Prospects for ultracold carbon via charge exchange reactions and laser cooled carbides

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Supplementary information

1. Ab initio introduction

The Hartree Fock (HF), Multi Configuration Self Consistent Field (MCSCF) and Multi Reference Configuration Interaction (MRCI) methods are employed to calculate potential energy surfaces for one or more electronic states in the four molecular systems investigated. HF is the basic method of *ab initio* electronic structure calculation, based on the Born-Oppenheimer approximation where the wavefunction can be given by a single Slater determinant. Therefore, it neglects electron-electron correlation, and is a poor method for calculating potential energy surfaces in general, but is very quick to run and is a mandatory precursor to post HF methods such as MCSCF. The MCSCF method[1] uses a linear combination of configuration state functions (CSF's, a symmetry adapted combination of slater determinants that satisfies the Pauli principle). The MRCI method[2] is a post-HF method that accounts for dynamic electron correlation and is based on a MCSCF wavefunction.

The theoretical study used two programs in order to calculate and evaluate the systems of interest for possible use in laser cooling. We used the Molpro[3] suite of computational chemistry programs in order to generate complete symmetry potential energy diagrams for the diatomic systems being investigated. The program also gives the transition dipole moments of the different energy levels as a function of internuclear separation. The potentials were then used as input into the LEVEL 8.0[4] program by R.J LeRoy in order to calculate Franck Condon Factors, ro-vibrational energy levels – including wavefunctions – and centrifugal distortions.

2. Atomic data and molecular symmetries

2.1 LiC

Atomic Limit	Level (cm^{-1})	Molecular Symmetry
C (^3P_g) + Li (^2S_g)	0	$^2\Pi$ $^2\Sigma^-$ $^4\Pi$ $^4\Sigma^-$
C (^1D_g) + Li (^2S_g)	10,192.63	$^2\Sigma^+$ $^2\Pi$ $^2\Delta$
C (^3P_g) + Li (^2P_u)	14,903.66	$^2\Sigma^+$ $^2\Sigma^-(2)$ $^2\Pi(2)$ $^2\Delta$
		$^4\Sigma^+$ $^4\Sigma^-(2)$ $^4\Pi(2)$ $^4\Delta$

Table 2.1

The ground and first excited state of the system will be calculated using the av6z basis set for carbon and the v5z basis set for lithium - the highest basis sets available to us - using the MRCI method. The MO diagram shows all the involved orbitals in the states being calculated. This provides the occupancy for the Molpro program as {occ,6,2,2,0}, including the 2p valence shell for lithium.

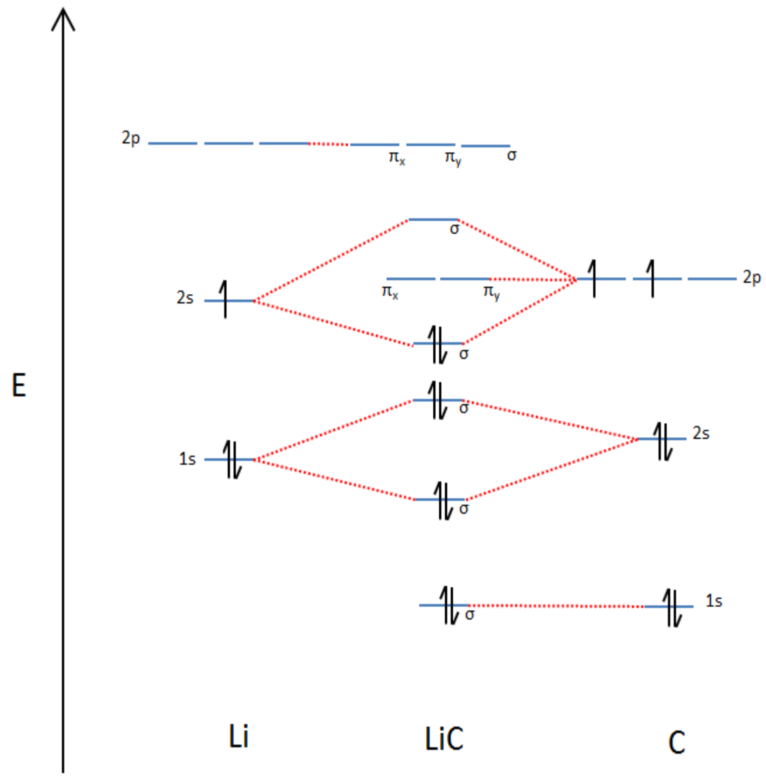


Figure 2.1a

LiC is a nine electron system and there are eight symmetry states (two states must be included for the Δ state) present in the ground and first excited state.

The energy level splitting diagram shown below illustrates clearly the expected asymptotic limits for the system[5].

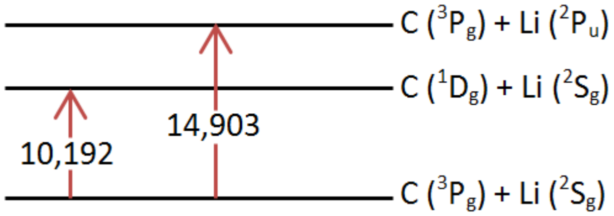


Figure 2.1b

2.2 CH

Atomic Limit	Level (cm^{-1})	Molecular Symmetry
C (^3P_g) + H (^2S_g)	0	$^2\Pi$ $^2\Sigma^-$ $^4\Pi$ $^4\Sigma^-$
C (^1D_g) + H (^2S_g)	10,192.63	$^2\Sigma^+$ $^2\Pi$ $^2\Delta$

Table 2.2

The ground and first excited state were calculated using an av6z basis set for both the carbon and hydrogen using the MRCI method. We also ran the program using an av5z basis set in order to compare the difference in result accuracy – and absolute energy difference as a function of distance - when using a smaller basis set.

The MO diagram shows all the involved orbitals in the states being calculated. This provides the occupancy for the Molpro program as {occ,4,1,1,0}.

CH is a seven electron system and there are eight symmetry states (two states must be included for the Δ state) present in the ground and first excited state.

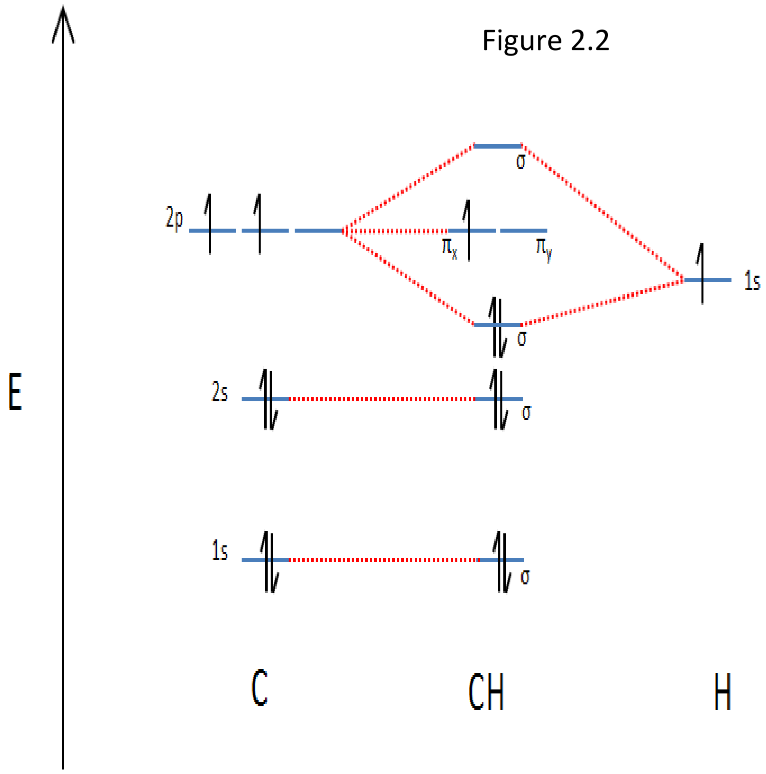


Figure 2.2

2.3 Diatomic molecular ions

The ionic systems investigate the potential for a charge transfer to take place when carbon ions are moved into a pre-prepared ultracold atomic gas. The calculated energy levels for each system include energy levels above and below the initial state, in order to identify a possible transition that could facilitate the proposed charge transfer.

Table 2.3a shows the ionisation energy for lithium, beryllium and carbon.

Atom	Ionisation Potential (eV)	Ionisation Potential (cm^{-1})
Li	5.391	43,481
Be	9.323	75,194
C	11.26	90,819

Table 2.3a

Table 2.3b shows the relevant atomic and ionic energy levels for lithium, beryllium and carbon.

Atom	Valence Configuration	Term Symbol	J	Level (cm^{-1})
Li	$1s^2 2s^1$	^2S	1/2	0
	$1s^2 2s^1$	^2P	1/2	14,903.66
			3/2	14,904.00
	$1s^2 2s^1$	^2S	1/2	27,206.12
	$1s^2 2s^1$	^2P	1/2	30,925.38
			3/2	30,925.38

Atom	Valence Configuration	Term Symbol	J	Level (cm^{-1})
Li^+	$1s^2$	^1S	0	0
	$1s^12s^1$	^3S	1	476,034.98
Be	$1s^22s^2$	^1S	0	0
	$1s^22s^12p^1$	^3P	0	21,978.28
			1	21,978.28
			2	21,981.27
Be^+	$1s^22s^1$	^2S	1/2	0
		^2P	1/2	31,928.744
			3/2	31,935.320
C	$2s^22p^2$	^3P	0	0
			1	16.40
			2	43.40
	$2s^22p^2$	^1D	2	10,192.63
	$2s^22p^2$	^1S	0	21,648.01
C^+	$2s^22p^1$	^2P	1/2	0
			3/2	63.42
		^4P	1/2	43,003.3
			3/2	43,025.3
			5/2	43,053.6

Table 2.3b

2.4 $[LiC]^+$

Atomic Limit	Level (cm^{-1})	Molecular Symmetry
C (^3P_g) + Li^+ (^1S_g)	0	$^3\Sigma^-$ $^3\Pi$
C (^1D_g) + Li^+ (^1S_g)	10,192.63	$^1\Sigma^+$ $^1\Pi$ $^1\Delta$
C (^1S_g) + Li^+ (^1S_g)	21,648.01	$^1\Sigma^+$
C (^5S_u) + Li^+ (^1S_g)	33,735.20	$^5\Sigma^-$
C^+ (^2P_u) + Li (^1S_g)	47,338	$^1\Sigma^+$ $^3\Sigma^+$ $^1\Pi$ $^3\Pi$

Table 2.4

The initial state in the entrance channel - C^+ (^2P_u) + Li (^1S_g) – is an excited state of the molecular system, with an asymptotic limit of 47,338 cm^{-1}, calculated as the difference in ionisation energies of carbon and lithium, with the carbocation being higher in energy.

The ground and first four excited states of the system (including the theoretical initial state) will be calculated using the av6z basis set for carbon and the v5z basis set for lithium - the highest basis sets available at the time - using the MRCI method.

