

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/239734842>

# Ab initio study of ternary radical–molecule complexes between HCN(HNC) and HO(HS) species

**DATASET** *in* STRUCTURAL CHEMISTRY · DECEMBER 2012

Impact Factor: 1.84 · DOI: 10.1007/s11224-012-0184-y

CITATION

1

READS

56

## 2 AUTHORS:



**Mohammad Solimannejad**

Arak University

167 PUBLICATIONS 1,589 CITATIONS

SEE PROFILE



**saber ghafari**

Arak University

3 PUBLICATIONS 27 CITATIONS

SEE PROFILE

# Ab initio study of ternary radical–molecule complexes between HCN(HNC) and HO(HS) species

Mohammad Solimannejad · Saber Ghafari

Received: 21 October 2012 / Accepted: 8 December 2012  
© Springer Science+Business Media New York 2012

**Abstract** MP2 calculations with the cc-pVTZ basis set were used to analyze the intermolecular interactions in ternary radical–molecule complexes between HCN(HNC) and HO(HS) species, in gas phase and in water media. Particular attention was given to parameters such as the cooperative energies and many-body interaction energies. The results indicate that hydrogen bonding between two HCN(HNC) molecules gives more stability to triads than hydrogen bonding between HCN(HNC) and OH(SH) species. The electronic properties of the complexes were analyzed using the parameters derived from the atoms in molecules methodology. The water media has an enhancing influence on the stabilities of studied clusters versus the ones obtained in gas phase.

**Keywords** Radical–molecule complexes · UMP2 calculations · Cooperativity effects · Solvent effects

## Introduction

Noncovalent intermolecular interactions have been the subject of a long and distinguished history of study [1]. These interactions are of course significant from a fundamental perspective, but are of a certain practical importance as well, in areas as diverse as atmospheric chemistry and catalysis, as well as in biochemically relevant processes.

Hydrogen bonding represents a unique sort of noncovalent interaction and has been studied extensively over the years, from both experimental and theoretical perspectives

[2, 3]; the vast majority of this body of work has been concerned with closed-shell systems. Information dealing with open-shell systems (such as radicals) remains far more limited. This paucity is due to both experimental and theoretical difficulties arising in the formation and characterization of the systems in question. One of the more intriguing areas of radical–molecule complex studies arise from the discovery of the formation of surprisingly stable complexes pairing radicals with other molecular moieties [4–25]. Bearing in mind the importance of free radicals in a number of fields (e.g., atmospheric chemistry and life sciences), fundamental information about the intermolecular interactions involving these open-shell systems is highly desirable.

OH is an important radical, which is generated mainly from the decomposition of hydroperoxides or the reaction of excited atomic oxygen with atmospheric water. It is of great importance in the atmospheric and biological sciences. The hydroxyl radical is often referred to as the “detergent” of the troposphere because it reacts with many pollutants through non-thermal plasma chemical reactions. It also plays an important role in eliminating greenhouse gases such as methane and ozone [26]. As an oxidant, it can damage all types of macromolecules, including carbohydrates, nucleic acids, lipids, and amino acids [27]. A number of systems combining OH radical with HCOOH [28], H<sub>2</sub>O [29], and H<sub>2</sub>S [30] have been reported in the literature. Like the OH, the SH radical also plays an important role in astrophysics and atmospheric chemistry and acts as the intermediate in the transformation between organic and inorganic sulfurs. Using coupled-cluster theory, Du and Francisco [31] studied the spectroscopic properties and stability of the H<sub>2</sub>O–HS open-shell complex. The results show that this complex is less stable than the H<sub>2</sub>O–HO counterpart.

Hydrogen cyanide (HCN) and its isomer, hydrogen isocyanide (HNC), have been detected in interstellar space

M. Solimannejad (✉) · S. Ghafari  
Quantum Chemistry Group, Department of Chemistry,  
Faculty of Sciences, Arak University, 38156-8-8349 Arak, Iran  
e-mail: m-solimannejad@araku.ac.ir

[32, 33] and may be involved in the synthesis of prebiotic compounds [34, 35]. Thus, much attention has been paid to the structures and properties of their complexes [36–39].

An ab initio study of the complexes formed between MH (M = O and S) and HXY (XY = CN and NC) was carried out at the UQCISD/6-311++G(2df,2p) level [40]. Considering that these molecules may exist simultaneously in interstellar space, we believe that the study of their triads is also important in providing useful information for their interaction in higher concentration of HCN (HNC) species. In the present work, we thus performed a study of a series of triads formed between HCN(HNC) and OH(SH) in the gas phase and solution media using quantum chemical calculations for the first time.

