

# Theoretical Calculation of the Low-Lying Electronic States of the Molecule BaS

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## Abstract

Complete Active Space Self Consistent Field (CASSCF) with Multireference Configuration Interaction (MRCI) and Rayleigh-Schrödinger Perturbation Theory (RSPT2-RS2) methods have been used to investigate the potential energy curves for the 12 low-lying singlet and triplet electronic states in the representation  $2s+1\Lambda^{(+/-)}$  of the molecule BaS with Davidson corrections. The harmonic frequency  $\omega_e$ , the internuclear distance  $R_e$ , the electronic energy with respect to the ground state  $T_e$ , the rotational constants  $B_e$  and the permanent dipole moment have been calculated for these electronic states. The eigenvalues  $E_v$ , the rotational constants  $B_v$ , the centrifugal distortion constant  $D_v$  and the abscissas of the turning points  $R_{\min}$  and  $R_{\max}$  have been investigated using the canonical functions approach. Nine new electronic states have been investigated here for the first time. The comparison between the values of the present work and those available in the literature for several electronic states shows a good agreement.

## Keywords

*Ab Initio* Calculation, Electronic Structure, Spectroscopic Constants, Potential Energy Curves, Dipole Moments, Vibration-Rotation Calculation

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## 1. Introduction

Examining the bonding of Alkaline earth sulfides molecules has been of both experimental and theoretical interest because of their promising variety of scientific areas including catalysis, biochemistry, material science [1] [2], astrophysical applications [3] [4] and its significant role in the electronic transition chemical laser [5]-[7]. Barium sulfide BaS is one of the Alkaline earth sulfides that have been first obtained in 17<sup>th</sup> century by the re-

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duction of the powder of barite  $\text{BaSO}_4$  with charcoal at high temperature [8]. Recently metal sulfide nanomaterials have attracted great attention because of their excellent properties and promising applications in electronic, optical and optoelectronic devices. Well-aligned nanostructure arrays on substrates are highly attractive for their enhanced properties and novel applications.

The rotational transitions of the main barium sulfide isotope have been recorded by Tiemann *et al.* [9]. In order to obtain the dipole moment for this molecule Melendres *et al.* [10] accomplished radio frequency Stark measurements of the  $J = 1$  rotational level. The absorption band system of the molecule BaS has been determined by Clements and Barrow [11]. Helms *et al.* [12] measured the millimeter-wave spectra of six isotopic species of BaS in the frequency range 55 - 339 GHz which allows the determination of Dunham coefficients. Additional measurements of the pure rotational spectrum of BaS in the range 358 - 394 GHz were recorded [13]. Recently, Janczyk and Ziurys performed a pure rotational study of BaS in the frequency range of 355 - 396 GHz [13]. High resolution laser excitation spectra of the  $A^1\Pi - X^1\Sigma^+$  and  $a^3\Pi - X^1\Sigma^+$  electronic transitions in the 12,100 - 12,765  $\text{cm}^{-1}$  spectral region were reported [14]. Rotational analysis of the electronic transitions  $B^1\Sigma^+ - X^1\Sigma^+$  has been done with the calculation of the molecular constants for each state. It was noticeably difficult to determine those constants for the electronic state  $A^1\Sigma^+$ , as it showed numerous perturbations [15].

The absence of theoretical calculation of higher excited states of the molecule BaS stimulate us to investigate, in the present work, more extensive *ab initio* calculation of barium sulfides molecule. Based on our previous theoretical calculations [16]-[24], the potential energy curves and spectroscopic constants of the low lying 12 singlet, and triplet electronic states have been calculated where 9 electronic states have been investigated here for the first time. The transition energy with respect to the minimum energy for the ground state  $T_e$ , the equilibrium internuclear distance  $R_e$ , the harmonic frequency  $\omega_e$ , the rotational constant  $B_e$ , and the permanent dipole moment have been calculated for the considered electronic states of this molecule. Taking advantage of the electronic structure of the investigated electronic states of the molecule BaS and by using the canonical functions approach [25]-[27], the eigenvalue  $E_v$ , the rotational constant  $B_v$ , and the abscissas of the turning points  $R_{\min}$  and  $R_{\max}$  have been calculated for several vibrational levels of the considered electronic states.

