

**Renormalized Triple Correction for Equation of Motion Coupled Cluster for Selected Transition Metal Compounds**

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**Summary**

Considering the calculations of molecules in GAMESS(US), in addition to the calculation of CCSD ground-state and EOM-CCSD excited-state energies, CR-EOMCCSD(T) and CR-EOMCC(2,3) (or CR-EOMCCSD(T)\_L ) methods are performed to obtain the non-iterative triple correction to CCSD and EOM-CCSD energies. DELTA-CR-EOMCCSD(T) and DELTA-CR-EOMCC(2,3) (or DELTA-CR-EOMCC(2,3)) approaches are used to calculate the vertical excitation energies.

In this project, investigations are pursued based on four transition metal compounds: Fe(CO)5, Ni(CO)4, CpNiNO, Cr(CO)6.

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1. **Introduction**

The calculation and exploration of excitation energies of transition metal complexes has been studied by using the multireference equation of motion coupled-cluster (MR-EOMCC) approach1-2, Brueckner based similarity transformed equation of motion (STEOM) approach3-5 and Brueckner based equation of motion coupled cluster (EOM-CCSD(T)6-9 .

In this work, we will employ the implementation of CR-EOMCCSD(T), CR-EOMCC(2,3), DELTA-CR-EOMCCSD(T) and DELTA-CR-EOMCC(2,3)10-13 in the GAMESS(US) package to calculate the excitation energies of transition mental complexes and also a small molecule ethylene.

The selected four transition metal compounds are Fe(CO)5, Ni(CO)4, CpNiNO, Cr(CO)6. Other computational approaches have been used to study these systems, the excitation energies of CR-EOMCCSD(T), CR-EOMCC(2,3), DELTA-CR-EOMCCSD(T) and DELTA-CR-EOMCC(2,3) approaches are printed in this work and will be compared with the previous studies results.

In Section 2, we will briefly view the four approaches that used in GAMESS(US) package. In Section 3, the computation strategy in GAMESS(US) is discussed. In Section 4, some variants of CR-EOMCCSD(T), CR-EOMCC(2,3), DELTA-CR-EOMCCSD(T) and DELTA-CR-EOMCC(2,3) are briefly described. In Section 5, the excitation energies of four approaches are printed and compared with MREOM in ACES(II) and ORCA , Brueckner based equation of motion coupled cluster (EOM-CCSD(T) and EOMCCSD in ACES(II). In Section 6, some concluding remarks are discussed.

1. **Background Theory**
2. Coupled-Cluster Theory14

The ground state wave function in CC theory is written as an exponential ansatz.

where is the cluster operator and is the Hartree-Fock ground state.

(2)

The exponential ansatz is essential because it can guarantee the size extensity.

The cluster operator is represented as

(3)

is the operator of all single excitations, and is defined as the operator of all double excitations, etc.

More generally, the n-orbital cluster operator can be witten as

where refer to occupied orbitals, while refer to virtual orbitals.

The nonrelativistic time-independent equation in CC theory can be written as

If we act with the excited state determinant ( and the ground state determinant on the left side of Eq.(37) respectively, the energy and t-amplitude can be obtained.

1. Equation of Motion Coupled Cluster Theory10

The equation of motion coupled cluster (EOMCC) method provides a useful extension of the ground-state CC theory to excited states.

The excited state wave function can be given as

whereis the excitation operator

The nonrelativistic time-independent equation in EOMCC theory can be written as

Two excitation operators and should commute. Eq. (16) can also be denoted as

The similarity transformed Hamiltonian can be denoted as

and have same eigenvalues but different eigenvectors.

The similarity transformed Hamiltonian is not hermitian, and is combined with two eigenvectors. So that, in addition to the right-side eigenstates , we can define the left-side eigenstates as .

whereis the excitation operator

In practice, one diagonalizes the CC similarity transformed Hamiltonian in the space of excited determinants included both excitation operators and to perform the standard EOMCC calculations.

