31 March 1995

ELSEVIER

Chemical Physics Letters 235 (1995) 430–435

CHEMICAL PHYSICS LETTERS

Multireference Møller–Plesset perturbation treatment for valence and Rydberg excited states of benzene

K. Hirao, H. Nakano, T. Hashimoto

Department of Applied Chemistry, Faculty of Engineering, University of Tokyo, Tokyo 113, Japan

Received 28 November 1994; in final form 9 January 1995

Abstract

State-specific multireference Møller–Plesset perturbation theory has been applied to the study of valence and Rydberg excitation energies of benzene. The results compare well with experiment. The calculated valence $\pi-\pi^*$ excitation energies (experimental values in parentheses) are $^1B_{2u}$, 4.77 (4.90), $^1B_{1u}$, 6.28 (6.20), $^1E_{1u}$, 6.98 (6.94) and $^1E_{2g}$, 7.88 (7.80) eV. Results of similar accuracy are obtained for the valence triplet excited states. The Rydberg excitation energies are also predicted with an accuracy of 0.18 eV or better.

1. Introduction

We are seeking theories that are quantitatively correct for all molecular states and all nuclear geometries. Despite the progress made so far, the present state of the art in accurate computations is still far from being satisfactory for larger systems.

Single-reference perturbation theory and cluster expansion theory such as symmetry-adapted cluster (SAC) [1] and coupled-cluster (CC) [2] theories are effective in describing dynamical correlation but fail badly in dealing with nondynamical correlation. CI is easily applied in multireference form and can handle nondynamical correlation but the CI expansion becomes less compact and less efficient as the number of electrons in the system grows. Therefore we have developed a multireference based Rayleigh–Schrödinger perturbation theory, called multireference Møller–Plesset (MRMP) theory [3]. The essential feature of the theory is that the multireference technique is used to include the nondynamical correlation effect due to the near-degeneracy problem. Once the state-specific nondynamical correlation is taken into account, the rest is primarily composed of dynamical pair correlation. Individual pair correlation can be calculated independently using second-order perturbation theory. The performance of perturbation theory depends critically on the choice of zeroth-order Hamiltonian. For closed shells, the best results are obtained with the MP partitioning, i.e. with the sum of one-electron Fock operators as the zeroth-order Hamiltonian. Thus, we have formulated our MRMP theory with a close analogue of MP partitioning. The second-order MRMP method has been successfully applied to various chemical problems [3]. The MRMP method is reliable and retains the attractive features of the single-reference MP method. The theory has conceptual simplicity due to the independent electron pair model. It is almost size consistent. It is efficient and cost effective. Neither iteration nor diagonalization is necessary in the calculation of the first-order correction to the wavefunction. The multireference

SSDI 0009-2614(95)00160-3

technique can dissociate a molecule correctly into its fragments. It is applicable to open shells and excited states.

This study has as its main objective to test the effectiveness of the MRMP approach for valence and Rydberg excited states of benzene. Benzene is a prototype of an intermediate case between large and small molecules. Our emphasis is on testing some of the unique features of state-specific MRMP theory to assess its capabilities, accuracy and limitations.