### Computational details

All calculations have been performed with the GAUSSIAN 03 quantum chemical package [41] using unrestricted second perturbation theory (labeled as UMP2) within the frozen core approximation. We have used cc-pVTZ basis set. In a very recent paper, Riley et al. [42] pointed out that this basis set combining with MP2 method provides very good estimates of geometries and energies for noncovalent complexes. Structures of the monomers and the complexes were optimized and characterized by frequency computations at the UMP2/cc-pVTZ computational level. Benchmark calculations at UQCISD/6-311++G(2df,2p) level are also carried out to confirm results that is obtained at UMP2/cc-pVTZ level.

The stabilization energy of the clusters in the present article was calculated as the difference between the energy of the supermolecule and the sum of the energies of the isolated monomers in their minimum configuration. The counterpoise (CP) method [43] has been used to take into account the basis set superposition error (BSSE) in the calculation of the binding energies since it has been shown that the BSSE corrected energies at MP2 level are closer to the MP2/CBS ones than the uncorrected ones [44]. The atoms in molecules (AIM) methodology [45] has been used with the AIM2000 [46] program to analyze the electron density calculated at the UMP2/cc-pVTZ computational level.

The energetic calculations in solutions were performed with the polarized continuum model (PCM) using the water parameters [47] at the UMP2/cc-pVTZ computational level.

### Results and discussion

The initial structures used to scan the potential energy surface have been generated using the geometry of the 1:1 complexes that previously reported for the dimers [40]. A total of 12

minima structures have been found for the trimers (Fig. 1). All complexes are formed through all the possible combination of a HCN(HNC) molecule with a HCN(HNC)⋯OH(HS) dimers. All trimers are assorted by three sets, in the first and second category the interacting OH(HS) radical act as hydrogen donor and hydrogen acceptor, respectively. In the third category, the OH(HS) radical plays a dual role as hydrogen donor and hydrogen acceptor simultaneously. Optimization of triads in the third category leads to cyclic structures as shown in Fig. 1. All complexes connected via O(S)H⋯N and CH⋯N(S,O) hydrogen bonds along with C⋯C and C⋯N weak interactions. The existence and characterization of weak N⋯C interaction in the CH<sub>3</sub>X⋯HNC⋯HCN and O<sub>2</sub>NX⋯HCN(HNC)⋯HCN(HNC) ternary complexes (X = Cl, Br) are reported in literature very recently [48, 49].

The stabilization energies of the 12 minima structures located in the potential energy surface of the trimer are reported in Table 1. Stabilization energies of the 1:2 complexes of HCN(HNC) and OH(SH) lie in the range of 33–65 and 31–55 kJ mol<sup>−1</sup> at UMP2/cc-pVTZ and UQCISD/6-311++G(2df,2p) computational levels, respectively. The results of UQCISD/6-311++G(2df,2p) calculations are compared with MP2 results, because this level of calculations gives very good results in 1:1 complexes [40]. Nice correlation between calculated stabilization energies at these two computational levels is established as shown in Fig. 2.

The stabilization energy in the dyads can be regarded as the energy difference between the complex and the monomers:  $\Delta E(AB) = E_{AB} - (E_A + E_B)$  and the corresponding value in the triads  $\Delta E(ABC)$  is calculated in the similar way.  $E_i(AB, T)$  and  $E_i(BC, T)$  are the interaction energies of AB and BC dyads while they are in the geometry of triads. Table 2 gives the stabilization energy of twelve studied triads and respective dyads. All results were corrected for BSSE by the full CP method. As shown in Table 2, the binding energy of the studied triads ranges from 20.28 to 57.92 kJ mol<sup>−1</sup>.

