Support Information

"Theoretical calculation of spectroscopy properties of selenium bromide cation"

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Spectroscopic constants of Λ-S states of $SeBr^+$

Tables S1 and S2 show the calculated spectrum data for all the low excited states and the electronic grouping at the equilibrium bond lengths.

S1: Spectroscopy constants of the $\Lambda - S$ states of $SeBr^+$

$\Lambda - S$ states	$T_{e/\mathrm{cm}^{-1}}$	$R_{e/\text{Å}}$	$\omega_{e/\mathrm{cm}^{-1}}$	$B_{e/\mathrm{cm}^{-1}}$	$\omega_e\chi_{e/\mathrm{cm}^{-1}}$
$X^3\Sigma^-$	0	2.1802	378.5	0.0905	1.0977
$1^1\Delta$	5733	2.1776	381.7	0.0907	1.0549
$1^1\Sigma^+$	10343	2.1890	366.1	0.0897	1.2493
$1^5\Pi$	19759	2.9854	130.5	0.0482	1.1235
$1^1\Sigma^-$	20145	2.4452	257.8	0.0719	0.8183
$1^3\Pi$	20402	2.9313	104.4	0.0500	0.8814
$1^3\Delta$	21263	2.4542	254.7	0.0714	0.8267
$1^3\Sigma^+$	21711	2.4633	251.3	0.0709	0.8224
$2^3\Sigma^-$	23885	2.5779	214.9	0.0647	0.5816
$1^1\Pi$	27575	2.6979	164.1	0.0591	0.1989
$2^1\Delta$	28564	2.6118	209.3	0.0630	0.7779
$2^3\Pi$	30579	2.8478	134.9	0.0530	0.6281
$3^3\Pi$	31027	2.8597	200.2	0.0526	2.2213

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$1^3\Phi$	32385	2.6194	248.8	0.0620	4.3734
$4^3\Pi$	33534	2.9264	154.8	0.0502	1.2145
$2^1\Pi$	33712	2.8983	137.5	0.0512	1.5400
$1^1\Phi$	34942	2.8506	67.1	0.0532	0.9840
$3^1\Pi$	37045	3.1107	98.9	0.0444	0.9914

S2: Main CSFs around the R_e of $SeBr^+$

$\Lambda-S$ states	Main CSFs at R_e(%)	$\Lambda-S$ states	Main CSFs at R_e(%)
$X^3\Sigma^-$	$11\sigma^2 12\sigma^0 4\pi^4 5\pi^4 6\pi^2 2\delta^2$(83.35)	$2^1\Delta$	$11\sigma^2 12\sigma^0 4\pi^4 5\pi^3 6\pi^3 2\delta^2$(70.75) $11\sigma^1 12\sigma^1 4\pi^4 5\pi^4 6\pi^2 2\delta^2$(8.96)
$1^1\Delta$	$11\sigma^2 12\sigma^0 4\pi^4 5\pi^4 6\pi^2 2\delta^2$(79.55)	$2^3\Pi$	$11\sigma^1 12\sigma^0 4\pi^4 5\pi^4 6\pi^3 2\delta^2$(86.0)
$1^1\Sigma^+$	$11\sigma^2 12\sigma^0 4\pi^4 5\pi^4 6\pi^2 2\delta^2$(74.12)	$3^3\Pi$	$11\sigma^2 12\sigma^1 4\pi^4 5\pi^3 6\pi^2 2\delta^2$(81.29)
$1^3\Pi$	$11\sigma^2 12\sigma^0 4\pi^4 5\pi^3 6\pi^3 2\delta^2$(9.0) $11\sigma^2 12\sigma^1 4\pi^4 5\pi^4 6\pi^1 2\delta^2$(66.73) $11\sigma^2 12\sigma^1 4\pi^4 5\pi^3 6\pi^2 2\delta^2$(15.59)	$4^3\Pi$	$11\sigma^2 12\sigma^1 4\pi^4 5\pi^3 6\pi^2 2\delta^2$(84.70)
$1^5\Pi$	$11\sigma^2 12\sigma^1 4\pi^4 5\pi^3 6\pi^2 2\delta^2$(88.88)	$2^1\Pi$	$11\sigma^1 12\sigma^0 4\pi^4 5\pi^4 6\pi^3 2\delta^2$(85.13)
$1^1\Sigma^-$	$11\sigma^2 12\sigma^0 4\pi^4 5\pi^3 6\pi^3 2\delta^2$(87.27)	$3^1\Pi$	$11\sigma^2 12\sigma^1 4\pi^4 5\pi^3 6\pi^2 2\delta^2$(87.66)
$1^3\Delta$	$11\sigma^2 12\sigma^0 4\pi^4 5\pi^3 6\pi^3 2\delta^2$(87.54)	$1^3\Phi$	$11\sigma^2 12\sigma^1 4\pi^4 5\pi^3 6\pi^2 2\delta^2$(86.96)
$1^3\Sigma^+$	$11\sigma^2 12\sigma^0 4\pi^4 5\pi^3 6\pi^3 2\delta^2$(87.49)	$1^1\Phi$	$11\sigma^2 12\sigma^1 4\pi^4 5\pi^3 6\pi^2 2\delta^2$(82.83)
$2^3\Sigma^-$	$11\sigma^2 12\sigma^0 4\pi^4 5\pi^3 6\pi^3 2\delta^2$(75.22)	$2^3\Delta$	$11\sigma^1 12\sigma^1 4\pi^4 5\pi^4 6\pi^2 2\delta^2$(84.34)
$1^1\Pi$	$11\sigma^2 12\sigma^1 4\pi^4 5\pi^4 6\pi^1 2\delta^2$(67.61) $11\sigma^2 12\sigma^1 4\pi^4 5\pi^3 6\pi^2 2\delta^2$(12.85)	$1^5\Sigma^-$	$11\sigma^1 12\sigma^1 4\pi^4 5\pi^4 6\pi^2 2\delta^2$(87.89)

