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An Accurate Description of the LiNe X $^2\Sigma^+$, A $^2\Pi$, and B $^2\Sigma^+$ States

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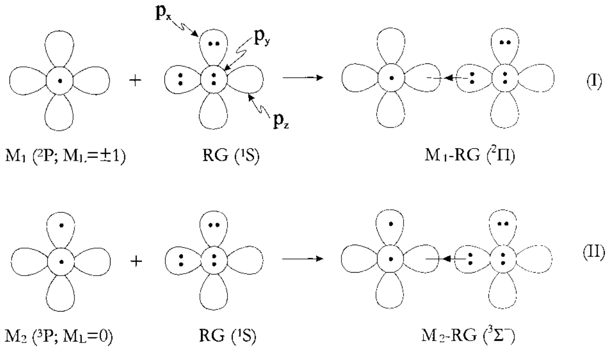
The X $^2\Sigma^+$, A $^2\Pi$, and B $^2\Sigma^+$ states of the LiNe molecule have been investigated by the coupled cluster approach, in conjunction with a series of increasing size augmented correlation-consistent basis sets of double through sextuple zeta quality. For the A $^2\Pi$ bound state the convergence properties of the binding energy and spectroscopic constants were examined as a function of the basis set size. It was found that at the extrapolated complete basis set limit all our findings are in excellent agreement with experiment, under the proviso, however, that basis set superposition effects have been carefully considered.

1. Introduction

The literature on the studies of the alkali metal[1] and alkaline earth metal−noble gas[2] diatomics has grown significantly in the last 20−30 years. The approach of a closed-shell (^{1}S) noble gas atom to a ground ^{2}S state alkali metal or a ^{1}S ground state alkaline earth metal leads necessarily to repulsive $^2\Sigma^+$ or $^1\Sigma^+$ interactions. However, the situation changes drastically when a “reaction channel” is created between the two interacting entities, that is, by considering the first excited ^{2}P ($^2\text{P} \leftarrow {}^2\text{S}$) state of the alkali metal atom or the doubly excited ^{3}P ($^3\text{P} \leftarrow {}^1\text{S}$) state of the alkaline earth metal atom. The ensuing bonding is captured pictorially by the following valence bond Lewis diagrams (M_1 = Li, Na, ...; M_2 = Be, Mg, ...; RG = (He), Ne, ...):



Obviously, the $M_L = 0$ component in the first diagram and the $M_L = \pm1$ in the second lead to the repulsive $^2\Sigma^+$ and $^3\Pi$ states, respectively. The interplay between the ability of the RG atom(s) to approach as close as possible to a given metal center, or the Pauli $p\pi-p\pi$ repulsion (with the exception of He), and the polarizability of the former dictates the bond strength of the M−RG systems in the $^2\Pi$ and $^3\Sigma^-$ states. For instance, in the Li−RG A $^2\Pi$ series, RG = He, Ne, Ar, Kr, and Xe, the (experimental) dissociation energies (D_e), bond distances (r_e), and polarizabilities (α)[7] are D_e (cm^{-1}), r_e (Å), α (Å^3) = (1020, 1.78, 0.204956),[3] (212, 2.31, 0.3946),[4] (925, 2.48, 1.64),[5] (1200, 3.27, 2.48),[6] and (1650, 3.17, 4.04),[6] respectively. Clearly, with the exception of LiHe, the bond strength increases monotonically as the polarizability increases. The dramatic 5-fold decrease of the LiNe bond strength as compared to LiHe is due to the Pauli $p\pi-p\pi$ repulsion switched on in LiNe, but absent in LiHe. The twice as large polarizability of Ne as compared to He cannot offset the Pauli repulsion, thus the plummeting of D_e in going from LiHe to LiNe. However, as we move from LiNe to LiXe, the polarizability takes over; therefore, the D_e values of the last two members of the series, i.e., LiKr and LiXe, are significantly larger than the LiHe D_e value. *Mutatis mutandis*, the same trend is followed by the series Na−RG ($^2\Pi$): RG = He,[8] Ne,[9,10] Ar,[11] Kr,[12] and Xe.[13]

