Accurate equilibrium inversion barrier of ammonia by extrapolation to the one-electron basis set limit*

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A scheme based on treating uniform singlet-pair and triplet-pair interactions is suggested to extrapolate electron correlation energy of ammonia, calculated at two basis-set levels of *ab initio* theory in the infinite one-electron basis-set limit. The dual-level method is tested on the extrapolation of the full correlation in coupled-cluster singles and doubles and in the case also a noniterative perturbative correction for connected triple energies for the C_{3v} and D_{3h} structures of ammonia, with correlation-consistent basis sets of the type cc-pVXZ ($X = \mathrm{D,T,Q,5,6}$) and aug-cc-pVXZ ($X = \mathrm{D,T,Q,5}$). For testing and comparison purposes, the energies reported by Klopper [*J. Comput. Chem.* **22** 1306 (2001)] have been taken. From a corresponding extrapolation of CCSD(T)/AVXZ energies for $X = 4$, 5, we obtain total inversion barriers of 1833.87 cm^{-1}/1832.33 cm^{-1} for the two/three-parameter extrapolation rules, which are in good agreement with other theoretical extrapolation and empirical values in the literature.

Keywords: inversion barrier, ammonia, complete basis set limit, low-cost

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1. Introduction

Ammonia is a challenging molecule for both the experimental spectroscopist and the theoretical spectroscopist. Of course the principle interest arises from its two distinct C_{3v} minima connected by a D_{3h} transition state.[1] A wealth of empirical and theoretical data are available for the inversion barrier.[1–19] The value generally accepted for the inversion barrier is 1885 cm^{-1} as reported by Špirko *et al.*,[5] who fitted the inversional experimental data[29] using their model Hamiltonian. This can be compared with the work by East and Radon who have recently published the value 1821(30) cm^{-1} with *ab initio* methods by investigating systematically the effect of diffuse functions on nitrogen and of core correlation in Mϕller Plesset techniques.[6] The highest quality *ab initio* results for the equilibrium inversion barrier of NH_3 have been obtained by Császár, Allen and Schaefer,[6] using the focal-point technique. These authors determined $B_e = 1810$ cm^{-1} for the barrier at the extrapolated nonrelativistic valence-only level.

An accurete potential energy surface (PES) is suitable for dynamics and kinetics studies.[21–24] Recently, Li and Varandas[25] reported a double many-body expansion (DMBE) global PES for the ground state of ammonia. The predicted DMBE inversion barrier of 2033.5 cm^{-1} is clearly in very good agreement with the result of 2029.4 cm^{-1} obtained by fitting the dense grid of *ab initio* points close to the equilibrium geometry and D_{3h} saddle point. However, the DMBE inversion barrier predicted is 199.5 cm^{-1} larger than the empirical value of 1834 cm^{-1} deduced from experimental data by Špirko *et al.*[20] This may be due to the fact that the DMBE PES of ammonia was employed at the multi-reference configuration interaction (MRCI) level with the AVTZ basis set, which is not accurate enough for obtaining an accurate inversion barrier. This situation prompts us to find an appropriate extrapolation scheme of extrapolating the *ab initio* energies of ammonia for obtaining the accurate corresponding inverse barrier. Of special interest for this work are the full correlation in coupled-cluster singles and doubles (CCSD), also a noniterative perturbative correction for connected triple excitations [CCSD(T)] energies for the C_{3v} and D_{3h} structures and the inversion barrier of ammonia with correlation-consistent basis sets of the type cc-pVXZ (VXZ) ($X = \mathrm{D,T,Q,5,6}$) and aug-cc-pVXZ (AVXZ) ($X = \mathrm{D,T,Q,5}$) reported by Klopper.[13] We choose here the former for testing purposes, as the set of reference energies has been taken from Ref. [13]. Note that we do not decompose the energy into singlet-pair and triplet-pair contributions for the following reasons, as reported by Varandas.[26] First, such a requirement is not necessary for accurate results. Second, because such a decomposition scheme cannot be implemented for open-shell CCSD calcu-

