BSSE-Free Description of the Formamide Dimers

A. BENDE,[1] Á. VIBÓK,[1] G. J. HALÁSZ,[2] S. SUHAI[3]

[1]*University of Debrecen, Department of Theoretical Physics, H-4010 Debrecen, Hungary*
[2]*University of Debrecen, Institute of Mathematics and Informatics, H-4010 Debrecen, Hungary*
[3]*Molecular Biophysics Department, German Cancer Research Center, Im Neuenheimer Feld 280, D-69120 Heidelberg, Germany*

ABSTRACT: The different configurations (linear, zig-zag, and cyclic) of formamide dimers have been studied at the level of both Hartree–Fock (HF) and second order Møller–Plesset perturbation theory (MP2). The widely used a posteriori Boys–Bernardi "counterpoise" (CP) correction scheme has been compared with our a priori methods utilizing the "chemical Hamiltonian approach" (CHA). The appropriate interaction energies have been calculated in six different basis sets (6-31G, 6-31G**, DZV, DZP, TZV, and cc-pVDZ).   © 2001 John Wiley & Sons, Inc. Int J Quantum Chem 84: 617–622, 2001

Key words: basis set superpositions error (BSSE); intermolecular interaction; chemical Hamiltonian approach (CHA); formamide dimer; binding energy

Introduction

Formamide molecules play a very important role in biophysics. Many recent papers [1–7] have studied this molecule from both the theoretical and experimental points of view. The monomers, as well as the different hydrogen bonds between them, are at the center of these studies.

The purpose of the present work is to calculate the interaction energy minima in three formamide dimers having different structures—linear, zig-zag, and cyclic, respectively—taking into account the basis set superposition error (BSSE) thoroughly. Different a posteriori and a priori schemes have been proposed in the literature for treating the BSSE problem. In 1969/1970, Jansen and Ross [8] and, independently, Boys and Bernardi [9], introduced an a posteriori correction scheme called "function counterpoise" (CP), or simply the Boys–Bernardi method. In this scheme, one compensates the monomer energy lowering taking place in the supermolecule by recalculating the monomer energies at each geometric arrangement of the system by using the whole supermolecule basis. In 1991,

Mayer and Surján extended this method to the case when relaxation of the monomer geometries is also taken into account [10]. It has been shown that in addition to the supermolecule energy calculation and the calculations of the free monomers, one has to perform four additional calculations for each geometric arrangement of the supersystem: one also needs the energies of each relaxed monomer in both supermolecule and monomer basis sets ("7 point formula"); this makes the general use of the CP method more complicated.

About 15 years ago, Mayer and his co-workers started to develop a conceptually different method to solve the BSSE problem, based on the so-called "chemical Hamiltonian approach" (CHA) [11]. In this a priori scheme, one identifies those terms of the Hamiltonian that actually cause BSSE. Omitting these terms, we can get a "physical" Hamiltonian, which leads to the wave functions that are free from the BSSE-caused nonphysical delocalizations. Several different approaches have been developed using the CHA scheme both at the HF level [12–18] and using second order perturbation theory [21].

According to the previous calculations, the results provided by the CP and CHA methods are very close to each other, despite of the fact that these schemes are conceptually very different. In this work we apply both methods in order to study the structure of the formamide dimers. As will be seen, the results give a further confirmation of the near equivalence of these BSSE correction methods. The calculations are performed at two different theoretical levels—Hartree–Fock (HF) and second order Møller–Plesset (MP2) perturbation theory—using six different basis sets (6-31G, 6-31G**, DZV, DZP, TZV, and cc-pVDZ).

The methods applied (CP, CHA/HF, and CHA/MP2) are briefly reviewed in the next section. In the third section, the results of the calculations performed on three different structures of formamide dimers are presented in six basis sets, and the interaction energies obtained are compared and discussed.

The Methods Applied (CP, CHA/HF, and CHA/MP2)

The simplest definition of the uncorrected interaction energy $\Delta E_{AB}^{unc.}$ between the "monomers" A and B is the difference of the supermolecule energy and the sum of the free monomer energies, each calculated in its own basis set:

$$\Delta E_{AB}^{unc.} = E_{AB}(AB) - E_A(A) - E_B(B), \qquad (1)$$

where $E_{AB}(AB)$, $E_A(A)$, and $E_B(B)$ denote the total energy of the AB "supermolecule" and of the A and B monomers, respectively. The notations in the parentheses indicate that basis sets corresponding to the (sub)system A, B, and AB, respectively, were used. The above definition would be the correct one if one were able to perform the calculations of the free monomers exactly; this would require the use of (nearly) complete basis sets on each monomer, which is usually far from feasible. Experience shows that the use of incomplete monomer basis sets leads to slightly overestimated interaction energies, i.e., to BSSE. It is important to realize that BSSE is not a physical phenomenon, but only an artifact of using finite basis sets. In the Boys–Bernardi method [8, 9], this "mathematical effect" is eliminated by introducing the so-called "counterpoise" (CP) corrected interaction energy which is defined as:

$$\Delta E_{AB}^{CP} = E_{AB}(AB) - E_A(AB) - A_B(AB). \qquad (2)$$

Here the monomer interaction energies $E_A(AB)$ and $E_B(AB)$ are calculated the same as a basis set used for the AB supermolecule. As can be seen from Eq. (2), the description of the monomers is adjusted to the dimer problem so the energies (and other properties) of the "free" monomers become distance-dependent. At the same time a new difficulty comes from the changes of the monomer geometry; namely, the internal geometries of the monomers are allowed to change during the dimer formation (it is called "monomer relaxation"). To take into account this effect, a new definition is needed calculating the appropriate BSSE-corrected interaction energy:

$$\Delta E_{AB}^{CP,rel.} = E_{AB}^{rel.}(AB) - E_A^{rel.}(AB) - E_B^{rel.}(AB)$$
$$+ \left[E_A^{rel.}(A) - E_A(A) \right] + \left[E_B^{rel.}(B) - E_B(B) \right], \quad (3)$$

where rel. indicates the relaxed internal monomer energies, and the differences $[E_A^{rel.}(A) - E_A(A)]$ and $[E_B^{rel.}(B) - E_B(B)]$ are the relaxation energies for monomers A and B, respectively [10]. As Eq. (3) shows, in order to calculate a single point on the CP corrected interaction energy surface of the relaxed monomers, one needs to perform five different calculations (in addition to the monomer energy calculations in the monomer basis sets).

In the alternative a priori CHA method, one omits those terms of the Hamiltonian which cause BSSE. The CHA scheme permits the supermolecule calculations to keep consistency with those for the free monomers performed in their original monomer basis sets. The only disadvantage of this procedure is that the resulting CHA Hamiltonian

is not Hermitian: as the BSSE is not a physical phenomenon, there cannot be any Hermitian operator associated with it—so one cannot expect the BSSE-free Hamiltonian $\hat{H}_{CHA}$ to be Hermitian either. Based on this CHA Hamiltonian, SCF-type equations and perturbational techniques have been developed [12, 21] which give the BSSE-free wave functions. However, it was established [13] that the energy of these BSSE-free wave functions should be calculated by using the usual Hermitian Hamiltonian. This follows from the requirement that the energy must be real and is supported by some analytical considerations [19] and a huge amount of the numerical results [14–16]. (This procedure of the energy calculations is often referred to by the acronym "CHA/CE"—CHA with conventional energy calculation.)

While the CHA generalization of the SCF procedure is a relatively straightforward one, the generalization to the correlated level has a number of difficulties. It was shown [20] that the appropriate second order energy can be obtained as follows. First, we have to calculate the first order CHA wave function χ by using the non-Hermitian CHA Hamiltonian partitioned as $\hat{H}_{CHA} = \hat{H}^0 + \hat{V}_{CHA}$, where $\hat{H}^0$ is a Møller–Plesset-type unperturbed Hamiltonian which is also non-Hermitian, as it is built up of the nonorthogonal eigenvectors of the non-Hermitian CHA-SCF equations [12]. The Hermitian conventional Hamiltonian $\hat{H}$ should also be taken as a sum of the same non-Hermitian unperturbed Hamiltonian $\hat{H}^0$ and of some (also non-Hermitian) perturbation $\hat{V}$, that is $\hat{V} = \hat{H} - \hat{H}^0$. In short, we use a Møller–Plesset-type partitioning of the conventional Hamiltonian, but the unperturbed $\hat{H}^0$ is built up of the eigenvalues and (nonorthogonal) eigenvectors of the non-Hermitian CHA-SCF equations. Then a detailed analysis shows that
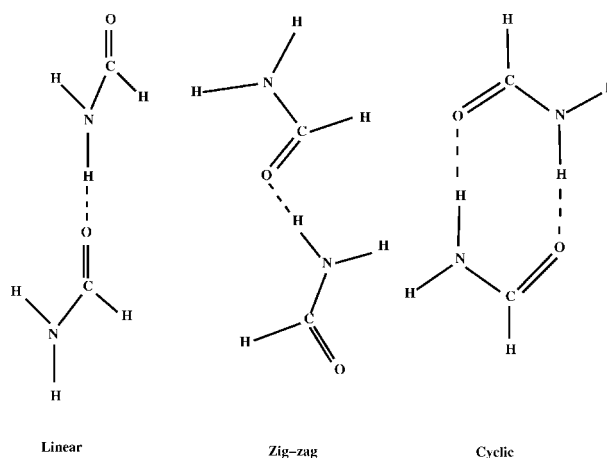