2. Calculated results

Calculations were carried out for the ground and low-lying singlet and triplet excited states of benzene. A regular hexagonal geometry was used for the ground and excited states with experimental C–C and C–H bond lengths of 1.397 and 1.084 Å [4], respectively. Thus, the excitation energies calculated are vertical in nature. All calculations were performed with a double-zeta plus polarization quality basis of Dunning's cc-pVDZ [5], augmented with Rydberg functions (8s8p8d/1s1p1d) placed at the center of the molecule. The universal Gaussian basis set devised by Kaufmann et al. [6] was employed for the Rydberg functions. We contracted the (8s8p8d) primitive set to a (1s1p1d) set by calculating the benzene cation with the primitive functions in the UHF approximation and selecting the lowest Rydberg-type virtual orbitals of each angular momentum component. Usually a CASSCF [7] calculation is carried out for each individual state with proper spin and symmetry to obtain an optimal reference function and then the MRMP procedure is applied to each state. Since the present calculations were carried out with D_{2h} molecular symmetry, we used the active space constructed from active orbitals obtained by CASSCF for an average energy of several lowest singlet states. Thus, the orbitals in the average CASSCF wavefunctions are optimized independently for each symmetry. The so determined active orbitals are used for the description of both the singlet and triplet excited states. The ground state of benzene is well described in a single Hartree–Fock configuration but the single configurational description is worsened for excited states, particularly for valence excited states due to severe quasi-degeneracy problems. The reference space should be chosen large enough such that all near degeneracy effects are included. Valence six π electrons are treated as active electrons and distributed among bonding π (a_{2u} and e_{1g}) and antibonding π^* (e_{2u} and b_{2g}) orbitals for the valence states. The contributions from σ electrons are included through second-order correlation effects. Carbon 1s orbitals were optimized in the CASSCF calculations but were uncorrelated in the MRMP calculations. For the calculations of the Rydberg excited states, we extended the active space by adding appropriate Rydberg orbitals in addition to valence π and π^* orbitals. We added $3d_\sigma$, $3d_\delta$ and 3s orbitals as active orbitals for the description of B_{1g}, E_{1g} and B_{2g} Rydberg states, $3d_\pi$ for A_{1g}, E_{2g} and A_{2g} states, $3p_\sigma$ for A_{1u}, E_{2u} and A_{2u} states and $3p_\pi$ for B_{1u}, E_{1u} and B_{2u} states. The method used was state-specific perturbation theory and each state was individually calculated. The transition energies were calculated as the difference of MRMP energies between the ground and the excited states which were calculated separately. At present the transition moments cannot be calculated at the same level of accuracy as used for the transition energies. The main difficulty is that the two wavefunctions involved in the transition are individually optimized and the orbitals are not orthonormal.

The results for the singlet and triplet valence π–π^* excitation energies are summarized in Table 1 and Fig. 1. It is well known that the $^1B_{2u}$ and $^1E_{2g}$ states are covalent excited states while $^1B_{1u}$ and $^1E_{1u}$ are singly excited states with strong ionic components. Moreover, analysis of the CASSCF wavefunctions shows that the $^1B_{2u}$ state is dominated by single excitations from the ground state but the $^1E_{2g}$ state is a mixed state of singly and doubly excited configurations. Thus, the correlation effects may be different in states of a different nature. The MRMP excitation energies are compared to the CASSCF, CASPT2, SAC/SAC-CI and CI results. The SAC/SAC-CI theories [1] are known to yield accurate total energies and excitation energies for the equilibrium geometry. The results of SAC/SAC-CI are cited from the study done by Kitao and Nakatsuji [9]. The SAC/SAC-CI reproduced the experimental excitation energies to within 0.5 eV. There are several CI works on the transition energies of benzene but we cited the study of MRD-CI results by Palmer

Table 1
Valence $\pi-\pi^*$ excitation energies (eV) of benzene [a]

State	CASSCF	MRMP (error)	Exp.	CASPT2 [b]	SAC-CI [c]	MRD-CI [d]	NO-CI [e]
singlet							
1^1B_{2u}	5.07	4.77 (−0.13)	4.90 [f]	4.70	5.25	5.19	5.17
1^1B_{1u}	8.10	6.28 (0.08)	6.20 [f,g]	6.10	6.60	6.67	6.38
1^1E_{1u}	9.37	6.98 (0.04)	6.94 [f]	7.06	7.47	7.55	7.32
1^1E_{2g}	8.17	7.88 (0.08)	7.80 [h]	7.77		8.17	
triplet							
1^3B_{1u}	4.58	4.11 (0.16)	3.95 [i]	3.89	4.06		3.90
1^3E_{1u}	5.62	4.81 (0.05)	4.76 [i]	4.50	5.02		4.57
1^3B_{2u}	7.41	5.34 (−0.26)	5.60 [i]	5.44	6.02		5.42
1^3E_{2g}	7.23	7.04 (0.21)	6.83 [j]	7.03			

