Theor Chim Acta (1988) 74: 185-194

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Electric properties of the chloride ion

Vladimir Kellö*, Björn O. Roos, and Andrzej J. Sadlej

Theoretical Chemistry, Chemical Centre, University of Lund, Box 124, S-221 00 Lund, Sweden

(Received December 9, 1987/Accepted January 30, 1988)

The dipole (α), quadrupole (C), and dipole-quadrupole (B) polarizabilities and the dipole hyperpolarizability (γ) of the chloride ion have been calculated by using the many-body perturbation theory approach and a series of large polarized GTO/CGTO basis sets. The complete fourth-order treatment of the electron correlation effects with a basis set comprising the s, p, d, f, and g functions gives: $\alpha = 38.01$ a.u., $C = 211.5$ a.u., $B = -5.14 \times 10^3$ a.u., and $\gamma = 128.5 \times 10^3$ a.u. as compared to the corresponding SCF values ($\alpha = 31.49$ a.u., $C = 158.9$ a.u., $B = -2.92 \times 10^3$ a.u., $\gamma = 57.7 \times 10^3$ a.u.). The quenching of polarizabilities of the Cl^- ion in solutions and ionic crystals is discussed.

Key words: Multipole polarizabilities - Properties of Cl^- — Polarized basis sets — MBPT calculations of properties

1. Introduction

The majority of physical effects arising from the ion-ion or ion-molecule interactions can be interpreted in terms of simple, basically electrostatic, models in which the electric properties of interacting species occur as parameters [1-3]. In the case of negative ions, the only reliable source of their electric properties follows from accurate theoretical calculations [4, 5]. The corresponding empirical estimates [6, 7] are considerably affected by the presence of the ionic and/or molecular environment. On the other hand, it has been found [8] that the electric properties of negative ions cannot be accurately predicted without a careful consideration of the electron correlation effects [4, 5].

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* *Permanent address*: Department of Physical Chemistry, Faculty of Sciences, Comenius University, CS-84215 Bratislava, Czechoslovakia

The most comprehensive studies of the electron correlation contribution to electric properties of negative ions have been carried out for the fluoride ion [4, 5, 8, 9-16]. The corresponding investigations for the chloride ion are less complete [15-18]. With a few exceptions [15, 17] most studies of electric properties of Cl^- have been carried out within the one-electron approximation.

In the present paper results will be reported for the dipole (α), quadrupole (C), and dipole-quadrupole (B) polarizabilities, and for the dipole hyperpolarizability (γ) of the chloride ion. All calculations have been performed with large GTO/CGTO basis sets generated by using the basis set polarization method [19]. The study of the electron correlation contribution to the electric properties of Cl^- has been carried out by using the many-body perturbation theory (MBPT) [20-21] within the finite-field perturbation scheme [8, 22, 23]. The electron correlation contributions to α, C, B and γ have been calculated through the complete fourth-order with respect to the correlation perturbation operator [24].

2. Computational details

Both the computational methods and certain details of numerical calculations are virtually the same as those described in Ref. [25]. The two major factors which determine the quality of the calculated electric properties are the amount of the electron correlation effects which are accounted for by the given computational method and the basis set choice. The first of them has already been widely discussed in other papers [4, 5, 13, 23-26]. As long as the reference function for the MBPT expansion is well approximated by a single HF SCF determinant, the complete fourth-order treatment of the electron correlation contribution to electric properties is known to be quite satisfactory [5, 23, 25, 26]. Far more important appear to be the basis set truncation effects and for this reason an extensive study of the basis set saturation has been carried out in the present paper.