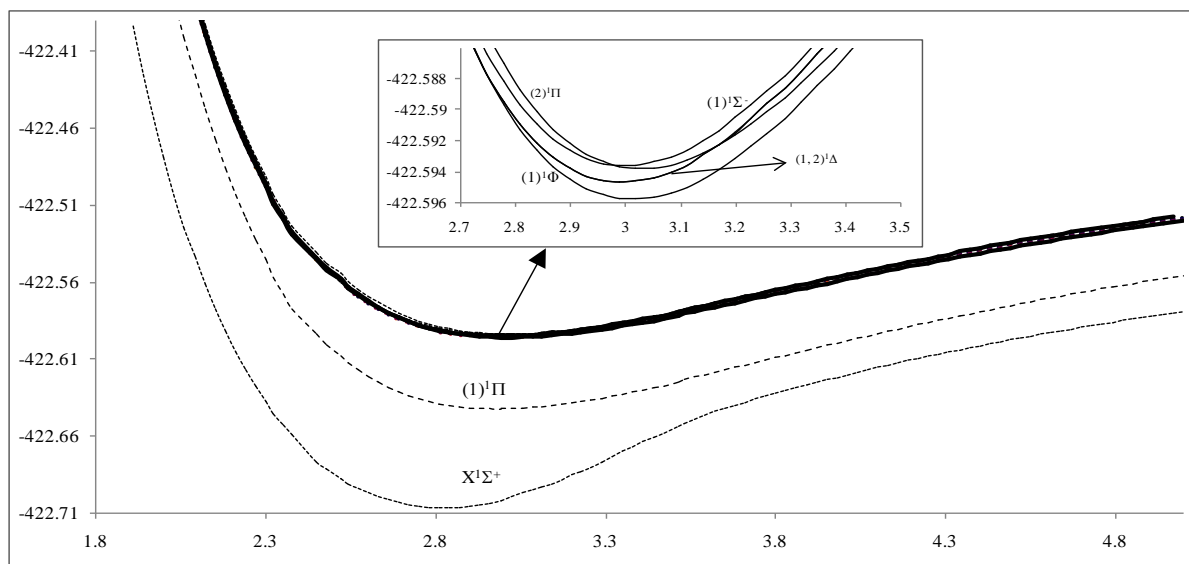
## 2. Method of Calculations

In the present work we investigated the low-lying singlet and triplet electronic states of the molecule BaS using complete active space self-consistent field (CASSCF) procedure followed by a multireference configuration interaction (MRCI with Davidson correction) treatment for the electron correlation and Rayleigh-Schrödinger Perturbation Theory (RSPT2-RS2). The entire CASSCF configuration space was used as the reference in the MRCI calculations, which were done via the computational chemistry program MOLPRO [28] taking advantage of the graphical user interface GABEDIT [29]. The Barium species is treated as a system of 56 electrons by using the ECP46MWB basis set for s, p, and d functions (with 46 core electrons). The 16 electrons of the sulfide atom are considered using the Rydberg5 basis set for s, p and d functions. Among the 26 electrons explicitly considered for BaS (10 electrons for Ba and 16 for S) 22 inner electrons were frozen in subsequent calculations so that four valence electrons were explicitly treated, corresponding to 16 active orbitals. All computations were performed in the  $C_{2v}$  symmetry.

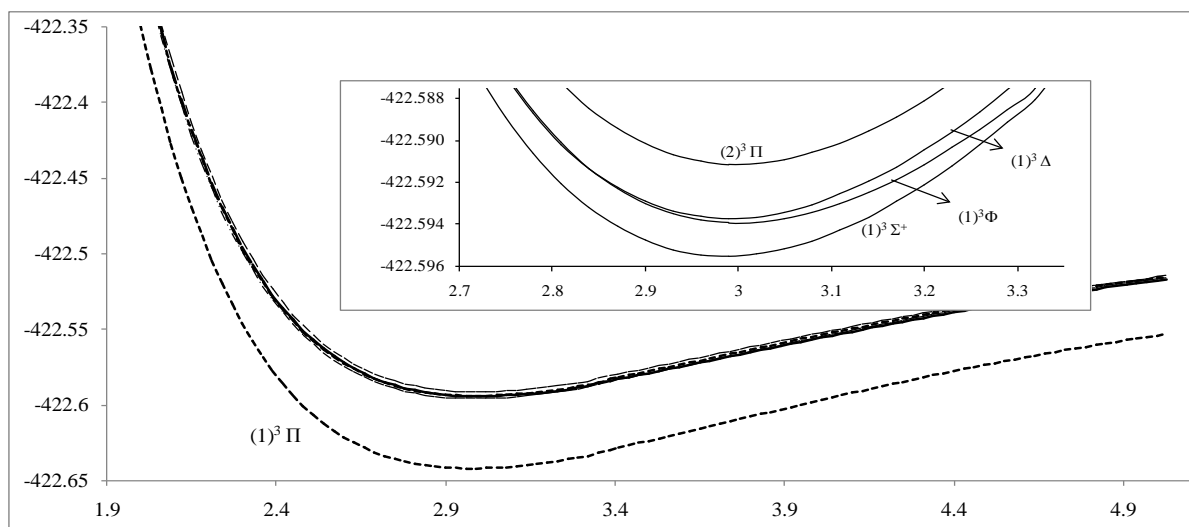
## 3. Results and Discussion

The potential energy curves (PECs) for the 12 singlet and triplet electronic states, in the representation  $^{2s+1}\Lambda^{(\pm)}$ , of the molecule BaS were generated using the MRCI for 105 internuclear distances calculations in the range  $1.9092\text{Å} \leq R_e \leq 4.9992\text{Å}$  (Figure 1, Figure 2)). By fitting the calculated energy values of the different investigated electronic states, into a polynomial in  $R$  around the internuclear distance at equilibrium  $R_e$ , the harmonic vibrational frequencies  $\omega_e$ , the relative energy separations  $T_e$ , and the rotational constants  $B_e$  have been calculated. These values with the available data in literature are given in Table 1.

One can notice the small difference between the values of  $T_e$  for the higher singlet and triplet electronic states. In literature there are fragmented experimental data for 3 lowest electronic states. By using the RSPT2-RS2 method we found that the ground state is  $(1)^1\Pi$ , by repeating the calculation with the MRCI technique we found that the ground state is  $X^1\Sigma^+$  which is confirmed experimentally. The comparison of our calculated values of  $T_e$  with the only value available in literature for the electronic state  $(1)^1\Pi$  shows an acceptable agreement. While by comparing the available data of  $R_e$  in literature for 3 electronic states with our investigated values one can find



**Figure 1.** Potential energy curves of the electronic states  ${}^1\Sigma^\pm$ ,  ${}^1\Delta$  and  ${}^1\Pi$  of the molecule BaS.



