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On the performance of diagrammatic complete active space perturbation theory

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Excited states of C_2, H_2O, CO, and formamide are studied to illustrate the performance and accuracy of second-order diagrammatic complete active space perturbation theory (D-CASPT2) [J. Chem. Phys. **108**, 1081 (1998)]. Comparisons are made with other *ab initio* methods and also full configuration interaction (FCI) calculations or experiment. Excitation energies computed by the D-CASPT2 method are quite accurate showing an average deviation of 0.1 eV from the FCI values for C_2 and H_2O. The CO and formamide excitation energies yield average deviations of 0.1 and 0.2 eV from experiment, respectively. The computational cost of this method is reduced to a great extent compared to the MRMP method. © *2000 American Institute of Physics.* [S0021-9606(00)31442-8]

I. INTRODUCTION

The second-order multireference Mϕller–Plesset (MRMP)[1–6] method and complete active space perturbation theory (CASPT2)[7–12] are two approaches that can compute the electronic spectra of medium-sized molecules. These approaches treat both the nondynamical and the dynamical correlation effects in a balanced way and do not suffer from near-degeneracy that can plague single-reference based methods. Hence, these methods are well suited to treat multiply-excited states and bond-breaking regions.

Although these *state-specific* methods have been quite successful, they do have some drawbacks. For example, the MRMP method has an energy expression with energy denominators that depend on the configuration state functions (CSFs) within the complete active space (CAS). This ket-dependence makes this method less efficient, since it then requires computational loops over the CSFs. The CASPT2 method avoids any ket-dependence by using a nonorthogonal, internally-contracted basis. However, this approach requires additional steps to orthogonalize a nonorthogonal basis and diagonalize the zeroth-order Hamiltonian (H_0). The effective Hamiltonian method,[13–16] H^ν, is an alternative to the *state-specific* methods that can also accurately compute electronic spectra.[17–19] Unlike the MRMP and CASPT2 methods, this *valence universal* approach is based on multireference perturbation theory[20–23] (MRPT) and possesses a linked diagrammatic expansion (LDE). However, the H^ν method is less efficient, since it requires a third-order treatment to obtain the accuracy of the second-order CASPT2 and MRMP methods and a final diagonalization step within the CAS using an effective Hamiltonian that has up to four-body terms.

The diagrammatic CASPT2 (D-CASPT2) method[24–26] is designed to have the best qualities of the H^ν , MRMP, and CASPT2 methods. As in the H^ν approach, this *hybrid* method is based on (valence universal) MRPT but with the addition of flexible energy denominators.[27] The D-CASPT2 wave-operator Ω_D is defined to be similar to the one employed in MRMP, but without the ket-dependence. It also possesses a LDE and requires no orthogonalization or diagonalization steps, even when it is computed using an internally contracted basis.[26] Calculations from D-CASPT2 are generally more efficient than those from H^ν, MRMP, and CASPT2, but are expected to be of similar accuracy. In a previous report, this was demonstrated by applications on N_2, benzene and LiF.[25]

Our purpose in this paper is to investigate the applicability and accuracy of the D-CASPT2 method for chemical problems. Specifically, we use the D-CASPT2 approach to compute the electronic spectra of C_2, H_2O, CO, and formamide. The C_2 is selected for study, since this system is a representative molecule that shows the significance of nondynamical correlation contributions: Its lowest-lying σ^* orbital—that is just above the HOMO π orbitals—yields a large amount of nondynamical, electron correlation. Also, this system has states dominated by doubly excited configurations that appear in the low-lying spectrum. Currently, only a few existing methods can describe both the singly- and doubly-excited low-lying states of C_2 with satisfactory accuracy.

The H_2O is selected because it is probably the most extensively studied molecule in *ab initio* quantum chemistry. Therefore, many benchmark calculations are available including calculations up to the FCI level.[28,29] The third system we considered is CO. In general, the correlation effect for multiply bonded system, including CO, is usually quite large, making them a challenge for any *ab initio* methods. Finally, formamide is examined in order to apply the D-CASPT2 method to a more chemically interesting system. This system is a model for proteins that possess an amide group. The amide is probably one of the most important functional groups in chemistry, since understanding the chemical property around the amide-linkage is indispensable for a compre-

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[a)] Author to whom correspondence should be addressed. Electronic mail: hirao@qcl.t.u-tokyo.ac.jp hension of protein structure and important biological process.