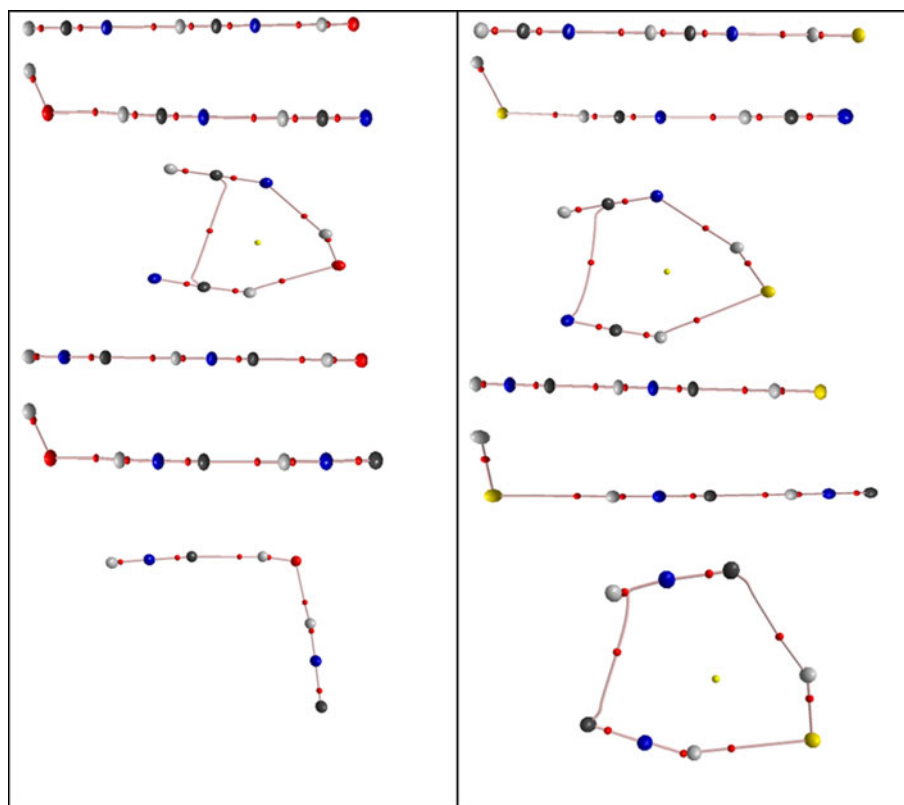
An energetic cooperativity parameter has been calculated using Eq. (1) [50, 51].

$$E_{\text{Coop}} = \Delta E(ABC) - \Delta E(AB) - \Delta E(BC) - E_i(AC) \quad (1)$$

where  $\Delta E(ABC)$  is the stabilization energy of the trimer,  $\Delta E(AB)$  and  $\Delta E(BC)$  are the stabilization energy of the isolated dimers within their corresponding minima configuration, and  $E_i(AC)$  is the interaction energy of the molecules A and C in the geometry they have in the trimer. In the title complexes, a favorable cooperativity is observed with values that range between −1.49 and −6.14 kJ mol<sup>−1</sup>. In the same way, diminutive effects are observed for a number of complexes in the ranges between 1.50 and 5.75 kJ mol<sup>−1</sup> (Table 2).

The two- and three-body contributions to total binding energy are obtained by many-body analysis [52, 53].

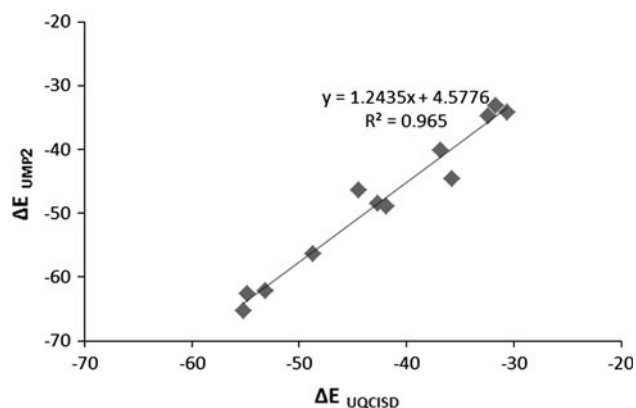
**Fig. 1** Molecular graphs of the complexes between HCN(HNC) and OH (left side) and SH (right side) species at the UMP2/cc-pVTZ computational level