The initial GTO/CGTO basis set of the structure [15.11.4/10.8.3] has been generated from the (12.8) GTO basis set of Huzinaga [27]. In order to increase the flexibility of the parent GTO basis set its orbital exponents have been slightly modified to form a geometric progression in the valence region. Moreover, some diffuse *s* and *p* functions have been added to allow for a proper description of the Cl^- ion. The *d* subset has been generated by using the concept of the basis set polarization [19]. The resulting [15.11.4/10.8.3] GTO/CGTO basis set, hereafter referred to as Basis 1, is presented in Table 1. This basis set has been first examined with respect to the saturation of its *d*-type subset and has led to the derived basis sets: [15.11.5/10.8.4] (Basis 2), [15.11.6/10.8.4] (Basis 3), and [15.11.7/10.8.5] (Basis 4). The four electric properties of the Cl^- ion have been calculated for each of those basis sets. According to the results presented in the next section, Basis 4 has been found to be sufficiently saturated in the *d* subset and has been used to investigate the effects of including the *f*-type GTO's. The following three (*spdf*) GTO/CGTO basis sets have been considered: [15.11.7.3/10.8.5.3] (Basis 5), [15.11.7.4/10.8.5.3] (Basis 6), and [15.11.7.5/10.8.5.4] (Basis 7). The orbital exponents and contraction coefficients

Table 1. GTP/CGTO basis sets used in calculations of electric properties of the Cl$^-$ ion

Basis set	CGTO	$\sum_i c_i$ GTO (α_i)
s subset (common for all basis sets)		
	1	0.000306(105747.0) + 0.002369(15855.3) +0.012204(3615.32) + 0.048447(1030.03) +0.149025(339.691)
	2	1.0(124.497)
	3	0.408846(49.5143) + 0.190191(20.8138)
	4	1.0(6.46497)
	5	1.0(2.52567)
	6	1.0(0.986704)
	7	1.0(0.385476)
	8	1.0(0.150594)
	9	1.0(0.058832)
	10	1.0(0.022984)
p subset (common for all basis sets)		
	1	0.002680(622.0274) + 0.022037(145.4972) +0.105186(45.00866) + 0.306826(15.90089)
	2	1.0(5.925944)
	3	1.0(2.294382)
	4	1.0(0.888329)
	5	1.0(0.343940)
	6	1.0(0.133165)
	7	1.0(0.051558)
	8	1.0(0.019962)
Basis 1 [15.11.4/10.8.3]		
d subset		
	1	0.310664(0.8883) + 0.785492(0.3439)
	2	1.0(0.1332)
	3	1.0(0.0516)
Basis 2 [15.11.5/10.8.4]		
d subset		
	1	0.310664(0.8883) + 0.785492(0.3439)
	2	1.0(0.1332)
	3	1.0(0.0516)
	4	1.0(0.0200)
Basis 3 [15.11.6/10.8.4]		
d subset		
	1	0.056936(5.9259) + 0.030368(2.2944)
	2	0.310664(0.8883) + 0.785492(0.3439)
	3	1.0(0.1332)
	4	1.0(0.0516)
Basis 4 [15.11.7/10.8.5]		
d subset		
	1	0.056936(5.9259) + 0.030368(2.2944)
	2	0.310664(0.8883) + 0.785492(0.3439)
	3	1.0(0.1332)
	4	1.0(0.0516)
	5	1.0(0.0200)

Table 1 (continued)

Basis set	CGTO	$\sum_i c_i$ GTO (α_i)
Basis 5 [15.11.7.3/10.8.5.3]		
f subset [a]		
	1	1.0(0.1332)
	2	1.0(0.0516)
	3	1.0(0.0200)
Basis 6 [15.11.7.4/10.8.5.3]		
f subset [a]		
	1	0.032962(0.8883) + 0.135650(0.3439)
	2	1.0(0.1332)
	3	1.0(0.0516)
Basis 7 [15.11.7.5/10.8.5.4]		
f subset[a]		
	1	0.032962(0.8883) + 0.135650(0.3439)
	2	1.0(0.1332)
	3	1.0(0.0516)
	4	1.0(0.0200)
Basis 8 [15.11.7.5.2/10.8.5.4.1]		
g subset[b]		
	1	0.6663(0.1332) + 0.9957(0.0516)

[a] The *s*, *p*, and *d* subsets are the same as in Basis 4

[b] The *s*, *p*, *d*, and *f* subsets are the same as in Basis 7

for the *f* subsets follow from the assumptions of the basis set polarization method [19] and all the relevant data are given in Table 1. The study of different electric properties of Cl^- has shown that Basis 7 can be considered as enough saturated through the *f* subset.