**Figure 2.** Potential energy curves of the electronic states  ${}^3\Sigma^\pm$ ,  ${}^3\Delta$  and  ${}^3\Pi$  of the molecule BaS.

that a very good agreement for the 2 electronic states  $(1)^1\Pi$  and  $(1)^3\Pi$  with an average relative difference  $\Delta R_e/R_e = 5.2\%$  and an acceptable agreement for the ground state. For the vibrational frequency  $\omega_e$  our calculated value is in excellent agreement with that given by Barrow *et al.* [33] for the electronic state  $(1)^3\Pi$  while this agreement becomes acceptable for the 2 electronic states  $X^1\Sigma^+$  and  $(1)^1\Pi$ . No comparison for the spectroscopic data for the other electronic states since they are given here for the first time.

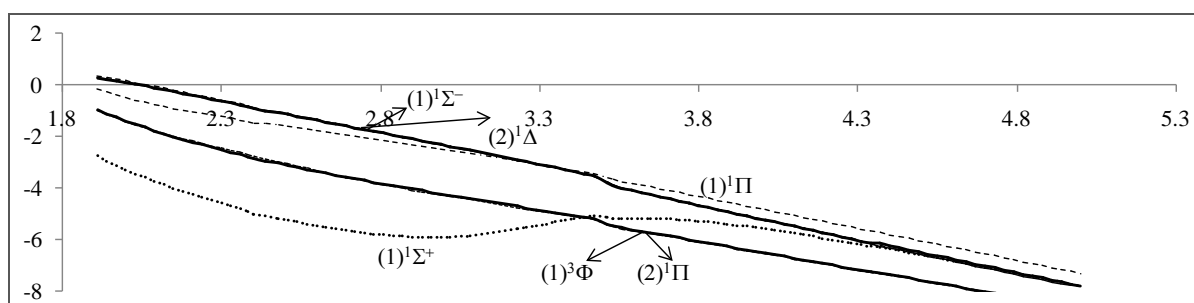
#### 4. Dipole Moment

The static dipole moment is a fundamental electrostatic property of a neutral molecule, its importance lying in the description of numerous physical phenomena. The expectation value of this operator is sensitive to the nature of the least energetic and most chemically relevant valence electrons. The calculated values of the dipole moments for the considered lowest-lying electronic states are plotted in term of the internuclear distance  $R$  in **Figure 3**, **Figure 4**. In our calculation we considered the Ba atom at the origin. Since the dipole moment have negative sign for the considered states where  $R \geq 2.0592\text{\AA}$  the dipole moment vector are directed from S to Ba atom.