If one considers the mapping over the ground-state, singly, doubly, triply excited determinants, the results can be represented as

X refers to large matrix elements and ~ represents small matrix elements due to three-particle operator in the similarity transformed Hamiltonian.15

1. CR-EOMCCSD(T) Approach10-13

The CR-EOMCCSD(T) approach is a single-reference method, which enables us to correct the ground-state CCSD and excited-state EOMCCSD energies based on non-iterative energy corrections due to triples.

The excited state wavefunction is written as234:

where , are the reference, singly excited, doubly excited components of the excitation operator. represents the approximate form of the triple excitation operator calculated by

are the triple excitation amplitudes, and can be given by

define the generalized moments of the EOMCCSD equations corresponding to projections on the triple excited determinants

represents the perturbative denominators for triple excitations.

we introduce two variants or the CR-EOMCCSD(T) theory, labeled as A and D. D refers to full treatment through the diagonal matrix elements of the triples-triples block of the CCSD similarity transformed Hamiltonian.

A means the roughest treatment based on bare orbital energies.4

For the D treatment, is expressed as

is the n-body component of the CCSD/EOMCCSD similarity transformed Hamiltonian , and is the EOMCCSD vertical excitation energy obtained through the diagonalization of the in the space of single and double excited determinants, and respectively.

For the A treatment, is expressed as

represents the Hartree-Fock spin-orbital energies.

The calculation of the CR-EOMCCSD(T) energies can be obtained by

1. CR-EOMCCSD(2,3) Approach 10-13

The key to this method is the use of the left eigenstates of the similarity transformed Hamiltonian.

We assume the exact operator can be given by

and it satisfies that

refers to the left eigenstateof the similarity transformed Hamiltonian represents the approximate form of the triple deexcitation operator calculated as

are the triple deexcitation amplitudes, and can be given by

defined by Eq. (27).

The correction energy is defined as

The final CR-EOMCCSD(2,3) energy is expressed as

1. DELTA-CR-EOMCCSD(T) and DELTA-CR-EOMCCSD(2,3) Approaches

These two methods calculate the vertical excitation energies by subtracting the CCSD ground-state energy from the excited-state CR-EOMCCSD(T)/CR-EOMCCSD(2,3) energy rather than correct the total CCSD/EOMCCSD energies by triple corrections.

1. **Computational Strategy**

In this project, the software program is GAMESS(US). Basis sets must be individually specified for each atom. For metals (Cr, Fe, Ni), the basis set is Wachters + F. CC-PVDZ basis set is used for carbon, oxygen, nitrogen and hydrogen atom.

GAMESS(US) is very strict about specifying the symmetry of the molecule, compared to other programs such as ORCA which does not require the symmetry. The point group of the molecule can only be Abelian (C1, Ci, Cs, C2, C2v, C2h, D2, or D2h).

The determined symmetries for Ni(CO)4, Fe(CO)5, CpNiNO, Cr(CO)6 are C2v, C2v, Cs, D2h respectively.

When the symmetry of the molecule is determined, only unique atoms are specified in the input.

The coordinates for those unique atoms are also need to be determined.

The standard orientation rule is that the principal rotation axis must lie along the z-axis; the axis must lie along the xz axis; the axis must lie along the xz axis.

1. **Methods**

Four approaches, labelled as CR-EOMCC(2,3) (or CR-EOMCCSD(T)\_L ), CR-EOMCCSD(T), DELTA--CR-EOMCCSD(T) and DELTA-CR-EOMCC(2,3) (or delta-CR-EOMCCSD(T)\_L ), are to be considered in GAMESS(US) when performing the non-iterative triples corrections to CCSD ground-state and EOM-CCSD excited-state energies.

The CR-EOMCCSD(T)2 method adds the state-selective non-iterative triple corrections to the ground-state and excited-state energies. GAMESS(US) also contains some different variants of the CR-EOMCCSD(T) method, labeled as CR-EOMCCSD(T), IX and CR-EOMCCSD(T), IIX approaches (X=A, B, C, D). Type I and II represent two different approximate wave functions that are used to obtain the CR-EOMCCSD(T) triple corrections to EOM-CCSD energies. Letters A-D indicate different treatments of perturbative denominators in calculating the triple corrections. D refers to full treatment through the diagonal matrix elements of the triples-triples block of the CCSD similarity transformed Hamiltonian.2 A means the roughest treatment based on bare orbital energies.

