Theor Chem Acc (2000) 104:484–490
DOI 10.1007/s002140000174

Theoretical
Chemistry Accounts

Regular article

The basis set convergence of the Hartree–Fock energy for H_3^+, Li_2 and N_2

Frank Jensen

Department of Chemistry, SDU, Odense University, 5230 Odense M, Denmark
e-mail: frj@dou.dk

Received: 14 February 2000 / Accepted: 12 April 2000 / Published online: 18 August 2000

Abstract. By using completely optimized basis functions it is shown that the convergence of the Hartree–Fock energy for the H_3^+, Li_2 and N_2 molecules is significantly better described by exponential behavior than by inverse power dependence. This is the case both with respect to the number of basis functions of a given type and with respect to the highest angular momentum function included. The Hartree–Fock limit for H_3^+ is estimated to be −1.300372125 hartree.

Key words: Basis set convergence – Hartree–Fock

1 Introduction

Contemporary ab initio methods for calculating accurate energetics and molecular properties have two major limiting factors: incomplete incorporation of electron correlation and incomplete description of the orbitals due to the use of finite basis sets [1]. Recovering substantial fractions of the correlation energy requires sophisticated wave functions and large basis sets, and obtaining microhartree accuracy for absolute energies is prohibitively expensive for all but the smallest systems. Recent research has focused on systematic hierarchies of electron correlation methods and basis sets and on extrapolation schemes for estimating the infinite basis, infinite correlation result [2, 3].

Although there are procedures for approaching the complete basis set limit by systematically enlarging a basis set (e.g. even-tempered basis set [4]), these prescriptions tend to be too slowly convergent to be of practical use. More recently the correlation-consistent polarized valence double (D)-, triple (T)-, quadruple (Q)-, quintuple (5)- and sextuple (6)- ζ basis sets (cc-pVXZ, X = D, T, Q, 5, 6) developed by Dunning and coworkers [5] have been employed extensively as hierarchial basis sets for systematically reducing the basis set truncation error. The cc-pVXZ basis sets have been developed for calculating the valence correlation energy in a systematic fashion. On the basis of a suitable number of s and p functions, the number and types of higher angular momentum functions, as well as their exponents, are selected from correlated calculations on atoms.

Both the Hartree–Fock (HF) and the correlation energies depend on the size of the basis set. The computationally difficult part is the correlation energy, although it only accounts for around 1% of the total energy. Theoretical analysis [6] indicates that for a basis set saturated up to angular momentum L ($L = 0$ is an s function, $L = 1$ a p function, $L = 2$ a d function, etc.) the correlation energy converges as an inverse power series, with the leading term being L^{-3}, i.e. $AL^{-3} + BL^{-4} + CL^{-5} + \cdots$. The HF energy converges significantly faster, but little is known about the actual convergence behavior.

For the cc-pVXZ basis sets, L^{-3} behavior for the correlation energy has been observed computationally [7], although other inverse power extrapolations have also been used [8–10]. The energy of the hydrogen atom has been shown to converge exponentially with the number of s functions [11, 12], and for molecular systems the HF energy calculated by the correlation-consistent basis sets can normally be fitted well by an exponential function of the type $E_\infty + Ae^{-BL}$ [13–15], although inverse power extrapolations have also been used [9, 10, 16]. Since the number and the types of higher angular momentum functions in the cc-pVXZ basis set have been chosen on the basis of atomic correlation energies, it is not obvious that they are also optimal for describing charge polarization for HF wave functions in molecular systems. The observed exponential behavior for the correlation-consistent basis sets therefore does not prove an inherent exponential convergence of the HF energy.

We have recently shown by using fully optimized basis functions that the HF energy for H_2 converges exponentially, both with respect to the number of s functions and with respect to the highest angular momentum functions included [17]. There are three main limitations in this study:

1. The molecular orbital in H_2 extends over only two nuclei.
2. H_2 has only two electrons and thus only one molecular orbital.

3. The individual atoms in H_2 only have electrons in an *s*-type orbital.

Presently we address these points by examining the convergence behavior of the HF energy for H_3^+, Li_2 and N_2. In order to rigorously probe the convergence all energies were converged to high accuracies, although such accuracies have little chemical significance.