Finally, in order to investigate the effect of the *g*-type functions, we have extended Basis 7 to the [15.11.7.5.2/10.8.5.4.1] GTO/CGTO basis set (Basis 8) with the parameters of the *g*-type OGTO determined by the basis set polarization scheme [19]. The details of Basis 8 are given in Table 1.

The calculations of electric properties of Cl^- have been carried out by using the integral, SCF, property, and 4-index transformation packages of this laboratory linked to the MBPT programs of the Bratislava group [28, 29]. The *s* components of the *d*-type cartesian GTO's, *p* components of the *f*-type GTO's, and *s* and *d* components of the *g* type GTO's have been removed from the basis set.

The finite-field perturbation method has been used to obtain the results for α, C, B, and γ. The numerical derivatives of the perturbation dependent energies have been calculated according to the formulae of Ref. [25] with the following values of the strength of the external electric field (F) and external electric field gradient (V): $F = 0.005$ a.u., 0.010 a.u., $V = \pm 0.001$ a.u. At the SCF level of approximation the energy derivatives have been checked against the corresponding derivatives of the induced multipole moments [25]. The agreement between those two sources of the polarizability data is assumed to approximately determine the numerical accuracy of our results.

Finally, let us mention that all definitions of polarizabilities used in the present paper follow those of Buckingham [1, 2]. It should be remarked that our quadrupole polarizability C is one half of the α_2 value which is usually considered in atomic physics [30].

3. Results and discussion

The major part of calculations reported in this paper has been carried out with the K- and L-shell electrons of Cl^- left uncorrelated. The results computed with those two shells frozen at the level of the MBPT approximation are collected in Table 2. In addition to the polarizability data obtained with different basis sets also the correlation energy values are presented.

The effect of correlating the L-shell electrons has been studied for some representative basis sets (Basis 4, Basis 7, and Basis 8) and the corresponding results are shown in Table 3.

The SCF values of α and C obtained in the present paper can be compared with the accurate SCF results of McEachran et al. ($\alpha = 31.55$ a.u., $C = 158.95$ a.u. [32]). This shows that our Basis 4 can be considered as well saturated for SCF calculations of the electric dipole polarizability. The same comment applies to Basis 7 with respect to the quadrupole polarizability C. It is obvious that in order to obtain a reasonable result for C at the SCF level of approximation one has to use a basis set which comprises the $s, p, d,$ and f GTO's. A similar minimum requirement as regards the basis set composition holds also for B and γ. To our knowledge there are no other values of B and γ of the Cl^- ion available for comparison.

The electron correlation contribution to the dipole polarizability has been previously studied [17] at the level of the fourth-order MBPT approximation limited to singly and doubly substituted intermediate states (SD-MBPT) and a GTO/CGTO basis set comprising the $s, p,$ and d functions only. The present complete fourth-order MBPT treatment indicates the importance of triply and quadruply substituted intermediate states. The previous result for the SD-MBPT (4) correlation correction to α was 5.31 a.u. (Basis II of Ref. [17]) while our value obtained in the complete fourth-order MBPT treatment (MBPT(4)) amounts to 6.60 a.u. (Basis 4). Both the f and g components of the basis set have a rather negligible effect on the calculated correlation corrections to α. At least formally the best present result for α is that obtained by the MBPT (4) method with Basis 8 and is equal to 38.01. However, the fourth-order contribution due to triply substituted intermediate states, which is given by the difference between the MBPT(4) and SDQ-MBPT(4) results, amounts to 2.09 a.u. (Basis 8) and shows that the MBPT(4) values of the dipole polarizability of Cl^- may be still affected by the higher-order terms in the correlation perturbation expansion.