**Table 1** Stabilization energies of studied triads at UMP2/cc-pVTZ and UQCISD/6-311++G(2df,2p) computational levels

Triads (A...B...C)	$\Delta E_{\text{UQCISD}}$ (gas)	$\Delta E_{\text{UMP2}}$ (gas)	$\Delta E_{\text{UMP2}}$ (PCM-water)
HCN...HCN...HO	-44.45	-46.44	-64.55
HO...HCN...HCN	-36.86	-40.14	-56.26
HCN...HO...HCN	-42.67	-48.45	-61.21
HNC...HNC...HO	-54.81	-62.61	-69.63
HO...HNC...HNC	-55.20	-65.36	-70.74
HNC...HO...HNC	-53.15	-62.25	-69.56
HCN...HCN...HS	-32.42	-34.74	-48.18
HS...HCN...HCN	-31.69	-33.19	-47.45
HCN...HS...HCN	-30.64	-34.13	-34.22
HNC...HNC...HS	-41.86	-48.86	-52.60
HS...HNC...HNC	-48.75	-56.30	-59.91
HNC...HS...HNC	-35.78	-44.63	-63.55

The two-body terms ( $\Delta E_{\text{A-B}}$ ,  $\Delta E_{\text{B-C}}$ , and  $\Delta E_{\text{A-C}}$ ) can be calculated as the interaction energy of each molecular pair in the geometry of triad minus the energy sum of the monomers, all of them frozen in the geometry of the triad. The three-body term  $\Delta E_{\text{A-B-C}}$  is calculated as the total binding energy of the triad minus the interaction energy of each pair of monomers, all of them frozen in the geometry of the triad using Eq. (2) [54].



**Fig. 2** Stabilization energy of triads at UMP2/cc-pVTZ versus UQCISD/6-311++G(2df,2p) results

$$\Delta E_{\text{A-B-C}} = E_{\text{i}}(\text{ABC})' - \Delta E_{\text{A-B}} - \Delta E_{\text{A-C}} - \Delta E_{\text{B-C}}. \quad (2)$$

$E_{\text{i}}(\text{ABC})'$  is obtained by subtracting the total energy of the optimized triads from the energy sum of the monomers frozen in the geometry of the triads. The total relaxation energy ( $E_{\text{R}}$ ) is defined as the energy sum of the monomers frozen in the geometry of the triads minus the energy sum of the optimized monomers. Thus, the total binding energy of the triad is obtained using Eq. (3) [54].

**Table 2** Stabilization and interaction energies ( $\Delta E$  and  $E_i$  kJ mol<sup>-1</sup>) of the investigated dyads and triads (T) at the UMP2/cc-pVTZ level

Triads (A...B...C)	$\Delta E(ABC)$	$\Delta E(AB)$	$\Delta E(BC)$	$E_i(AB, T)$	$E_i(BC, T)$	$E_i(AC, T)$	$E_{Coop}$
HCN...HCN...HO	-40.90	-18.75	-18.26	-18.49	-17.93	-1.30	-2.59
HO...HCN...HCN	-34.12	-12.33	-18.75	-12.46	-18.56	-0.79	-2.25
HCN...HO...HCN	-40.05	-14.82	-8.88	-14.78	-8.84	-10.21	-6.14
HNC...HNC...HO	-56.77	-31.40	-19.81	-31.02	-18.57	-1.34	-4.23
HO...HNC...HNC	-57.92	-21.27	-31.40	-20.69	-30.69	-0.29	-4.96
HNC...HO...HNC	-44.67	-20.59	-19.15	-17.97	-19.15	-7.16	2.23
HCN...HCN...HS	-30.90	-18.75	-9.82	-18.63	-9.55	-0.70	-1.63
HS...HCN...HCN	-29.69	-9.08	-18.75	-8.90	-18.60	-0.38	-1.49
HCN...HS...HCN	-20.28	-7.92	-7.60	-7.92	-7.60	-10.51	5.75
HNC...HNC...HS	-45.02	-31.40	-10.24	-31.22	-9.18	-0.66	-2.72
HS...HNC...HNC	-51.71	-16.14	-31.40	-15.61	-30.81	0.11	-4.28
HNC...HS...HNC	-29.79	-5.95	-14.47	-5.95	-14.47	-10.88	1.50