2 Basis set optimization

Analogous to the previous study [17], basis set exponents were optimized by a pseudo-Newton–Raphson approach with ln ζ as the variables and using gradients generated by central finite differences [18][1]. The target accuracy for terminating an optimization was around 0.01 nanohartree for H_3^+, around 0.1 nanohartree for Li_2 and around 10 nanohartree for N_2. The residual error compared to the numerical HF value is around 12 nanohartree for Li_2 and is most likely due to errors from the use of numerical gradients. The corresponding error for H_3^+ is estimated to be around 1 nanohartree on the basis of results for Li_2 and H_2 [17]. It was checked that all results can be reproduced to the reported accuracy using independent program packages [19, 20].

The primary interest is how the energy converges as a function of maximum angular momentum functions included in the basis set, but for H_3^+ and Li_2 the convergence behavior as a function of s functions only is also of interest. As discussed later, the corresponding sp behavior for N_2 could not be investigated. The angular momentum convergence can be established by determining the energy limit for using s functions only, using s and p functions only (sp limit), using s, p and d functions only (spd limit), etc. The L-limit energy was determined by sequentially optimizing larger and larger basis sets, until the energy became stable to within the target accuracy. In some cases, as discussed later, optimization resulted in variational collapse, i.e. two basis exponents having the same L value converge toward the same value, causing the overlap matrix to become singular. This indicates a lack of higher angular momentum functions, and the problem disappears when higher angular momentum functions are added.

All basis functions were centered on the nuclei, and only the spherical components of the polarization functions were used. For Li_2 the experimental distance of 5.051 au was chosen [21], N_2 was taken to have a bond length of 2.068 au, which is the value used in a numerical calculation of the HF energy [22], while H_3^+ was assumed to be a regular triangle with an internuclear distance of 1.65 au.

3 Results and discussion

3.1 Results for H_3^+

The energy convergence as a function of s functions for H_3^+ is shown in Table 1. With a basis set consisting of 15 functions on each center, an energy of −1.281035206 hartree is obtained, and addition of additional s functions lowers the energy by less than 0.1 nanohartree. The corresponding optimized exponents are shown as a ln ζ plot in Fig. 1. The pattern is slightly different from H_2 [17], since the ratio between ζ_1 and ζ_2 of 7.0 (ζ_i are labeled according to increasing exponents, i.e. ζ_1 is the most diffuse function) is significantly larger than between ζ_2 and ζ_3, 3.4. For H_2 the ratios between successive exponents decrease monotonically as the exponents become smaller, but this is not the case for H_3^+. The $M = 15$ basis set has exponents in the range 7×10^5–3×10^{-2}. By comparing with the basis set exponents for H_2 [17] it can be seen that there is a clear trend for the optimal exponents for a given number of s functions to be larger (tighter) for H_3^+ than for H_2, except for the most diffuse exponent first appearing for the $M = 9$ solution for H_3^+. This is as expected since the wave function for H_3^+ is more compact than for H_2.

The corresponding sp, spd, spdf, spdfg and spdfgh limits are given in Table 2. The energy-lowering by addition of an i function to the 21s11p8d5f3g1h basis is 0.1 nanohartree, i.e. at this point the energy is essentially converged to the HF limit. On the basis of the observed agreement between numerical and basis set energy limits for H_2 and Li_2 (5×10^{-8} and 8×10^{-8}%, respectively), we estimate the HF limit for H_3^+ to be −1.300372125 hartree, with probable error bars of ±0.4 nanohartree. Two fully numerical studies of the HF energy of H_3^+ have been published, producing energies of −1.30040 [23] and −1.30041 ± 0.00004 hartree [24] for a triangular geometry with $R = 1.6405$ au. Using this geometry with our 21s11p8d5f3g1h basis set gives an energy of −1.300400141 hartree. Reoptimization of the exponents of the 21s11p8d4f basis (spdf limit) at the $R = 1.6405$ au geometry gave an energy lowering of 0.2 nanohartree,

Table 1. Hartree–Fock (HF) energy convergence for H_3^+ as a function of the number of s functions (M)

M	Energy (hartree)
1	−1.166879804
2	−1.257028247
3	−1.275759647
4	−1.280259159
5	−1.280910242
6	−1.281011417
7	−1.281029568
8	−1.281033199
9	−1.281034224
10	−1.281034982
11	−1.281035153
12	−1.281035193
13	−1.281035203
14	−1.281035205
15	−1.281035206

---

[1] The numerical differentiation used a step size corresponding to energy changes of around 0.1 nanohartree for H_3^+, around 1.0 nanohartree for Li_2 and around 10 nanohartree for N_2

