy is lowered and the scattering angle increased (Fig.1). The excitation occurs in two molecular orbitals: 6a₁, non-bonding mixed valence and Rydberg orbital, and 3b₂, anti-bonding valence orbital. Theoretical calculation of the excitation energies of these states is given in Table 1.

Table 1

transition:	mixed & Rydberg states 2b ₁ → 6a ₁	valence states (4sa ₁)	valence states 2b ₁ → 3b ₂	states
authors	³ B ₁	¹ B ₁	³ A ₂	¹ A ₂
[2] Shih <i>et al.</i> (1976)	5.75	6.13	5.88	6.30
[3] Hatano (1978)	6.14	6.62	6.48	7.02
[4] Roberge and Salahub (1979)	5.39	6.08	5.60	6.89

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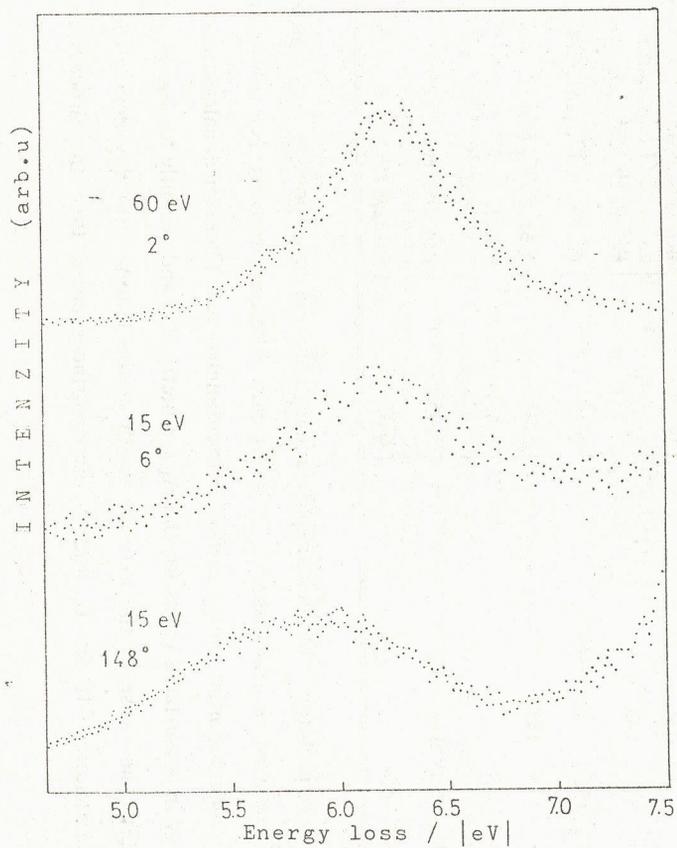


Figure 1.

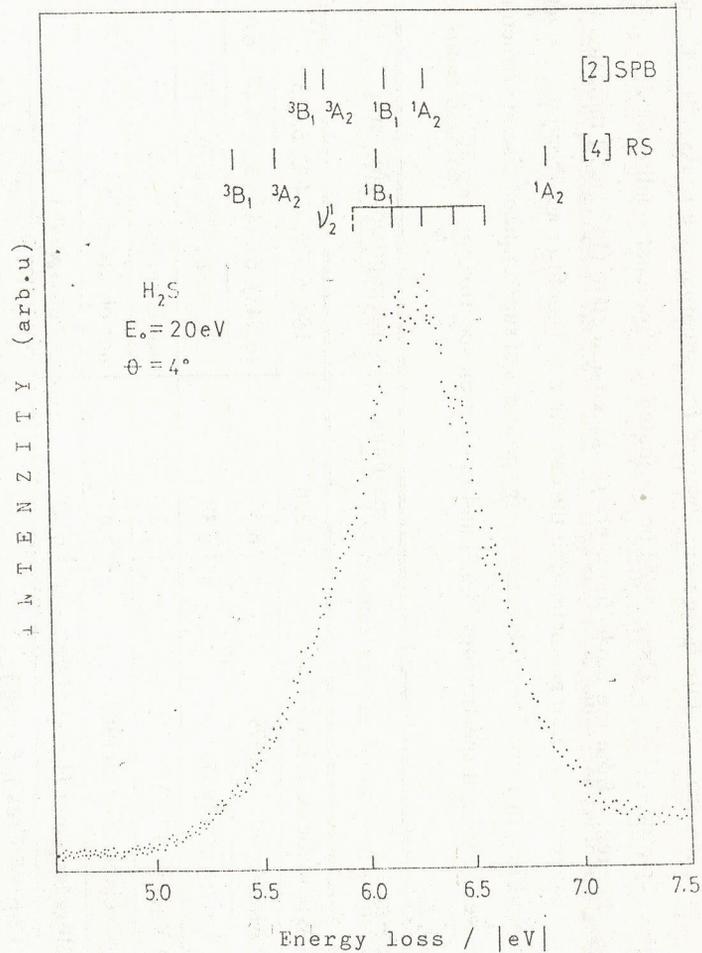


Figure 2.

On the broad feature there were observed four superimposed peaks with 142 meV energy separation (Fig.2). These could be attributed to vibrational bending mode v'_2 . The small difference from the mode frequency of the ground state (147 meV) indicates very small change of molecular geometry after the excitation and confirms non-bonding character of the orbital. In Table 2 are presented energy positions of superimposed discrete structures observed in optical spectroscopy [5,6,7] and in electron spectroscopy [8,9,10].

Table 2.

authors	maximum (eV)	superimposed structures
[5] Watanabe & Jursa(1964)	6.326	6.184, 6.326, 6.468, 6.613
[6] Masuko <i>et al.</i> (1979)	6.47	(6.045), 6.184, 6.326, 6.471, 6.616
[7] Lee <i>et al.</i> (1987)	6.38	6.20, 6.38, 6.57, 6.76, 6.89
[8] Knoop (1972)	5.8	not observed
[9] Cvejanović <i>et al.</i> (1982)	5.6	not observed
[10]Pradeep and Hegde (1988)	6.30	not observed
PRESENT E(eV), θ (deg.)		
10 6	6.15	not observed
10 148	5.91	not observed
15 4	6.17	(6.10), 6.17, 6.31, 6.43, 6.58
15 148	5.95	5.81, 5.95, (6.11)
20 4	6.25	(5.94), 6.12, 6.25, 6.40, 6.57
20 148	5.95	not observed
60 2	6.30	6.15, 6.30

In polyatomic molecular spectra many continua correspond to dissociation processes as there exist several dissociation limits with different products. For nonlinear triatomic molecules potential energy surface is fourdimensional. Theoretical calculation of potential energy hypersurfaces exists for the A_1 symmetry [11] and recently for the B_1 and A_2 states [12,13]. The cause of the extreme width of the feature probably lies in the process of predissociation. If the B_1 and A_2 hypersurfaces cross, then the process is heterogen

predissociation of type I with the lower B_1 state having vibrational progression and dissociative limit $H_2 + S^*$ and the upper A_2 state with dissociative limit $SH - H$. If dissociation process occurs via vibrational progression of the same electronic hypersurface then predissociation is of type II.

Acknowledgement

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