**Table 1.** Spectroscopic constants for the singlet and triplet electronic states of the molecule BaS.

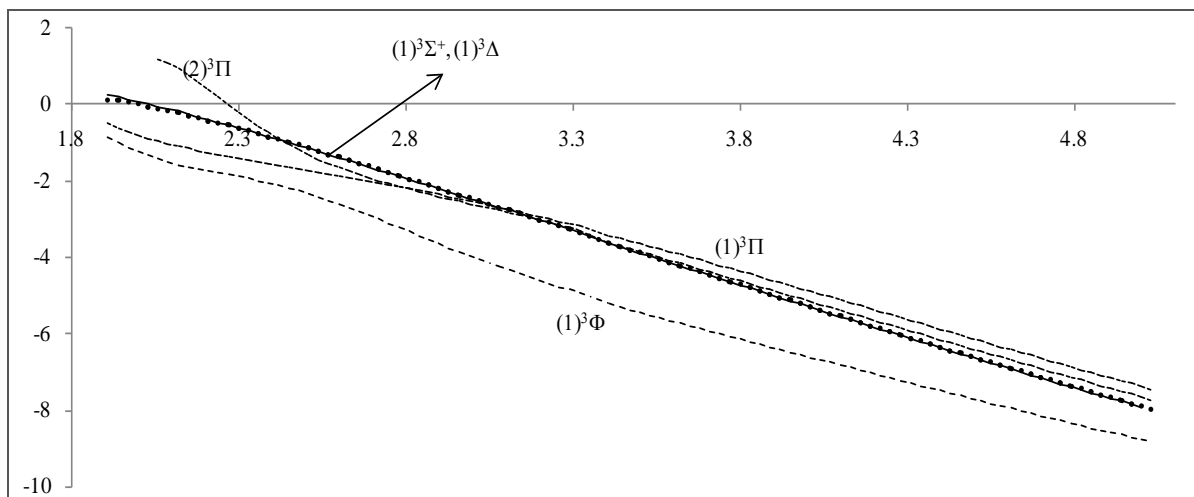
States	$T_e$ (cm <sup>-1</sup> )	$R_e$ (Å)	$\omega_e$ (cm <sup>-1</sup> )	$B_e \times 10^2$ (cm <sup>-1</sup> )
$X^1\Sigma^+$	0.0 <sup>a</sup>	2.8234 <sup>a</sup>	324.127 <sup>a</sup>	7.963 <sup>a</sup>
	0.0 <sup>b</sup>	2.9797 <sup>b</sup>	224.078 <sup>b</sup>	7.197 <sup>b</sup>
	0.0 <sup>c</sup>	2.5067 <sup>c</sup>	379.42 <sup>c</sup>	10.330 <sup>c</sup>
	0.0 <sup>d</sup>	2.5070 <sup>d</sup>	379.50 <sup>d</sup>	10.334 <sup>d</sup>
	0.0 <sup>e</sup>	2.5037 <sup>e</sup>	379.57 <sup>e</sup>	10.331 <sup>e</sup>
$(1)^1\Pi$	14125.32 <sup>a</sup>	2.9784 <sup>a</sup>	236.064 <sup>a</sup>	7.203 <sup>a</sup>
	-8897.92 <sup>b</sup>	2.9864 <sup>b</sup>	228.903 <sup>b</sup>	7.165 <sup>b</sup>
	12095.00 <sup>d</sup>	2.8130 <sup>d</sup>	258.900 <sup>d</sup>	8.210 <sup>d</sup>
	12175.23 <sup>f</sup>	2.8217 <sup>f</sup>	260.961 <sup>f</sup>	8.157 <sup>f</sup>
$(4)^1\Pi$	2352.42 <sup>b</sup>	3.0290 <sup>b</sup>	219.527 <sup>b</sup>	6.964 <sup>b</sup>
$(1)^3\Sigma^+$	24257.29 <sup>a</sup>	2.9855 <sup>a</sup>	228.526 <sup>a</sup>	7.169 <sup>a</sup>
	1653.48 <sup>b</sup>	2.9944 <sup>b</sup>	224.55 <sup>1b</sup>	7.127 <sup>b</sup>
$(4)^3\Sigma^+$	25819.48 <sup>b</sup>	3.8045 <sup>b</sup>	74.819 <sup>b</sup>	4.398 <sup>b</sup>
$(1)^3\Pi$	14116.28 <sup>a</sup>	2.9752 <sup>a</sup>	231.908 <sup>a</sup>	7.219 <sup>a</sup>
	-	2.9803 <sup>b</sup>	233.785 <sup>b</sup>	7.194 <sup>b</sup>
	$\leq 14500$ <sup>c</sup>	$\leq 2.8800$ <sup>c</sup>	$\geq 235$ <sup>c</sup>	7.800 <sup>c</sup>
	11835.00 <sup>d</sup>	2.8130 <sup>d</sup>	259.600 <sup>d</sup>	8.210 <sup>d</sup>
-	-	-	8.191 <sup>f</sup>	
$(2)^3\Pi$	1687.73 <sup>b</sup>	3.0053 <sup>b</sup>	221.312 <sup>b</sup>	7.097 <sup>b</sup>
$(3)^3\Pi$	25221.54 <sup>a</sup>	2.9973 <sup>a</sup>	225.757 <sup>a</sup>	7.113 <sup>a</sup>
$(4)^3\Pi$	2884.08 <sup>b</sup>	3.0184 <sup>b</sup>	215.933 <sup>b</sup>	7.0154 <sup>b</sup>
$(1)^3\Sigma^-$	2106.21 <sup>b</sup>	3.0011 <sup>b</sup>	222.118 <sup>b</sup>	7.0952 <sup>b</sup>
$(2)^3\Sigma^-$	2467.88 <sup>b</sup>	3.0078 <sup>b</sup>	220.573 <sup>b</sup>	7.0631 <sup>b</sup>
$(4)^3\Sigma^-$	22022.49 <sup>b</sup>	3.7518 <sup>b</sup>	398.470 <sup>b</sup>	4.539 <sup>b</sup>

<sup>a</sup> and <sup>b</sup> are for present work using respectively MRCI and RSPT2-RS2 methods. <sup>c</sup>Ref. [30], <sup>d</sup>Ref. [31], <sup>e</sup>Ref. [32], <sup>f</sup>Ref. [14].

**Figure 3.** Static dipole moment curves of the electronic states  $^1\Sigma^+$ ,  $^1\Delta$  and  $^1\Pi$  of the molecule BaS.

## 5. Vibration-Rotation Calculation

The vibrational calculation of a diatomic molecule is a promising approach for realizing a quantum computer. The vibrational states of these molecules represent the qubits and tailored the femtosecond laser pulses to implement quantum gate operations [30]. These vibrational states of molecules are stable over the time scales of interest, therefore the number of qubits is not limited to ten and by using more vibrational states, it may be possible to represent quantum information units having more than two states  $|0\rangle$ ,  $|1\rangle$ ,  $|2\rangle$ ,  $|3\rangle \dots$  [31]. This vibrational state approach has a number of qubits proportional to the number of vibrational degrees of freedom and more qubits can be realized using a N-atom molecule. Using the canonical functions approach [25]-[27] the radial Schrödinger equation can be replaced by the system of equations



**Figure 4.** Static dipole moment curves of the electronic states  $^3\Sigma^+$ ,  $^3\Delta$  and  $^3\Pi$  and  $^3\Phi$  of the molecule BaS.

$$\phi_0''(r) + [e_0 - U(r)]\phi_0(r) = 0 \quad (1)$$

$$\phi_1''(r) + [e_0 - U(r)]\phi_1(r) = -[e_1 - R(r)]\phi_0(r) \quad (2-1)$$

$$\phi_2''(r) + [e_0 - U(r)]\phi_2(r) = -[e_1 - R(r)]\phi_1(r) - e_2\phi_0(r) \quad (2-2)$$

...