Mixed approximations such as CR-EOMCCD(T), ID/IA can also be printed in GAMESS(US). The ID/IA refers to the excitation energy obtaining by subtracting the CR-EOMCCSD(T), IA ground-state energy from the CR-EOMCCSD(T), ID excited-state energy. Other approximations (IID/IA, IID/IB, etc.) can also be obtained analogously.

The DELTA-CR-EOMCCSD(T) method calculates the vertical excitation energies obtained by directly correcting the EOMCCSD excitation energies rather than the total CCSD/EOMCCSD energies by triple corrections. Mixed approximations (IIA, IB, etc.) are also considered in this method. For instance, the del(IA) means that the vertical excitation energy is obtained by subtracting the CCSD ground-state energy from the excited-state CR-EOMCCSD(T), IA energy.

The CR-EOMCCSD(2,3) approach employs both left-side eigenstates and right-sight eigenstate when performing the triple corrections. Different variants of this method are denoted as CR-EOMCCSD(2,3), X (X=A, B, C, D).

The DELTA-CR-EOMCCSD(2,3) approach calculate the vertical excitation energy directly by subtracting the CCSD ground-state energy from the excited-state CR-EOMCCSD(2,3), X (X=A, B, C, D) energy.

The D variants use a better treatment of perturbative deominators in evaluating the triple corrections, so that, in this project, we print CR-EOMCCSD ID/IA , DELTA-CR-EOMCCSD DEL(ID), CR-EOMCCSD(2,3), D and DELTA-CR-EOMCCSD(2,3), D calculations for these four molecules.

1. **Results**

We use Brueckner EOM-CCSD(T) as the reference method when we explore the error bars for various approaches.

*Figure 1. Comparison of Ni(CO)4 Excitation Energies to Benchmark Values*

*Figure 2. Comparison of Fe(CO)5 Excitation Energies to Benchmark Values*

*Figure 3. Comparison of Cr(CO)6 Excitation Energies to Benchmark Values*

*Figure 4. Comparison of CpNiNO Excitation Energies to Benchmark Values*

*Figure 5. Comparison of Ni(CO)4 Excitation Energies in GAMESS(US)*

*Figure 6. Comparison of Fe(CO)5 Excitation Energies in GAMESS(US)*

*Figure 7. Comparison of Cr(CO)6 Excitation Energies in GAMESS(US)*

*Figure 8. Comparison of CpNiNO Excitation Energies in GAMESS(US)*

We use Brueckner EOM-CCSD(T) as the reference approaches when we explore the energy difference for different states for various approaches.

*Table 1. Energy Differences between Benchmark Values and EOM-CCSD in GAMESS(US) for Ni(CO)4*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| State | EOM-CCSD(no rel.) (ACESII) | MREOM T|SXD (ACESSII) | MREOMTT†|  SXD-h-v (ORCA) | EOM-CCSD  (GAMESS-US) |
| 1T1 | 0.09 | 0.24 | 0.15 | 0.091 |
| 1E | 0.15 | 0.35 | 0.25 | 0.152 |
| 1T2 | 0.15 | N/A | N/A | 0.151 |
| 1T1 | 0.23 | 0.41 | 0.43 | 0.229 |

*Table 2. Energy Differences between Benchmark Values and EOM-CCSD in GAMESS(US) for Fe(CO)5*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| State | EOM-CCSD(no rel.) (ACESII) | MREOM T|SXD (ACESSII) | MREOMTT†|  SXD-h-v (ORCA) | EOM-CCSD  (GAMESS-US) |
| 1A1" | 0.13 | 0.01 | 0.12 | 0.127 |
| 1E" | 0.13 | 0.13 | 0.01 | 0.129 |
| 1A2" | 0.01 | 0.03 | 0.21 | 0.011 |
| 1A' | N/A | N/A | N/A | N/A |
| 1E' | 0.04 | 0.35 | 0.59 | 0.041 |