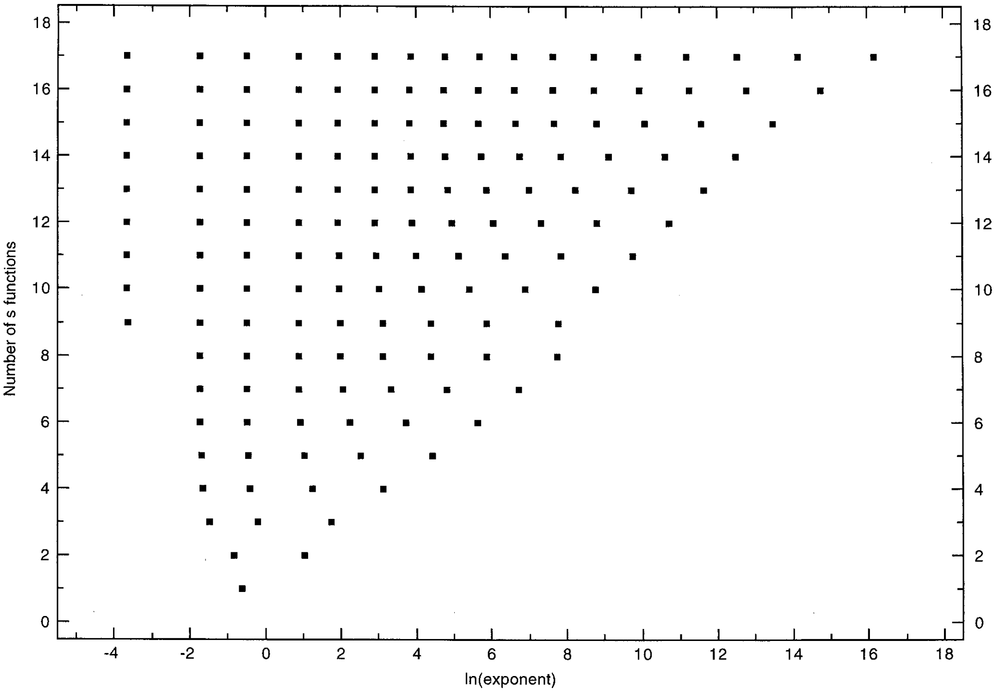

Fig. 1. Logarithmic value of optimized exponents for H_3^+ as a function of the number of s functions per atom

Table 2. HF energy convergence for H_3^+ as a function of the highest angular momentum basis functions (L)

L	Basis	Composition	Energy (hartree)
0	s limit	(17s)	−1.281035206
1	sp limit	(18s,8p)	−1.300177173
2	spd limit	(19s,10p,6d)	−1.300369780
3	spdf limit	(21s,11p,8d,4f)	−1.300372065
4	spdfg limit	(21s,11p,8d,5f,3g)	−1.300372122
5	spdfgh limit	(21s,11p,8d,5f,3g,1h)	−1.300372124
∞	Estimated HF limit		−1.300372125

i.e. the above value is essentially the HF limit, and it agrees well with the numerical results. The HF limit for H_3^+ allows the correlation energy to be estimated as −0.043463 hartree on the basis of explicitly correlated Gaussian function calculations [25]. This is larger than the value of −0.040846 hartree for H_2 [26], in agreement with expectations.

The convergence behavior can be investigated by plotting $\ln(E_x - E_\infty)$ as a function of either x or $\ln x$, where x denotes either the number of basis functions or the highest angular momentum functions in the basis set ($x = M$ or L). An exponential convergence should give a straight line as a function of x, while an inverse power dependence should give a straight line as a function of $\ln x$.

$$\begin{aligned} E_x &= E_\infty + Ae^{-Bx} \Leftrightarrow \ln(E_x - E_\infty) = \ln A - Bx \\ E_x &= E_\infty + Ax^{-B} \Leftrightarrow \ln(E_x - E_\infty) = \ln A - B\ln x \end{aligned} \tag{1}$$

Both types of plots are shown for the energy dependence on the number of s functions in Fig. 2. The points are better fitted by an exponential function ($\ln A = 1.4$, $B = 1.4$ in Eq. 1, correlation coefficient = 0.997) than by an inverse power form ($\ln A = 1.6$, $B = 7.7$, correlation coefficient = 0.956). Also shown is the corresponding convergence for the hydrogen atom, and it is clear that the s convergence for H_3^+ largely reflects the atomic behavior.