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lations (Note that the wave function is not a spin eigenfunction in practical implementations of CCSD theory) and is not commonly implemented in most CC codes. Specifically, it is shown in this work that the previously reported dual-level scheme[27] can be modified to yield accurate extrapolated results for Klopper's[13] data set. We focus on the inversion barrier of ammonia energy values and try to find an appropriate extrapolation scheme of extrapolating the *ab initio* energies to the complete basis set limit. Such a work will pave the way for improving the global DMBE PES for the ground state of ammonia by providing a proper extrapolation method to extrapolate the *ab initio* energies for obtaining the accurate corresponding inverse barrier in future work.

The rest of the paper is organized as follows. In Section 2, a brief survey on the extrapolation scheme and its presentation is provided. In Section 3, the results and their discussion are presented, while the conclusions are drawn from this study in Section 4.

2. Extrapolation scheme

Built in a systematic manner, which is intended to relate the correlation energy to the cardinal number X, Dunning's correlation consistent basis sets[28] allow the raw energies to be extrapolated to the one-electron CBS limit.[29–31] To perform the extrapolation, by carrying out calculations for several values of X, one may then exploit the X dependence of the calculated energy E_X to obtain its value E_∞ in the CBS limit. While convergence to this limit is exponentially fast at the Hartree–Fock self-consistent field level of theory,[32–34] dynamical correlation energies, such as CCSD, converge rather slowly, that is, with an inverse power of X. The CCSD or CCSD(T) electronic energy is then best treated in split form by writing

$$E_X = E_X^{\mathrm{CAS}} + E_X^{\mathrm{dc}}, \tag{1}$$

where the subscript X indicates that the energy is calculated in the VXZ or AVXZ basis, while the superscripts CAS and dc denote the complete-active-space and dynamical correlation energies, respectively. A similar partition is applied to single reference calculations, with CAS replaced by the Hartree–Fock energy and dc replaced by the full correlation.

To extrapolate the CAS energy, a proposed[26] generalization of the protocol adopted by Karton and Martin[35] (KM) to extrapolate single-reference self-consistent-field energies is utilized

$$E_X^{\mathrm{CAS}} = E_\infty^{\mathrm{CAS}} + B/X^\alpha, \tag{2}$$

where α is a predefined constant. As a two-parameter protocol $(E_\infty^{\mathrm{CAS}}, B)$, a minimum of two raw energies will be required for the extrapolation. Specifically, equation (2) will be calibrated from the CAS/AVXZ energy pairs, using a value of $\alpha = 5.34$, which has been found to be optimal when extrapolating HF energies to the HF limit.

For the extrapolation of the correlation energy, the simplest and most popular two-parameter law for extrapolation of the correlation energy is[26,36–40]

$$E_X^{\mathrm{cor}} = E_\infty^{\mathrm{cor}} + \frac{A_3}{(X+\alpha)^3}, \tag{3}$$

where E_X^{cor} is the correlation energy obtained with the X-tuple basis set of (aug)cc quality, E_∞^{cor} and A_3 are parameters usually determined from the calculations for the two highest affordable values of X, while α is an offset parameter fixed from some auxiliary condition. Although equation (3) is known to perform accurately when being extrapolated from energies based on large cardinal number pairs, its performance is significantly less satisfactory when the pair of (T,Q) is used. A more reliable scheme is the recently suggested uniform singlet-pair and triplet-pair extrapolation (USTE)[26] model. This has its basis on the three-parameter protocol, i.e.,

$$E_X^{\mathrm{cor}} = E_\infty^{\mathrm{cor}} + \frac{A_3}{(X+\alpha)^3} + \frac{A_n}{(X+\alpha)^n}. \tag{4}$$

With $n = 5$ and $\alpha = -3/8$, i.e. the auxiliary relation is assumed to be in the form of

$$A_5 = A_5(0) + cA_3^n, \tag{5}$$

where $A_5(0)$ is the basis-set error in the energy for a pure pair-triplet interaction and c and n are least-squares parameters, with $n = 1$, $A_5(0) = 0.16606993$ and $c = 1.42225121$ for CCSD and CCSD(T) energies. Recently, Li *et al.* used Eqs. (2) and (4) to extrapolate the MRCI(Q)/AV(T,Q)Z *ab initio* energies and successfully obtain a DMBE/CBS PES for the first[41] and second[42] excited states of NH_2.