FIGURE 1. Structure of the linear, zig-zag, and cyclic dimers of formamide.

the second order energy contribution can be calculated as using the generalized Hylleraas functional J_2 [20] with the first order CHA wave function χ:

$$J_2 = \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \left[2Re\left(\langle \hat{Q}\chi | \hat{V} | \Psi_0 \rangle \right) + Re\left(\langle \chi | \hat{H}^0 - E_0 | \chi \rangle \right) \right].$$

(4)

Here Ψ_0 is the unperturbed wave function, E_0 is the zero order energy ($\hat{H}^0\Psi_0 = E_0\Psi_0$), and $\hat{Q}$ is the projection operator on the orthogonal complement to Ψ_0. This generalized Hylleraas-functional represents the appropriate application of the CHA scheme with conventional energy calculation for the perturbational problem. This formalism is called ("CHA/MP2") [21]. In this perturbation theory, the zero order energy is the sum of the occupied orbital energies. Although the CHA Hamiltonian is not Hermitian, the occupied orbital energies where found to be real in all cases studied, providing E_0 is real. Complex virtual orbital energies do occur

TABLE I

Interaction energies for formamide dimers in different conformations (Fig. 1) computed at the Hartree–Fock (HF) level, using 6-31G and 6-31G** basis sets. $\Delta E_{HF}^{unc.}$ with uncorrected interaction energy; ΔE_{HF}^{CP} with "counterpoise" (CP) corrected interaction energy for rigid monomers; $\Delta E_{HF}^{CP,rel.}$ with "counterpoise" (CP) corrected interaction energy for relaxed monomers, and ΔE_{HF}^{CHA} with CHA correction (in kcal/mol).

	6-31G				6-31G**			
Dimer	$\Delta E_{HF}^{unc.}$	ΔE_{HF}^{CP}	$\Delta E_{HF}^{CP,rel.}$	ΔE_{HF}^{CHA}	$\Delta E_{HF}^{unc.}$	ΔE_{HF}^{CP}	$\Delta E_{HF}^{CP,rel.}$	ΔE_{HF}^{CHA}
Linear	−8.199	−7.659	−7.459	−7.065	−6.332	−5.812	−5.644	−6.134
Zig-zag	−8.265	−7.748	−7.544	−7.225	−6.358	−5.856	−5.703	−6.264
Cyclic	−16.441	−14.939	−14.001	−14.236	−13.390	−12.018	−11.196	−12.436

TABLE II

Interaction energies for formamide dimers in different conformations (Fig. 1) computed at the Hartree–Fock (HF) level, using DZV and DZP basis sets. $\Delta E_{HF}^{unc.}$ with uncorrected interaction energy; ΔE_{HF}^{CP} with "counterpoise" (CP) corrected interaction energy for rigid monomers; $\Delta E_{HF}^{CP,rel.}$ with "counterpoise" (CP) corrected interaction energy for relaxed monomers, and ΔE_{HF}^{CHA} with CHA correction (in kcal/mol).

Dimer	DZV				DZP			
	$\Delta E_{HF}^{unc.}$	ΔE_{HF}^{CP}	$\Delta E_{HF}^{CP,rel.}$	ΔE_{HF}^{CHA}	$\Delta E_{HF}^{unc.}$	ΔE_{HF}^{CP}	$\Delta E_{HF}^{CP,rel.}$	ΔE_{HF}^{CHA}
Linear	−8.592	−8.027	−7.832	−8.019	−6.338	−5.901	−5.759	−5.927
Zig-zag	−8.612	−8.085	−7.873	−8.069	−6.360	−5.942	−5.796	−5.971
Cyclic	−16.072	−15.152	−14.199	−15.307	−12.159	−11.884	−11.130	−12.065

in practice; as they always appear in complex conjugate pairs, the CHA/MP2 energy corrections are always real [21].

Results and Discussion

The calculation has been carried out partly in Heidelberg (on an IBM SP2 cluster) and partly in Debrecen (on a Pentium 200 PC running Linux). In the standard HF and MP2 calculations, the Gaussian 98 computer code [23] was utilized, while the CHA- type calculation was performed by a slightly modified version of HONDO-8 [22].