In Sec. II, the D-CASPT2 formalism is presented. The results and discussions are given in Sec. III. Comparisons are made with MRMP and, when available, other theoretical methods and/or the FCI results. In Sec. III we also compare the efficiency of D-CASPT2 with MRMP.

II. D-CASPT2 THEORY

D-CASPT2 is based on MRPT[20–23] with flexible energy denominators.[27] This formalism permits one-body shifts Δ_w^r to be introduced into the one-body, energy denominator factors $(\epsilon_w - \epsilon_r)$, two-body shifts Δ_{wx}^{rs} into the two-body, energy-denominator factors $(\epsilon_w + \epsilon_x - \epsilon_r - \epsilon_s)$, and so on, where some restrictions are imposed on wave-operator diagrams with disconnected products, so that the linked diagram expansion (LDE) is preserved. These shifts result in additional (diagonal) diagrams that first appears in third order from an additional perturbation. Nevertheless, energy denominator shifts—if chosen properly–can enhance convergence. For D-CASPT2, they are chosen so that the first-order wave function and second-order energy is similar to MRMP. However, other choices are possible.[30]

The first-order wave operator $\Omega^{(1)}$ for MRPT, which is needed for a second-order treatment, can be obtained by solving the first-order, generalized, Bloch equation,[23]

$$Q[\Omega^{(1)}, H_0]P = QVP, \tag{2.1}$$

where P is the projection operator for the model space, which is chosen to be a CAS, and Q is the space orthogonal to P,

$$P = \sum_p |p\rangle\langle p|, \tag{2.2}$$

$$Q = 1 - P. \tag{2.3}$$

The sum over p in Eq. (2.2) includes all determinantal states from the CAS. The second-order energies for MRPT are computed by diagonalizing the effective Hamiltonian H_{eff} within the reference space. Through the second order, it is given by

$$H_{\text{eff}} = PHP + PH\Omega^{(1)}P, \tag{2.4}$$

where the diagonalization of the first term, *PHP*, gives the CASSCF energies if CASSCF orbitals are used. If the CASSCF state of interest, $|\alpha\rangle$, is well separated from the other CASSCF states, then H_{eff} is approximately diagonal,

$$H_{\text{eff}} \approx PHP + |\alpha\rangle\langle\alpha|H\Omega_D^{(1)}|\alpha\rangle\langle\alpha| + K^{(\alpha)}H\Omega_{\text{D}}^{(1)}K^{(\alpha)}, \tag{2.5}$$

where $K^{(\alpha)}$ is spanned by the CASSCF states orthogonal to $|\alpha\rangle$. Using this approximation, the second-order energy for the state of interest in D-CASPT2 can be obtained, in an identical manner as in MRMP or CASPT2,

$$E^{(2)} = \langle\alpha|H|\alpha\rangle + \langle\alpha|H|\Psi^{(1)}\rangle, \tag{2.6}$$

where the first-order wave function is given by

$$|\Psi_D^{(1)}\rangle = \Omega_D^{(1)}|\alpha\rangle. \tag{2.7}$$

In contrast to D-CASPT2, the first-order wave operator for MRMP, denoted by $\Omega_{\text{MP}}^{(1)}$, is ket-dependent and given by

$$\Omega_{\text{MP}}^{(1)} = \sum_p \Omega_{\text{MP}}^{(p)}|p\rangle\langle p|, \tag{2.8}$$

where we permit it to act within the CAS. Its first-order wave function $|\Psi_{\text{MP}}^{(1)}\rangle$, however, is obtained in an identical manner as in the D-CASPT2:

$$|\Psi_{\text{MP}}^{(1)}\rangle = \Omega_{\text{MP}}^{(1)}|\alpha\rangle. \tag{2.9}$$