$$\phi_n''(r) + [e_0 - U(r)]\phi_n(r) = R(r)\phi_{n-1} - \sum_{m=1}^n e_m\phi_{n-m}(r) \quad (2-n)$$

where  $R(r) = 1/r^2$ , Equation (1) represents the pure vibrational Schrödinger equation and the remaining equations are the pure rotational Schrödinger equations. Once  $e_0 = E_v$  is calculated,  $e_1 = B_v$ ,  $e_2 = D_v$ , ... can be obtained by using alternatively Equations (2-n). By using the cubic spline interpolation between each two consecutive points of the potential energy curves obtained from the *ab initio* calculation the abscissas of the turning points  $R_{\min}$  and  $R_{\max}$  have been calculated (**Table A1** in **Appendix**). By comparing our calculated values of  $B_v$  with those given in literature for the 3 electronic states  $X^1\Sigma^+$ ,  $(1)^1\Pi$ , and  $(1)^3\Pi$  given in literature [13]-[15] [33] [34], one can find that, these experimental values are systematically greater than our calculated values by  $\approx 0.02 \text{ cm}^{-1}$  for the ground state and by  $\approx 0.01 \text{ cm}^{-1}$  for the  $(1)^1\Pi$ , and  $(1)^3\Pi$  states for the investigated vibrational levels. The comparison of our calculated values of  $E_v$  with those given in literature [13]-[15] [33] [34] is not possible since the origin of energy in these references is considered at  $v = 0$  while in our calculation this origin is at the minimum of the potential energy curve for each electronic state. But we compared the difference of energy  $\Delta E_v = E_n - E_{n-1}$  between each 2 consecutive vibrational levels of our calculated values with those given in literature [13]-[15] [33] [34], we found that this difference varies from one vibrational level to another and depend on the considered electronic state, but an overall good agreement can be considered where the relative difference is  $4.5\% \leq \Delta E_v/E_v \leq 12\%$ .

## 6. Conclusion

In the present work, an *ab initio* calculation of 12 singlet and triplet lowest electronic states in the  $^{2s+1}\Lambda^\pm$  representation has been performed via CASSCF/MRCI methods. The potential energy curves have been calculated along with the spectroscopic constants  $T_e$ ,  $R_e$ ,  $B_e$ , and  $\omega_e$  for these states and the static dipole moment  $\mu$ . In literature there is a limited number of data for the investigated values either theoretically or experimentally. The comparison of our calculated values with either the theoretical or the experimental data available in the literature demonstrated an overall good agreement. Nine new electronic states have been investigated here for the first time. The investigated data in the present work may help for more experimental or theoretical studies in the future for higher electronic states.

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## Appendix

**Table A1.** Values of the eigenvalues  $E_v$ , the rotational constants  $B_v$ , and the abscissas of the turning points  $R_{\min}$  and  $R_{\max}$  for the different vibrational levels of  $X^1\Sigma^+$ ,  $(1)^1\Pi$ ,  $(1)^3\Sigma^+$ ,  $(1)^3\Pi$ , and  $(3)^3\Pi$  states of the BaS molecule.

		$X^1\Sigma^+$				$(1)^1\Pi$				$(1)^3\Sigma^+$			
V	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{Å}$ )	$R_{\max}$ ( $\text{Å}$ )	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{Å}$ )	$R_{\max}$ ( $\text{Å}$ )	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{Å}$ )	$R_{\max}$ ( $\text{Å}$ )	
0	164	7.990 <sup>a</sup>	2.803	2.867	118	7.187	2.906	3.026	114	7.153	2.912	3.035	
1	488	8.010	2.718	2.906	351	7.161	2.858	3.085	341	7.126	2.863	3.094	
2	814	8.032	2.686	2.937	584 <sup>a</sup>	7.135 <sup>a</sup>	2.826	3.128	566	7.099	2.831	3.138	
3	1141	8.049	2.660	2.961	815	7.109 <sup>a</sup>	2.800	3.164	791	7.071	2.805	3.175	
4	1470	8.066	2.637	2.982	1045	7.084 <sup>a</sup>	2.779	3.196	1014	7.043	2.784	3.208	
5	1799	8.076	2.617	2.999	1274	7.057 <sup>a</sup>	2.761	3.226	1237	7.016	2.766	3.238	
6	2126	8.073	2.599	3.016	1502	7.032	2.744	3.254	1459	6.990	2.749	3.266	
7	2448	8.053	2.583	3.039	1729	7.006	2.729	3.280	1680	6.971	2.734	3.294	
8	2762	8.022	2.568	3.064	1955	6.980	2.715	3.305	1903	6.965	2.720	3.318	
9	3070	8.003	2.554	3.084	2180	6.955	2.702	3.329	2129	6.979	2.707	3.330	
10	3375	7.995	2.542	3.102	2404	6.929	2.691	3.352	2363	7.003	2.694	3.341	
11	3678	7.980	2.530	3.120	2626	6.904	2.679	3.374	2602	7.016	2.682	3.357	
12	3978	7.966	2.519	3.135	2848	6.880	2.669	3.395	2843	6.977	2.670	3.387	
13	4279	7.978	2.508	3.147	3069	6.860	2.659	3.419	3073	6.856	2.660	3.410	
14	4584	7.993	2.497	3.159	3290	6.849	2.649	3.438	3286	6.779	2.651	3.431	
15	4888	7.969	2.487	3.175	3513	6.851	2.640	3.451	3503	6.831	2.642	3.453	
16	5188	7.925	2.477	3.200	3740	6.864	2.631	3.462	3726	6.796	2.633	3.475	
17	5480	7.895	2.469	3.217	3976	6.873	2.622	3.477	3940	6.706	2.624	3.496	
18	5778	7.879	2.461	3.229	4203	6.849	2.614	3.499	4151	6.722	2.617	3.517	
19	6076	7.866	2.454	3.239	4430	6.773	2.606	3.519	4366	6.694	2.609	3.538	
20	6378	7.858	2.448	3.249	4647	6.689	2.598	3.538	4575	6.635	2.602	3.558	
21	6684	7.837	2.443	3.260	4869	6.690	2.591	3.557	4784	6.636	2.595	3.578	
22	6991	7.804	2.437	3.274	5079	6.703	2.584	3.576	4993	6.593	2.588	3.597	
23	7299	7.776	2.433	3.288	5296	6.642	2.578	3.595	5198	6.564	2.581	3.617	
24	7610	7.749	2.428	3.301	5507	6.592	2.571	3.614	5403	6.544	2.575	3.636	
25	7921	7.717	2.424	3.314	5718	6.600	2.565	3.632	5606	6.507	2.569	3.655	
26	8232	7.680	2.419	3.327	5937	6.569	2.559	3.650	5809	6.486	2.563	3.674	
27	8541	7.648	2.415	3.340	6346	6.513	2.547	3.686	6010	6.453	2.557	3.693	
28	8849	7.621	2.410	3.354	6554	6.485	2.542	3.704	6209	6.429	2.551	3.712	
29	9155	7.594	2.406	3.367	6759	6.452	2.536	3.722	6408	6.399	2.546	3.730	
30	9459	7.571	2.401	3.381	6963	6.434	2.531	3.739	6605	6.373	2.544	3.749	
31	9759	7.551	2.395	3.394	7166	6.404	2.526	3.757	6800	6.345	2.536	3.767	