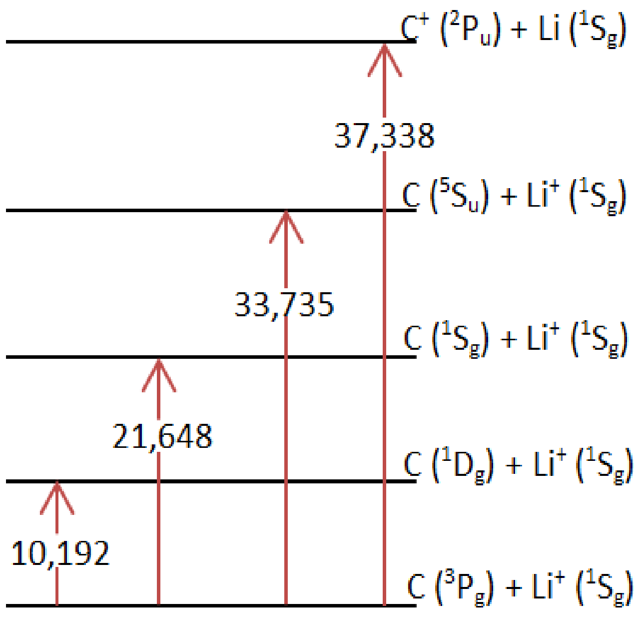


Figure 2.4

Due to the nature of carbons excited states – namely that the electrons only occupy up to the 2p valence orbital for all the excited states of interest in the system – the occupancy for Molpro will remain the same as that already shown {occ,6,2,2,0}.

The energy level splitting diagram to the left shows clearly the expected asymptotic limits for the system.

2.5 $[BeC]^+$

Atomic Limit	Level (cm^{-1})	Molecular Symmetry
Be^+ (^2S_g) + C (^3P_g)	0	$^2\Sigma^-$ $^2\Pi$ $^4\Sigma^-$ $^4\Pi$
Be^+ (^2S_g) + C (^1D_g)	10,192.63	$^2\Sigma^+$ $^2\Pi$ $^2\Delta$
Be (^1S_g) + C^+ (^2P_u)	15,624.343	$^2\Sigma^+$ $^2\Pi$
Be^+ (^2S_g) + C (^1S_g)	21,648.01	$^2\Sigma^+$
Be^+ (^2P_u) + C (^3P_g)	31,928.74	$^2\Sigma^+$ $^2\Pi(2)$ $^2\Sigma^-(2)$ $^2\Delta$
		$^4\Sigma^+$ $^4\Pi(2)$ $^4\Sigma^-(2)$ $^4\Delta$

Table 2.5

The initial state in the entrance channel - C^+ (^2P_u) + Be (^1S_g) - is again an excited state of the molecular system, with an asymptotic limit of 15,624.343 cm^{-1}, calculated as the difference in ionisation energies of carbon and beryllium, with the carbocation being higher in energy.

The ground and first four excited states of the system (including the theoretical initial state) will be calculated using an av6z basis set for carbon and an avqz basis set for lithium – the highest basis sets available at the time – using the MRCI method.

The MO diagram shows the theoretical initial state, including any orbitals to be occupied by the excited states, and shows the occupancy for the Molpro program to be {occ,6,2,2,0}.

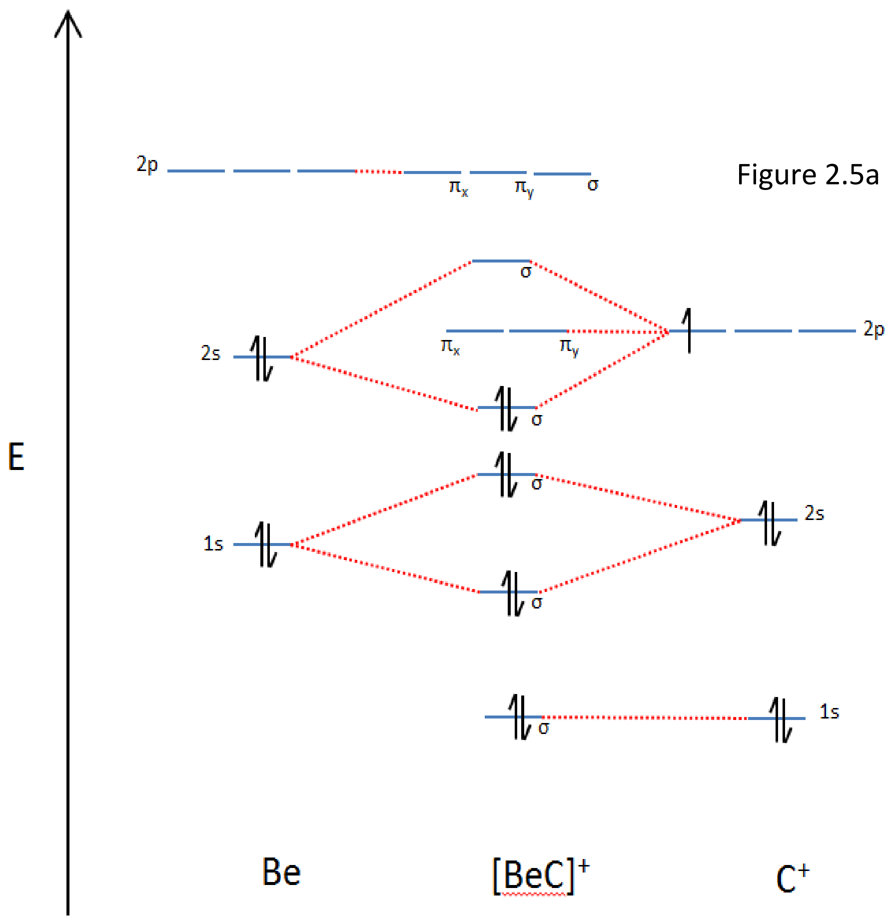


Figure 2.5a

$[BeC]^+$ is a nine electron system with 25 symmetry states (including a Σ^+ and Σ^- for each Δ state) for the ground and first four excited states.

The energy level splitting diagram shows clearly the expected energy level splitting for the system.

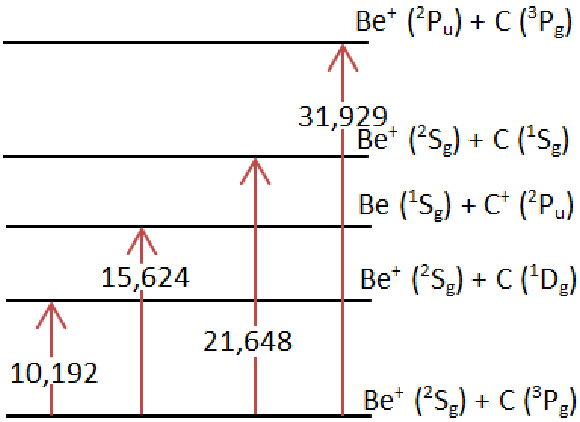


Figure 2.5b

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

3. Potential energy curves

3.1 CH

3.1.1 av5z Potential Energy Surface

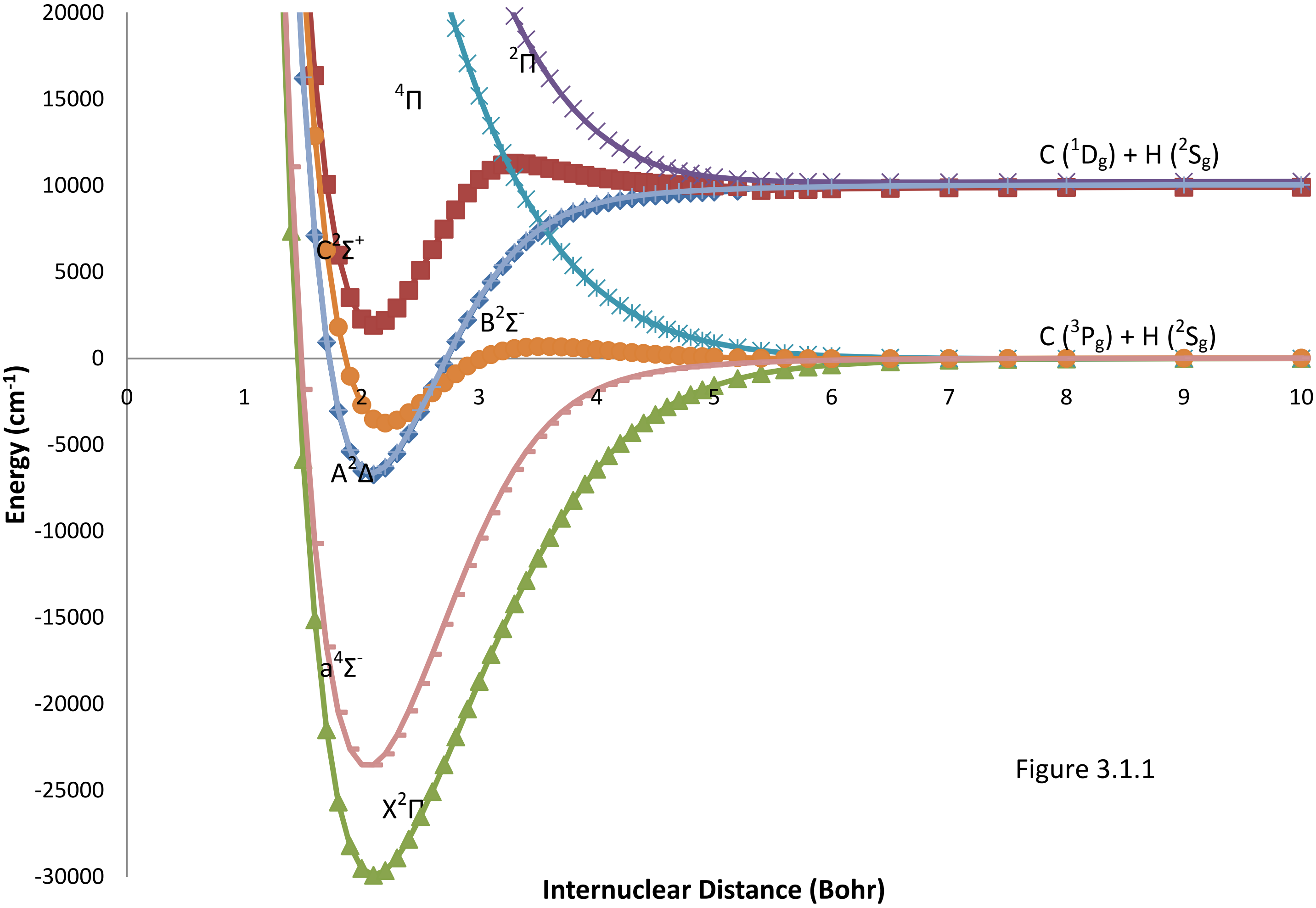


Figure 3.1.1

Molecular Symmetry	Calculated Asymptotic Limit	Experimental Asymptotic Limit	Difference (wavenumbers)	Difference (percentage)
$X^2\Pi$	0	0	0	-
$a^4\Sigma^-$	22.87	0	22.87	-
$A^2\Delta$	10,047.54	10,192.63	145.09	1.42%
$B^2\Sigma^-$	23.11	0	23.11	-
$C^2\Sigma^+$	9,912.77	10192.63	279.86	2.75%
$^4\Pi$	-0.08	0	0.08	-
$^2\Pi$	10,240.34	10,192.63	47.71	0.47%