The *p*th component of the wave operator for MRMP is given by[31]

$$\Omega_{\text{MP}}^{(p)} = \sum_{wr} \frac{(r|h^0|w)}{\epsilon_w^r + \Delta_p}\hat{E}_{rw} + \frac{1}{2}\sum_{rswx}\frac{(rw|sx)}{\epsilon_{wx}^{rs} + \Delta_p}\hat{E}_{rwsx}, \tag{2.10}$$

where

$$\hat{E}_{rw} = \sum_\sigma a_{r\sigma}^+ a_{w\sigma}, \tag{2.11}$$

$$\hat{E}_{rwsx} = \sum_\sigma \sum_{\sigma'} a_{r\sigma}^+ a_{s\sigma'}^+ a_{x\sigma'} a_{w\sigma}, \tag{2.12}$$

w and x denote inactive and active orbitals, r, s denote active and secondary orbitals and σ denotes a spin. In Eq. (2.10), the summation indices are restricted so that all indices are not simultaneously active. (No internal excitations are permitted.) The terms in the denominator and numerator in Eq. (2.10) are defined as follows:

$$\epsilon_w^r = \epsilon_w - \epsilon_r, \tag{2.13}$$

$$\epsilon_{wx}^{rs} = \epsilon_w + \epsilon_x - \epsilon_r - \epsilon_s, \tag{2.14}$$

$$(i|h^0|j) = (i|h|j) + \sum_a [2(ij|aa) - (ia|aj)], \tag{2.15}$$

where $(ij|kl)$ are two-electron integrals written in chemist notations.[32] Furthermore, the orbital energies ϵ_i are eigenvalues of a diagonal, one-body, zeroth-order Hamiltonian which is given by

$$H_0 = \sum_{ab} f_{ab}\hat{E}_{ab} + \sum_{uv} f_{uv}\hat{E}_{uv} + \sum_{ef} f_{ef}\hat{E}_{ef}, \tag{2.16}$$

where a, b denotes inactive; u, v active; and e, f secondary orbitals. The matrix elements f_{ij} are given by

$$f_{ij} = (i|h|j) + \frac{1}{2}\sum_{ww'} D_{ww'}[2(ij|ww') - (iw'|wj)], \tag{2.17}$$

where $D_{ww'}$ is the one-particle density matrix with respect to the CASSCF state of interest $|\alpha\rangle$,

$$D_{ww'} = \langle\alpha|\hat{E}_{ww'}|\alpha\rangle. \tag{2.18}$$

MRMP uses orbitals that diagonalize f_{ij} within the inactive, active, and secondary subspaces resulting in H_0, given by Eq. (2.16), to be diagonal, where the orbitals energies are then given by $\epsilon_i = f_{ij}\delta_{ij}$.

The ket-dependent shifts Δ_p are given by

$$\Delta_p = E_\alpha^0 - E_p^0, \tag{2.19}$$

TABLE I. (a) Excitation energies (eV) for C_2. (b) Ground state total energies (eV) for C_2.

(a)

State	FCI[a]	D-CASPT2	MRMP	CC3[a]
$^1\Pi_u$	1.385	1.49	1.48	1.316
$^1\Delta_g$	2.293	2.47	2.47	3.152
$^1\Sigma_u^+$	5.602	5.64	5.59	5.555
$^1\Pi_g$	4.494	4.56	4.52	4.990
	Average deviation	0.097	0.076	0.37

(b)

	FCI[a]	D-CASPT2	MRMP	CC3[a]
Ground state	−75.730 209	−75.720 375	−75.721 547	−75.728 669

[a] Reference 35.

where the zeroth-order energies are

$$E_i^0=\langle i|H_0|i\rangle, \quad i=\alpha,p. \tag{2.20}$$

Note that the second-order energy expression given by Eq. (2.6) has a ket-dependence in the denominators since $\Omega_{\mathrm{MP}}^{(1)}$, given by Eq. (2.10), is ket-dependent.

For D-CASPT2, the first-order wave operator, denoted by $\Omega_D^{(1)}$, is given by

$$\Omega_D^{(1)}=\sum_{wr}\frac{(r|h^0|w)}{\epsilon_w^r+\Delta_x^r}\hat{E}_{rw}+\frac{1}{2}\sum_{rswx}\frac{(rw|sx)}{\epsilon_{wx}^{rs}+\Delta_{wx}^{rs}}\hat{E}_{rwsx}, \tag{2.21}$$

where its zeroth-order Hamiltonian is given by Eq. (2.16), as in MRMP. It is seen in Eq. (2.21) that the ket-dependent shifts Δ_p in MRMP are replaced by one- and two-body shifts, Δ_w^r and Δ_{wx}^{rs}, in D-CASPT2. These shifts are defined in a manner so that the wave operator for D-CASPT2 is similar to the one for MRMP. One significant aspect of D-CASPT2 is that, by introducing a ket-independent shift, the D-CASPT2 method avoids the calculation of the loop over determinants or CSFs, which usually leads to a more efficient computation of the second-order energy compared to MRMP, since the number of CSFs or determinants is frequently large.