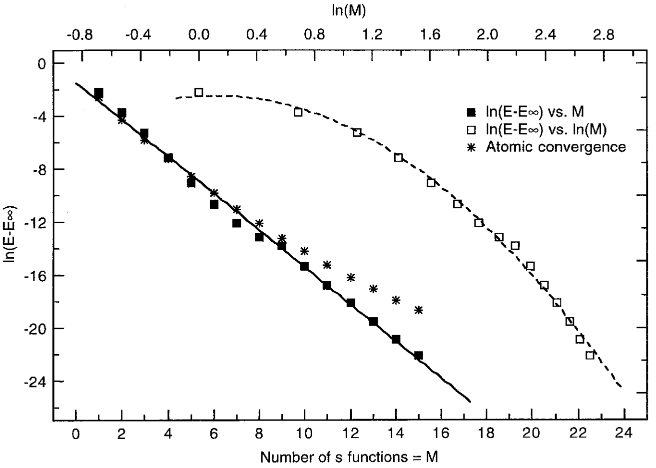

Fig. 2. Convergence of the Hartree–Fock energy for H_3^+ as a function of the number of s functions per atom

Using the estimated HF limit in Eq. (1), the corresponding plots as a function of highest angular momentum are shown in Fig. 3. For the $L = 4$ and $L = 5$ points (spdfg and spdfgh limits), $E_L - E_\infty$ is comparable to the residual error of around 1 nanohartree, and these points will deviate systematically from the expected behavior. This is partly artificial, as the around 1 nanohartree error presumably is evenly distributed, but appears localized in the energies for the highest L limits. The plots of $\ln(E_L - E_\infty)$ against L or $\ln L$ for the first four points (s, sp, spd and spdf limits) indicate that the

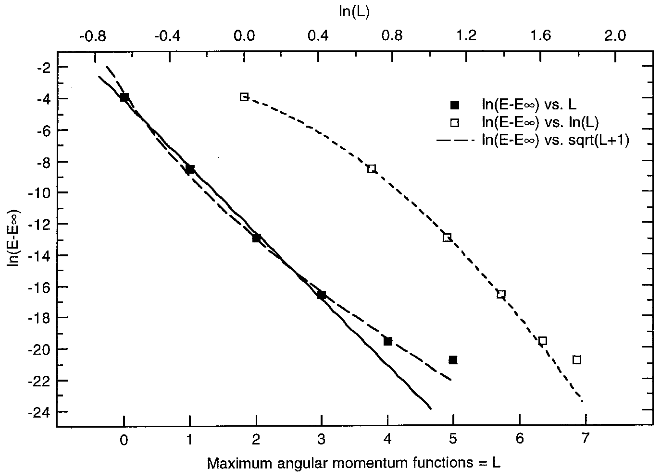

Fig. 3. Convergence of the Hartree–Fock energy for H_3^+ as a function of the highest angular momentum functions

behavior is better described by an exponential function (ln $A = -4.1$, $B = 4.2$ in Eq. 1, correlation coefficient = 0.9987) than by an inverse power form (ln $A = -3.4$, $B = 9.0$, correlation coefficient = 0.988). Motivated by the results for the hydrogen atom [12] we also investigated an alternative exponential form depending on the square root of $(L + 1)$, as shown in Eq. (2). It provides a statistical fit similar to Eq. (1) (ln $A = -12.7$, $B = 9.1$, correlation coefficient = 0.9984), but reproduces the $L = 4$ point better.

$$E_L = E_\infty + Ae^{-B\sqrt{L+1}} \Leftrightarrow \ln(E_L - E_\infty) = \ln A - B\sqrt{L+1} \tag{2}$$

3.2 Results for Li_2

The energy convergence as a function of s functions for Li_2 is shown in Table 3. With a basis set consisting of 25 functions on each center an energy of −14.861396057 hartree is obtained. Addition of one additional tight function lowers the energy by 0.2 nanohartree, and by rounding we estimate the s limit for the energy to be −14.861396058 hartree. The corresponding optimized exponents are shown in Fig. 4. The exponents show a clear pattern resembling the 1*s* and 2*s* atomic orbitals. As found for the H_2 and H_3^+ systems, the valence exponents become stable beyond $M \sim 20$, as additional tight functions are added. The $M = 25$ basis set has exponents in the range 25×10^6–8×10^{-3}.