[a] Ground state energy; CASSCF = −230.79492 E_h, MRMP = −231.51027 E_h.
[b] Ref. [8]. [c] Ref. [9]. [d] Ref. [19]. [e] Ref. [11]. [f] Ref. [12]. [g] Ref. [13]. [h] Ref. [14]. [i] Ref. [15]. [j] Ref. [16].

and Walker [10] and the work by Yamamoto et al. [11]. The former predicted the line position for the singlet valence states with an accuracy of 0.61 eV. The latter is a single-reference CI based on composite natural orbitals with extended basis set although the $^1B_{2u}$ state is computed in a MRCI treatment starting with three reference functions. The calculation predicted the experiment to within 0.38 eV. The CASPT2 results of Roos et al. [8] are also listed for comparison. CASPT2 achieved an accuracy of 0.26 eV or better. MRMP and CASPT2 [17] are similar in a sense that both are perturbation theory based on the multireference functions. The difference between the two methods is the choice of the zeroth-order Hamiltonian, H_0. CASPT2 uses an internally contracted scheme to generate the first-order wavefunction and therefore a large set of linear equations must be solved. MRMP expands the first-order wavefunction in the full set of Slater determinants in the reference set. This space is much larger than the interacting space used in CASPT2, but H_0 is diagonal in this space so the denominator in the perturbation expression, $(H_0 - E_0)^{-1}$, is easily formed in the MRMP calculations.

We observe that CASSCF tends to overestimate the excitation energies compared to the experimental values. Fig. 1 shows that the largest errors are found in the states with the largest ionic character: $^1B_{1u}$, $^1E_{1u}$ and $^3B_{2u}$. For instance, the CASSCF excitation energy for the strongly ionic state, $^1E_{1u}$, is 9.37 eV,

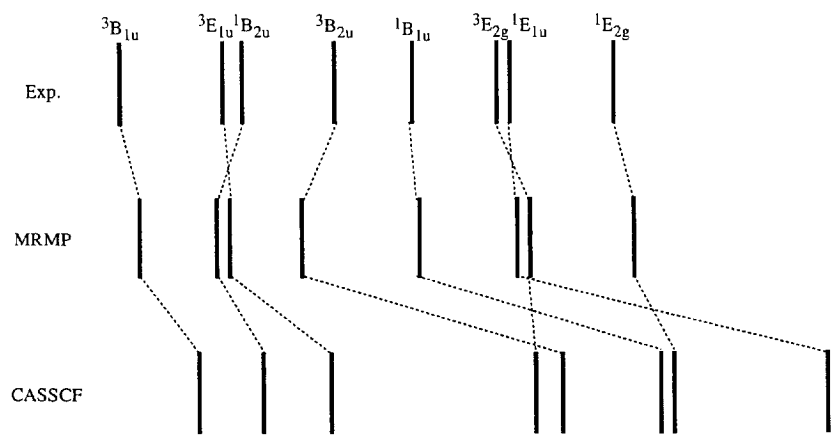

Fig. 1. Schematic summary of the calculated results of the valence $\pi-\pi^*$ excitation energies of benzene.

which is 2.4 eV too high compared to the experimental value of 6.94 eV. The present CASSCF active space contains only π orbitals and is not adequate for the description of the ionic states, the so-called V states. An adequate description of V states cannot be obtained before the $\sigma-\sigma$ and $\sigma-\pi$ interactions are correctly taken into account. These interactions can be included through the second-order correlation energies. The previous CI and SAC-CI studies also have difficulties in describing these ionic states, placing transitions at higher energies. For the covalent states, the CASSCF excitation energies are still too high compared to experiment but the deviation is much smaller than that for ionic states. A multiconfigurational treatment can handle such covalent excited states involving double excitations as $^1E_{2g}$ as well as those characterized as single excitations.