Table 2. Correlation energies and polarizabilities of the chloride ion. SCF and MBPT results for different GTO/CGTO basis sets. The *K*- and *L*-shell electrons left uncorrelated. All values in a.u.

Method[a]	Basis 1[b]	Basis 2	Basis 3	Basis 4	Basis 5	Basis 6	Basis 7	Basis 8
Correlation energy [c]								
MBPT(2)	−0.165286	−0.165533	−0.167607	−0.167840	−0.172228	−0.193972	−0.194048	−0.194412
MBPT(3)	−0.176875	−0.173137	−0.180006	−0.180253	−0.185180	−0.210442	−0.210521	−0.210890
SDQ-MBPT(4)	−0.175974	−0.176230	−0.179161	−0.179403	−0.184357	−0.209416	−0.209491	−0.209875
MBPT(4)	−0.180288	−0.180567	−0.183777	−0.184044	−0.189894	−0.217348	−0.217429	−0.217869
Dipole polarizability α								
SCF	31.20	31.40	31.29	31.50	31.49	31.49	31.49	31.49
MBPT(2)	36.48	36.94	36.55	37.02	37.58	37.14	37.49	37.23
MBPT(3)	35.14	35.48	35.21	35.55	35.96	35.47	35.46	35.50
SDQ-MBPT(4)	35.73	36.13	35.77	36.17	36.61	35.85	35.84	35.92
MBPT(4)	37.52	38.03	37.58	38.10	38.73	37.90	37.89	38.01
Quadrupole polarizability C								
SCF	71.1	71.1	71.2	71.2	156.7	153.3	158.9	158.9
MBPT(2)	91.7	91.6	91.9	91.9	208.5	195.7	205.8	207.6
MBPT(3)	86.0	86.0	86.2	86.2	192.3	181.9	189.1	190.2
SDQ-MBPT(4)	88.3	88.3	88.5	88.5	197.3	184.2	192.3	193.7
MBPT(4)	95.0	95.1	95.3	95.3	215.2	198.8	209.3	211.5
Dipole-quadrupole polarizability B ($\times 10^3$)								
SCF	−1.72	−2.00	−1.73	−2.00	−2.90	−2.69	−2.91	−2.92
MBPT(2)	−2.62	−3.23	−2.62	−3.23	−4.85	−4.24	−4.75	−4.81
MBPT(3)	−2.34	−2.81	−2.35	−2.81	−4.09	−3.63	−3.99	−4.02
SDQ-MBPT(4)	−2.48	−3.03	−2.48	−3.02	−4.48	−3.84	−4.27	−4.32
MBPT(4)	−2.81	−3.50	−2.81	−3.50	−5.29	−4.50	−5.07	−5.14
Dipole hyperpolarizability $\gamma (\times 10^3)$								
SCF	34.6	44.7	34.6	44.8	57.6	53.7	57.6	57.7
MBPT(2)	63.0	87.9	63.3	88.4	114.3	101.5	111.8	112.4
MBPT(3)	51.9	69.8	52.3	70.2	89.3	79.8	86.8	86.8
SDQ-MBPT(4)	59.2	81.9	59.4	81.9	105.3	90.6	99.1	99.6
MBPT(4)	72.7	102.9	73.0	101.1	133.8	115.7	127.5	128.5

[a] The abbreviation MBPT (*n*) corresponds to the MBPT treatment of correlation effects through the *n*th order in the electron correlation perturbation [21–26]

[b] For the basis set description see Table 1

[c] The SCF energy is the same for all basis sets used in the present study and equal to −459.566893 a.u. The estimated Hartree-Fock energy is −459.57670 a.u. [31]

Table 3. Correlation corrections to the SCF energy and polarizabilities of the chloride ion. A study of the *L*-shell correlation contribution. All values in a.u.