One- and two-body shifts that appear in Eq. (2.21) are arbitrary[27] but are chosen so that the difference between Ω_D and Ω_{MP} is as small as possible. A reasonable choice is a weighted average of the shifts Δ_p. Explicitly, the one-body shifts, for P space states that can have $w \rightarrow r$ excitations, are given by

$$\Delta_w^r=\frac{1}{N_w^r}\sum_p \eta_w^{(p)}(2-\eta_r^{(p)})\Delta_p|C_p|^2, \tag{2.22}$$

where

$$N_w^r=\sum_p \eta_w^{(p)}(2-\eta_r^{(p)})|C_p|^2, \tag{2.23}$$

$\eta_i^{(p)}$ is the occupation—0,1 or 2—of the ith orbital in $|p\rangle$, and C_p is the CI coefficient of $|p\rangle$ in the CASSCF state of interest;

$$|\alpha\rangle=\sum_p C_p|p\rangle. \tag{2.24}$$

The two-body shift corresponds to single excitations whenever either w or x is an active orbital, say m, and either r or s is the same active orbital. These excitations are defined by

$$\Delta_{mw}^{mr}=\Delta_{mw}^{rm}=\Delta_{wm}^{mr}=\Delta_{wm}^{rm}=\Delta_w^r. \tag{2.25}$$

Similarly, the remaining two-body shift, corresponding to double excitations, are given by

$$\Delta_{wx}^{rs}=\frac{1}{N_{wx}^{rs}}\sum_p \eta_w^{(p)}\eta_x^{(p)}(2-\eta_r^{(p)})(2-\eta_s^{(p)})\Delta_p|C_p|^2, \tag{2.26}$$

$$N_{wx}^{rs}=\sum_p \eta_w^{(p)}\eta_x^{(p)}(2-\eta_r^{(p)})(2-\eta_s^{(p)})|C_p|^2. \tag{2.27}$$

III. RESULTS AND DISCUSSIONS

A. Excitation energies of C_2

Calculations are carried out using the D-CASPT2 and MRMP methods for the ground and single-excited states of C_2. Dunning's aug-cc-pVDZ basis set[33,34] with only an s diffuse function is used in order to make a direct comparison with the FCI results of Christiansen and co-workers.[35] The internuclear distance is fixed to 2.348 bohr. The 1s orbitals of carbon are kept frozen during the CASSCF computations and not correlated in the D-CASPT2 and MRMP computations. To obtain the second-order energy by perturbation theory, we compute the CASSCF reference wave functions for each state of interest. For the CASSCF calculations, eight active electrons that come from 2s and 2p orbitals of carbon are distributed among the eight active orbitals. Perturbation calculations are then made with D-CASPT2 and MRMP for each state. All the CASSCF[36,37] calculations reported in this paper are performed by the MOLPRO[38] suite program package. The MR2D[39,40] code and its modified version for D-CASPT2 are used for the perturbative calculations.

One characteristic feature of this molecule is that the ground state of C_2 has a large nondynamical correlation con-

TABLE II. (a) Excitation energies (eV) for H_2O. (b) Ground state total energies (eV) for H_2O.

(a)

State	FCI[a]	D-CASPT2	MRMP	CC3[a]
2 $^1A_1$	9.874	9.84	9.80	9.858
1 $^1B_1$	7.447	7.38	7.42	7.427
1 $^1B_2$	11.612	11.62	11.60	11.591
1 $^1A_2$	9.2111	9.20	9.21	9.187
	Average deviation	0.030	0.029	0.020

(b)

	FCI[a]	D-CASPT2	MRMP	CC3[a]
Ground state	−76.258 208	−76.246 879	−76.247 155	−76.257 757

[a] Reference 35.

TABLE III. Excitation energies (eV) for CO.