**Continued**

32	10,056	7.532	2.390	3.409	7368	6.380	2.521	3.774	6995	6.318	2.530	3.786
33	10,350	7.519	2.384	3.426	7569	6.355	2.516	3.791	7188	6.290	2.526	3.804
34	10,641	7.507	2.379	3.438	7769	6.328	2.511	3.809	7381	6.263	2.521	3.822
35	10,929	7.500	2.374	3.446	7967	6.304	2.507	3.826	7572	6.236	2.516	3.840
36	11,216	7.498	2.370	3.454	8165	6.277	2.502	3.843	7761	6.209	2.512	3.858
37	11,503	7.492	2.365	3.461	8361	6.252	2.498	3.860	7950	6.182	2.507	3.876
38	11,789	7.473	2.360	3.475	8556	6.226	2.494	3.877	8137	6.155	2.503	3.894
39	12,074	7.438	2.355	3.514	8751	6.202	2.490	3.894	8324	6.128	2.499	3.912
40	12,354	7.399	2.350	3.522	8944	6.177	2.485	3.911	8509	6.102	2.494	3.930
41	12,632	7.379	2.345	3.529	9136	6.152	2.481	3.927	8693	6.075	2.490	3.948
42	12,908	7.381	2.339	3.538	9327	6.129	2.477	3.944	8876	6.048	2.486	3.965
43	13,183	7.377	2.334	3.552	9517	6.106	2.472	3.961	9058	6.022	2.482	3.983
44	13,454	7.337	2.329	3.570	9705	6.083	2.468	3.978	9238	5.995	2.479	4.001
45	13,716	7.265	2.324	3.587	9893	6.059	2.463	3.994	9418	5.969	2.475	4.019
46	13,970	7.207	2.320	3.603	10,080	6.035	2.460	4.011	9596	5.942	2.471	4.036
47	14,220	7.188	2.316	3.620	10,265	6.010	2.456	4.027	9773	5.916	2.468	4.054
48	14,470	7.157	2.312	3.637	10,450	5.982	2.453	4.044	9950	5.890	2.464	4.072
49	14,716	7.099	2.308	3.654	10,633	5.954	2.450	4.061	10,125	5.864	2.461	4.089
50	14,959	7.055	2.304	3.670	10,816	5.923	2.448	4.077	10,299	5.838	2.457	4.107
51	15,200	7.020	2.300	3.687	10,998	5.890	2.446	4.094	10,472	5.812	2.454	4.125
52	15,439	6.973	2.296	3.704	11,180	5.857	2.443	4.111	10,643	5.786	2.451	4.142
53	15,674	6.942	2.293	3.721	11,361	5.823	2.441	4.127	10,814	5.760	2.447	4.160
54	15,908	6.910	2.289	3.737	11,541	5.789	2.439	4.144	10,984	5.734	2.444	4.178
55	16,138	6.868	2.286	3.754	11,720	5.756	2.437	4.161	11,153	5.708	2.441	4.195
56	16,366	6.841	2.283	3.771	11,899	5.724	2.435	4.177	11,320	5.682	2.438	4.213
57	16,593	6.803	2.279	3.788	12,077	5.693	2.433	4.194	11,487	5.657	2.435	4.230
58	16,816	6.766	2.276	3.805	12,254	5.663	2.431	4.211	11,652	5.631	2.432	4.248
59	17,038	6.734	2.273	3.822	12,430	5.635	2.429	4.228	11,817	5.606	2.429	4.266
60	17,257	6.696	2.270	3.839	12,605	5.609	2.427	4.244	11,980	5.580	2.426	4.283
61	17,474	6.666	2.267	3.856	12,779	5.585	2.425	4.261	12,143	5.555	2.424	4.301
62	17,690	6.629	2.264	3.873	12,952	5.562	2.423	4.278	12,304	5.530	2.421	4.319
63	17,903	6.598	2.261	3.890	13,124	5.540	2.420	4.295	12,464	5.504	2.418	4.337
64	18,114	6.562	2.258	3.900	13,295	5.518	2.417	4.321	12,624	5.479	2.415	4.354
65	18,323	6.530	2.256	3.924	13,464	5.496	2.414	4.332	12,782	5.454	2.413	4.372
66	18,531	6.494	2.253	3.941	13,630	5.475	2.410	4.350	12,940	5.429	2.410	4.390
67	18,737	6.462	2.250	3.958	13,795	5.464	2.405	4.366	13,096	5.404	2.408	4.408
68	18,941	6.428	2.248	3.975	13,958	5.466	2.399	4.382	13,251	5.379	2.405	4.426