Correlation contribution[a]	Basis 4[a]		Basis 7		Basis 8	
	K shell frozen	*K*, *L*-shells frozen	*K*-shell frozen	*K*, *L*-shells frozen	*K*-shell frozen	*K*, *L*-shells frozen
Energy						
MBPT(2)	−0.359491	−0.167840	−0.386230	−0.194048	−0.386593	−0.194412
MBPT(3)	−0.368672	−0.180253	−0.399503	−0.210521	−0.399872	−0.210890
SDQ-MBPT(4)	−0.367779	−0.179403	−0.398301	−0.209491	−0.398682	−0.209875
MBPT(4)	−0.374059	−0.184044	−0.408043	−0.217429	−0.408481	−0.217869
Dipole polarizability						
MBPT(2)	5.61	5.52	5.72	5.64	5.82	5.74
MBPT(3)	4.13	4.06	4.03	3.97	4.07	4.01
SDQ-MBPT(4)	4.65	4.67	4.32	4.35	4.39	4.43
MBPT(4)	6.70	6.60	6.49	6.40	6.60	6.52
Quadrupole polarizability						
MBPT(2)	21.1	20.7	47.5	46.8	49.3	48.7
MBPT(3)	15.3	15.1	30.6	30.2	31.6	31.2
SDQ-MBPT(4)	17.2	17.3	33.0	33.4	34.4	34.8
MBPT(4)	24.5	24.2	51.1	50.4	53.2	52.6
Dipole-quadrupole polarizability ($\times 10^3$)						
MBPT(2)	−1.25	−1.23	−1.87	−1.84	−1.91	−1.88
MBPT(3)	−0.82	−0.81	−1.09	−1.08	−1.11	−1.09
SDQ-MBPT(4)	−1.01	−1.01	−1.34	−1.36	−1.37	−1.39
MBPT(4)	−1.52	−1.50	−2.19	−2.24	−2.24	−2.22
Dipole hyperpolarizability ($\times 10^3$)						
MBPT(2)	44.2	43.6	55.1	54.2	55.7	54.7
MBPT(3)	25.7	25.4	29.9	29.2	29.8	29.1
SDQ-MBPT(4)	36.7	37.1	41.1	41.4	41.6	42.0
MBPT(4)	59.0	56.3	70.9	69.9	71.9	70.8

[a] See the corresponding footnotes to Table 2

The complete fourth-order MBPT treatment of the electron correlation contribution to the dipole polarizability of systems similar to the Cl^- ion is known to overshoot a little the estimated exact results [25, 26]. Hence, one can conclude that the exact correlated value of α for the Cl^- ion is a little lower than our most accurate MBPT(4) result calculated with Basis 8.

The importance of f functions for accurate calculations of the quadrupole polarizability is also manifested at the level of the MBPT approximation. The major part of the electron correlation correction to C follows from the second-order treatment. Since the convergence pattern for correlation corrections to C is similar to that for the dipole polarizability, one can expect that the best MBPT (4) values of C computed in this paper (Basis 7, Basis 8) may be a little too high. The percentage of the electron correlation contribution to C in the MBPT(4) calculation with Basis 8 amounts to about 25% and is slightly higher than that for the dipole polarizability (about 17% in MBPT(4) calculations with Basis 8). However, these values are much higher than those obtained in similar calculations for the Ar atom (about 5% for α and about 2.6% for C [26]). On the other hand they are much lower than the corresponding results for the fluoride ion [5, 13].

The importance of the electron correlation contribution to B and γ has already been stressed in our previous studies of atomic systems [25, 26]. As shown by the data of Table 2 the electron correlation effects account for about 40% of the calculated value of B (Basis 8, MBPT(4)) and about 60% of the corresponding result for γ. In the case of the Ar atom [26] the correlation contribution to B and γ have been found to account for about 14 and 25% of their MBPT(4) values, respectively.