State	Expt.[a]	D-CASPT2	MRMP	MRCI[b]	STEOM-CC[a]
$^1\Pi$	8.51	8.52	8.56	8.65	8.59
$^1\Sigma^-$	9.88	9.99	9.90	10.16	10.06
$^1\Delta$	10.23	10.20	9.92	10.28	10.21
$^3\Pi$	6.32	6.07	5.88	6.36	6.55
$^3\Sigma^+$	8.54	8.33	8.22	8.53	8.43
$^3\Delta$	9.36	9.28	9.23	9.43	9.33
$^3\Sigma^-$	9.88	9.67	9.62	9.95	9.96
	Average deviation	0.12	0.21	0.09	0.10

[a] Reference 44.

[b] The Davidson correction is included.

tribution. Table I(a) shows D-CASPT2 and MRMP results compared with the FCI values of Christiansen and co-workers.[35] The total ground state energies are listed in Table I(b). The energy difference for the ground state of D-CASPT2 and MRMP is very small. D-CASPT2 gives very similar accuracy compared with MRMP, differing, on average, by only 0.025 eV for the excited states considered. In comparison to the FCI results, the average deviations for D-CASPT2 and MRMP are less than 0.1eV. CC3 calculations made by Christiansen and co-workers are significantly less accurate with a 0.37 eV average deviation from the FCI values. Not surprisingly, the $^1\Delta_g$ and $^1\Pi_g$ states are not properly described within the coupled-cluster linear response framework, since two of the states are dominated by doubly excited configurations.[35] In contrast, both D-CASPT2 and MRMP can treat these states.

B. Excitation energies of H_2O

Calculations are performed on excitation energies of H_2O and compared to the FCI results of Christiansen and co-workers.[35] The same geometry and basis sets are employed for H_2O as used in the FCI benchmark calculations. The eight active electrons are distributed among the eight active orbitals for the CASSCF calculations. The 1*s* canonical Hartree–Fock orbitals are frozen.

Table II(a) gives the results of D-CASPT2 and MRMP for the low-lying excited states of H_2O. Also, the total ground state energies are given in Table II(b). It is seen that both D-CASPT2 and MRMP are of almost the same accuracy for both ground and excited states. The average deviation from the FCI values for D-CASPT2 is again quite small, being only 0.03 eV. CC3 calculations by Christiansen and co-workers also show very good agreement with the FCI for all the states considered. This is anticipated, since none of these states have a doubly excited state character.

C. Valence excitation energies of CO

Valence excitation energies of CO are computed. We employ a Sadlej's pVTZ basis set.[41] Ten electrons distributed among eight active orbitals define the active space for the CASSCF calculations. They constitute the two σ, two σ^*, two π, and two π^* orbitals. The lowest two σ orbitals are canonical Hartree–Fock orbitals and are frozen. The internuclear distance is 1.1282 Å . Internally contracted multireference configuration interaction (MRCI) calculations[42,43] are also preformed with the same active space employed in the D-CASPT2 and MRMP calculations.

Valence excited energies of CO are listed in Table III. The average deviation of D-CASPT2 from the experiment is 0.12 eV. The overall accuracy of D-CASPT2 for this system is again good, which is similar to the accuracy obtained by MRCI and STEOM-CC.[44] In this system, D-CASPT2 and MRMP give slightly different results for some states. For example, the difference of D-CASPT2 and MRMP for the $^1\Delta$ state is about 0.3 eV. Such a significant difference between these methods has also been reported in the previous application on N_2.[25] Furthermore, the excitation energy for the $^3\Pi$ state by MRMP is rather poor, deviating 0.44 eV from the experimental value. This poor MRMP result may be caused by an intruder state that is also known to cause difficulties for CASPT2 in some systems.[45] Recently, we have coded the program to identify intruder states and developed a new approach to treat this problem.[46] The intruder state problem is discussed in the following subsection.

D. Valence excited states of formamide

The low-lying valence absorption spectra of formamide are computed. The geometrical parameters are optimized using cc-pVQZ[33] basis sets at the CCSD(T) level of theory using Gaussian 98[47] within the C_s symmetry. We use aug-cc-pVDZ quality basis sets for C, N, O and cc-pVDZ for H.[33] The two σ and four π orbitals are active: six electrons are distributed among the six active orbitals. The MRMP and D-CASPT2 calculations are carried out for the low-lying valence excited states.