MRMP theory corrects the deficiency and represents a great improvement over CASSCF. The inclusion of second-order correlation effects changes the situation dramatically and the MRMP excitation energies become quite close to the experimental values both for ionic and covalent states. The calculated valence singlet $\pi-\pi^*$ excitation energies with MRMP (experimental values in parentheses) are $^1B_{2u}$, 4.77 (4.90), $^1B_{1u}$, 6.28 (6.20), $^1E_{1u}$, 6.98 (6.94) and $^1E_{2g}$, 7.88 (7.80) eV. The deviation of the excitation energy from experiment is within 0.13 eV for all the singlet excited states calculated. It is worth noting that second-order correlation effects are important especially for the ionic states (see Fig. 1).

Table 2
Singlet Rydberg excitation energies (eV) of benzene

State	CASSCF	MRMP (error)	Exp.	SAC-CI [a]
1^1E_{1g} (3s)	6.01	6.39 (0.06)	6.33 [b]	6.31
1^1A_{2u} (3pσ)	6.48	6.84 (−0.09)	6.93 [c,d]	6.88
1^1E_{2u} (3pσ)	6.54	6.92 (−0.03)	6.95 [d]	6.99
1^1A_{1u} (3pσ)	6.61	6.93		7.10
2^1E_{1u} (3pπ)	7.01	7.27 (−0.14)	7.41 [d]	6.91
1^1B_{1g} (3dσ)	7.16	7.51 (0.05)	7.46 [e]	7.42
1^1B_{2g} (3dσ)	7.00	7.53 (0.07)	7.46 [e]	7.42
2^1E_{1g} (3dδ)	6.99	7.56		7.44
3^1E_{1g} (3dδ)	7.05	7.61 (0.07)	7.54 [f]	7.35
2^1A_{1g} (3dπ)	7.26	7.62 (−0.18)	7.80 [c,f]	7.64
2^1E_{2g} (3dπ)	7.24	7.63 (−0.18)	7.81 [c,f]	7.64
1^1A_{2g} (3dπ)	7.27	7.66		7.57

[a] Ref. [9]. [b] Ref. [18]. [c] Ref. [19]. [d] Ref. [20].
[e] Ref. [21]. [f] Ref. [22].

Table 3
Triplet Rydberg excitation energies (eV) of benzene

State	CASSCF	MRMP	Exp. (singlet)	SAC-CI [a]
1^3E_{1g} (3s)	5.98	6.36	6.33 [b]	6.28
1^3A_{2u} (3pσ)	6.45	6.81	6.93 [c,d]	6.82
1^3E_{2u} (3pσ)	6.53	6.87	6.95 [d]	7.02
1^3A_{1u} (3pσ)	6.61	6.93		7.15
2^3E_{1u} (3pπ)	7.00	7.27	7.41 [d]	6.89
1^3B_{1g} (3dσ)	7.15	7.51	7.46 [e]	7.43
1^3B_{2g} (3dσ)	6.99	7.53	7.46 [e]	7.42
2^3E_{1g} (3dδ)	6.99	7.55		7.42
3^3E_{1g} (3dδ)	7.04	7.61	7.54 [f]	7.33
1^3E_{2g} (3dπ)	7.23	7.61	7.81 [c,f]	7.71
1^3A_{1g} (3dπ)	7.23	7.62	7.80 [c,f]	7.66
1^3A_{2g} (3dπ)	7.27	7.66		7.57

[a] Ref. [9]. [b] Ref. [18]. [c] Ref. [19]. [d] Ref. [20].
[e] Ref. [21]. [f] Ref. [22].