Table 3.1.1

3.1.2 av6z Potential Energy Surface

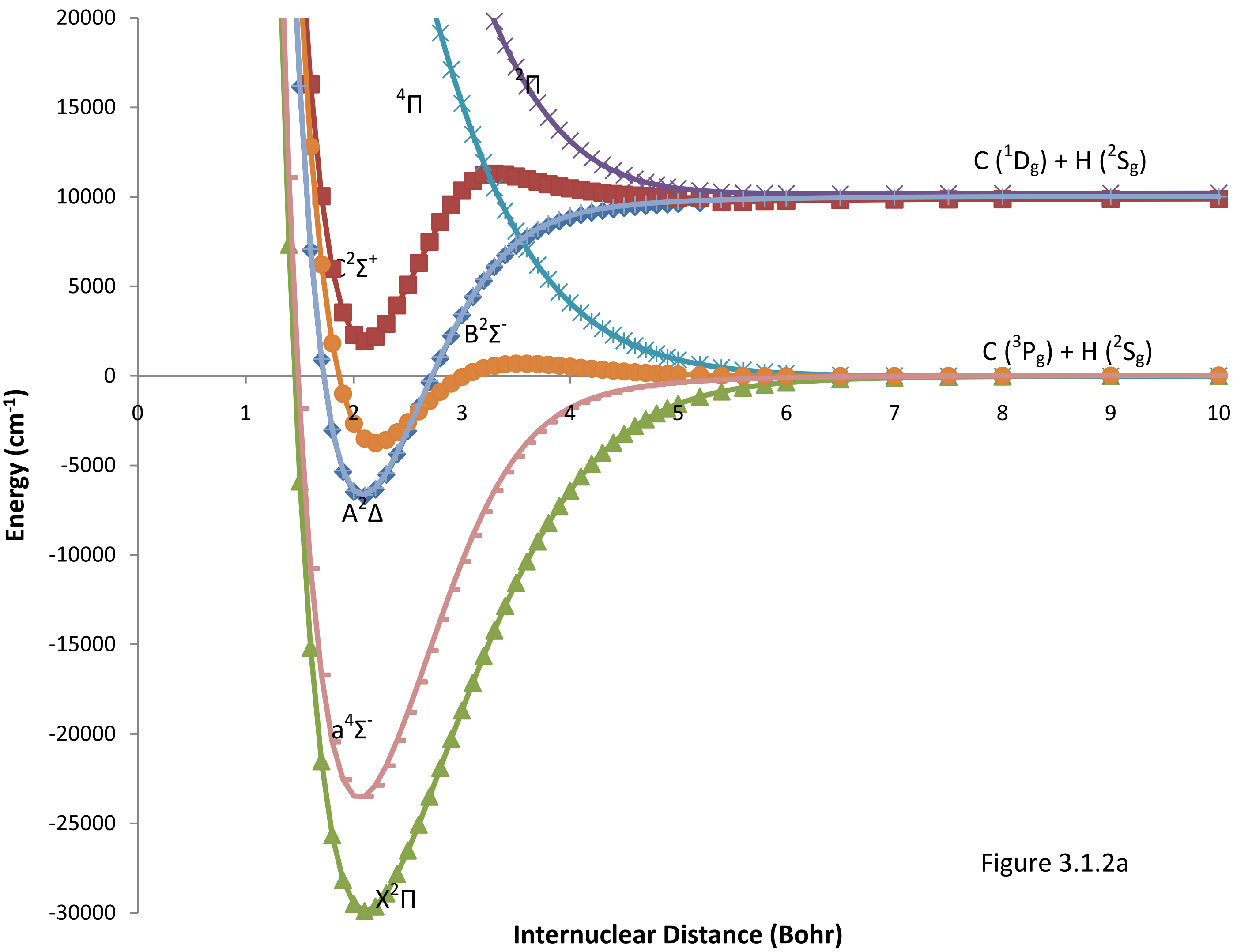


Figure 3.1.2a

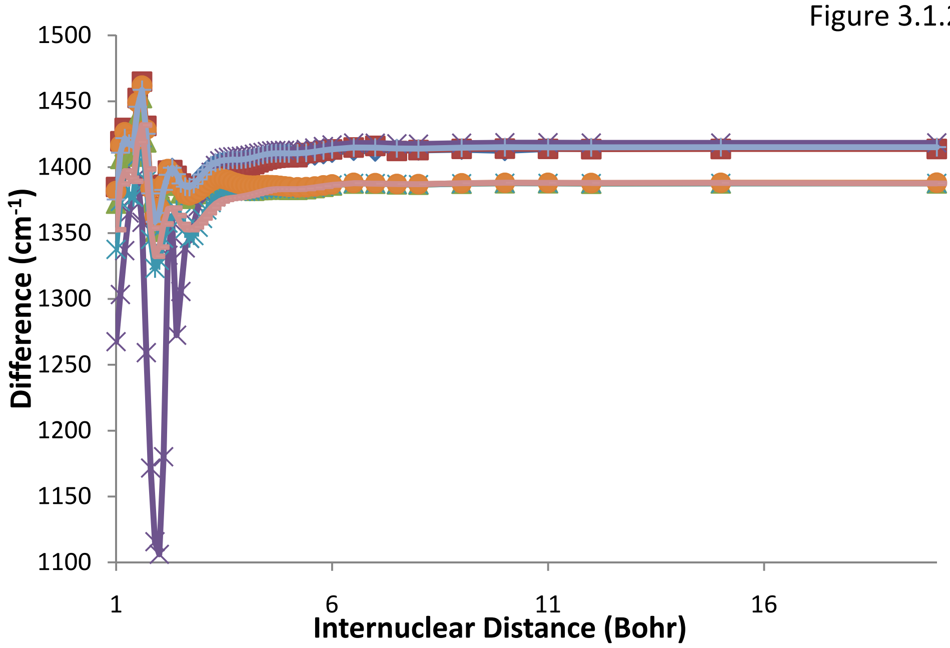
Molecular Symmetry	Calculated Asymptotic Limit	Experimental Asymptotic Limit	Difference (wavenumbers)	Difference (percentage)
$X^2\Pi$	0	0	0	-
$a^4\Sigma^-$	22.87	0	22.87	-
$A^2\Delta$	10,020.05	10,192.63	172.58	1.69%
$B^2\Sigma^-$	22.67	0	22.67	-
$C^2\Sigma^+$	9,886.65	10192.63	305.98	3.00%
$^4\Pi$	-0.08	0	0.08	-
$^2\Pi$	10,209.64	10,192.63	16.96	0.17%

Table 3.1.2

Figure 3.1.2b below shows the absolute energy difference in wavenumbers as a function of internuclear distance for the two basis sets.

With both basis sets, the calculated asymptotic limits are in excellent agreement with experimental data.

Figure 3.1.2b



The $v' = 0 \leftarrow v = 0$ transition has a good transition of 0.9957, higher that seen by Shuman *et al* in their production of ultracold SrF[6]. Figure 3.1.2b shows proposed laser driven transitions (solid red) and radiative decay (solid blue) for the CH $A^2\Delta \leftarrow X^2\Pi$ transition based on the calculated FCF's and Shuman's experimental setup.

As the FCF's are so similar to those present in the SrF $A^2\Pi \leftarrow X^2\Pi$ transition, it is logical to propose a similar set up. There is a strong possibility that CH can be cooled using just one vibronic transition, but a more efficient scheme would use three transitions as detailed (Figure 3.1.2c). The rotational structure is more difficult to deal with than SrF and requires five wavelengths per vibronic transition.

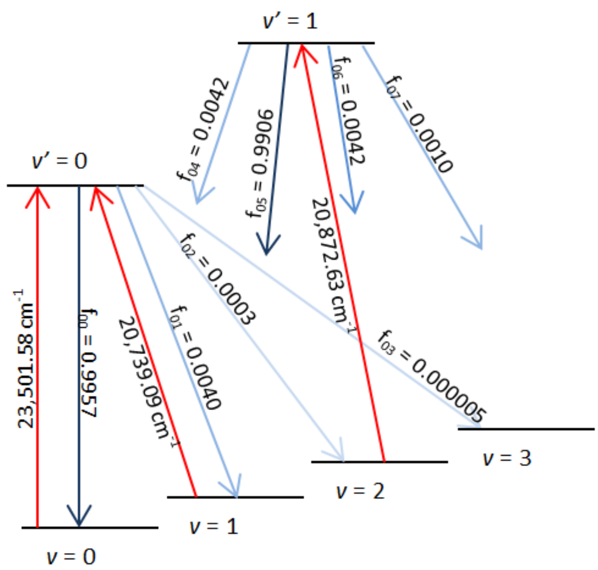


Figure 3.1.2c

Although the $X^2\Pi \leftarrow C^2\Sigma^+$ transition has slightly more favourable FCF's ($0 \leftarrow 0 = 0.998$), it is a predissociating state, and so cooling on it would be inefficient.