3. Results and discussion

As the set of reference energies of ammonia has been taken from Ref. [13], the dual-level method is tested on extrapolating the CCSD and CCSSD(T) energies for the C_{3v} and D_{3h} structures of ammonia, with correlation-consistent basis sets of the type XVZ (X = D, T, Q, 5, 6) and AVXZ (X = D, T, Q, 5), respectively. Figures 1 and 2 illustrate the extrapolatons as a function of the cardinal number X for the C_{3v} and D_{3h} structures of ammonia, respectively. Shown in the above panel are the CAS extrapolating energies based on Eq. (2), while the bottom panel illustrates the dc extrapolating energies based

on Eqs. (3) and (4). Two observations are highlighted from Figs. 1 and 2. First, the CBS/(4,5) results nearly overlap the CBS/(3,4) extrapolations at $X = \infty$ where the exact value lies. Second, the bottom panels in both Figs. 1 and 2 show very small dc/CBS(4,5) extrapolating energy differences between using Eq. (3) and Eq. (4), which they should be for the two methods to be consistent when using two large cardinal number pairs for the extrapolation. This may be best appreciated from Fig. 3, which shows the inversion barriers of ammonia of the (D, T), (T, Q) (Q, 5) and (5, 6) extrapolations for CCSD/VXZ, CCSD/AVXZ, CCSD(T)/VXZ and CCSD(T)/AVXZ energies and the comparison with the corresponding explicitly correlated target value (results are cited from CCSD-R12/B and CCSD[T]-R12/B energies in Ref. [13]).

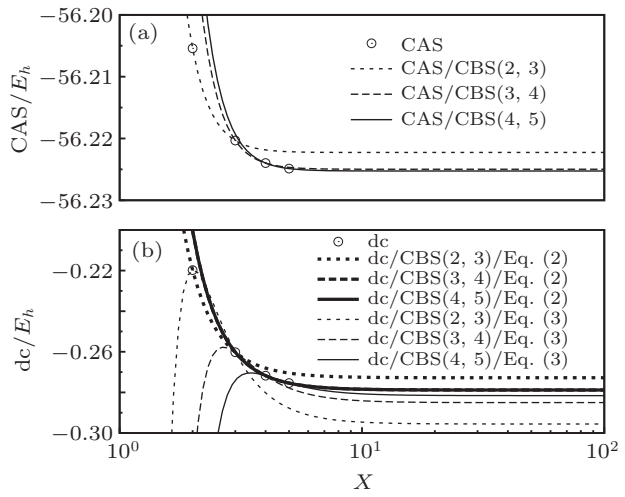


Fig. 1. The extrapolated CCSD(T)/AVXZ energies for the C_{3v} structures of ammonia. Shown are the CAS (a) and dc (b) extrapolating energies, each as a function of cardinal number X. The lines indicate fittings obtained from two different cardinal numbers: dotted line, CBS/(2, 3); dashed line, CBS/(3, 4); solid line, CBS/(4, 5). The thin line fits Eq. (3) and the dark line fits Eq. (4) in the bottom panel.