The significance to the binding on the ability of the RG atom to approach the positively charged core of the metal is dramatically demonstrated by the recent (quadratic configuration interaction)[14] QCISD(T)/6-311++G**(3df,3dp)/$_{\text{Be}}$aug-cc-pVQZ/$_{\text{He,Ne}}$ calculations of Leung and Breckenridge[15] on the BeHe and BeNe $^3\Pi$ and $^3\Sigma^-$ states. In the $^3\Pi$ state of the BeHe system, the in situ Be atom is in a *singly* ^{3}P (2s^{1}2p^1) excited state, so the access of the He (^{1}S) atom to the Be core is hindered by the intervening 2s^1 electron distribution. The resulting $^3\Pi$ state is characterized by $D_e = 12$ cm^{-1} and $r_e = 3.80$ Å.[15] However, in the $^3\Sigma^-$ state where the in situ Be atom finds itself in the *doubly* excited ^{3}P (2p^2) state (see diagram II), the He atom penetrates unobstructed to the Be atom, thus facing the +2 charged Be core. The result is a stunning binding energy D_e = 6251 cm^{-1} (=17.87 kcal/mol) at $r_e = 1.35$ Å. Corresponding results for the BeNe system are[15] $^3\Pi$: $r_e = 3.75$ Å, $D_e = 25$ cm^{-1}; $^3\Sigma^-$: $r_e = 1.88$ Å, $D_e = 1294$ cm^{-1}. No experimental results are available for the Be−RG molecular systems.

Continuing our studies toward a quantitative description of the Li−RG molecules,[16] the present report focuses on the A $^2\Pi$, X $^2\Sigma^+$, and B $^2\Sigma^+$ states of the LiNe system. Table 1 lists existing experimental and all ab initio results published so far on the A $^2\Pi$ state of the LiNe molecule. Preliminary experimental results of Havey et al.,[17] extracted by observation of the red wing intensity of the Li D lines perturbed by Ne, gave a $D_e = 225 \pm 30$ cm^{-1}. A few years later Lee and Havey[4] using accurate rotationally resolved absorption spectra narrowed down the A $^2\Pi$ D_e to 212 ± 5 cm^{-1} at $r_e = 4.36 \pm 0.02$ b (=2.307 ± 0.011 Å). An anomalously large fine-structure constant $A = 2.77 \pm 0.03$ cm^{-1} was also determined experimentally for the $v'' = 0$ vibrational level.[4] Sohlberg and Yarkony[18] confirmed this result theoretically via multireference

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TABLE 1: Existing Experimental and Theoretical Results of the LiNe A $^2\Pi$ State: Total Energies *E*, Dissociation Energies D_e, Bond Distances r_e, and Harmonic Frequencies and Anharmonic Corrections ω_e, $\omega_e x_e$

method	E (hartree)	D_e[a] ($\mathrm{cm^{-1}}$)	r_e (Å)	ω_e ($\mathrm{cm^{-1}}$)	$\omega_e x_e$ ($\mathrm{cm^{-1}}$)
expt[b]		212 ± 5	2.307 ± 0.011	108.1 ± 1.3	21.0 ± 0.6
ACPF[c]	−136.20304	214	2.26	131	−18.21
MRCI[d]		200	2.47		
SOCI +Q[e]		340	2.32	112	15
CEPA-0[f]	−136.26024	168	2.32	90	14

[a] With respect to Li (^{2}P) + Ne (^{1}S). [b] Rotationally resolved absorption spectroscopy, ref 4. [c] Averaged coupled-pair functional, $[5s4p3d2f]_{\mathrm{Li,Ne}}$ basis, ref 19. [d] Multireference CI, effective core potentials, BSSE-corrected, ref 1. [e] Second-order CI + Davidson correction, $[(4s3p2d1f)_{\mathrm{Li}}/(5s4p3d2f)_{\mathrm{Ne}}]$ basis, ref 18. [f] Coupled electron-pair approximation, $[(8s5p3d3f2g)_{\mathrm{Li}}/(11s7p5d4f3g)_{\mathrm{Ne}}]$ basis, BSSE-corrected, ref 22.