Table 3. HF energy convergence for Li_2 as a function of *M*

M	Energy (hartree)
2	−12.345957084
3	−14.362093828
4	−14.750570434
5	−14.833274371
6	−14.852738204
7	−14.857716890
8	−14.859411575
9	−14.860783827
10	−14.861193674
11	−14.861323067
12	−14.861366135
13	−14.861381396
14	−14.861387806
15	−14.861392312
16	−14.861394252
17	−14.861395190
18	−14.861395636
19	−14.861395818
20	−14.861395446
21	−14.861396015
22	−14.861396043
23	−14.861396052
24	−14.861396057
25	−14.861396057
26	−14.861396058

For Li_2 the problem of variational collapse is more pronounced than for H_2 and H_3^+. The largest sp basis which could be completely optimized was 25s8p. Although extension of the p function space by adding additional tight functions provided an energy-lowering of around 30 nanohartree, subsequent full optimization caused variational collapse of the p functions. Consequently two additional tight p functions were added to the 25s8p basis, and only these two exponents were allowed to relax. The 25s10p basis gives an energy of −14.871468854 hartree, which is taken as the sp limit. Similar problems were encountered for the spd and spdf limits, with the results indicated in Table 4. Once g functions were included, the problem of variational collapse disappeared, and the spdfg and spdfgh limits are obtained from fully optimized basis sets. A 25s12p7d4f2g1h basis provides an energy of −14.871562846 hartree, and further extension of any of the function spaces gives changes of less than 0.2 nanohartree. Addition of an i function causes an energy-lowering of 0.2 nanohartree; thus the above energy is effectively converged to the basis set limit.

The numerical HF value for Li_2 was reported as −14.871563 hartree in Ref. [27] and has been refined with larger grids to −14.871562858 hartree [28][2]. This is around 12 nanohartree below the present basis set limit, with the discrepancy most likely due to errors associated with the use of numerical gradients.

Plots for the s function convergence according to Eq. (1) are shown in Fig. 5. The points are better fitted by an exponential function (ln $A = 1.0$ and $B = 0.9$ in Eq. (1), correlation coefficient = 0.994, neglecting the $M = 24$ and 25 points) than by a power form (ln $A = 9.3$ and $B = 8.2$, correlation coefficient = 0.978). The s convergence again mainly reflects the corresponding atomic convergence.

The corresponding plots as a function of highest angular momentum are shown in Fig. 6. For the $L = 4$ and $L = 5$ points (spdfg and spdfgh limits), $E_L - E_\infty$ is comparable to the residual error of around 12 nanohartree, and these points will deviate systematically from

---

[2] The largest grid was 319 × 595 and used a cutoff distance of 65 au, (J. Kobus, privat communication)

Fig. 4. Logarithmic value of optimized exponents for Li_2 as a function of the number of s functions per atom