Results of similar accuracy are obtained for the triplet excited states. The triplet $\pi-\pi^*$ excitation energies with MRMP (experimental values in parentheses) are $^3B_{1u}$, 4.11 (3.95), $^3E_{1u}$, 4.81 (4.76), $^3B_{2u}$, 5.34 (5.60) and $^3E_{2g}$, 7.04 (6.83) eV. The maximum error is 0.26 eV in the case of ionic $^3B_{2u}$. We used the same orbitals optimized for the singlet excited states to compute the corresponding triplet states, which may lead to a slightly poor description for the triplet states compared to the singlet states. The imbalance of the singlet and triplet treatments may lead to incorrect ordering between $^3E_{1u}$ and $^1B_{2u}$ and between $^3E_{2g}$ and $^1E_{1u}$, which are close in energy.

The calculated Rydberg excitation energies are listed in Tables 2 and 3 with the SAC/SAC-CI results. The Rydberg excitation energies are usually calculated to reasonable accuracy even at a low level of theory if the basis set is chosen adequately. For Rydberg excitation energies, CASSCF shows the reverse trend as that in the valence excitation energies. That is, CASSCF produces too small excitation energies compared to experiment although the deviation is much smaller than that of the valence excitation energies. The addition of second-order correlation effects again remedies this and MRMP excitation energies become fairly close to experiment. The MRMP Rydberg excitation energies agree with the experimental values to within 0.18 eV. Since correlation effects in Rydberg states are similar to those in the ground state, SAC/SAC-CI also reproduced the

Rydberg excitation energies quite well with an accuracy of 0.3 eV. The difference between the singlet and triplet excitation energies for each Rydberg state is expected to be small. The present theory predicts that the triplet state is lower than the corresponding singlet state for all the Rydberg excited states studied here.

In terms of the Fermi sea determined by the reference function the first-order corrections to the wavefunction may be classified in terms of the number (0, 1 or 2) of external orbitals introduced as internal, semi-internal and external. In Table 4 we show second-order correlation energies partitioned into external, semi-internal and internal contributions for the singlet states. The differential correlation contributions with respect to the ground state are also listed in the table. The internal contribution is found to be small within 4 mE_h for all the states. The semi-internal term includes significant single excitations which arise from the failure of the reference function to satisfy the Brillouin theorem. Physically, the semi-internal contribution represents the dynamical polarization effects. The external term resembles the dynamical pair correlation of the closed-shell theory. For the Rydberg states, the second-order electron correlation has the same simple structure and is insensitive to the state. The total differential correlation effect is positive, which means that second-order correlation is smaller in the Rydberg states than in the ground state. The external correlation is dominant and the semi-internal correlation is almost one third in magnitude of the external correlation. On the other hand, the second-order correlation is state-specific for the valence excited states. The total differential correlation energies are negative, indicating that the second-order correlation energy is larger in magnitude for valence excited states compared to the ground state. However, the magnitude and origin of the correlation effects differ significantly between the covalent ($^1B_{2u}$ and $^1E_{2g}$) and ionic ($^1B_{1u}$ and $^1E_{1u}$) states. The wavefunction for the covalent states is dominated by covalent valence bond structures and the dynamical correlation is usually of the same order as that of the ground state. The total differential correlation energies are only -10 mE_h for the covalent states. However, second-order correlation effects are large in the ionic states. For instance, the differential

Table 4
Second-order correlation energy ($-E$) partitioned into external, semi-internal and internal contributions [a]