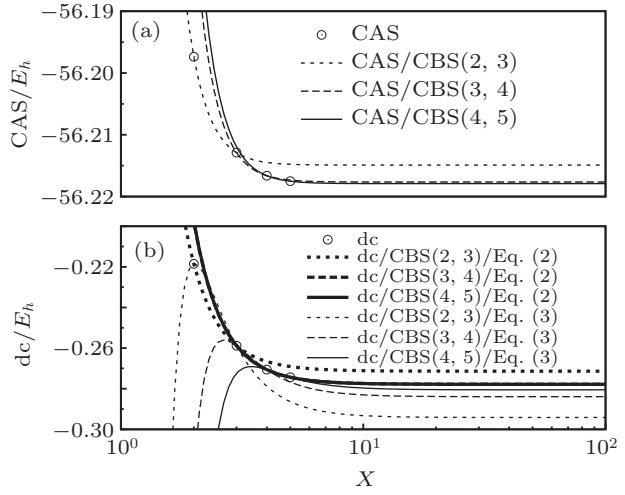


Fig. 2. The same as Fig. 1 but for D_{3h} structures of ammonia.

The calculated and extrapolated energies of the C_{3v} and D_{3h} structures and the corresponding inversion barriers are collected in Tables 1–4. We now address the extrapolated inversion barriers obtained from fitting the CCSD and CCSD(T) energies. From Tables 1–4 and Fig. 3, it follows that our extrapolation scheme attains the same accuracy as the traditional one based on Eq. (3) when the two largest affordable basis sets are used. This reveals that the convergence to the exact value will be expected when the USTE scheme utilizes the increasing pairs of cardinal numbers for the extrapolation. By correspondingly fitting the RHF/AVXZ energies for $X = 4,\ 5$, we obtain an inversion barrier of 1615.33 cm^{-1} with Eq. (2), which is in good agreement with the results of 1613/1614 cm^{-1} from VXZ ($X = 4,5,6$)/AVXZ ($X = 3,\ 4,\ 5$) of Klopper's RHF inversion barrier prediction.[13] While, by correspondingly fitting the CCSD/AVXZ energies for $X = 4,\ 5$, we obtain extrapolated inversion barriers of 1792.17 cm^{-1}/1790.63 cm^{-1} with Eq. (3)/Eq. (4), which are in good agreement with the result of 1791 cm^{-1} from Klopper's CCSD inversion barrier prediction[13] on the average value of the extrapolated CCSD(FC)/cc-pV(56)Z, extrapolated CCSD(FC)/aug-cc-pV(Q5)Z and CCSD(FC)-R12/B pair energies. By correspondingly fitting the CCSD(T)/AVXZ energies for $X = 4,\ 5$, we obtain extrapolated inversion barriers of 1833.87 cm^{-1}/1832.33 cm^{-1} with Eq. (3)/Eq. (4), in good agreement with 1831 cm^{-1}, which is Klopper's[13] best estimate of the CCSD(T) inversion barrier, and in very good agreement with the empirical value of 1834 cm^{-1}, deduced from experimental data by Špirko *et al.*[20] This suggests that the CBS scheme can be used to fit more accurate global DMBE PES for the ground state of ammonia.

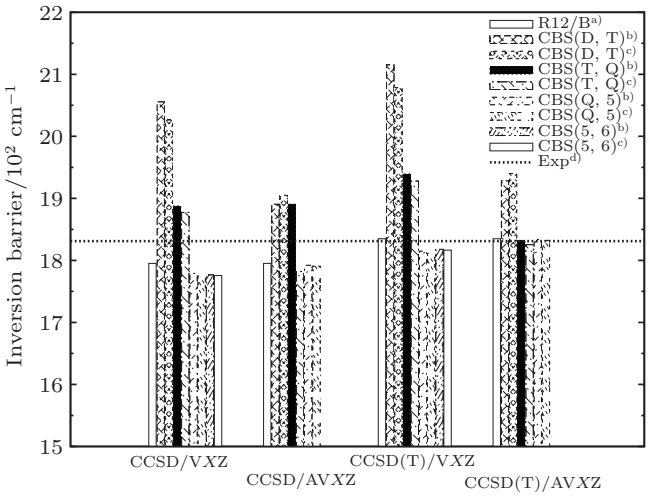


Fig. 3. Extrapolated inversion barriers of ammonia: a) CCSD-R12/B and CCSD[T]-R12/B results in Ref. [13]; b) the dc energies extrapolated using Eq. (3), which indicate the X^{-3} results; c) the dc energies extrapolated using Eq. (4), which indicate USTE results; d) the experimental value by Špirko *et al.*[20]

Table 1. Extrapolated CCSD/V*XZ* energies of the C_{3v} and D_{3h} structures (in E_h) and inversion barrier (in cm^{-1}) for the geometries considered in Ref. [13], headings Eq. (3) and Eq. (4) indicate the X^{-3} and USTE results, respectively.