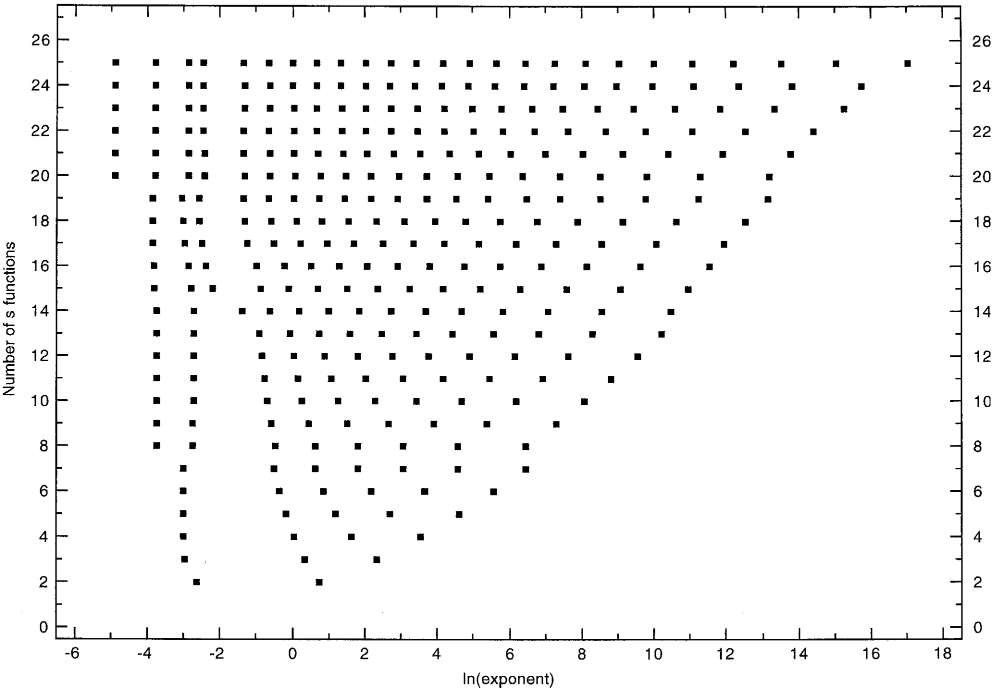

Table 4. HF energy convergence for Li_2 as a function of L

L	Basis	Composition	Energy (hartree)
0	s limit	(26s)	−14.861396058
		(25s,8p)	−14.871468456
1	sp limit	(25s,10p)[a]	−14.871468485
		(25s,10p,5d)	−14.871560836
2	spd limit	(25s,11p,6d)[a]	−14.871560844
		(25s,12p,6d,3f)	−14.871562784
3	spdf limit	(25s,12p,7d,4f)[a]	−14.871562787
4	spdfg limit	(25s,12p,7d,4f,2g)	−14.871562843
5	spdfgh limit	(25s,12p,7d,4f,2g,1h)	−14.871562846
∞	HF limit[b]		−14.871562858

[a] Only the additional basis functions with respect to the previous entry were optimized

[b] Refs. [27, 28]

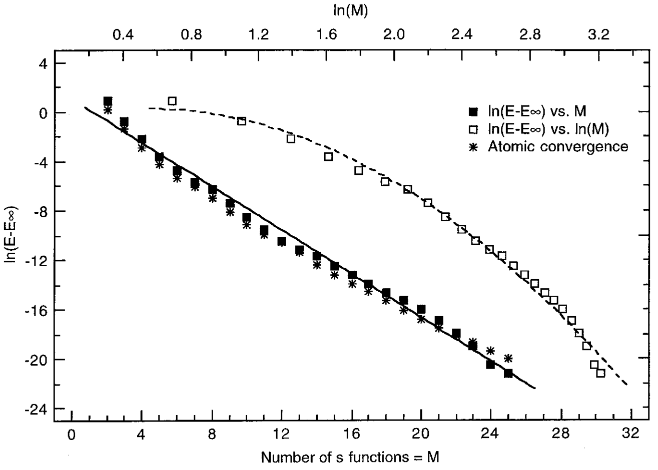

Fig. 5. Convergence of the Hartree–Fock energy for Li_2 as a function of the number of s functions per atom

the expected behavior. The plots of $\ln(E_L - E_\infty)$ against L or $\ln L$ for the first four points (s, sp, spd and spdf limits) indicate that the behavior is slightly better described by an exponential function ($\ln A = -1.0$ and $B = 3.9$ in Eq. (1), correlation coefficient = 0.997) than by an inverse power form ($\ln A = -4.2$ and $B = 8.4$, correlation coefficient = 0.992). A somewhat better fit ($\ln A = -11.9$ and $B = 7.4$, correlation coefficient = 0.9997) can be obtained by an exponential function of the type shown in Eq. (2).

3.3 Results for N_2

For N_2 the problem of variational collapse is significantly worse than for Li_2. With only s and p functions, the largest basis set which could be completely optimized was 15s8p. The energy with this basis is −108.910828 hartree, and the last s function added gave an energy-lowering of −0.000048 hartree. A constrained optimization of the 16s9p basis (addition of one s and p function to the 15s8p basis) gave an energy of −108.910851 hartree, but further extensions caused variational collapse. Our best estimate of the sp limit is thus −108.910851 hartree, but it is clear that this is a somewhat crude upper limit and a convergence plot corresponding to Figs. 2 and 4 is therefore not justified.

Similar problems of variational collapse were encountered for the spd, spdf and spdfg limits, with the results shown in Table 5. The spdfg limit is −108.993813 hartree, and addition of a single h function lowers the energy to −108.993824, in good agreement with the numerical HF value of −108.993826 hartree [22]. A fully

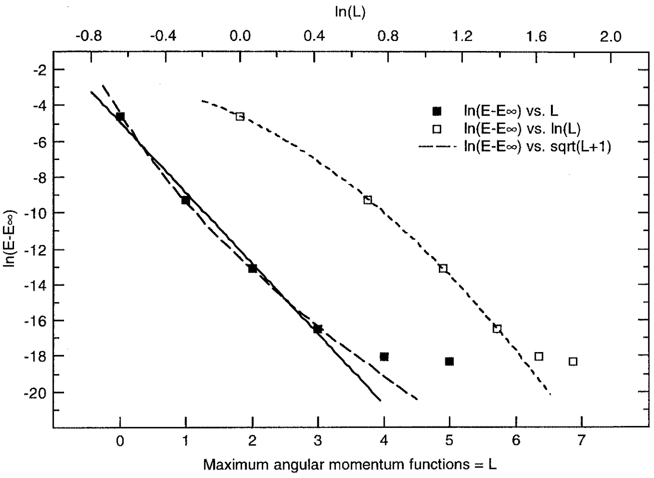

Fig. 6. Convergence of the Hartree–Fock energy for Li_2 as a function of the highest angular momentum functions