*Table 3. Energy Differences between Benchmark Values and EOM-CCSD in GAMESS(US) for Cr(CO)6*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| State | EOM-CCSD(no rel.) (ACESII) | MREOM T|SXD (ACESSII) | MREOMTT†|  SXD-h-v (ORCA) | EOM-CCSD  (GAMESS-US) |
| 1A2u | N/A | N/A | N/A | N/A |
| 1Eu | 0.14 | 0.86 | 0.03 | 0.14 |
| 1T2u | 0.16 | 0.88 | 0.02 | 0.157 |
| 1T1u | 0.16 | 0.99 | 0.01 | 0.164 |

*Table 4. Energy Differences between Benchmark Values and EOM-CCSD in GAMESS(US) for CpNiNO*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| State | EOM-CCSD(no rel.) (ACESII) | MREOM T|SXD (ACESSII) | MREOMTT†|  SXD-h-v (ORCA) | EOM-CCSD  (GAMESS-US) |
| 1E1 | 0.24 | 0.14 | 0.01 | 0.241 |
| 1E2 | 0.35 | 0.13 | 0.04 | 0.345 |
| 1A2 | 0.03 | 0.22 | 0.33 | 0.027 |
| 1E1 | 0.14 | 0.31 | 0.43 | 0.139 |

*Table 5. Energy Differences between Benchmark Values and Corrections for Ni(CO)4 in GAMESS(US)*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| State | CR-EOMCCSD(T) | Δ-CR-EOMCCSD(T) | CR-EOMCC(2,3) | Δ-CR-EOMCC(2,3) | EOMCCSD |
| 1T1 | 1.291 | 0.018 | 2.486 | 0.738 | 0.091 |
| 1E | 1.362 | 0.053 | 2.538 | 0.686 | 0.152 |
| 1T2 | 1.347 | 0.038 | 2.494 | 0.731 | 0.151 |
| 1T1 | 1.592 | 0.283 | 2.622 | 0.603 | 0.229 |

Table 6. *Energy Differences between Benchmark Values and Corrections for Fe(CO)5 in GAMESS(US)*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| State | CR-EOMCCSD(T) | Δ-CR-EOMCCSD(T) | CR-EOMCC(2,3) | Δ-CR-EOMCC(2,3) | EOMCCSD |
| 1A1" | 0.705 | 0.58 | 2.177 | 1.185 | 0.127 |
| 1E" | 0.773 | 0.512 | 2.256 | 1.106 | 0.129 |
| 1A2" | 0.735 | 0.549 | 2.097 | 1.265 | 0.011 |
| 1A' | N/A | N/A | N/A | N/A | N/A |
| 1E' | 0.755 | 0.53 | 2.143 | 1.219 | 0.041 |

Table 7. *Energy Differences between Benchmark Values and Corrections for Cr(CO)6 in GAMESS(US)*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| State | CR-EOMCCSD(T) | Δ-CR-EOMCCSD(T) | CR-EOMCC(2,3) | Δ-CR-EOMCC(2,3) | EOMCCSD |
| 1A2u | N/A | N/A | N/A | N/A | N/A |
| 1Eu | 1.044 | 0.388 | 2.739 | 0.974 | 0.140 |
| 1T2u | 1.059 | 0.373 | 2.748 | 0.965 | 0.157 |
| 1T1u | 1.040 | 0.392 | 2.693 | 1.020 | 0.164 |

Table 8. *Energy Differences between Benchmark Values and Corrections for cpNiNOin GAMESS(US)*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| State | CR-EOMCCSD(T) | Δ-CR-EOMCCSD(T) | CR-EOMCC(2,3) | Δ-CR-EOMCC(2,3) | EOMCCSD |
| 1E1 | 1.203 | 0.17 | 2.285 | 0.818 | 0.241 |
| 1E2 | 1.318 | 0.055 | 2.349 | 0.753 | 0.345 |
| 1A2 | 0.616 | 0.757 | 1.704 | 1.399 | 0.027 |
| 1E1 | 0.72 | 0.659 | 1.769 | 1.311 | 0.139 |
| 1E2 | 1.344 | 0.029 | 2.313 | 0.789 | 0.399 |