	CAS/CBS		dc/CBS		Total/CBS	
Basis	Eq. (2)	Others[a]	Eq. (3)	Eq. (4)	Eq. (3)	Eq. (4)
			C_{3v}			
(2, 3)	–56.220768	–0.26316	–0.261679	–0.270903	–56.482448	–56.491671
(3, 4)	–56.224541	–0.27002	–0.269566	–0.270833	–56.494107	–56.495374
(4, 5)	–56.225437	–0.26983	–0.269745	–0.270020	–56.495182	–56.495457
(5, 6)	–56.225067	–0.26949	–0.269433	–0.269510	–56.494500	–56.494577
(4, 5, 6)[b]	–56.224977					
			D_{3h}			
(2, 3)	–56.212764	–0.26189	–0.260318	–0.269674	–56.474443	–56.482438
(3, 4)	–56.216829	–0.26915	–0.268676	–0.269991	–56.486395	–56.486820
(4, 5)	–56.218151	–0.26902	–0.268924	–0.269213	–56.487896	–56.487364
(5, 6)	–56.217752	–0.26870	–0.268653	–0.268735	–56.487185	–56.486488
(4, 5, 6)[b]	–56.217625					
			inversion barrier			
(2, 3)	1756.83	280	298.74	269.68	2055.57	2026.51
(3, 4)	1692.57	191	195.25	184.81	1887.82	1877.39
(4, 5)	1598.98	179	180.12	177.24	1779.11	1776.22
(5, 6)	1605.54	173	171.16	169.99	1776.70	1775.53
(4, 5, 6)[b]	1613					

[a]Extrapolated CAS energies using Eqs. (6) and (7) in Ref. [13] by Klopper *et al.*

[b]Extrapolated dc energies using Eq. (8) in Ref. [13] by Klopper *et al.*

Table 2. Calculated and extrapolated CCSD/AV*XZ* energies of the C_{3v} and D_{3h} structures (in E_h) and inversion barrier (in cm^{-1}) for the geometries considered in Ref. [13], headings Eq. (3) and Eq. (4) indicate the X^{-3} and USTE results, respectively.

	CAS/CBS		dc/CBS		Total/CBS	
Basis	Eq. (2)	Others[a]	Eq. (3)	Eq. (4)	Eq. (3)	Eq. (4)
			C_{3v}			
(2, 3)	–56.222264	–0.26509	–0.263552	–0.269908	–56.485815	–56.492172
(3, 4)	–56.224981	–0.26998	–0.269475	–0.270388	–56.494456	–56.495369
(4, 5)	–56.225258	–0.26963	–0.269463	–0.269655	–56.494721	–56.494913
(3, 4, 5)[b]	–56.225148					
			D_{3h}			
(2, 3)	–56.214901	–0.26384	–0.262299	–0.268591	–56.478453	–56.483492
(3, 4)	–56.217643	–0.26918	–0.268662	–0.269607	–56.487118	–56.487250
(4, 5)	–56.217898	–0.26882	–0.268657	–0.268856	–56.487361	–56.486754
(3, 4, 5)[b]	–56.217793					
			inversion barrier			
(2, 3)	1615.83	276	274.97	289.09	1890.80	1904.91
(3, 4)	1610.52	176	178.45	171.49	1788.97	1782.01
(4, 5)	1615.33	177	176.83	175.29	1792.17	1790.63
(3, 4, 5)[b]	1614					

[a]Extrapolated CAS energies using Eqs. (6) and (7) in Ref. [13] by Klopper *et al.*

[b]Extrapolated dc energies using Eq. (8) in Ref. [13] by Klopper *et al.*

Table 3. Calculated and extrapolated CCSD(T)/VXZ energies of the C_{3v} and D_{3h} structures (in E_h) and inversion barrier (in cm^{-1}) for the geometries considered in Ref. [13], headings Eq. (3) and Eq. (4) indicate the X^{-3} and USTE results, respectively.