3.2 LiC

av6z/5z Potential Energy Surface

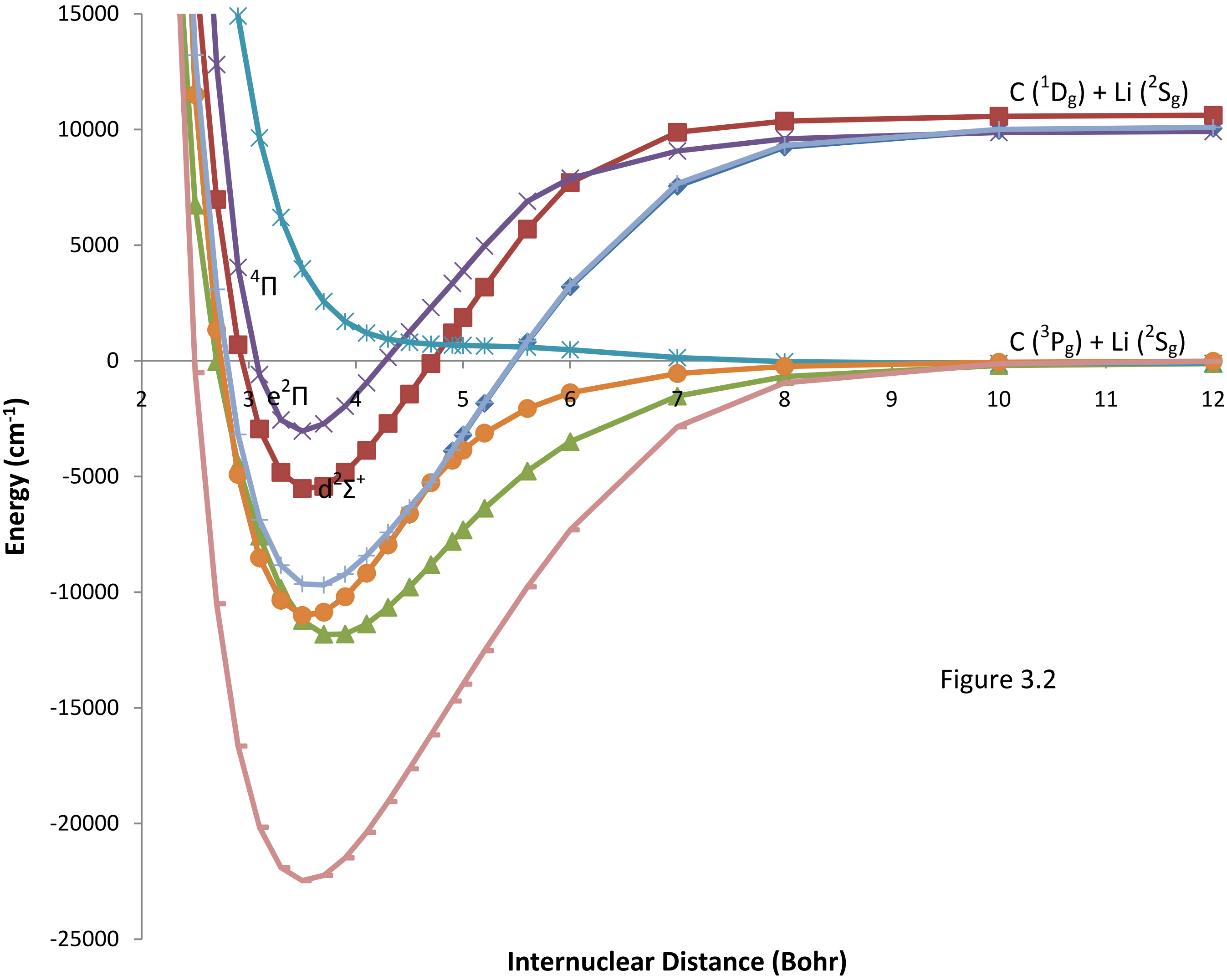


Figure 3.2

Molecular Symmetry	Calculated Asymptotic Limit	Experimental Asymptotic Limit	Difference (wavenumbers)	Difference (percentage)
$X^4\Sigma^-$	0	0	0	-
$a^2\Pi$	-83.50	0	83.50	-
$b^2\Sigma^-$	-0.14	0	0.14	-
$c^2\Delta$	10,116.50	10,192.63	76.13	0.75%
$d^2\Sigma^+$	10,637.88	10,192.63	445.25	4.37%
$e^2\Pi$	9,930.03	10,192.63	262.60	2.58%
$^4\Pi$	-83.33	0	83.33	-

Table 3.2

3.3 $[LiC]^+$

av6z/5z Potential Energy Surface

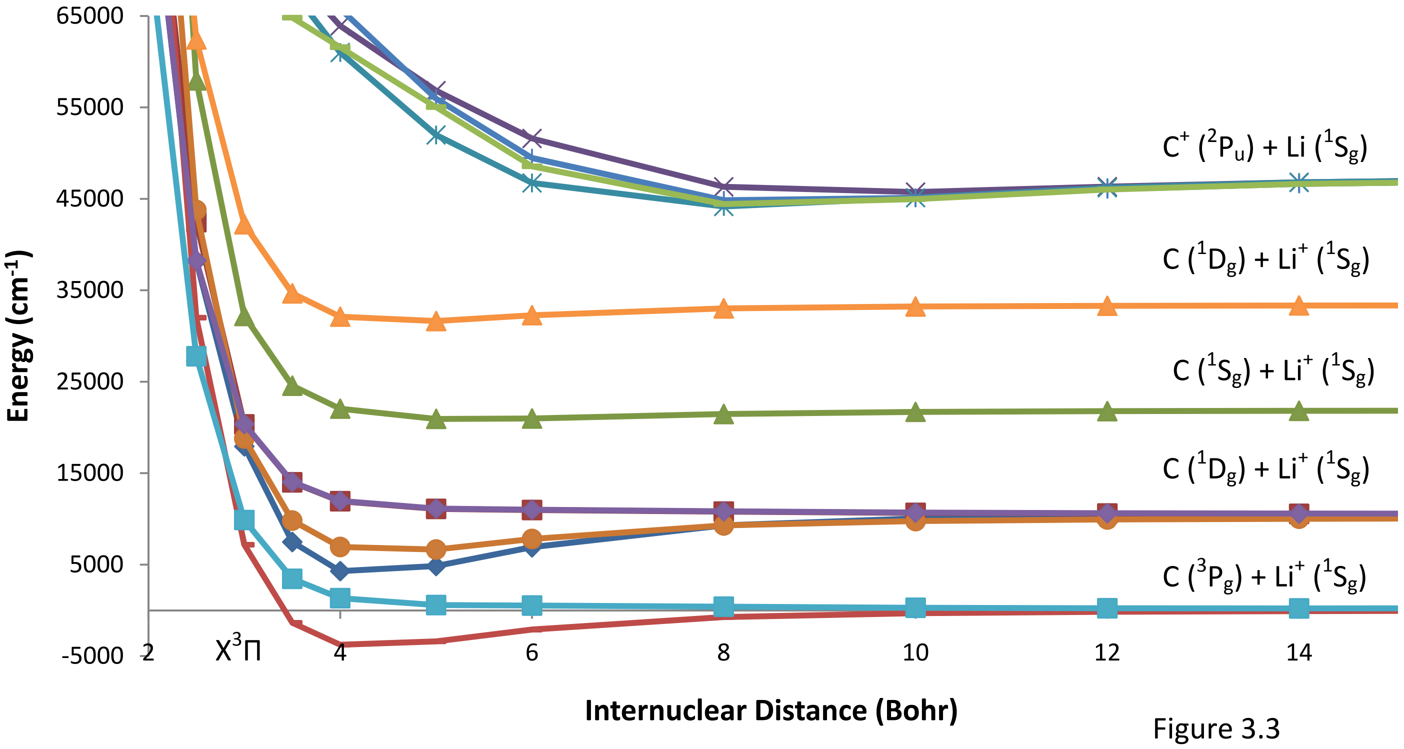


Figure 3.3

Atomic Limit	Calculated Asymptotic Limit	Experimental Asymptotic Limit	Difference (wavenumbers)	Difference (percentage)
C (^3P_g) + Li^+ (^1S_g)	0	0	0	-
C (^1D_g) + Li^+ (^1S_g)	10,098.86	10,192.63	93.77	0.92%
C (^1S_g) + Li^+ (^1S_g)	21,849.96	21,648.01	201.95	0.93%
C (^1D_g) + Li^+ (^1S_g)	33,364.04	33,735.20	371.16	1.10%
C^+ (^2P_u) + Li (^1S_g)	47,230.43	47,338	107.57	0.23%

Table 3.3

The calculated asymptotic limits agree with experimental values with a very high degree of accuracy. However, there are no instances of curve crossings, making non-radiative charge transfer extremely unlikely. The $^5\Sigma^-$ state removed from the published potentials (figure 2) is presented above.

3.4 $[BeC]^+$

3.4.1 av6z/qz Potential Energy Surface

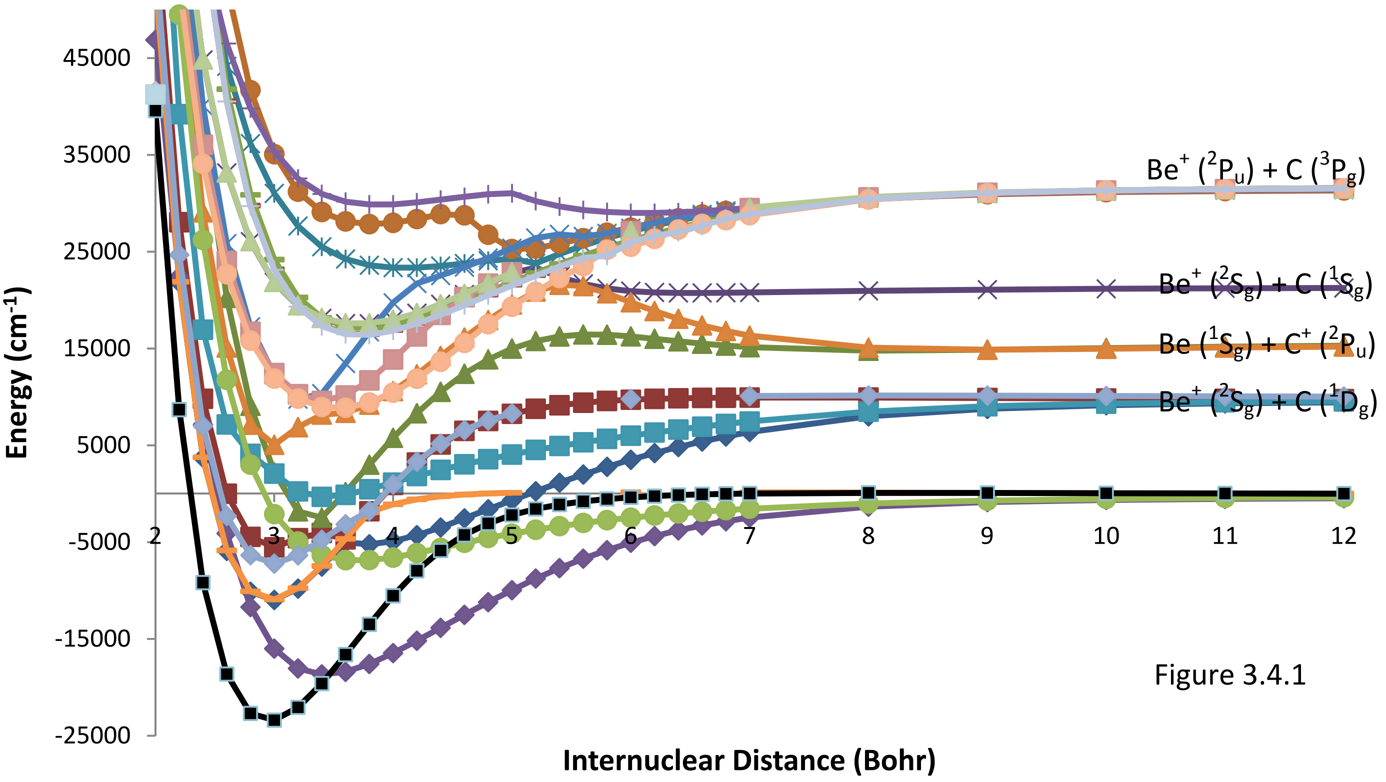


Figure 3.4.1

Atomic Limit	Calculated Asymptotic Limit	Experimental Asymptotic Limit	Difference (wavenumbers)	Difference (percentage)
Be^+ (^2S_g) + C (^3P_g)	0	0	0	-
Be^+ (^2S_g) + C (^1D_g)	10,024.70	10,192.63	167.93	1.65%
Be (^1S_g) + C^+ (^2P_u)	15,277.13	15,624.34	347.21	2.22%
Be^+ (^2S_g) + C (^1S_g)	21,252.13	21,648.01	395.88	1.83%
Be^+ (^2P_u) + C (^3P_g)	31,534.99	31,928.74	393.75	1.23%

Table 3.4.1

The calculated asymptotic limits agree very well with experimental values with a high degree of accuracy. Due to the amount of molecular states present however, we will present separate diagrams for each molecular symmetry. The two molecular symmetries corresponding to the initial collision channel - Be (^1S_g) + C^+ (^2P_u) – both have a repulsive wall before a potential well that falls below the dissociation limit of the system ground state, forming a barrier on the surface.