Spectroscopy constants of Ω states of $SeBr^+$

Table S3 shows all calculated SO matrix elements.

S3: Notation of spin-orbit matrix element

$SO_1 = -i\left\langle 1^1\Pi \middle\| \hat{H}_{SO}^{BP} \middle\| 1^3\Sigma_x^+ \right\rangle$	$SO_2 = \left\langle 1^1\Pi \middle\| \hat{H}_{SO}^{BP} \middle\| 1^3\Sigma_y^+ \right\rangle$	$SO_3 = -i\left\langle 2^1\Pi \middle\| \hat{H}_{SO}^{BP} \middle\| 1^3\Sigma_x^+ \right\rangle$
$SO_4 = \left\langle 2^1\Pi \middle\| \hat{H}_{SO}^{BP} \middle\| 1^3\Sigma_y^+ \right\rangle$	$SO_5 = -i\left\langle X^3\Sigma^- \middle\| \hat{H}_{SO}^{BP} \middle\| 1^1\Pi_x \right\rangle$	$SO_6 = \left\langle X^3\Sigma^- \middle\| \hat{H}_{SO}^{BP} \middle\| 1^1\Pi_y \right\rangle$

$SO_7 = -i\left\langle X^3\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 2^1\Pi_x \right\rangle$ $SO_8 = \left\langle X^3\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 2^1\Pi_y \right\rangle$ $SO_9 = -i\left\langle X^3\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_x \right\rangle$

$SO_{10} = \left\langle X^3\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_y \right\rangle$ $SO_{11} = -i\left\langle X^3\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 2^3\Pi_x \right\rangle$ $SO_{12} = \left\langle X^3\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 2^3\Pi_y \right\rangle$

$SO_{13} = -i\left\langle X^3\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^5\Pi_x \right\rangle$ $SO_{14} = \left\langle X^3\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^5\Pi_y \right\rangle$ $SO_{15} = -i\left\langle 1^5\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^5\Pi_x \right\rangle$

$SO_{16} = \left\langle 1^5\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^5\Pi_y \right\rangle$ $SO_{17} = -i\left\langle 1^5\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_x \right\rangle$ $SO_{18} = \left\langle 1^5\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_y \right\rangle$

$SO_{19} = -i\left\langle 1^3\Delta \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_x \right\rangle$ $SO_{20} = \left\langle 1^3\Delta \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_y \right\rangle$ $SO_{21} = -i\left\langle 1^3\Sigma^+ \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_x \right\rangle$

$SO_{22} = \left\langle 1^3\Sigma^+ \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_y \right\rangle$ $SO_{23} = -i\left\langle 1^1\Sigma^+ \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_x \right\rangle$ $SO_{24} = \left\langle 1^1\Sigma^+ \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_y \right\rangle$

$SO_{25} = -i\left\langle 1^1\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_x \right\rangle$ $SO_{26} = \left\langle 1^1\Sigma^- \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_y \right\rangle$ $SO_{27} = -i\left\langle 1^1\Pi \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_x \right\rangle$

$SO_{28} = \left\langle 1^1\Pi \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_y \right\rangle$ $SO_{29} = -i\left\langle 1^3\Pi_x \middle| \hat{H}_{SO}^{BP} \middle| 1^3\Pi_y \right\rangle$