	CAS/CBS	dc/CBS		Total/CBS	
Basis	Eq. (2)	Eq. (3)	Eq. (4)	Eq. (3)	Eq. (4)
			C_{3v}		
(2, 3)	–56.220768	–0.270503	–0.281180	–56.491272	–56.501948
(3, 4)	–56.224541	–0.278921	–0.280329	–56.503462	–56.504871
(4, 5)	–56.225437	–0.279159	–0.279466	–56.504595	–56.504903
(5, 6)	–56.225067	–0.278795	–0.278881	–56.503863	–56.503949
			D_{3h}		
(2, 3)	–56.212764	–0.268870	–0.279713	–56.483267	–56.492477
(3, 4)	–56.216829	–0.277795	–0.279257	–56.495750	–56.496087
(4, 5)	–56.218151	–0.278174	–0.278500	–56.497310	–56.496651
(5, 6)	–56.217752	–0.277828	–0.277920	–56.496547	–56.495672
			inversion barrier		
(2, 3)	1756.83	358.44	321.91	2115.27	2078.74
(3, 4)	1692.57	246.94	235.34	1939.51	1927.91
(4, 5)	1598.98	216.02	212.18	1815.01	1811.16
(5, 6)	1605.54	212.31	210.99	1817.85	1816.53

Table 4. Calculated and extrapolated CCSD(T)/AVXZ energies of the C_{3v} and D_{3h} structures (in E_h) and inversion barrier (in cm^{-1}) for the geometries considered in Ref. [13], headings Eq. (3) and Eq. (4) indicate the X^{-3} and USTE results, respectively.

	CAS/CBS	dc/CBS		Total/CBS	
Basis	Eq. (2)	Eq. (3)	Eq. (4)	Eq. (3)	Eq. (4)
			C_{3v}		
(2,3)	–56.222264	–0.272777	–0.280223	–56.495041	–56.502487
(3,4)	–56.224981	–0.278805	–0.279800	–56.503785	–56.504781
(4,5)	–56.225258	–0.278818	–0.279028	–56.504076	–56.504287
			D_{3h}		
(2,3)	–56.214901	–0.271354	–0.278747	–56.487679	–56.493648
(3,4)	–56.217643	–0.277795	–0.278821	–56.496447	–56.496464
(4,5)	–56.217898	–0.277822	–0.278040	–56.496716	–56.495938
			inversion barrier		
(2,3)	1615.83	312.43	324.05	1928.26	1939.88
(3,4)	1610.52	221.49	214.83	1832.01	1825.34
(4,5)	1615.33	218.53	216.99	1833.87	1832.33

4. Conclusions

We have extrapolated the CCSD and CCSD(T) energies for the C_{3v} and D_{3h} structures of ammonia to the complete one-electron basis-set limit, with correlation-consistent basis sets of the type cc-pVXZ ($X = \mathrm{D,T,Q,5,6}$) and aug-cc-pVXZ ($X = \mathrm{D,T,Q,5}$). The KM protocol is employed to extrapolate the CAS energies; our inversion barrier is obtained by fitting the RHF/AVXZ energies for the two cardinal numbers, which accords well with the extrapolating inversion barrier of ammonia using the three largest sets given by Klopper *et al*. While the USTE is used to extrapolate the correlation energy, the results are found to compare favorably with those obtained from traditional schemes. As a result, our extrapolating inversion barrier of ammonia obtained by fitting the CCSD(T) energies for $X = 4,\ 5$ agrees well with Klopper's theoretical result and other experimental results. Thus, in order to obtain the accurate inversion barrier, we expect to improve our global DMBE PES for the ground state of ammonia obtained by the CCSD(T) *ab initio* energies in future work.

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