3.4.2 av6z/qz $^2\Sigma^+$

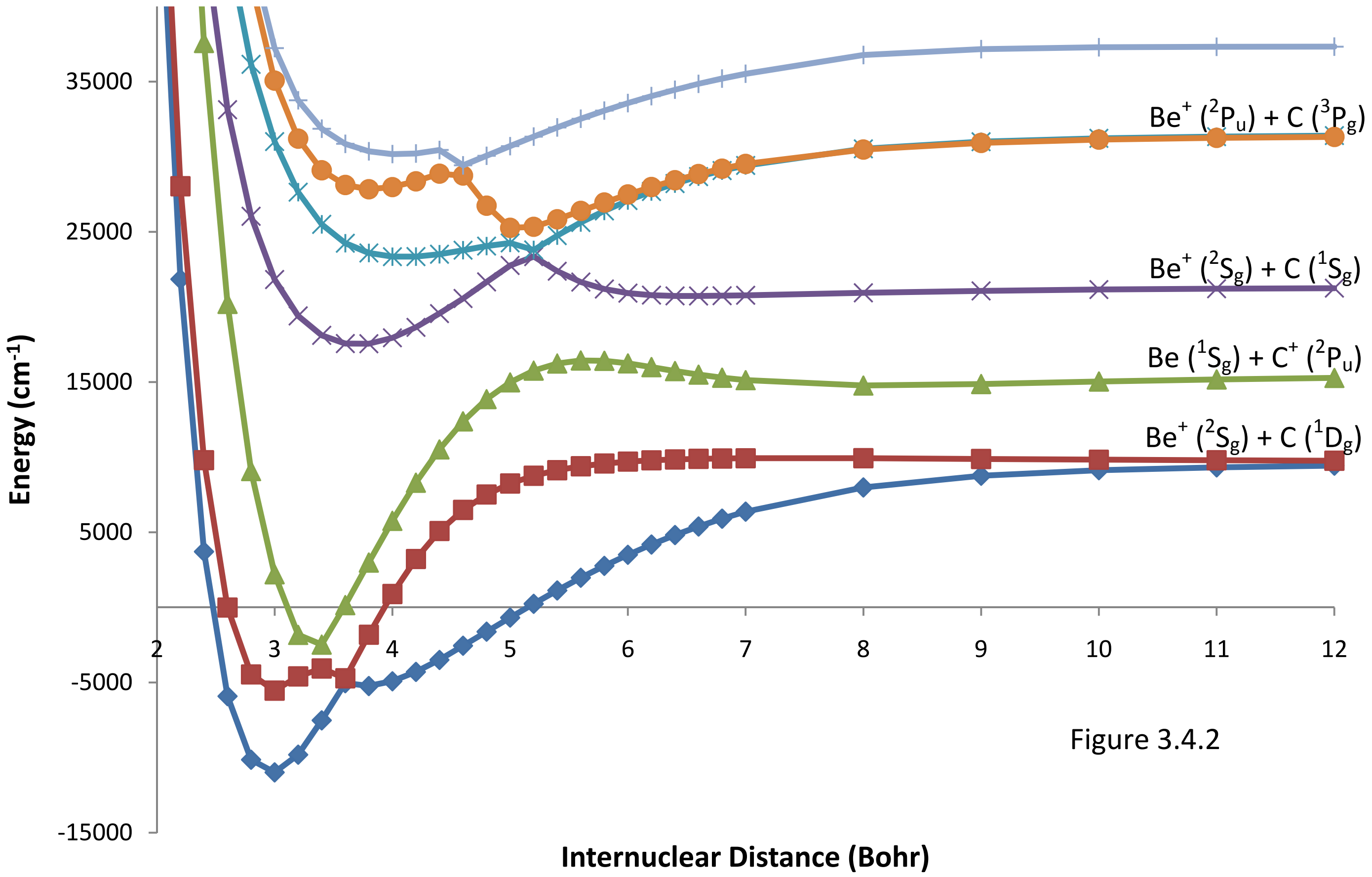


Figure 3.4.2

Atomic Limit	Calculated Asymptotic Limit	Experimental Asymptotic Limit	Difference (wavenumbers)	Difference (percentage)
Be^+ (^2S_g) + C (^1D_g)	9,763.46	10,192.63	429.17	4.21%
Be (^1S_g) + C^+ (^2P_u)	15,277.13	15,624.34	347.50	2.22%
Be^+ (^2S_g) + C (^1S_g)	21,252.15	21,648.01	395.86	1.83%
Be^+ (^2P_u) + C (^3P_g)	31,409.66	31,928.74	519.08	1.63%

Table 3.4.2

The calculated asymptotic limits agree well with experimental data. By showing just the $^2\Sigma^+$ symmetries, it can be clearly seen that there are many instances of avoided crossings (note one of these potentials is the $^2\Sigma^+$ component of a $^2\Delta$ state). The theoretical initial state - Be (^1S_g) + C^+ (^2P_u) – is involved in the avoided crossings of the upper excited states between 5 and 6 Bohr, and the lower excited states between 3 and 4 Bohr. Because the other molecular symmetries are instances of the Be atom carrying the positive charge and the entrance channel has the carbon carry the positive charge, the avoided crossing areas have the potential to facilitate a charge transfer. However, strong radiative charge exchange in the entrance channel again dominates.

3.4.3 av6z/qz quartet states

The $^4\Sigma^+$ and $^4\Sigma^-$ are grouped together in order to show clearly the $^4\Delta$ state.

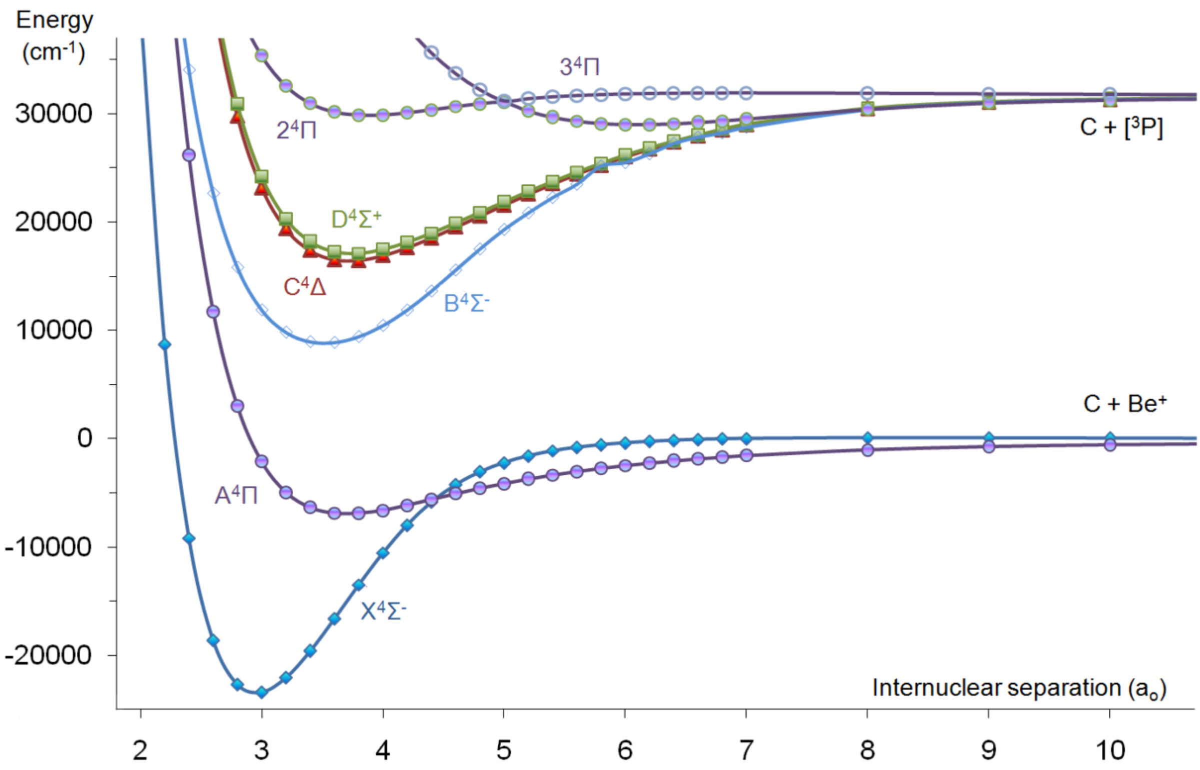


Figure 3.4.3

Molecular Symmetry	Calculated Asymptotic Limit	Experimental Asymptotic Limit	Difference (wavenumbers)	Difference (percentage)
$X^4\Sigma^-$	0	0	0	-
$^4\Sigma^-$	31,528.61	31,928.74	400.13	1.25%
$^4\Delta$	31,564.63	31,928.74	364.11	1.14%
$^4\Sigma^+$	31,566.62	31,928.74	362.12	1.13%

Table 3.4.3

The calculated asymptotic limits agree very well with the expected experimental values.