**Table 3** Decomposition of interaction energy (kJ mol<sup>-1</sup>) of the investigated triads

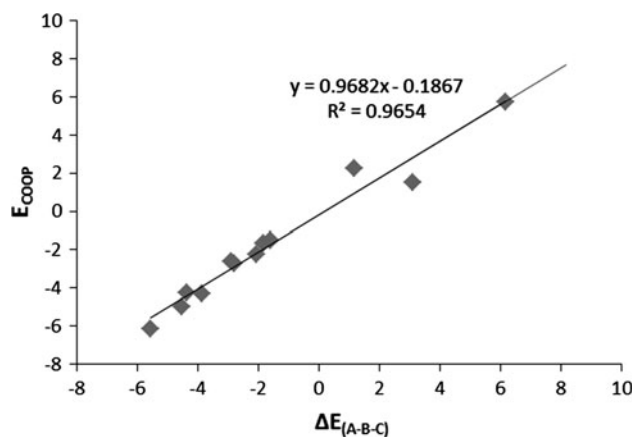
Triads (A...B...C)	$\Delta E_{A-B}$	$\Delta E_{B-C}$	$\Delta E_{A-C}$	$\Delta E_{A-B-C}$	$E_R$
HCN...HCN...HO	-18.67	-18.16	-1.40	-2.92	0.26
HO...HCN...HCN	-12.58	-18.78	-0.91	-2.08	0.23
HCN...HO...HCN	-15.02	-9.43	-10.67	-5.58	0.65
HNC...HNC...HO	-32.33	-19.86	-1.69	-4.37	1.48
HO...HNC...HNC	-21.49	-32.39	-1.23	-4.53	1.71
HNC...HO...HNC	-18.64	-20.55	-8.22	1.17	1.57
HCN...HCN...HS	-18.78	-9.70	-0.74	-1.85	0.17
HS...HCN...HCN	-9.01	-18.80	-0.48	-1.60	0.21
HCN...HS...HCN	-8.05	-7.92	-10.87	6.15	0.40
HNC...HNC...HS	-32.3	-10.15	-0.89	-2.82	1.15
HS...HNC...HNC	-16.31	-32.34	-0.74	-3.86	1.54
HNC...HS...HNC	-6.46	-15.61	-12.42	3.10	1.60

$$\Delta E(ABC) = \Delta E_{A-B} + \Delta E_{A-C} + \Delta E_{B-C} + \Delta E_{A-B-C} + E_R. \quad (3)$$

The results are presented in Table 3, in which all energies are corrected for BSSE. As seen in Table 3, the main contribution of stabilization energy is coming from the two-body terms.

For all triads, the two-body interaction  $\Delta E_{A-B}$ ,  $\Delta E_{B-C}$ , and  $\Delta E_{A-C}$  are attractive. For all triads  $\Delta E_{A-C}$  is the smallest two-body interaction term, consistent with the largest distance between them. Analysis of two-body terms in studied complexes leads to the following conclusions:

- (1) Hydrogen bonding between two HCN(HNC) molecules gives more stability to triads than hydrogen bonding between HCN(HNC) and OH(SH) species.
- (2) In complexes involving HCN, hydrogen donor ability of OH(SH) radicals is more important in stability of

**Fig. 3**  $E_{Coop}$  versus  $\Delta E_{A-B-C}$  in studied complexes

triads while in complexes involving HNC, hydrogen acceptor ability of OH(SH) radicals is more prominent in stability of triads.

- (3) OH radical is a better hydrogen donor and hydrogen acceptor than SH radical.

The three-body interaction energy  $\Delta E_{A-B-C}$  is attractive in triads with cooperativity and repulsive for triads with diminutive effect. The contribution of the three-body interaction energy is much smaller than that of two-body interaction energy. Nice correlation between three-body terms and cooperativity energy established in studied complexes as shown in Fig. 3.

The relaxation energy can be taken as a measure of the degree of strain that drives the distortion of the ternary system. As seen in Table 3, the relaxation energy is positive, so makes a destabilizing contribution to the total stabilization energy of the triads. The relaxation energy is larger for HNC complexes than HCN complexes.

**Table 4** Changes in the AIM parameters of the triads relative to the respective dyads

Triads (A...B...C)	$\Delta\rho_{AB}$	$\Delta\nabla_{AB}^2$	$\Delta\rho_{BC}$	$\Delta\nabla_{BC}^2$
HCN...HCN...HO	0.0019	0.0048	0.0020	0.0035
HO...HCN...HCN	0.0022	0.0054	0.0012	0.0031
HCN...HO...HCN	0.0019	0.0039	0.0019	0.0009
HNC...HNC...HO	0.0030	0.0009	0.0026	0.0025
HO...HNC...HNC	0.0042	0.0062	0.0023	0.0007
HNC...HO...HNC	0.0072	0.0061	0.0081	0.0081
HCN...HCN...HS	0.0012	0.0029	0.0015	0.0046
HS...HCN...HCN	0.0014	0.0025	0.0009	0.0023
HCN...HS...HCN	0.0010	0.0023	−0.0001	−0.0003
HNC...HNC...HS	0.0018	0.0007	0.0022	0.0046
HS...HNC...HNC	0.0030	0.0020	0.0019	0.0006
HNC...HS...HNC	−0.0004	−0.0025	0.0022	0.0016