## Continued

69	19,143	6.396	2.245	3.992	14,121	5.480	2.394	4.399	13,406	5.355	2.403	4.443
70	19,343	6.363	2.243	4.009	14,283	5.488	2.390	4.416	13,559	5.330	2.400	4.461
71	19,542	6.332	2.240	4.026	14,444	5.479	2.386	4.433	13,712	5.305	2.398	4.479
72	19,739	6.298	2.238	4.043	14,602	5.466	2.384	4.449	13,863	5.280	2.395	4.497
73	19,934	6.267	2.236	4.061	14,758	5.464	2.381	4.466	14,014	5.256	2.393	4.515
74	20,128	6.234	2.233	4.078	15,069	5.433	2.376	4.499	14,163	5.231	2.391	4.533
75	20,320	6.203	2.231	4.095	15,224	5.390	2.374	4.515	14,312	5.207	2.388	4.551
76	20,511	6.171	2.229	4.112	15,377	5.356	2.372	4.532	14,460	5.182	2.386	4.569
77	20,700	6.140	2.226	4.130	15,531	5.323	2.370	4.548	14,606	5.158	2.384	4.587
78	20,888	6.110	2.224	4.147	15,684	5.278	2.368	4.565	14,752	5.134	2.382	4.605
79	21,074	6.078	2.222	4.164	15,836	5.236	2.366	4.582	14,897	5.110	2.380	4.624
80	21,258	6.049	2.220	4.180	15,988	5.206	2.364	4.599	15,041	5.085	2.378	4.642
81	21,441	6.017	2.218	4.199	16,140	5.172	2.362	4.616	15,184	5.062	2.376	4.660
82	21,623	5.987	2.216	4.216	16,291	5.140	2.360	4.633	15,326	5.037	2.373	4.678
83	21,803	5.957	2.214	4.234	16,441	5.115	2.358	4.650	15,467	5.013	2.371	4.697
84	21,982	5.927	2.212	4.251	16,590	5.090	2.357	4.668				
85	22,159	5.897	2.210	4.269	16,738	5.066	2.355	4.685				
86	22,335	5.865	2.208	4.286								
87	22,510	5.833	2.206	4.303								
88	22,683	5.796	2.204	4.323								
89	22,853	5.757	2.202	4.343								
90	23,022	5.720	2.201	4.360								
91	23,189	5.693	2.199	4.377								
92	23,356	5.680	2.197	4.395								
93	23,523	5.664	2.195	4.413								
94	23,688	5.629	2.193	4.431								
95	23,852	5.587	2.192	4.448								
96	24,014	5.562	2.190	4.466								
97	24,175	5.549	2.188	4.484								
98	24,336	5.519	2.187	4.502								
99	24,495	5.480	2.185	4.520								
100	24,653	5.459	2.184	4.538								
101	24,809	5.437	2.182	4.556								
102	24,965	5.402	2.180	4.574								
103	25,120	5.376	2.179	4.592								
104	25,273	5.354	2.177	4.610								
105	25,426	5.323	2.176	4.628								
106	25,577	5.297	2.174	4.646								
107	25,727	5.272	2.173	4.664								