3.4.4 av6z/qz $^2\Pi$

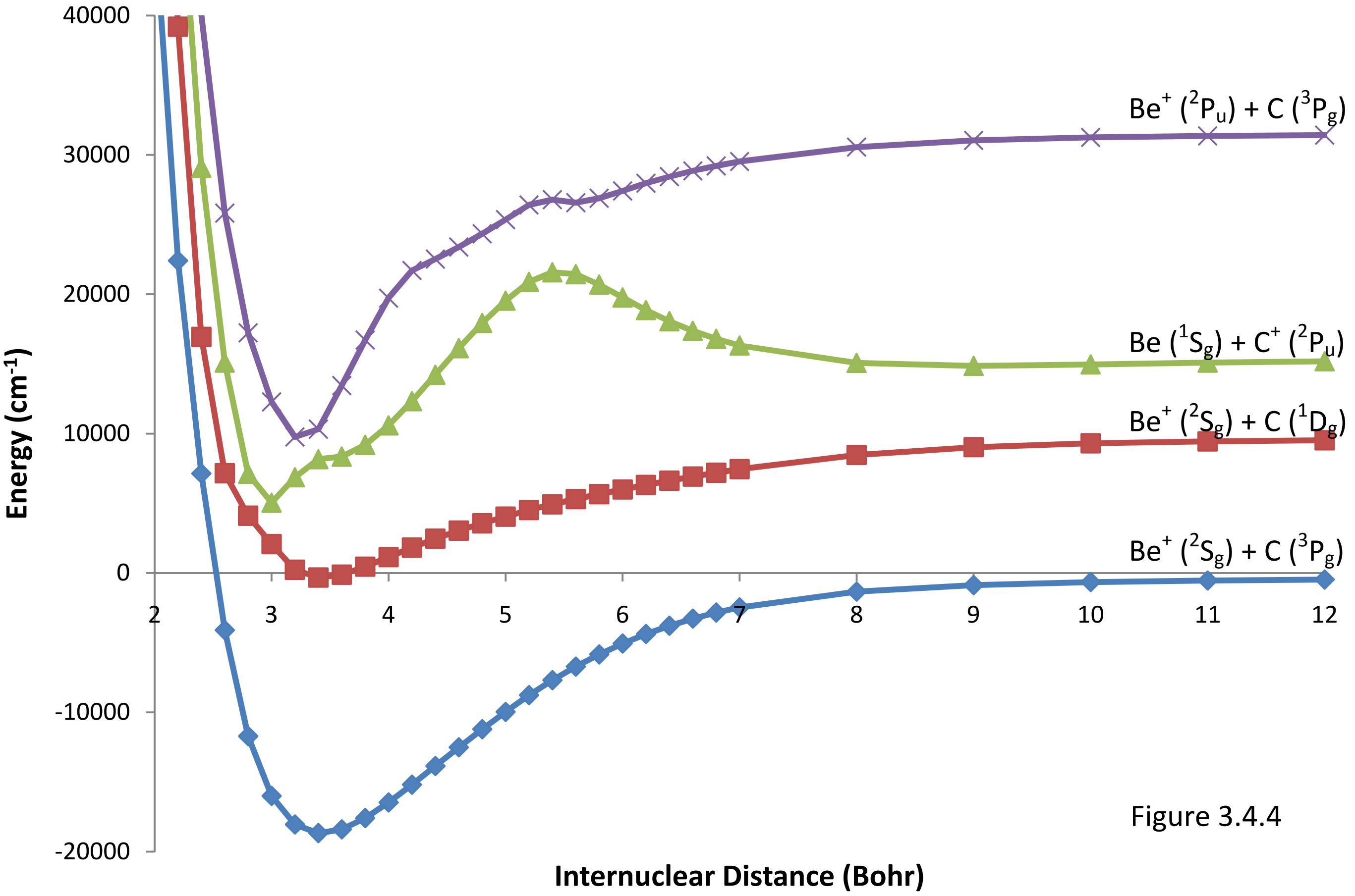


Figure 3.4.4

Atomic Limit	Calculated Asymptotic Limit	Experimental Asymptotic Limit	Difference (wavenumbers)	Difference (percentage)
Be^+ (^2S_g) + C (^3P_g)	-475.33	0	475.33	-
Be^+ (^2S_g) + C (^1D_g)	9,522.31	10,192.63	670.32	6.58%
Be (^1S_g) + C^+ (^2P_u)	15,190.23	15,624.34	434.11	2.78%
Be^+ (^2P_u) + C (^3P_g)	31,421.03	31,928.74	507.71	1.59%

Table 3.4.4

Similarly to the $^2\Sigma^+$ states shown earlier, there are many instances of avoided crossings in the system. The theoretical initial state - Be (^1S_g) + C^+ (^2P_u) – has an avoided crossing with the 4th excited state of the system - Be^+ (^2P_u) + C (^3P_g) – at between 5 and 6 Bohr as well at near the potential well minima between 3 and 3.5 Bohr.

3.4.5 av6z/qz $^2\Sigma^-$

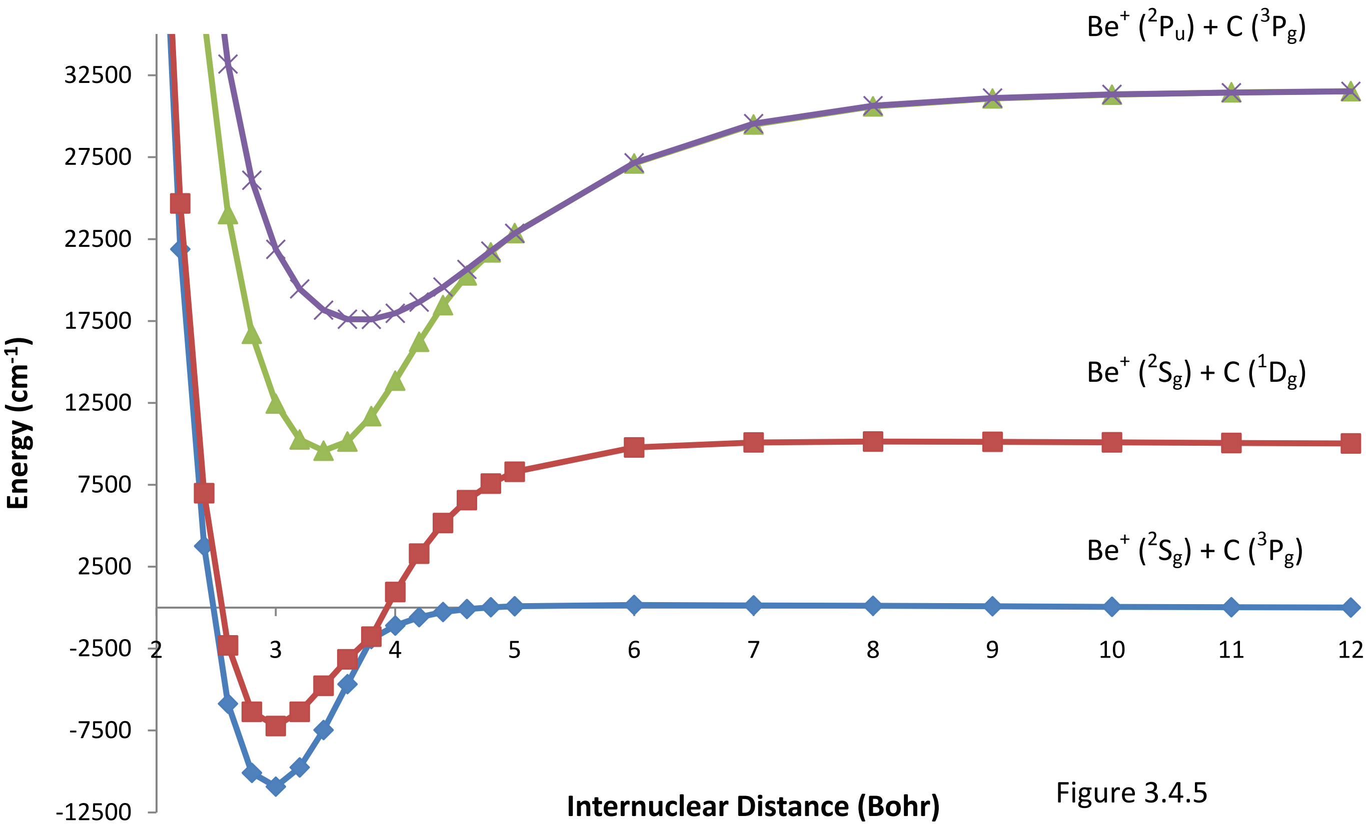


Figure 3.4.5

Atomic Limit	Calculated Asymptotic Limit	Experimental Asymptotic Limit	Difference (wavenumbers)	Difference (percentage)
Be^+ (^2S_g) + C (^3P_g)	4.50	0	4.50	-
Be^+ (^2S_g) + C (^1D_g)	10,024.70	10,192.63	167.93	1.65%
Be (^1S_g) + C^+ (^2P_u)	31,528.61	31,928.74	400.13	1.25%

Table 3.4.5

The calculated asymptotic limits are in excellent agreement with experimental data. Note one of these potentials is the $^2\Sigma^-$ component of a $^2\Delta$ state

4. *Ab initio* data points

CH	$^{2}\Delta$	$^{2}\Sigma^{+}$	$^{2}\Pi$	$^{2}\Pi$	$^{4}\Pi$	$^{2}\Sigma^{-}$	$^{4}\Sigma^{-}$
Distance (Bohr)	1st Excited	1st Excited	Ground	1st Excited	Ground	Ground	Ground
1	158916.2057	168848.3139	136764.9779	203996.7044	204716.5792	166584.5621	139874.8107
1.1	109296.4507	119118.6045	87332.34955	153334.0016	154499.8504	116728.7956	90496.18957
1.2	73506.26189	83220.69542	51633.175	116294.6576	118211.4757	80677.1303	54923.44729
1.3	47728.27478	57334.97487	25864.78531	89330.40663	91994.75048	54606.18804	29349.18759
1.4	29265.83069	38761.03783	7336.535337	70011.94395	73131.26667	35813.37357	11086.32294
1.5	16153.70967	25533.58971	-5899.939585	56290.09576	59631.30265	22334.14727	-1828.485774
1.6	7029.338789	16289.73937	-15191.94384	46864.06117	50102.82386	12803.70642	-10759.76036
1.7	893.4250601	10031.54134	-21523.2978	40784.25495	43514.83924	6225.115116	-16705.51211
1.8	-3038.3756	5978.303543	-25657.52662	37121.28309	39043.78981	1821.102803	-20442.70653
1.9	-5355.197487	3542.105339	-28170.19695	35116.45537	36046.47705	-998.039825	-22555.21282
2	-6483.960228	2294.850745	-29482.13594	34356.97943	34016.02181	-2667.43838	-23469.16491
2.1	-6737.024501	1924.157136	-29897.07689	34492.35072	32524.02745	-3504.275295	-23494.78364
2.2	-6352.699611	2191.609862	-29641.39873	34951.12423	31180.3926	-3749.539604	-22868.05633
2.3	-5520.625194	2909.452338	-28906.94457	35079.74462	29657.93579	-3578.763413	-21777.50112
2.4	-4382.148711	3936.348079	-27821.64347	34365.64191	27782.8719	-3148.042565	-20374.0629
2.5	-3077.9219	5096.804483	-26510.04905	34361.56197	25707.17951	-2591.600521	-18781.98582
2.6	-1720.774287	6297.048603	-25062.21863	33106.65665	23516.63627	-1981.638524	-17087.69937
2.7	-353.807587	7486.332391	-23504.31742	31086.07317	21304.73202	-1402.283813	-15349.79106
2.8	975.8645762	8600.219456	-21893.30228	28920.18739	19144.64902	-880.9569694	-13619.92413
2.9	2229.565004	9571.947022	-20279.96075	26813.47511	17107.05223	-431.3595062	-11946.97455
3	3378.332436	10347.84809	-18688.70229	24828.42163	15218.48435	-63.3105109	-10367.71452
3.1	4405.425699	10891.99104	-17137.74292	22993.17837	13487.68906	221.3508579	-8908.111724
3.2	5304.205828	11198.4348	-15641.1309	21318.92734	11915.2348	427.7404459	-7585.045608
3.3	6075.906242	11299.38222	-14209.02111	19807.18506	10496.85725	565.2164539	-6407.266437
3.4	6727.52145	11257.08597	-12848.71094	18453.81013	9224.714757	645.8804577	-5376.50583
3.5	7270.499009	11137.59113	-11565.93073	17250.08083	8088.852161	681.6365101	-4488.622387
3.6	7718.461421	10989.75395	-10364.59585	16186.40631	7078.324493	683.3439867	-3734.551998
3.7	8085.259437	10840.826	-9247.258715	15252.10935	6182.03096	660.6310364	-3101.87705
3.8	8383.960302	10702.73547	-8214.999128	14436.3657	5389.15608	620.9530551	-2576.272737
3.9	8626.41759	10579.50087	-7268.00583	13728.49594	4689.41549	570.6615046	-2142.733893
4	8823.027594	10471.46896	-6404.483557	13118.21351	4073.21396	514.5869196	-1786.841341
4.1	8982.555948	10377.96377	-5622.582178	12595.58521	3531.469823	456.3637233	-1495.512474