State	Total	External	Semi-internal	Internal
ground state				
1^1A_{1g}	0.71535 (0.0)	0.55592 (0.0)	0.15525 (0.0)	0.00418 (0.0)
valence states				
1^1B_{2u}	0.72621 (−10.9)	0.57883 (−22.9)	0.14283 (12.4)	0.00455 (−0.4)
1^1B_{1u}	0.78239 (−67.0)	0.59474 (−38.8)	0.18191 (−26.7)	0.00571 (−1.5)
1^1E_{1u}	0.79845 (−83.1)	0.58545 (−29.5)	0.20696 (−51.7)	0.00604 (−1.9)
1^1E_{2g}	0.72617 (−10.8)	0.58059 (−24.7)	0.14178 (13.5)	0.00379 (0.4)
Rydberg states				
1^1E_{1g} (3s)	0.70166 (13.7)	0.52560 (30.3)	0.16826 (−13.0)	0.00780 (−3.8)
1^1B_{2g} (3dσ)	0.69555 (19.8)	0.52005 (35.2)	0.16748 (−12.2)	0.00801 (−3.8)
1^1B_{1g} (3dσ)	0.70221 (13.1)	0.52075 (35.2)	0.17346 (−18.2)	0.00799 (−3.8)
2^1E_{1g} (3dδ)	0.69447 (20.7)	0.51995 (36.0)	0.16669 (−11.4)	0.00797 (−3.8)
3^1E_{1g} (3dδ)	0.69447 (20.9)	0.51982 (36.1)	0.16664 (−11.4)	0.00801 (−3.8)
1^1A_{2u} (3pσ)	0.70228 (13.1)	0.52518 (30.7)	0.16930 (−14.1)	0.00780 (−3.6)
1^1A_{1u} (3pσ)	0.70377 (11.6)	0.52523 (30.7)	0.17086 (−15.6)	0.00768 (−3.5)
1^1E_{2u} (3pσ)	0.70131 (14.0)	0.52368 (32.2)	0.16991 (−14.7)	0.00772 (−3.5)
2^1E_{1u} (3pπ)	0.70584 (9.5)	0.52853 (27.4)	0.17043 (−15.2)	0.00687 (−2.7)
2^1A_{1g} (3dπ)	0.70228 (13.7)	0.52496 (31.0)	0.17023 (−15.0)	0.00709 (−2.9)
2^1E_{2g} (3dπ)	0.70107 (14.3)	0.52426 (31.7)	0.16971 (−14.5)	0.00711 (−2.9)
1^1A_{2g} (3dπ)	0.70103 (14.3)	0.52406 (31.9)	0.16988 (−14.6)	0.00710 (−2.9)

[a] Energies are in hartree. Values in parentheses are differential second-order energies in millihartree with respect to the ground state.

correlation energy for the $^1E_{1u}$ state is -83 mE_h, which comes mainly from the semi-internal term. This indicates that dynamical polarization effects due to the reorganization of σ electrons are important for ionic states.

Single-reference truncated CI usually gives too high excitation energies since the convergence of the CI expansions is rather slow for excited states compared to the ground state. Single-reference CI works well when the correlation effects in excited states are similar to those in the ground state. However, stable accuracy is not reached with this approach in situations where the correlation effects are significantly different in the ground and excited states. SAC/SAC-CI also gives too high excitation energies for valence states. In the multireference based perturbation theory, the quasi-degeneracy effects are fully included in advance in the reference space and the remaining dynamical correlation effects and the coupling between the dynamical and nondynamical correlation are estimated by the perturbation treatment. Thus, the present approach can account for a proper balance of the correlation energy difference between the two states involved. This leads to success in the calculation of transition energies.

To conclude, the MRMP method appears to work quite well for covalent and ionic valence excited states as well as for Rydberg excited states. MRMP was able to predict the valence $\pi-\pi^*$ excitation energies and Rydberg excitation energies of benzene with an accuracy of 0.26 and 0.18 eV, respectively. The MRMP method may be one of the most promising approaches for calculating the low-lying excited states for larger systems. The reliability of the present method, however, depends on the reference functions and/or the active orbitals. Since the number of active orbitals must be limited, it may be difficult to handle many states of the same symmetry. This is the only unfavorable feature of the present approach. A more detailed test of the method will be reported in forthcoming publications.

Acknowledgement

The present research is supported in part by a Grant-in-Aid for Scientific Research on Priority Area 'Theory of Chemical Reactions' from the Ministry of Education, Science and Culture. The authors also thank the Sumitomo Foundation for partial financial support for the project. The CASSCF wavefunctions were calculated with the HONDO8 program [23].

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