Continued

		(1) <sup>3</sup> Π			(3) <sup>3</sup> Π			
0	116	7.155	2.902	3.023	113	7.097	2.924	3.045
1	349	7.130	2.854	3.082	338	7.070	2.875	3.106
2	581	7.104	2.822	3.125	562	7.043	2.842	3.150
3	812	7.079	2.796	3.161	785	7.015	2.817	3.187
4	1042	7.053	2.775	3.193	1007	6.987	2.795	3.220
5	1271	7.028	2.757	3.222	1228	6.960	2.777	3.251
6	1499	7.003	2.740	3.250	1448	6.936	2.760	3.278
7	1727	6.981	2.725	3.275	1668	6.923	2.745	3.310
8	1954	6.966	2.711	3.303	1892	6.928	2.731	3.325
9	2184	6.966	2.698	3.321	2121	6.950	2.717	3.336
10	2418	6.983	2.686	3.332	2358	6.973	2.704	3.349
11	2659	7.007	2.674	3.343	2599	6.962	2.692	3.374
12	2905	7.016	2.662	3.360	2834	6.871	2.681	3.401
13	3151	6.970	2.652	3.388	3051	6.744	2.671	3.424
14	3385	6.853	2.642	3.409	263	6.768	2.661	3.446
15	3606	6.791	2.633	3.429	484	6.783	2.652	3.469
16	3830	6.840	2.624	3.450	700	6.682	2.643	3.491
17	4059	6.808	2.615	3.471	908	6.667	2.635	3.512
18	4281	6.725	2.607	3.491	122	6.670	2.627	3.534
19	4499	6.734	2.600	3.510	331	6.597	2.620	3.555
20	4721	6.717	2.592	3.530	537	6.591	2.612	3.575
21	4938	6.659	2.585	3.549	744	6.560	2.605	3.596
22	5154	6.655	2.578	3.568	4947	6.519	2.599	3.616
23	5370	6.625	2.572	3.586	5151	6.505	2.592	3.635
24	5583	6.591	2.565	3.605	5352	6.464	2.586	3.655
25	5796	6.576	2.559	3.623	5552	6.443	2.580	3.675
26	6008	6.542	2.553	3.641	5751	6.410	2.574	3.694
27	6218	6.521	2.547	3.659	5948	6.384	2.568	3.713
28	6427	6.494	2.541	3.677	6144	6.354	2.563	3.733
29	6635	6.468	2.536	3.694	6339	6.326	2.557	3.752
30	6842	6.444	2.530	3.712	6532	6.298	2.552	3.771
31	7047	6.417	2.525	3.729	6724	6.269	2.547	3.789
32	7252	6.393	2.520	3.747	6915	6.242	2.542	3.808
33	7455	6.367	2.515	3.764	7105	6.214	2.537	3.827
34	7657	6.343	2.510	3.781	7293	6.185	2.532	3.846
35	7858	6.317	2.506	3.798	7480	6.158	2.528	3.864
36	8058	6.293	2.501	3.815	7666	6.130	2.523	3.883
37	8257	6.268	2.496	3.832	8034	6.074	2.514	3.919
38	8455	6.243	2.492	3.849	8216	6.047	2.510	3.938
39	8652	6.218	2.488	3.866	8398	6.020	2.506	3.956
40	8847	6.194	2.483	3.883	8577	5.993	2.502	3.974
41	9042	6.169	2.479	3.900	8756	5.965	2.498	3.993
42	9235	6.144	2.475	3.916	8934	5.938	2.494	4.011
43	9427	6.120	2.471	3.933	9110	5.911	2.490	4.029
44	9619	6.095	2.467	3.950	9285	5.884	2.487	4.047
45	9809	6.071	2.464	3.966	9459	5.857	2.483	4.066
46	9998	6.046	2.460	3.983	9632	5.830	2.479	4.084

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47	10,186	6.022	2.456	3.999	9804	5.803	2.476	4.102
48	10,373	5.998	2.453	4.016	9975	5.777	2.473	4.120
49	10,560	5.974	2.449	4.032	10,144	5.750	2.469	4.138
50	10,745	5.949	2.445	4.049	10,313	5.723	2.466	4.156
51	10,929	5.925	2.442	4.066	10,480	5.697	2.463	4.175
52	11,112	5.901	2.439	4.082	10,646	5.670	2.459	4.193
53	11,294	5.877	2.435	4.099	10,812	5.644	2.456	4.211
54	11,475	5.853	2.432	4.115	10,976	5.618	2.453	4.229
55	11,654	5.829	2.429	4.132	11,139	5.592	2.450	4.247
56	11,833	5.805	2.426	4.148	11,301	5.566	2.447	4.265
57	12,011	5.781	2.423	4.165	11,462	5.539	2.444	4.283
58	12,188	5.757	2.420	4.185	11,623	5.514	2.441	4.302
59	12,364	5.733	2.417	4.198	11,781	5.488	2.439	4.320
60	12,539	5.709	2.414	4.214	11,938	5.462	2.436	4.338
61	12,713	5.686	2.411	4.231	12,095	5.436	2.433	4.356
62	12,886	5.662	2.408	4.247	12,251	5.411	2.430	4.375
63	13,058	5.638	2.405	4.264	12,406	5.385	2.428	4.393
64	13,229	5.614	2.402	4.280	12,559	5.360	2.425	4.411
65	13,399	5.590	2.400	4.297	12,712	5.334	2.423	4.430
66	13,568	5.567	2.397	4.313	12,864	5.309	2.420	4.448
67	13,736	5.544	2.394	4.330	13,015	5.284	2.418	4.466
68	13,903	5.520	2.392	4.347	13,164	5.259	2.415	4.485
69	14,069	5.496	2.389	4.363	13,313	5.234	2.413	4.503
70	14,234	5.473	2.387	4.380	13,461	5.209	2.410	4.521
71	14,398	5.450	2.384	4.397	13,608	5.184	2.408	4.540
72	14,561	5.426	2.382	4.413	13,754	5.159	2.406	4.558
73	14,723	5.403	2.379	4.430	13,899	5.135	2.403	4.577
74	14,885	5.380	2.377	4.447	14,043	5.110	2.401	4.596
75	15,045	5.357	2.375	4.464	14,186	5.085	2.399	4.614
76	15,204	5.334	2.372	4.480	14,328	5.061	2.397	4.633
77	15,363	5.310	2.370	4.497	14,469	5.036	2.395	4.651
78	15,677	5.264	2.366	4.531	14,609	5.011	2.393	4.670
79	15,833	5.241	2.363	4.548	14,748	4.987	2.390	4.689
80	15,987	5.218	2.361	4.565	14,887	4.963	2.388	4.708
81	16,141	5.195	2.359	4.582				
82	16,294	5.172	2.357	4.599				
83	16,446	5.149	2.355	4.616				
84	16,597	5.127	2.353	4.633				
85	16,747	5.104	2.351	4.650				
86	16,896	5.080	2.349	4.668				
87	17,045	5.058	2.347	4.685				
88	17,192	5.035	2.345	4.702				