Though formamide is the simplest amide, an exact assignment of its excited states is not trivial, since there are many Rydberg states. Nevertheless, a reliable assignment has been made by Serrano-Andrés and Fülscher[48] using the CASPT2 method. The calculated energies for the valence-excited states are seen in Table IV along with the CASPT2 results.[48] The D-CASPT2 method produces reliable results for all the states in comparison with available experimental observations,[49–53] deviating 0.14 eV from the experimental values. The CASPT2 method is slightly more accurate than D-CASPT2 for this system.

TABLE IV. Valence excitation energies (eV) for formamide.

State character	Expt.[b]	D-CASPT2	MRMP	CASPT2[b]
$1\,^1A''(n\rightarrow\pi^*)$	5.5	5.79	5.59	5.61
$2\,^1A'(\pi\rightarrow\pi^*)$	7.4	7.34	6.50	7.41
$1\,^3A''(n\rightarrow\pi^*)$	5.30	5.49	5.22	5.34
	Average deviation	0.14	0.39	0.05

[a] References 49–53.

[b] Reference 48. A value of 0.3 a.u. has been used for the level shift in all the computed states.

The MRMP results shows that the $2\,^1A'$ state is unsatisfactory with a large deviation of 0.9 eV from the experimental value. As in the $^3\Pi$ state of CO, this large deviation from experiment may be caused by an intruder state.[46] Intruder states may appear when an orthogonal, zeroth-order state—an intruder state—is quasidegenerate in zeroth order with the CASSCF reference state, producing a small energy-denominator factor.[45] As discussed in the Sec. II, since D-CASPT2 is a ket-independent formalism, there are less energy denominators in D-CASPT2 than MRMP. Hence, the probability of encountering a small energy denominator is reduced. This may be the reason that our D-CASPT2 calculations in this report show better results, compared to MRMP, for the $^3\Pi$ state of CO and the $2\,^1A'$ state of formamide. The CASPT2 method has the same number of energy denominators as D-CASPT2. Following the above statistical reasoning, the probability of encountering a small energy denominator for CASPT2 may, therefore, be less than MRMP and similar to D-CASPT2. Intruder states can also appear for this method,[45] and can be treated by a level-shift technique.[9] A similar approach should be useful when D-CASPT2 encounters the same problem. Since CASPT2 uses an internally contracted basis, any orthogonal state responsible for a small energy denominator—an intruder state—is a multiconfigurational state. In contrast, a D-CASPT2 intruder state, like MRMP, is a single CSF outside the CAS. Because of this difference, it should be easier to identify and treat an intruder state for MRMP and D-CASPT2 than for CASPT2 *before* doing a perturbative calculation. Future work will focus on analyzing the intruder state problem for MRMP and D-CASPT2.[46]

E. Computational costs

From a mathematical point of view, it is quite apparent that the D-CASPT2 method is more efficient than MRMP since, for D-CASPT2, it is not necessary to compute the loops over the CSFs. We have modified the existing MR2D program[54] to perform D-CASPT2 calculations. Since we can use same routines for MRMP and D-CASPT2, a direct comparison between the D-CASPT2 and MRMP is possible. The above tested systems are relatively small for comparing computational times. Therefore, in this section, we employ a larger system. Table V shows a comparison of CPU times for both methods using the thiophene molecule. The total number of basis functions is 149 and the number of active orbitals is 7. Due to technical reasons, the three-body terms have not yet been optimized, so we only compare the zero-, one-, and two-body terms. As expected, the D-CASPT2 method shows a better efficiency, especially, for the costly two-body terms. Although, the D-CASPT2 calculations also require a routine to calculate the denominator shifts defined in Eqs. (2.22) and (2.26), these calculations are very trivial since they only depend on, at most, three active indices. Since D-CASPT2 does not require a loop over CSFs, it is expected to be even more efficient in cases where the CAS is very large.

TABLE V. A comparison of CPU time (s) for thiophene.

	D-CASPT2	MRMP
0-body term	0.20	1.430
1-body term	0.50	1.390
2-body term	0.40	3.480

IV. CONCLUSION

In this report, we apply the D-CASPT2 method to C_2, H_2O, CO, and formamide. The electronic spectra computed by D-CASPT2 are in good agreement with available FCI data or experiments. The D-CASPT2 method is demonstrated to be more efficient than MRMP. Furthermore, unlike MRMP, the systems tested by D-CASPT2 are not deteriorated by intruder states.

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