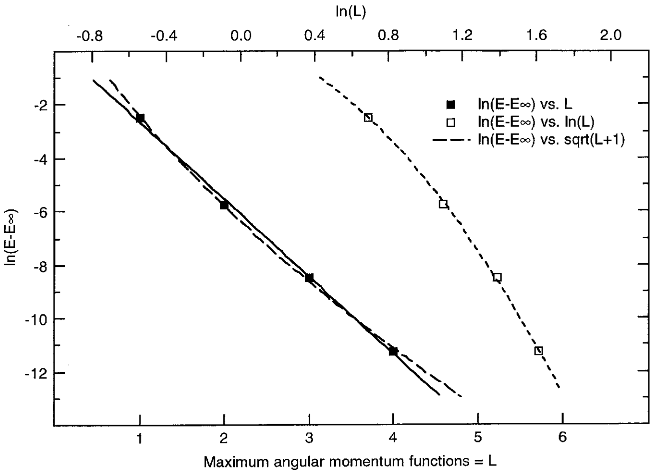

Fig. 7. Convergence of the Hartree–Fock energy for N_2 as a function of the highest angular momentum functions

Table 5. HF energy convergence for N_2 as a function of L

L	Basis	Composition	Energy (hartree)
		(15s,8p)	−108.910828
1	sp limit	(16s,9p)[a]	−108.910851
		(20s,10p,5d)	−108.990675
2	spd limit	(20s,12p,7d)[a]	−108.990691
		(21s,12p,7d,3f)	−108.993620
3	spdf limit	(21s,12p,7d,4f)[a]	−108.993623
		(23s,13p,9d,4f,2g)	−108.993812
4	spdfg limit	(23s,13p,9d,5f,3g)[a]	−108.993813
∞	HF limit[b]		−108.993826

[a] Only the additional basis functions with respect to the previous entry were optimized
[b] Ref. [22]

optimized spdfgh basis will presumably be able to reproduce the HF limit, but this was not attempted owing to the high computational cost. Plots corresponding to Figs. 3 and 6 are shown in Fig. 7. The convergence is again better described by an exponential function ($\ln A = 0.3$ and $B = 2.9$ in Eq. 1, correlation coefficient = 0.9990; $\ln A = -2.1$ and $B = 6.2$, correlation coefficient = 0.9996 in Eq. 2) than by an inverse power form ($\ln A = 12.6$ and $B = 10.6$, correlation coefficient = 0.988).

4 Conclusion

For the H_2, H_3^+ and Li_2 systems the convergence behavior as a function of s functions only is markedly better described by an exponential dependence (correlation coefficients = 0.994–0.998) than by a power form (correlation coefficients = 0.956–0.978). The s functions primarily describe the atomic structure within the molecule, and the convergence is clearly best described by an exponential function, in agreement with the findings for the hydrogen atom [11, 12]. Higher angular momentum functions describe charge polarization, which is a purely molecular effect. The preference for exponential versus power convergence as a function of angular momentum is less pronounced, i.e. correlation coefficients of 0.997–0.999 versus 0.984–0.992; however, an exponential form depending on the square root of ($L + 1$) improves the fit, with correlation coefficients of 0.998–0.999.

The total polarization energies are 5, 10, 19 and 83 millihartree for H_2, Li_2, H_3^+ and N_2, respectively. The large majority (96–99%) of this can be recovered by the first set of polarization functions (p or d functions). Basis sets including angular momentum functions two higher than necessary for describing the atoms are capable of providing results which reduce the HF error below 1 kcal/mol, which in the majority of cases will be of sufficient accuracy.

Acknowledgement. This work was supported by grants from the Danish Natural Science Research Council. The author thanks J. Kobus for performing additional finite difference calculations for estimating the HF limit for Li_2.

References

1. (a) Hehre WH, Radom L, Schleyer PvR, Pople JA (1986) Ab initio molecular orbital theory. Wiley, New York; (b) Jensen F (1998) Introduction to computational chemistry. Wiley, New York
2. Martin JML, de Oliveira G (1999) J Chem Phys 111: 1843
3. Feller D, Peterson KA (1998) J Chem Phys 108: 154
4. Schmidt MW, Ruedenberg K (1979) J Chem Phys 71: 3951
5. (a) Dunning TH Jr (1989) J Chem Phys 90: 1007; (b) Wilson AK, van Mourik T, Dunning TH Jr (1996) J Mol Struct 388: 339
6. (a) Schwartz C (1962) Phys Rev 126: 1015; (b) Hill RN (1985) J Chem Phys 83: 1173; (c) Kutzelnigg W (1985) Theor Chim Acta 68: 445; (d) Kutzelnigg W, Morgan JD III (1992) J Chem Phys 96: 4484; (e) Kutzelnigg W, Morgan JD III (1992) J Chem Phys 97: 8821
7. (a) Helgaker T, Klopper W, Koch W, Noga J (1997) J Chem Phys 106: 9639; (b) Halkier A, Helgaker T, Jørgensen P, Klopper W, Koch H, Olsen J, Wilson AK (1998) Chem Phys Lett 286: 243