The convergence of the correlation perturbation series for B and γ appears to be slightly poorer than for the other polarizabilities. The large fourth-order contribution due to triply substituted intermediate states makes also the MBPT(4) results more uncertain than those obtained for α and C. However, one can safely conclude that the B value for the Cl^- ion is close to -5×10^3 a.u. while the dipole hyperpolarizability γ is larger than 10^5 a.u.

According to the present investigation of the effect of g functions on the correlation contribution to electric properties of Cl^-, their presence in the basis set does not seem to considerably affect the computed correlation correction. Though the study of this problem has been limited to only one set of g functions (Basis 8), the method of their choice [19] suggests that they should be able to recover the major part of the pertinent correlation effects. As shown by the data of Table 2, the results obtained with Basis 8 are only marginally different from those calculated with the best (*spdf*) basis set (Basis 7).

The results including the electron correlation contribution due to the L shell electrons are shown in Table 3. Their comparison with the corresponding MBPT data calculated with both the K- and L-shells frozen indicates that the contribution of the intra- and inter-shell effects to electric properties of the Cl^- ion is practically negligible. Including the L shell electrons in MBPT(4) calculations increases slightly the polarizabilities computed within the valence shell approximation. The numerical data of Table 3 obtained with freezing only the *K*-shell electrons in MBPT treatment may be to some extent affected by the present choice of polarization functions [19]. This choice corresponds mostly to polarizaing the valence orbitals of Cl^-. However, the qualitative conclusions based on the data of Table 3 are unlikely to be considerably affected by the basis set extension.

4. Summary and conclusions

Four basic electric properties of the chloride ion, α, C, B and γ, have been calculated by using the complete fourth-order MBPT method. The basis set truncation effects on those properties have been investigated by a systematic extension of the initial polarized basis set. The two largest GTO/CGTO basis sets employed in the present study (Basis 7, Basis 8) have been found to be nearly saturated with respect to the calculated properties. The effect of extending the basis set beyond the *f*-type functions is almost negligible. Also the *L*-shell and *LM*-intershell correlation contribution to the studied electric properties is relatively unimportant.

The calculations have been carried out for the isolated chloride ion, which is a somewhat artificial system and so far can be studied only theoretically. Under the experimental conditions its electronic structure is significantly affected by the ionic or molecular environment. This leads to the well known quenching of electric polarizabilities of the Cl^- ion in solutions [6, 7] and ionic crystals [15, 16]. The isolated Cl^- appears then as the result of some extrapolation procedures [6, 7].

The polarizability quenching effects can be easily interpreted in terms of the modification of the effective nuclear charge [9]. For this purpose it is instructive to compare the present results for the Cl^- ion (MBPT(4), Basis 8) with those calculated recently for the Ar atom [26]. The corresponding data are given in Table 4 and show the magnitude of the quenching effect upon changing the nuclear charge from 17 (Cl^-) to 18 (Ar).

On the basis of our previous calculations for the fluoride ion [9] one can expect that the nuclear charge (Z) dependence of the electric polarizabilities is strongly

Table 4. Polarizabilities of Cl^- and Ar calculated by the fourth-order MBPT approach. All values in a.u.

	Cl^- This work[a]	Ar Ref. [26]
α	38.01	11.23
C	211.5	26.89
B	-5.14×10^3	-164.3
γ	128.5×10^3	1329

[a] Basis 8

non-linear and steeply increases in the vicinity of $Z = 17$. Hence, a relatively small charge transfer from the Cl^- ion to its surrounding brings about a very large reduction of polarizabilities. On the other hand, the size of the quenching effect can be considered as a qualitative measure of the departure from the purely electrostatic model of ion–ion or ion–molecule interactions.

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