CH (Continued)	$^2\Delta$	$^2\Sigma^+$	$^2\Pi$	$^2\Pi$	$^4\Pi$	$^2\Sigma^-$	$^4\Sigma^-$
Internuclear Distance (Bohr)	1st Excited	1st Excited	Ground	1st Excited	Ground	Ground	Ground
4.2	9112.359285	10297.37438	-4918.924048	12151.21114	3056.097803	398.6036087	-1257.192196
4.3	9218.484003	10228.18427	-4290.776766	11776.27956	2639.741266	343.1786549	-1061.969241
4.4	9305.8594	10168.97785	-3730.180156	11464.19103	2275.800749	291.4276289	-901.538866
4.5	9378.442518	10118.33515	-3237.406359	11204.00934	1958.326421	244.182322	-769.0755528
4.6	9439.283991	10075.38487	-2804.530315	10990.05023	1682.061974	201.7719392	-659.0925517
4.7	9490.776043	10038.9704	-2426.085026	10815.61767	1441.891564	164.2711003	-567.2377726
4.8	9534.742468	10008.15243	-2096.623246	10674.59064	1233.548693	131.5239816	-490.0743153
4.9	9572.601043	9981.952098	-1810.767961	10561.41435	1053.093875	103.2474668	-424.8917253
5	9606.162395	9959.840495	-1563.646935	10471.35045	897.0287575	79.2242806	-369.5457807
5.2	9659.085391	9925.611954	-1166.825423	10344.25098	646.0121397	41.6312643	-281.865321
5.4	9901.540484	9700.771523	-873.073607	10266.72979	459.8598804	15.9137697	-216.9285374
5.6	9884.726888	9734.510646	-656.0419187	10220.72009	322.7021039	-0.109735	-168.0350108
5.8	9873.709494	9759.852847	-495.453525	10194.34638	222.4130927	-9.8520083	-130.6109864
6	9866.804967	9782.150999	-376.303262	10179.81308	149.6522036	-14.5464716	-101.5334061
6.5	9861.669369	9820.944516	-193.8644351	10170.36709	46.8831814	-13.9912125	-52.5915961
7	9865.229173	9845.294713	-103.4559633	10175.18446	5.9542211	-7.058155199	-24.0275756
7.5	9876.213646	9858.026167	-57.347511	10182.72325	-7.962371599	0.3621255	-7.207394799
8	9883.844618	9866.741321	-33.337493	10189.41709	-11.0349516	6.434860401	3.085748201
9	9893.442041	9876.678923	-13.0716332	10198.53168	-8.829278099	14.0614429	13.3328025
10	9898.977075	9881.540183	-6.0837084	10203.58168	-5.394572599	18.0536022	17.8582739
11	9900.427771	9883.897291	-3.134031599	10206.39968	-3.120863399	20.2614704	20.0617527
12	9902.872667	9884.979278	-1.703087199	10207.78892	-1.7667335	21.3193158	21.1393504
15	9904.187293	9886.206115	-0.4345506	10209.17597	-0.513559799	22.276205	22.4759227
20	9904.663542	9886.645055	0	10209.63686	-0.081203899	22.671251	22.868774

LiC	$^2\Delta$	$^2\Sigma^+$	$^2\Pi$	$^2\Pi$	$^4\Pi$	$^2\Sigma^-$	$^4\Sigma^-$
Internuclear Distance (Bohr)	1st Excited	1st Excited	Ground	1st Excited	Ground	Ground	Ground
2	66772.6567	71346.3413	42485.0838	96842.169	91757.6066	72313.8133	53769.1295
2.5	11492.6848	17098.4117	6728.48053	28096.8698	34900.1348	11500.8513	-514.86126
2.7	1330.21425	6968.48415	-39.278546	12804.5448	22891.2719	1339.88849	-10503.547
2.9	-4929.6671	693.59543	-4470.7488	4038.10754	14901.5411	-4913.2486	-16649.269
3.1	-8536.0662	-2947.289	-7585.7874	-595.44625	9635.41336	-8516.6189	-20156.599
3.3	-10365.658	-4822.1444	-9839.9945	-2559.8213	6196.06387	-10353.475	-21902.674
3.5	-11011.938	-5521.2309	-11224.925	-3038.1649	3973.39461	-11006.561	-22469.648
3.7	-10867.426	-5434.2199	-11822.954	-2723.017	2563.20549	-10868.051	-22244.244
3.9	-10194.044	-4821.8744	-11813.256	-1960.5672	1700.90347	-10199.05	-21485.516
4.1	-9184.6637	-3871.679	-11375.707	-955.03248	1203.83245	-9182.2407	-20377.067
4.3	-7968.9316	-2711.0076	-10659.803	150.26233	935.831054	-7955.4715	-19058.705
4.5	-6642.1081	-1437.4495	-9781.6287	1251.00314	796.689268	-6621.6513	-17634.893
4.7	-5272.5495	-120.44953	-8816.0484	2301.9484	722.0563	-5268.3598	-16172.731
4.9	-3894.0408	1206.11275	-7807.9218	3346.51806	679.485704	-4298.9125	-14704.988
5	-3204.9555	1870.01389	-7309.0731	3888.73845	665.474739	-3864.5726	-13973.106
5.2	-1837.269	3187.43743	-6375.3577	4965.4056	644.078609	-3126.0934	-12527.848
5.6	812.77203	5694.50689	-4770.9683	6893.24983	587.70774	-2062.8666	-9772.9179
6	3197.06997	7700.59437	-3495.9113	7892.91154	478.686017	-1378.2782	-7305.1489
7	7545.06915	9879.59129	-1524.961	9067.67519	138.189286	-548.06487	-2855.2542
8	9234.92889	10358.883	-678.8646	9595.32497	-37.186997	-243.82239	-950.91303
10	9956.08756	10566.6597	-200.36075	9870.77298	-114.35923	-61.561335	-126.58371
12	10049.5291	10611.7849	-120.24322	9912.33182	-110.82357	-20.869402	-26.786314
15	10073.2955	10632.4765	-93.876098	9925.54172	-93.443742	-4.0645844	-3.7858575
20	10078.0053	10637.8777	-83.495167	9930.0255	-83.334954	-0.1426555	0

$[BeC]^+$	$^2\Sigma^+$	$^2\Delta$	$^2\Sigma^+$	$^2\Sigma^+$	$^2\Sigma^+$	$^2\Delta$	$^2\Sigma^+$	$^4\Delta$	$^4\Sigma^+$
Internuclear Distance (Bohr)	1st Excited	1st Excited	2nd Excited	3rd Excited	4th Excited	4th Excited	5th Excited	4th Excited	4th Excited
2	53130.4762	59229.7976	93754.5948	98204.6739	118502.688	116855.873	137011.847	126074.66	127661.0133
2.2	21846.1184	28040.049	63315.2822	63703.4171	78920.9401	95971.5557	95904.749	84668.3217	86135.96372
2.4	3712.17045	9801.10443	37577.6841	44806.238	57013.6554	69551.542	70926.6137	57767.8838	59119.81684
2.6	-5910.6387	-11.447555	20209.309	33131.6784	44135.1624	52495.9203	54053.1302	40552.6636	41784.69578
2.8	-10137.622	-4462.7644	9074.90015	26036.1343	36154.3312	41683.7264	43473.6206	29753.5281	30866.89726
3	-10982.033	-5541.7667	2209.5647	21824.4984	31011.6728	35067.5267	37234.6613	23180.8691	24180.00849
3.2	-9804.7564	-4596.5928	-1829.0454	19407.6904	27642.771	31203.6608	33757.4993	19374.8752	20266.70695
3.4	-7519.2244	-4066.744	-2477.8975	18113.7063	25502.313	29102.2992	31866.5831	17364.5564	18156.74213
3.6	-5040.5192	-4721.3879	153.536823	17566.798	24242.9832	28120.994	30859.1412	16532.0825	17232.56712
3.8	-5230.7097	-1819.5446	2990.01319	17555.5019	23595.1648	27840.2874	30360.9619	16472.9617	17089.50122
4	-4914.2493	892.43525	5763.36121	17945.9609	23347.8419	27980.5727	30178.9642	16906.9088	17447.64553
4.2	-4292.087	3222.16197	8304.90721	18642.5302	23351.3424	28361.8425	30218.3985	17639.5545	18111.83418
4.4	-3493.6573	5082.62892	10518.6857	19558.5782	23513.0852	28873.956	30447.782	18541.721	18952.70056
4.6	-2548.9004	6491.80409	12388.6294	20566.6017	23777.6037	28747.5677	29429.0791	19530.3851	19886.79561
4.8	-1617.1493	7515.21903	13866.7489	21670.6609	24053.6421	26742.8672	30063.9553	20552.3252	20860.15822
5	-680.79155	8245.92465	14982.9162	22762.6164	24263.0911	25271.8125	30706.2803	21576.3547	21841.50077
5.2	239.417628	8765.60327	15763.4591	23355.6901	23798.8901	25336.4881	31339.967	22572.4324	22800.12598
5.4	1128.09116	9134.99762	16238.6643	22380.4906	24755.4391	25834.3141	31951.8933	23526.699	23721.94168
5.6	1973.16479	9396.15155	16440.5767	21660.1483	25621.7003	26392.479	32531.766	24425.8895	24592.76791
5.8	2766.95486	9578.39725	16420.4074	21194.7578	26396.3175	26951.8356	33073.5277	25263.5933	25406.04911
6	3505.06539	9704.07455	16245.819	20924.2983	27083.0633	27487.7791	33574.5886	26038.8601	26160.61989
6.2	4187.4064	9790.25822	15998.0747	20789.1487	27687.2642	27985.1025	34036.742	26736.4324	26840.34921
6.4	4814.4256	9848.89841	15737.0151	20736.8951	28217.113	28438.859	34462.4545	27356.5295	27445.61455
6.6	5386.89554	9888.04308	15497.2134	20730.9431	28678.5904	28845.9736	34853.1616	27939.5559	28015.64617
6.8	5905.76432	9913.19215	15293.4575	20749.0735	29077.4179	29205.8715	35207.7922	28481.7851	28547.43515
7	6371.93835	9928.22804	15128.6158	20778.1181	29420.9323	29521.1621	35526.6053	28956.7269	29013.69039
8	7984.78827	9931.19966	14769.4795	20944.0155	30528.2243	30478.8962	36777.4372	30458.6896	30488.05473
9	8763.05961	9877.00374	14870.9075	21072.197	31000.8947	30924.653	37163.6825	31069.0708	31085.71763
10	9131.88992	9832.26697	15040.7905	21158.6725	31223.7884	31142.0578	37291.5106	31327.466	31336.90324
11	9324.23782	9795.93371	15178.3894	21215.2607	31337.9786	31255.7432	37324.9008	31457.5788	31461.21544
12	9437.4997	9763.46313	15277.1267	21252.147	31409.6554	31321.0619	37328.5528	31564.5309	31566.6181