In these calculations, we have used the same CHA/HF and CHA/MP2 programs as in [12, 21]. In this work we have considered three different configuration of formamide dimers—linear, zig-zag, and cyclic—as shown on Figure 1. The dimer geometries were opimized at two theoretical levels—Hartree–Fock (HF) and second order Møller–Plesset perturbation theory (MP2) for each basis set.

Six different basis sets were used: 6-31G, 6-31G**, DZV, DZP, TZV, and cc-pVDZ. 6-31G and 6-31G** are standard Pople's basis sets; DZV, DZP, and TZV are the built-in basis sets of HONDO-8 system. They were read into the Gaussian system. At the same time, we had to input externally the cc-pVDZ basis to the HONDO. A small difficulty should be noted in this connection: HONDO-8 only performs calculations by using 6d and 10f functions, while the cc-pVDZ basis is assumed to use pure d and f functions. This may cause minor discrepancies in the comparisons.

Tables I–III display the results obtained for the interaction energies using for different methods at the Hartree–Fock level. Results marked ($\Delta E_{HF}^{unc.}$, ΔE_{HF}^{CP}, and $\Delta E_{HF}^{CP,rel.}$) represent the results obtained in calculations with no BSSE correction, the standard CP corrected results obtained without admitting geometry relaxation and the CP corrected results with geometry relaxation, as prescribed by the "7-point" formula Eq. (3). The fourth type of the results (ΔE_{HF}^{CHA}) is those given by the CHA calculations.

TABLE III

Interaction energies for formamide dimers in different conformations (Fig. 1) computed at the Hartree–Fock (HF) level, using TZV and cc-pVDZ basis sets. $\Delta E_{HF}^{unc.}$ with uncorrected interaction energy; ΔE_{HF}^{CP} with "counterpoise" (CP) corrected interaction energy for rigid monomers; $\Delta E_{HF}^{CP,rel.}$ with "counterpoise" (CP) corrected interaction energy for relaxed monomers, and ΔE_{HF}^{CHA} with CHA correction (in kcal/mol).

Dimer	TZV				cc-pVDZ			
	$\Delta E_{HF}^{unc.}$	ΔE_{HF}^{CP}	$\Delta E_{HF}^{CP,rel.}$	ΔE_{HF}^{CHA}	$\Delta E_{HF}^{unc.}$	ΔE_{HF}^{CP}	$\Delta E_{HF}^{CP,rel.}$	ΔE_{HF}^{CHA}
Linear	−7.885	−7.401	−7.220	−7.387	−6.508	−5.480	−5.295	−5.637
Zig-zag	−7.901	−7.464	−7.274	−7.451	−6.530	−5.511	−5.342	−5.691
Cyclic	−14.385	−14.369	−13.529	−14.306	−13.538	−11.074	−10.218	−11.897

TABLE IV

Interaction energies for formamide dimers in different conformations (Fig. 1) computed at the second order Møller–Plesset perturbation theory (MP2) level, using 6-31G and 6-31G** basis sets. $\Delta E_{MP2}^{unc.}$ with uncorrected interaction energy; ΔE_{MP2}^{CP} with "counterpoise" (CP) corrected interaction energy for rigid monomers; $\Delta E_{MP2}^{CP,rel.}$ with "counterpoise" (CP) corrected interaction energy for relaxed monomers, and ΔE_{MP2}^{CHA} with CHA correction (in kcal/mol).

	6-31G				6-31G**			
Dimer	$\Delta E_{MP2}^{unc.}$	ΔE_{MP2}^{CP}	$\Delta E_{MP2}^{CP,rel.}$	ΔE_{MP2}^{CHA}	$\Delta E_{MP2}^{unc.}$	ΔE_{MP2}^{CP}	$\Delta E_{MP2}^{CP,rel.}$	ΔE_{MP2}^{CHA}
Linear	−8.322	−6.474	−6.277	−6.389	−7.792	−6.071	−5.840	−5.817
Zig-zag	−8.051	−6.369	−6.206	−6.186	−7.423	−5.822	−5.642	−5.894
Cyclic	−17.848	−13.591	−12.649	−12.710	−17.157	−13.379	−12.201	−12.264

Tables IV–VI display the results obtained for the interaction energies using different methods at the second order Møller–Plesset perturbation theory level. Results marked $\Delta E_{MP2}^{unc.}$, ΔE_{MP2}^{CP}, and $\Delta E_{MP2}^{CP,rel.}$ were obtained in calculations with no BSSE correction, the standard CP corrected results obtained without admitting geometry relaxation, and the CP corrected results with geometry relaxation, as prescribed by the "7-point" formula Eq. (3). The fourth type of result (ΔE_{MP2}^{CHA}) is given by the CHA calculations.