configuration interaction (MRCI) methods giving $A = 3.20$ $\mathrm{cm^{-1}}$. Sadlej and Edwards[19] using complete active space perturbation theory (CASPT2),[20] MRCI, and coupled-pair functional (CPF)[21] methods coupled with nearly quadruple-ζ quality basis sets obtained $D_e = 214$ $\mathrm{cm^{-1}}$, in complete accordance with the experimental value of Lee and Havey,[17,4] but, on the other hand, their r_e, ω_e, and $\omega_e x_e$ values deviate significantly from experiment, Table 1. Sohlberg and Yarkony[18] and Behmenburg et al.[22] pointed out that the neglect of the basis set superposition error (BSSE) correction was the most probable cause of the inconsistent results of Sadlej and Edwards.[19] Our calculations prove that, indeed, there exists a severe BSSE problem in the LiNe (A $^2\Pi$) system, which can only be remedied by using very large basis sets (vide infra). Bililign et al.,[1] performing BSSE-corrected MRCI-effective core potential (ECP) calculations, obtained satisfactory D_e agreement with experiment (Table 1) but with an r_e value ∼0.16 Å longer, probably due to their ECP approach. Finally, the recent BSSE-corrected coupled electron-pair approximation (CEPA-0)[23] calculations of Behmenburg et al.,[22] the largest so far in the literature, give $D_e = 168$ $\mathrm{cm^{-1}}$ while their r_e, ω_e, and $\omega_e x_e$ values are toward the correct direction.

The above results indicate that more accurate calculations are needed for the quantitative description of the LiNe problem, while care is required in coping with the BSSE correction.

2. Methods

The well-known correlation-consistent basis sets of Dunning and co-workers were used.[24] The convergence characteristics of the cc-basis sets allow the estimation of complete basis (CBS) limit properties.[25−26] For the Li atom the aug-cc-pCV*n*Z, $n =$ 2(D), 3(T), 4(Q), 5 series, was employed, with n the cardinal number defining the quality of the plain (nonaugmented by diffuse functions) cc-pV*n*Z bases. The core (C) functions used ($(n-1)$s, $(n-1)$p, $(n-2)$d, $(n-3)$f, ... contracted Gaussians) are as in ref 16. Our previous experience on LiHe[16] has shown that core (C) functions on Li are absolutely necessary for achieving a quantitative description of that system, while the addition of the diffuse functions makes the convergence to the CBS limit smoother. For the Ne atom, the aug-cc-pV*n*Z, $n = 2-6$, was used; thus our largest generally contracted basis set, $[(11s10p8d6f4g2h)_{\mathrm{Li}}/(8s7p6d5f4g3h2i)_{\mathrm{Ne}}]$ contains 370 contracted spherical Gaussian functions (5d, 7f, 9g, 11h, 13i).

Recognizing the single-reference nature of the Li−RG interaction, the coupled-cluster plus single and double excitations with a perturbative estimate of the connected triple excitations from a restricted Hartree−Fock (RHF) reference wave function [RCCSD(T)][27−28] methodology was used. We remind the reader that the CCSD(T) approach is size-extensive, size-consistent for this particular problem at hand, but not variational. With the exception of the Ne 1s^2 electrons, which were always constrained to be doubly occupied, the rest of the 11 electrons were allowed to correlate.

CBS limits for the properties E, D_e, r_e, ω_e and $\omega_e x_e$ were estimated in two ways using the simple exponential formula[25]

$$P_n = P_\infty + A\mathrm{e}^{-Bn} \tag{1}$$

and the mixed exponential/Gaussian function[29]

$$P_n = P_\infty + A\mathrm{e}^{-(n-1)} + B\mathrm{e}^{-(n-1)^2} \tag{2}$$

where n is the cardinal basis set number and A and B are fitting constants. A recent study of CBS extrapolations in CCSD(T) and CCSDT calculated properties of diatomic molecules by Feller and Sordo[26] shows that the mixed exponential/Gaussian formula performs slightly better than the simple one in most cases, although, as they point out, care should be taken in deciding which extrapolation scheme to use. Following their designation, we will refer to these two extrapolation schemes as "CBS/e^{-n}" and "CBS/mixed", respectively.