$[BeC]^+$ (Continued)	$^2\Pi$	$^2\Pi$	$^2\Pi$	$^2\Pi$	$^4\Pi$	$^4\Pi$	$^2\Sigma^-$	$^2\Delta$
Internuclear Distance (Bohr)	Ground	1st Excited	2nd Excited	4th Excited	Ground	4th Excited	Ground	1st Excited
2	46869.94516	77775.8247	89175.4147	99825.811	86326.7183	97958.9114	53177.2167	55357.9452
2.2	22412.71095	39197.8731	52162.0362	63141.5761	49478.4251	72238.5681	21887.0605	24679.8053
2.4	7134.726088	16935.6154	29074.0205	40069.8406	26201.8298	56442.307	3755.12292	6987.00522
2.6	-4105.941327	7153.50614	15093.8583	25824.6069	11764.9637	46488.5326	-5867.0344	-2307.6502
2.8	-11716.82953	4106.59096	7115.41931	17232.0184	3004.59258	39798.7249	-10087.601	-6355.8556
3	-16004.90242	2069.6833	5039.49867	12271.3819	-2116.1627	35340.1063	-10930.701	-7229.3725
3.2	-18053.06011	231.145804	6865.98946	9761.98829	-4941.1629	32561.6512	-9755.0157	-6358.34
3.4	-18671.0174	-328.36004	8165.30234	10321.1298	-6346.5983	30961.2869	-7471.5796	-4765.7033
3.6	-18402.95674	-121.86072	8350.90373	13444.7958	-6872.7974	30158.4108	-4673.8726	-3158.1053
3.8	-17593.92887	450.927451	9195.68765	16716.7621	-6861.8042	29878.964	-1918.181	-1768.3203
4	-16473.45332	1141.14304	10590.3624	19721.1418	-6604.2803	29884.1655	-1097.3259	952.515163
4.2	-15195.10202	1825.07302	12327.992	21709.7222	-6130.4643	30090.1315	-583.93066	3295.22134
4.4	-13855.73367	2459.47519	14222.8411	22524.2456	-5603.8746	30369.5651	-268.55227	5166.12189
4.6	-12515.96369	3035.5598	16129.9433	23390.5683	-5076.9051	30662.6256	-85.755708	6562.67095
4.8	-11214.53293	3559.19547	17939.1815	24342.2319	-4577.2246	30928.4235	21.3149264	7571.32654
5	-9974.090682	4042.65715	19537.3291	25352.5818	-4133.6494	31028.1309	86.2912146	8293.32358
5.2	-8772.027156	4518.97509	20887.1618	26408.6912	-3724.3006	30226.7362		
5.4	-7696.810705	4925.88564	21574.296	26787.4811	-3355.5778	29664.1512		
5.6	-6719.708318	5303.97758	21441.5057	26573.5944	-3026.9763	29304.8612		
5.8	-5843.505069	5657.78736	20695.4745	26892.9715	-2737.1201	29094.7055		
6	-5067.072882	5992.27939	19766.5282	27415.6174	-2481.3344	29001.2333	160.700323	9779.63368
6.2	-4385.063273	6312.3303	18866.0736	27967.7534	-2253.834	28998.0619		
6.4	-3791.939014	6619.77265	18064.286	28438.2905	-2049.9156	29064.1443		
6.6	-3281.061137	6913.99194	17376.3661	28854.8424	-1866.5046	29180.6588		
6.8	-2844.816229	7193.20387	16799.8184	29215.2758	-1701.5882	29332.1721		
7	-2475.14535	7455.27519	16324.9841	29525.9487	-1553.5403	29505.4415	137.195086	10086.4308
8	-1345.320374	8469.83891	15078.5174	30558.1447	-1018.3474	30397.8921	111.284458	10138.4188
9	-872.9441197	9026.02637	14862.1375	31039.9581	-717.75688	30980.7364	80.8198275	10125.9946
10	-653.7967406	9302.7122	14964.2152	31254.8983	-546.17524	31247.9894	49.6155829	10089.33
11	-541.9789703	9442.38949	15093.5006	31359.7479	-444.51893	31374.3229	23.0026507	10051.6426
12	-475.3347101	9522.31169	15190.2276	31421.0327	-378.93032	31443.2321	4.5035244	10024.6983

$[BeC]^+$ (continued)	$^2\Sigma^-$	$^2\Sigma^-$	$^4\Sigma^-$	$^4\Sigma^-$	$^4\Sigma^-$
Internuclear Distance (Bohr)	4^{th} Excited	4th Excited	Ground	4^{th} Excited	4th Excited
2	85563.9481	93755.7339	39564.40338	82174.9121	120803.131
2.2	55262.2717	63748.2987	8679.467878	52646.5668	85709.1121
2.4	36023.1167	44854.9955	-9187.36974	34070.2353	57746.3472
2.6	24029.6759	33187.3119	-18631.6335	22665.5623	40517.1534
2.8	16715.8974	26091.342	-22705.1174	15810.7329	29705.9317
3	12461.5922	21877.3402	-23402.1037	11886.7256	23125.5034
3.2	10269.7277	19458.3112	-22074.1851	9821.48441	19314.769
3.4	9586.08309	18162.2596	-19621.1381	8944.62714	17301.1537
3.6	10143.4491	17612.744	-16629.1695	8878.88271	16465.728
3.8	11695.9557	17595.5003	-13504.2722	9417.58499	16404.2961
4	13862.7106	17974.0619	-10547.5197	10441.4608	16837.4224
4.2	16232.4379	18656.3327	-7967.45014	11872.1638	17570.4851
4.4	18471.1724	19575.3896	-5870.34625	13628.7095	18474.2516
4.6	20285.3005	20649.7304	-4262.90408	15571.6313	19464.8777
4.8	21691.3306	21766.4376	-3075.99056	17513.8157	20488.3146
5	22867.512	22857.0324	-2211.79452	19319.4503	21509.6512
5.2			-1583.51775	20854.9261	22506.0954
5.4			-1126.22786	22274.6424	23460.3269
5.6			-794.378249	23506.488	24358.9621
5.8			-554.736761	25193.5758	24575.4013
6	27114.6275	27158.4205	-381.002115	25506.0616	25959.4515
6.2			-251.83963	26317.7867	26654.7149
6.4			-148.390251	27276.5897	27022.8978
6.6			-67.6077335	27859.7215	27663.7655
6.8			-18.5188786	28248.8901	28405.5237
7	29494.1892	29550.4174	14.0943634	28765.9197	28892.9051
8	30602.234	30641.969	82.5119412	30391.207	30440.6975
9	31083.6875	31114.1763	67.0283327	31043.2985	31066.4065
10	31312.2524	31335.0509	39.7855216	31313.6833	31326.2941
11	31455.4609	31439.703	17.0857395	31444.7749	31452.6254
12	31528.6103	31521.1154	0	31530.5438	31534.9947

$[LiC]^+$	$^1\Sigma^+$	$^1\Delta$	$^1\Sigma^+$	$^1\Sigma^+$	$^3\Sigma^+$	$^1\Pi$
Internuclear Distance (Bohr)	1st Excited	1st Excited	2nd Excited	4th Excited	4th Excited	1st Excited
2	83883.3961	89822.2038	140432.5	179709.7	147809.6	109256
2.5	38190.1569	42444.0034	57949.16	109417.6	94365.17	43771.99
3	17929.3405	20326.4445	32193.04	81311.85	73262.41	18789.88
3.5	7472.8723	13993.3589	24557.28	69683.38	67753.25	9811.24
4	4290.81627	11930.9445	22045.11	63916.2	60994.8	6929.258
5	4846.3519	11095.8567	20933.3	56831.34	51987.06	6648.519
6	6904.07629	10963.5602	20976.28	51601.38	46733.89	7799.799
8	9285.01853	10790.045	21462.07	46309.19	44164.73	9286.452
10	10041.7401	10661.6309	21695.91	45735.33	45116.87	9757.739
12	10322.0889	10590.6719	21778.08	46332.88	46209.81	9933.95
14	10450.6698	10548.7246	21814.36	46801.7	46795.08	10014.88
16	10518.6484	10522.4628	21833.59	47042.55	47049.73	10058.36
20	10580.9603	10492.5973	21849.96	47229.84	47230.43	10098.66

$[LiC]^+$ (Continued)	$^1\Pi$	$^3\Pi$	$^3\Pi$	$^3\Sigma^-$	$^5\Sigma^-$	$^5\Sigma^-$
Internuclear Distance (Bohr)	4th Excited	Ground	4th Excited	Ground	3rd Excited	4th Excited
2	156801.5	97313.97	127473.6	73002.79	114508.8	156801.5
2.5	106438.3	32003.49	93115.08	27786.9	62432.73	106438.3
3	83951.39	7177.922	74465.32	9873.87	42218.96	83951.39
3.5	72777.25	-1371.18	64804.53	3439.494	34655.73	72777.25
4	65784	-3767.01	61579.59	1328.676	32107.78	65784
5	55950.19	-3400.46	55033.95	572.7245	31625.63	55950.19
6	49454.57	-2108.16	48547.79	519.7379	32265.94	49454.57
8	44836.01	-736.785	44421.59	396.6591	33014.17	44836.01
10	45097.64	-318.699	44967.67	281.2991	33225.08	45097.64
12	46045.96	-160.088	46022.95	222.3648	33302.22	46045.96
14	46622.46	-85.128	46624.01	203.903	33336.12	46622.46
16	46890.2	-40.9794	46892.07	224.2698	33352.05	46890.2
20	47086.27	0	47086.44	231.2819	33364.04	47086.27

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