8. (a) Martin JML (1996) Chem Phys Lett 259: 669; (b) Martin JML, Taylor PR (1997) J Chem Phys 106: 8620
9. Fast PL, Sanchez ML, Truhlar DG (1999) J Chem Phys 111: 2921
10. (a) Truhlar DG (1998) Chem Phys Lett 294: 45; (b) Chuang V, Truhlar DG (1999) J Phys Chem A 103: 65
11. van Duijneveldt FB (1971) IBM Publ RI 945. Yorktown Heights, New York
12. Klopper W, Kutzelnigg W (1986) J Mol Struct 135: 339
13. (a) Feller D (1992) J Chem Phys 96: 6104; (b) Feller D (1993) J Chem Phys 98: 7059; (c) Petersson KA, Kendall RA, Dunning TH Jr (1993) J Chem Phys 99: 9790
14. Halkier A, Helgaker T, Jørgensen P, Klopper W, Olsen J (1999) Chem Phys Lett 302: 437
15. (a) Woon DE, Dunning TH Jr (1993) J Chem Phys 99: 1914; (b) Petersson KA, Kendall RA, Dunning TH Jr (1993) J Chem Phys 99: 1930
16. (a) Petersson GA, Bennett A, Tensfeldt TG, Braunstein M, Al-Laham MA, Shirley WA, Mantzaris J (1988) J Chem Phys 89: 2193; (b) Montgomery JA Jr, Petersson GA (1994) J Chem Phys 101: 5900
17. Jensen F (1999) J Chem Phys 110: 6601
18. Frisch MJ, Trucks GW, Schlegel HB, Gill PMW, Johnson BG, Robb MA, Cheeseman JR, Keith T, Petersson GA, Montgomery JA, Raghavachari K, Al-Laham MA, Zakrzewski VG, Ortiz JV, Foresman JB, Cioslowski J, Stefanov BB, Nanayakkara A, Challacombe M, Peng CY, Ayala PY, Chen W, Wong MW, Andres JL, Replogle ES, Gomperts R, Martin RL, Fox DJ, Binkley JS, Defrees DJ, Baker J, Stewart JJP, Head-Gordon M, Gonzalez C, Pople JA (1995) Gaussian 94. Gaussian, Pittsburgh, Pa
19. Helgaker T, Jensen HJAa, Jørgensen P, Olsen J, Ruud K, Ågren H, Andersen T, Bak KL, Bakken V, Christiansen O, Dahle P, Dalskov EK, Enevoldsen T, Fernandez B, Heiberg H, Hettema H, Jonsson D, Kirpekar S, Kobayashi R, Koch H, Mikkelsen KV, Norman P, Packer MJ, Saue T, Taylor PR, Vahtras O (1997) DALTON 1.0
20. Schmidt MW, Baldridge KK, Boatz JA, Elbert ST, Gordon MS, Jensen JH, Koseki S, Matsunaga N, Nguyen KA, Su SJ, Windus TL, Dupuis M, Montgomery JA (1993) J Comput Chem 14: 1347
21. Harmony MD, Laurie VW, Kuczkowski RL, Schwendeman RH, Ramsay DA, Lovas FJ, Lafferty WJ, Maki AG (1979) J Phys Chem Ref Data 8: 619
22. Kobus J (1993) Chem Phys Lett 202: 7
23. Becke AD, Dickson RM (1992) J Chem Phys 92: 3610
24. Alexander SA, Coldwell RL, Monkhorst HJ (1988) J Comput Phys 76: 263
25. Cencek W, Komasa J, Rychlewski J (1995) Chem Phys Lett 246: 417
26. Rychlewski J, Cencek W, Komasa J (1994) Chem Phys Lett 229: 657
27. Sundholm D, Pyykkö P, Laaksonen L (1985) Mol Phys 56: 1411
28. Kobus J, Laaksonen L, Sundholm D (1996) Comput Phys Commun 98: 346