All our reported results have been BSSE-corrected[30] following the counterpoise technique.[31−32] BSSEs were calculated point-by-point along the A $^2\Pi$ curve and around "equilibrium" in the repulsive (van der Waals) X $^2\Sigma^+$ and B $^2\Sigma^+$ states. Interatomic distances for the A $^2\Pi$ state of LiNe were determined by fitting the three lowest-energy points of the corresponding potential energy curve (PEC) and then recalculating the energy at the determined r_e. Spectroscopic constants for the same state were extracted by a standard Dunham analysis by always fitting 28 energy points of the PEC up to an interatomic distance of 5.5 b. In our largest basis set $[(\text{aug-cc-pCV5Z})_{\mathrm{Li}}/(\text{aug-cc-pV6Z})_{\mathrm{Ne}}]$, the Dunham analysis was performed by fitting 17 points up to $r_{\mathrm{Li-Ne}} = 6$ b.

All calculations were performed with the MOLPRO 2000 suite of codes.[33]

3. Results and Discussion

The Li and Ne Atoms. Table 2 summarizes the results of our calculations on Li (^{2}S) and Ne (^{1}S) atoms at the RHF and RCCSD(T) levels of theory, coupled with a series of increasing quality (n) basis sets, double through sextuple (Ne). The RHF values are a mere 0.9 (Li) and 9 (Ne) $\mathrm{cm^{-1}}$ higher that the numerical Hartree−Fock results.[34] Our best RCCSD(T) number for the total energy of the Li atom is just 0.714 mh higher than the "exact" nonrelativistic energy.[35] Finally, the RCCSD(T) atomic energy gap $^2\mathrm{P} \leftarrow {}^2\mathrm{S}$ in Li is in practical agreement with the experimental (averaged over M_J) value.[36]

LiNe X $^2\Sigma^+$ and B $^2\Sigma^+$ Repulsive States. Figure 1 shows the PECs of the repulsive X $^2\Sigma^+$ and B $^2\Sigma^+$ states at the RCCSD(T)/$(\text{aug-cc-pCV5Z})_{\mathrm{Li}}/(\text{aug-cc-pV6Z})_{\mathrm{Ne}}$ level correlating to Li (^{2}S), Li (^{2}P, $M_L = 0$) + Ne (^{1}S) fragments, respectively. Similarly to the LiHe case,[16] these repulsive states exhibit weak van der Waals minima at large internuclear distances. Our results for the van der Waals interactions (ΔE) and distances (r_{vdW}) of the X $^2\Sigma^+$ and B $^2\Sigma^+$ states are presented in Table 3, along with existing experimental values;[37−38] for comparison ab initio results from ref 19 are also included. Taking into account the weakness of the van der Waals interaction, our values for the X $^2\Sigma^+$ state can be considered in good agreement with the experimental values. Corresponding theoretical (experimental)

TABLE 2: Absolute Energies of the Ground States of the Li (^{2}S) and Ne (^{1}S) Atoms and Energy Gaps of the First Excited State of Li at the RHF, RCCSD(T)/(aug-cc-pCV*n*Z)$_{\mathrm{Li}}$/(aug-cc-pV*n*Z)$_{\mathrm{Ne}}$, $n = 2, 3, 4, 5$, and 6 (Ne), Level

	Li				Ne	
	E (^{2}S; 2s^1) (hartree)		^{2}P (2p^1) ← ^{2}S (2s^1) (cm^{-1})		E (^{1}S; 1s^{2}2s^{2}2p^6) (hartree)	
basis set (n)	RHF	RCCSD(T)	RHF	RCCSD(T)	RHF	RCCSD(T)
2	−7.432426	−7.466114	14883.7	14908.8	−128.496350	−128.709295
3	−7.432681	−7.474267	14855.1	14924.4	−128.533273	−128.812648
4	−7.432696	−7.476370	14850.6	14911.0	−128.543756	−128.847459
5	−7.432723	−7.477346	14849.7	14907.8	−128.546786	−128.859837
6					−128.547062	−128.864036
NHF[a]	−7.432727				−128.547098	
exact[b]	−7.4780603					
expt	−7.4780604[c]		14903.89[d]			

[a] Numerical Hartree−Fock, ref 34. [b] Nonrelativistic "exact" calculation, ref 35. [c] Nonrelativistic "experimental" estimate, ref 35. [d] Averaged over M_J values, ref 36.