The AIM treatment of electron density has emerged as a useful tool to analyze the strengths of intermolecular interactions such as H-bonds. Table 4 shows the variation in electron density and the Laplacian of the electron density at two bond critical points located between molecules A, B, and C. An enhancement in electron density and the Laplacian of electron density at the bond critical point is observed for all triads excepting HCN(HNC)...HS...HCN(HNC) cyclic complexes. The variations in topological parameters of electron density are consistent with cooperative and diminutive energetic effects in investigated triads.

On most occasions, hydrogen bonds take place in liquid phase. Thus it is interesting to consider the effect of the solvent on the strength of hydrogen bonds in title complexes. The interaction energy of the studied complexes was recalculated using a continuum solvent model, PCM, with the water parameters at the UMP2/cc-pVTZ level (Table 1). Comparison of stabilities in gas phase and in solution shows that the solvent has an enhancing influence on the stabilities of studied clusters. Similar solvent effect has been described for the hydrogen bonds [55–57]. A more detailed analysis shows that the average percentage increment in stability from gas phase to PCM-water is about 23.

## Conclusion

This work reports a study of the structural and electronic properties of complexes between one OH(SH) radical and two HCN(HNC) molecules. The investigated complexes show that the molecules involved approach to each other through a number of possible interactions, namely O(S)H...N and CH...(O)N hydrogen bonds along with C...C(N) weak interactions. The solvent has been

considered by means of a continuum solvent model, PCM-water. The results indicate an enhancing influence on the stabilities of studied clusters in solution versus the ones obtained in gas phase. The most favorable interaction energies obtained for the studied triads range between 20 and 58 kJ mol<sup>−1</sup>. Finally, we hope that the results of the present study motivate experimentalists for matrix isolation study of title complexes.

## References

- Muller-Dethlefs K, Hobza P (2000) Chem Rev 100:143
- Scheiner S (1997) Hydrogen bonding. A theoretical perspective. Oxford University Press, Oxford; and references therein
- Hobza P, Havlas Z (2000) Chem Rev 100:4253
- Johnson ER, Dilabio GA (2009) Interdiscip Sci Comput Life Sci 1:133
- Hammerum S (2009) J Am Chem Soc 131:8627
- Franchi P, Lucarini M, Pedrielli P, Pedulli GF (2002) ChemPhysChem 3:789
- Alkorta I, Rozas I, Elguero J (1998) J Phys Chem 102:429
- Wang B, Li Z, Wu D, Hao X, Li R, Sun C (2003) Chem Phys Lett 375:91
- Tang K, Shi FQ (2007) Int J Quantum Chem 107:665
- An X, Liu H, Li Q, Gong B, Cheng J (2008) J Phys Chem A 112:5258
- Li Q, Zhu H, An X, Gong B (2009) Int J Quantum Chem 109:605
- Hansen JC, Francisco JS (2002) ChemPhysChem 3:833
- Solimannejad M, Azimi G, Pejov Lj (2004) Chem Phys Lett 400:185
- Solimannejad M, Azimi G, Pejov Lj (2004) Chem Phys Lett 391:201
- Solimannejad M, Alikhani ME (2005) Chem Phys Lett 406:351
- Solimannejad M, Alkorta I (2006) J Phys Chem A 110:10817
- Solimannejad M, Scheiner S (2006) Chem Phys Lett 429:38
- Solimannejad M, Scheiner S (2006) J Phys Chem A 110:5948
- Solimannejad M, Shirazi SG, Scheiner S (2007) J Phys Chem A 111:10717
- Solimannejad M, Nielsen CJ, Scheiner S (2008) Chem Phys Lett 466:136
- Solimannejad M, Massahi S, Scheiner S (2009) J Mol Struct (Theochem) 913:50
- Solimannejad M, Scheiner S (2009) Mol Phys 107:713
- Solimannejad M, Jamshidi FH, Amani S (2010) Struct Chem 913:50
- Qi XJ, Liu L, Fu Y, Guo QX (2005) Struct Chem 16:347
- Bil A, Latajka Z (2006) J Comput Chem 27:287
- Helmut S (1993) Eur J Biochem 215:213
- Hiraoka W, Kuwabara M, Sato F, Matsuda A, Ueda T (1990) Nucleic Acids Res 18:1217
- Torrent-Sucarrat M, Anglada JM (2004) ChemPhysChem 5:183
- Lai CH, Chou PT (2007) J Comput Chem 28:1357
- Wang BS (2000) J Mol Struct (Theochem) 505:241
- Du ST, Francisco JS (2009) J Chem Phys 130:124304
- Matthews CN, Minard RD (2006) Faraday Discuss 133:393
- Brown RD, Godfrey PD, Storey JWV, Clark FO (1976) Nature 262:672
- Ferris JP, Hagan WJ Jr (1984) Tetrahedron 40:1093
- Liebman SA, Pesce-Rodriguez RAP (1994) Adv Space Res 15:71
- McDowell Sean AC (2001) J Chem Phys 115:15