*Table 9. Sample Calculation Output for Large Molecules (Ni(CO)4)*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| STATE | EOMCCSD | (2,3),D | (2,3),A | (2,3),B | (2,3),C |
| A2 | 4.821 | 7.216 | 7.341 | 6.939 | 7.225 |
| A1 | 4.852 | 7.238 | 7.367 | 6.967 | 7.247 |
| A1 | 5.161 | 7.504 | 7.633 | 7.240 | 7.513 |
| A2 | 5.202 | 7.574 | 7.712 | 7.312 | 7.583 |
| A2 | 5.529 | 7.922 | 8.063 | 7.658 | 7.930 |
| A1 | 5.654 | 7.930 | 8.060 | 7.681 | 7.938 |
| A1 | 5.740 | 8.010 | 8.131 | 7.758 | 8.019 |

*Table 10. Sample Calculation Output for Small Molecule (Ethylene)*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| STATE | EOMCCSD | (2,3),D | (2,3),A | (2,3),B | (2,3),C |
| B3U | 7.646 | 7.541 | 7.602 | 7.622 | 7.518 |
| B1U | 8.846 | 8.903 | 8.904 | 8.906 | 8.902 |
| B2G | 8.919 | 8.969 | 8.977 | 8.978 | 8.967 |
| B3G | 9.154 | 9.227 | 9.223 | 9.221 | 9.228 |
| B2G | 9.901 | 9.933 | 9.939 | 9.942 | 9.932 |
| AU | 11.165 | 11.065 | 11.106 | 11.114 | 11.064 |

Considering the Energy Differences between Benchmark Valuesand EOM-CCSD in GAMESS(US) for these four molecules (Table 1-4):

For all the four molecules, the EOMCCSD values in GAMESS(US) and ACESII are almost exactly the same. The energy difference is 0.001eV.

For Ni(CO)4, the MREOM T|SXD (ACESSII) yields the highest value, the energy difference is large than 0.2 eV for all states.

For Fe(CO)5, the MREOMTT†|SXD-h-v (ORCA) yields the highest value.

For Cr(CO)6 and CpNiNO, the MREOMTT†|SXD-h-v (ORCA) obtains the lowest value when compared to other three approaches.

Considering the Energy Differences between Benchmark Valuesand EOM-CCSD in GAMESS(US) for these four molecules (Table 5-8):

All triple corrections are very bad compared to EOMCCSD energy.

For all the four molecules, DELTA-CR-EOMCCSD(T) has the most accurate triple corrections. CR-EOMCC(2,3) always obtains the highest energy, the energy difference is always larger than 2.0 eV.

For CR-EOMCC(2,3) approach, the triple corrections for different variants are around 2.4 eV larger than EOMCCD energies for Ni(CO)4. For ethylene, the triple corrections for different variants are pretty good, as the energy difference are around or much less than 0.1 eV.

1. **Concluding Remarks**

There is little difference between the EOMCCSD values calculated in GAMESS(US) and benchmark values (Huntington, Nooijen) and the overall average difference in energy is no greater than 0.6 eV. This observation is consistent for all states in each of the selected compounds, and we can therefore consider these calculations to be accurate.

There are substantial differences in energies calculated using triples corrections, which can exceed 2 eV. These values are not considered accurate compared to the benchmark and calculated EOM-CCSD values.

However, when compared to the respective Brueckner values in GAMESS(US) we concluded that the most accurate correction to be

DELTA-CR-EOMCCSD(T), with an average absolute difference of 0.094eV, 0.449 eV, 0.536 eV and 0.564 eV for Ni(CO)4, Fe(CO)5, Cr(CO)6 ,CpNiNO, respectively. And the least accurate being CR-EOMCCSD(2,3) with an average absolute difference of 2.379 eV, 2.260 eV, 2.578 eV and 1.854 eV for Ni(CO)4, Fe(CO)5, Cr(CO)6 ,CpNiNO, respectively.

Triples corrections produce accurate results for small systems (such as ethylene) but not for complex systems such as transition metal compounds.

Future work will not be pursued in GAMESS(US), and other methods should be explored for any further calculations.

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