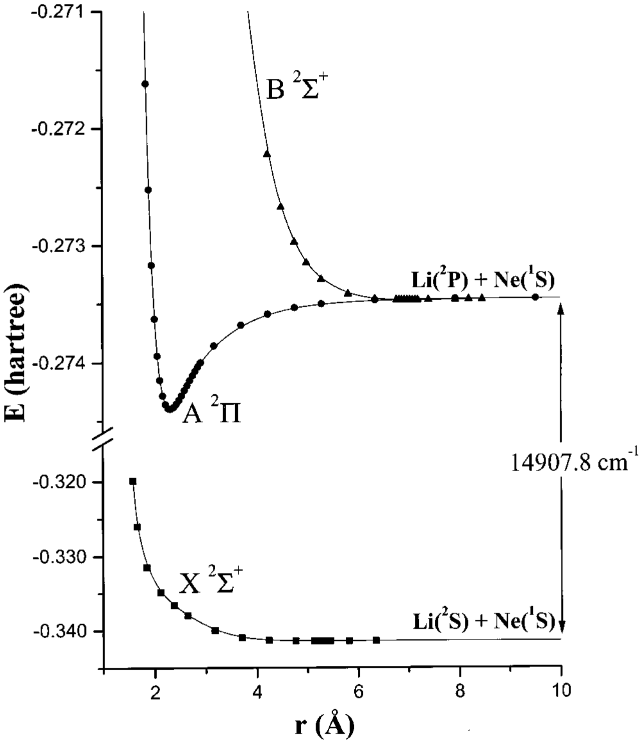

Figure 1. Potential energy curves of the LiNe X $^2\Sigma^+$, A $^2\Pi$, and B $^2\Sigma^+$ states at the RCCSD(T)/(aug-cc-pCV5Z)$_{\mathrm{Li}}$/(aug-cc-pV6Z)$_{\mathrm{Ne}}$ level of theory. Energies have been shifted by 136 hartrees.

TABLE 3: Interaction Energies Δ*E* and van der Waals Distances r_{vdW} of the Repulsive X $^2\Sigma^+$ and B $^2\Sigma^+$ States of the LiNe Molecule

method	ΔE (cm^{-1})	ΔE(BSSE)[a] (cm^{-1})	r_{vdW} (Å)
	X $^2\Sigma^+$		
RCCSD(T)[b]	−7.68	−6.96	5.2
ACPF[c]	−15.8		5.28
expt[d]	−8.95		5.05
expt[e]	−9.61 ± 2.11[f]		4.979 ± 0.217[f]
	−9.43 ± 0.16[g]		4.924 ± 0.016[g]
	−8.78 ± 0.44[h]		5.116 ± 0.114[h]
	B $^2\Sigma^+$		
RCCSD(T)[b]	−3.70	−3.47	7.1

[a] BSSE-corrected. [b] This work, (aug-cc-pCV5Z)$_{\mathrm{Li}}$/(aug-cc-pV6Z)$_{\mathrm{Ne}}$ basis set. [c] Ref 19, averaged coupled-pair functional. [d] From velocity dependence of the total scattering cross section, fit to Lennard−Jones (12,6) potential, ref 37. [e] From absolute total scattering cross sections, ref 38. [f] Fit to Buckingham−Corner (6,8) potential. [g] Fit to Lennard−Jones (12,6) potential. [h] Fit to Morse−Spline−van der Waals potential.

values for the LiHe (X $^2\Sigma^+$) system[16] are −1.42 (−1.14) cm^{-1} and 6.1 (6.01) Å.

The LiNe A $^2\Pi$ State. This is the first excited state of the LiNe system bound "strongly" with respect to Li (^{2}P, $M_L = \pm1$) + Ne (^{1}S) fragments. Diagram I in the Introduction describes pictorially the bonding type, Figure 1 shows the CCSD(T)/(aug-cc-pCV5Z)$_{\mathrm{Li}}$/(aug-cc-pV6Z)$_{\mathrm{Ne}}$ potential energy curve, and Table 4 presents calculated properties, their BSSE-corrected values, and CBS limits. Notice that BSSE corrections were applied for every calculated point of the corresponding potential energy curve. Table 5 presents BSSE-corrected harmonic frequencies and anharmonic corrections (ω_e(BSSE), $\omega_e x_e$(BSSE)) and their CBS limits of the isotopic species ^{6}Li^{20}Ne, ^{6}Li^{22}Ne, ^{7}Li^{20}Ne, and ^{7}Li^{22}Ne, along with some experimental findings.[4]

