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0247 пик

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Equation (21) should be written:

$$n^{\nu}_{nlm}(E) = [N_n(E)/\Delta] \sum_{E-\delta}^{E+\delta} |c^{\nu}_{nklm}|^2 I^{\nu}_l(E), \tag{21}$$

with

$$I^{\nu}_l(E) = \int_0^{r^{\nu}_{MT}} [rR^{\nu}_l(r)]^2 \, dr + \int_{r^{\nu}_{MT}}^{r^{\nu}_{WS}} [rv^{\nu}_l(r)]^2 \, dr. \tag{22}$$

The numbers in Table I were calculated according to Eqs. (21) and (22) and are therefore correct as reported. We are grateful to L. Kopp for calling this to our attention.

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130: 30779f **Experimental and Theoretical Studies of Vanadium Sulfide Cation.** Kretzschmar, Ilona; Schroeder, Detlef; Schwarz, Helmut; Rue, Chad; Armentrout, P. B. (Institut fuer Organische Chemie, Technischen Universitaet Berlin, D-10623 Berlin, Germany). *J. Phys. Chem. A* **1998**, 102(49), 10060-10073 (Eng), American Chemical Society. The reactions of V^+ (^5D) with CS_2 and COS and the reactions of VS^+ with Xe, CO, COS, CO_2, and D_2 are studied as a function of translational energy in a guided-ion-beam (GIB) mass spectrometer. From these expts., $D_0(V^+-S) = 3.78 \pm 0.10$ eV, $D_0(V^+-CS) = 1.70 \pm 0.08$ eV, and $D_0(V^+-SD) = 2.57 \pm 0.15$ eV are derived. Verification of $D_0(V^+-S)$ is achieved by probing reactions of V^+ and VS^+ in a Fourier transform ICR mass spectrometer. The good agreement between the thermochem. obtained in the V^+/CS_2 system and that from the other systems studied shows that the formally spin-forbidden formation of ground-state VS^+ ($^3\Sigma^-$) from V^+ (^5D) and CS_2 has no activation barrier in excess of the

$D_0(V^+-S)$

$D_0(V^+-SD)$

VS^+

(расщепление $^3\Sigma^- - {}^5\Pi$)

$D_0(V^+-CS)$,

~~$D_0(V^+$~~

С. А. 1999, 130, № 3

reaction endothermicity. At higher energies, the spin–gave VS^+ ($^5\Pi$) competes efficiently, giving rise to a composite shape of the VS^+ cross section. The adiabatic and vertical splittings between the $^3\Sigma^-$ and $^5\Pi$ states of VS^+ are calcd. as 1.37 and 1.87 eV at the MR–ACPF level of theory. These values agree well with the splittings obtained in GIB and sector–field mass spectrometric expts.

V8

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