Considering the results, the following conclusion can be drawn. In all calculations, the cyclic structure is roughly twice as stable as the other two, which is in agreement with the fact that it contains two hydrogen bonds. No significant tendencies could be observed as far as the small differences in the strength of individual hydrogen bonds in the different isomers/structures—the basis set effects, etc., are bigger than these tiny effects and vary quite randomly.

Concerning the comparison of the different methods, we make the following observations. (1) As expected, the BSSE-free ΔE_{HF}^{CHA} and the BSSE-corrected CP interaction energies (ΔE_{HF}^{CP} and $\Delta E_{HF}^{CP,rel.}$) exhibit less deep minima than those given by the usual uncorrected ($\Delta E_{HF}^{unc.}$) HF one. Exactly the same effect can be seen in correlated level, namely, the BSSE-free ΔE_{MP2}^{CHA} and the BSSE-corrected CP interaction energies (ΔE_{MP2}^{CP} and $\Delta E_{MP2}^{CP,rel.}$) are higher than the uncorrected ($\Delta E_{MP2}^{unc.}$) MP2 one. The difference between the CP and CHA results is essentially not significant, while the uncorrected interaction energies differ appreciably from these three corrected results in all cases. (2) The use of larger basis sets (adding polarization function to a given basis) in the calculations provides a better description for the dimer structure. (3) Turning to the correlated level, the amount of the BSSE content in the intermolecular interaction energies is much higher than those in Hartree–Fock level. Most probably, BSSE correction remains imperative even for the largest basis sets.

TABLE V

Interaction energies for formamide dimers in different conformations (Fig. 1) computed at the second order Møller–Plesset perturbation theory (MP2) level, using DZV and DZP basis sets. $\Delta E_{MP2}^{unc.}$ with uncorrected interaction energy; ΔE_{MP2}^{CP} with "counterpoise" (CP) corrected interaction energy for rigid monomers; $\Delta E_{MP2}^{CP,rel.}$ with "counterpoise" (CP) corrected interaction energy for relaxed monomers, and ΔE_{MP2}^{CHA} with CHA correction (in kcal/mol).

	DZV				DZP			
Dimer	$\Delta E_{MP2}^{unc.}$	ΔE_{MP2}^{CP}	$\Delta E_{MP2}^{CP,rel.}$	ΔE_{MP2}^{CHA}	$\Delta E_{MP2}^{unc.}$	ΔE_{MP2}^{CP}	$\Delta E_{MP2}^{CP,rel.}$	ΔE_{MP2}^{CHA}
Linear	−8.709	−6.784	−6.577	−6.988	−7.524	−6.089	−5.884	−6.352
Zig-zag	−8.604	−6.798	−6.616	−6.839	−7.391	−5.956	−5.800	−6.065
Cyclic	−17.362	−13.815	−12.795	−13.732	−15.788	−13.445	−12.316	−13.901

TABLE VI

Interaction energies for formamide dimers in different conformations (Fig. 1) computed at the second order Møller–Plesset perturbation theory (MP2) level, using TZV and cc-pVDZ basis sets. $\Delta E_{MP2}^{unc.}$ with uncorrected interaction energy; ΔE_{MP2}^{CP} with "counterpoise" (CP) corrected interaction energy for rigid monomers; $\Delta E_{MP2}^{CP,rel.}$ with "counterpoise" (CP) corrected interaction energy for relaxed monomers, and ΔE_{MP2}^{CHA} with CHA correction (in kcal/mol).

Dimer	TZV				cc-pVDZ			
	$\Delta E_{MP2}^{unc.}$	ΔE_{MP2}^{CP}	$\Delta E_{MP2}^{CP,rel.}$	ΔE_{MP2}^{CHA}	$\Delta E_{MP2}^{unc.}$	ΔE_{MP2}^{CP}	$\Delta E_{MP2}^{CP,rel.}$	ΔE_{MP2}^{CHA}
Linear	−7.697	−6.421	−6.284	−6.551	−7.959	−5.478	−5.220	−6.054
Zig-zag	−7.686	−6.403	−6.271	−6.529	−7.489	−5.252	−5.055	−5.670
Cyclic	−14.744	−13.151	−12.372	−13.438	−17.114	−12.001	−10.663	−13.701

In this article, we applied BSSE-free methods in order to investigate the structure of the formamide dimers. It can be concluded that the results also give a further confirmation of the near equivalence of the a posteriori CP and a priori CHA methods. The interaction energies are strongly dependent upon the basis sets applied, so our next aim will be to perform a more extensive study for the basis set dependence of the structure of formamide dimers. In orde to achieve this, one needs to first build the CHA codes into the Gaussian system.

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