The first conclusion that can be drawn from Table 4 is the essentially complete agreement of all BSSE-corrected CBS limit values with experiment. However, the painful convergence with increasing basis set quality (n) should be noticed, as well as the absolute necessity for BSSE corrections, even for the largest bases. The role of the BSSE correction is graphically illustrated in Figure 2, where D_e, r_e and D_e(BSSE), r_e(BSSE) values are plotted as a function of basis set size n. It is interesting that uncorrected BSSE D_e, ω_e, and $\omega_e x_e$ values present a maximum for the quadruple ($n = 4$) zeta quality basis, while r_e shows a minimum for $n = 4$. This means that extrapolation CBS limit formulae cannot be applied to uncorrected values. In light of the above, the rather conflicting results of Table 1 are easily explained, in particular the excellent $D_e = 214$ cm^{-1} and very short $r_e = 2.26$ Å ACPF results of ref 19 (Table 1).

It is also of interest to observe that even at the highest basis set level, i.e., aug-cc-pCV5Z/aug-cc-pV6Z, the BSSE is 10 cm^{-1} or about 5% of the "true" binding interaction. At this level we also calculate a dipole moment, $\mu = 0.441$ D; no experimental μ values are reported at the literature so far for the LiNe system.

Concerning the simple exponential versus the mixed exponential/Gaussian extrapolation function, Table 4 suggests that the latter performs slightly better, in agreement with the conclusions of Feller and Sordo.[26]

Given now the excellent agreement between theory and experiment at the CBS(BSSE) limit, one could raise some doubts as to the ability of the counterpoise (CP) technique used to remedy *rigorously* BSSEs. It seems that a definite answer to such criticisms has been given by van Duijneveldt and coworkers[39] who argue persuasively that the CP approach is a rigorous, fundamentally sound method for taking care of BSSE.

In conclusion, we would like to stress that for van der Waals or weakly interacting systems, reliable results can only be obtained by using highly correlated methods and very large basis

TABLE 4: RCCSD(T) Results on the A $^2\Pi$ State of $^7Li^{20}Ne$: Energies E, Dissociation Energies D_e, Equilibrium Bond Distances r_e, Harmonic Frequencies and Anharmonic Corrections ω_e, $\omega_e x_e$, Rotational−Vibrational Coupling Constants α_e, and CBS Limits, in a Series of Increasing Size Basis Sets

basis set (n)[a]	E (hartree)	D_e (cm^{-1})	D_e(BSSE)[b] (cm^{-1})	r_e (Å)	r_e(BSSE)[b] (Å)	ω_e (cm^{-1})	ω_e(BSSE)[b] (cm^{-1})	$\omega_e x_e$ (cm^{-1})	$\omega_e x_e$(BSSE)[b] (cm^{-1})	α_e(BSSE)[b] (cm^{-1})
expt[c]		212 ± 5		2.307 ± 0.011		108.1 ± 1.3		21.0 ± 0.6		0.110 ± 0.008
2	−136.108148	151.4	56.1	2.453	2.560	80.9	59.7	18.4	11.8	0.063
3	−136.219987	242.1	146.0	2.329	2.424	107.2	82.9	17.8	14.8	0.109
4	−136.257101	268.0	185.1	2.279	2.327	119.2	101.8	20.8	20.6	0.102
5	−136.270302	229.3	204.9	2.300	2.315	109.1	104.0	20.2	21.0	0.104
6	−136.274445	216.6	206.6	2.307	2.314	107.4	104.9	18.9	22.1	0.100
CBS/e^{-n} [d,e]	−136.2766		211.8 (5.5)		2.314		104.7 (0.3)		21.8 (0.6)	
CBS/mixed[d,f]	−136.2777		212.0 (3.2)		2.311 (0.002)		105.3 (0.1)		22.0 (0.5)	

[a] (aug-cc-pCVnZ)$_{Li}$/(aug-cc-pVnZ)$_{Ne}$, $n = 2, 3, 4, 5$, and 6 (Ne). [b] BSSE-corrected values. [c] Experimental values, ref 4. [d] $n = 2$ (DZ quality) results have not been used in the extrapolations. [e] Simple exponential CBS extrapolation, see text. [f] Mixed exponential/Gaussian CBS extrapolation, see text.