37. Heikkilä A, Lundell J (2000) *J Phys Chem A* 104:6637
38. Heikkilä A, Pettersson M (1999) *J Phys Chem A* 103:2945
39. Li RJ, Li ZR (2003) *J Phys Chem A* 107:6306
40. Jing B, Li Q, Gong B, Cheng J, Li W, Liu Z (2010) *Mol Phys* 108:1655
41. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Montgomery JA Jr., Vreven T, Kudin KN, Burant JC, Millam JM, Iyengar SS, Tomasi J, Barone V, Mennucci B, Cossi M, Scalmani G, Rega N, Petersson GA, Nakatsuji H, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Klene M, Li X, Knox JE, Hratchian HP, Cross JB, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Ayala PY, Morokuma K, Voth GA, Salvador P, Dannenberg JJ, Zakrzewski VG, Dapprich S, Daniels AD, Strain MC, Farkas O, Malick DK, Rabuck AD, Raghavachari K, Foresman JB, Ortiz JV, Cui Q, Baboul AG, Clifford S, Cioslowski J, Stefanov BB, Liu G, Liashenko A, Piskorz P, Komaromi I, Martin RL, Fox DJ, Keith T, Al-Laham MA, Peng CY, Nanayakkara A, Challacombe M, Gill PMW, Johnson B, Chen W, Wong MW, Gonzalez C, Pople JA (2003) GAUSSIAN03, revision B.03. Gaussian Inc, Pittsburgh
42. Riley KE, Pitonak M, Jcerny J, Hobza P (2010) *Chem Theory Comput* 6:66
43. Boys SF, Bernardi F (1970) *Mol Phys* 19:553
44. Alkorta I, Trujillo C, Elguero J, Solimannejad M (2011) *Comput Theor Chem* 967:147
45. Bader RFW (1990) In: Halpen J, Green MLH (eds) *The international series of monographs of chemistry*. Clarendon Press, Oxford
46. Biegler-König F, Schönbohm J (2002) AIM2000 Program Package, Ver. 2.0. University of Applied Sciences, Bielefeld, Germany
47. Tomasi J, Mennucci B, Cammi R (1993) *Chem Rev* 105:2999
48. Domagała M, Matczak P, Palusiak M (2012) *Comput Theor Chem* 998:26
49. Solimannejad M, Nassirinia N, Amani S (2012) *Struct Chem*. doi: [10.1007/s11224-012-0116-x](https://doi.org/10.1007/s11224-012-0116-x)
50. Lucas X, Estarellas C, Escudero D, Frontera A, Quiñonero D, Deyà PM (2009) *Chem Phys Chem* 10:2256
51. Gong B, Jing B, Li Q, Liu Z, Li W, Cheng J, Zheng Q, Sun J (2010) *Theor Chem Acc* 127:303
52. White JC, Davidson ER (1990) *J Chem Phys* 93:8029
53. Valiron P, Mayer I (1997) *Chem Phys Lett* 275:46
54. Hankins D, Moskowitz JW, Stillinger FH (1970) *J Chem Phys* 53:4544
55. Li QZ, Wang NN, Yu ZW (2007) *J Mol Struct (Theochem)* 847:68
56. Li QZ, An XL, Gong BA, Cheng JB (2007) *J Phys Chem A* 111:10166
57. Solimannejad M, Gharabaghi M, Alkorta I (2012) *Struct Chem*. doi: [10.1007/s11224-012-0099-7](https://doi.org/10.1007/s11224-012-0099-7)