TABLE 5: BSSE-Corrected Harmonic ω_e and Anharmonic $\omega_e x_e$ Frequencies for the Four Most Abundant Isotopic Species of the LiNe Molecule in a Series of Basis Sets at the RCCSD(T) Level of Theory[a]

	$^6Li^{20}Ne$		$^6Li^{22}Ne$		$^7Li^{20}Ne$		$^7Li^{22}Ne$	
basis set (n)[b]	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})
2	63.3	13.0	62.6	12.8	59.7	11.8	59.0	11.6
3	87.9	16.8	87.0	16.5	82.9	14.8	81.9	14.4
4	107.9	23.1	106.7	22.7	101.8	20.6	100.6	20.1
5	110.2	24.1	109.1	23.5	104.0	21.0	102.8	20.4
6	111.2	25.1	110.0	24.5	104.9	22.1	103.7	21.6
CBS/e^{-n} [c]	111.0 (0.4)	25.0 (0.5)	109.8 (0.3)	24.3 (0.5)	104.7 (0.3)	21.8 (0.6)	103.5 (0.3)	21.2 (0.7)
CBS/mixed[d]	111.6 (0.1)	25.2 (0.4)	110.5	24.5 (0.4)	105.3 (0.1)	22.0 (0.5)	104.1 (0.1)	21.4 (0.6)
expt[e]	114.1 (1.3)	23.2 (0.6)			108.1 (1.3)	21.0 (0.6)		

[a] The following reduced masses were used (in g/mol): $^6Li^{20}Ne$, 4.62392; $^6Li^{22}Ne$, 4.72322; $^7Li^{20}Ne$, 5.19345; $^7Li^{22}Ne$, 5.31905. [b] (aug-cc-pCVnZ)$_{Li}$/(aug-cc-pVnZ)$_{Ne}$, $n = 2, 3, 4, 5$, and 6 (Ne). [c,d] CBS limit values, see Table 4. [e] Experimental values, ref 4.

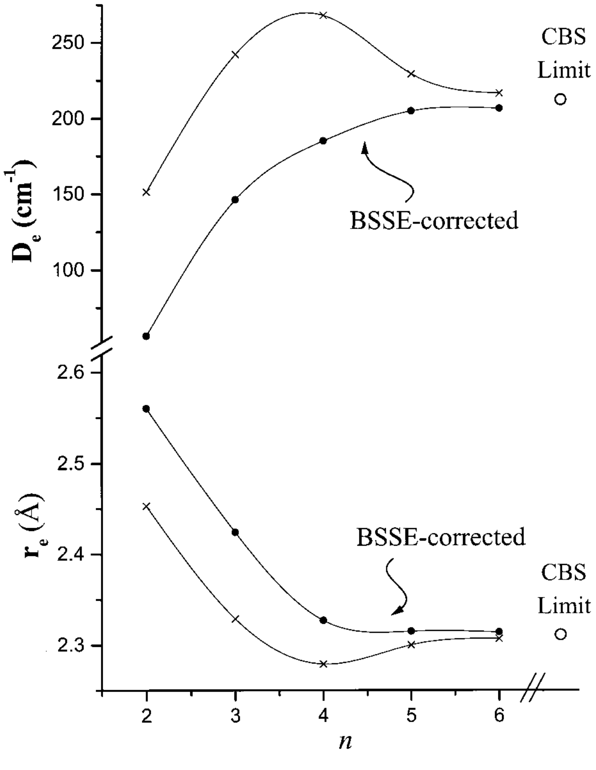

Figure 2. Spline fitting to dissociation energies (D_e) and bond lengths (r_e) of the A $^2\Pi$ state of LiNe as a function of the basis set size (n) at the RCCSD(T)/(aug-cc-pCVnZ)$_{Li}$/(aug-cc-pVnZ)$_{Ne}$ level of theory, $n = 2, 3, 4, 5$, and 6 (Ne).

sets, while special care should be taken for the ever present BSSE effects.

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