ORIGINAL PAPER

Structures and energies of the radicals and anions generated from chlorpyrifos

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Abstract The radicals and anions generated from chlorpyrifos by removing a hydrogen atom have been investigated using the hybrid density functional B3PW91 method. The results show that all the radicals have been classified as three groups and their stability order is methylene (radical **1**, **3**, **5**, and **7**) > methyl (radical **9**, **11** and **13**) > ring (**15**); the anions have the relative energetic order: methyl > methylene > ring. Moreover, some decomposition reactions are also reported. The large HOMO-LUMO gaps indicate that both radicals and anions are predicted to be high-kinetic stable molecules. We also find that radicals **9**, **11** and **13** have the highest AEAs and anions **2**, **4** and **6** have higher VDEs. Additionally, natural population analysis charges show that there is the lowest Δq (0.14) for the C7 and C9 atoms. We hope that our theoretical results may provide a reference for further experiment and practical application.

Keywords Adiabatic electron affinity · Chlorpyrifos · Density functional theory · HOMO-LUMO gap · Relative stability · Vertical detachment energy

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Introduction

In recent years, computer-aided investigations for drug molecules and biomolecules have been extensively reported in the literature. These calculations have greatly performed in the role of some important properties, such as the bond dissociation energy, the molecular adiabatic electron affinity (AEA), the vertical detachment energy (VDE), and photoelectron spectra [1–7]. For understanding these properties, more detailed information about molecular geometries is an essential prerequisite. Now many theoretical and experimental studies have been carried out at the molecular level. For example, Lacaze-Dufaure et al. [8] studied the G3-Factor and two derivatives (G3Me and G3F), and found that their geometric parameters obtained by the density functional theory (DFT) calculations are in agreement with available experimental results. O'Malley [9] predicted the geometry and electron affinity of hydrogen bonded 1,4-benzoquinone. It was found that the two electron reduction of 1,4-benzoquinone (BQ) to the dianion (BQ^{2-}) via the semi-quinone radical anion (BQ^{-}) form is accompanied by a gradual change in the internal geometry of the quinone from quinonoid to benzenoid form. Teberekidis et al. [10] reported the theoretical study of hydrogen bond interactions of felodipine with polyvinylpyrrolidone and polyethyleneglycol at the density functional level of theory with the B3LYP exchange correlation functional. It was shown that the vibrational properties as well as the ^{1}H and ^{13}C NMR spectroscopic properties calculated for the most stable isomer are in satisfactory agreement with the experimental data. Baranovski et al. [11] calculated the electron affinities of several aromatic compounds and their diimino-derivatives by means of quantum chemical method. They concluded that addition of imino groups increases the electron affinities of

the molecules up to 2–2.5 eV. Wolken and Turecek [12] also investigated the isomeric radicals corresponding to hydrogen atom adducts to 2-hydroxypyridine and 2-pyridone using neutralization-reionization mass spectrometry and ab initio and density functional theory calculations. Additionally, a number of other radicals and the analogous anions are interesting both theoretically and experimentally [13–18].

In this research, we investigate the electron affinities of the radicals generated from chlorpyrifos by removing a hydrogen atom. As we know, there are no experimental and theoretical values for the electron affinities of these radicals. However, the knowledge of the electron affinity is essential for the understanding of their properties as environmental protection. Moreover, the chlorpyrifos has played a key role in the environment to control domestic and agricultural pests [19–24]. Therefore, it is of essential interest to explore structures and a variety of physical and chemical properties, and the investigations on the radicals and anions are also indispensable for understanding chemical reactivity and making predictions about inter-mediates and reaction mechanism. With this motivation, we have performed a detailed study of structures and electron affinities of these radicals and their anions using density functional theory.

Computational details

Density functional theory method has been widely used to study the structures and properties of molecules, requiring much less computational effort than convergent quantum mechanical methods. In this study, all structures were fully optimized using the hybrid density functional B3PW91 method, which is a linear combination of Becke's three-parameter (B3) hybrid exchange functional [25] with the correlation functional of Perdew and Wang (PW91) [26]. The method was also checked to be more accurate to provide reliable results [27, 28]. Considering the high computational costs and accuracy, the 6-31G(d,p) basis set was utilized here. Meanwhile, the natural population analysis method of Weinhold and coworkers [29] was carried out to reveal the difference of natural charges between the radical and anion species. So the optimized structures, relative energies, the HOMO-LUMO gaps, zero-point corrected adiabatic electron affinities, vertical detachment energies, and natural charges of the radicals and anions generated from chlorpyrifos by removing a hydrogen atom were investigated at the B3PW91/6-31G (d,p) level of theory. All the quantum chemical calcu-lations were performed with the Gaussian 09 software package [30]. Vibrational frequency evaluations were done on all the stable radicals and anions at the same theoretical level.

The adiabatic electron affinities were evaluated as the difference between the absolute energies of the radical and the corresponding anion species in the following manner: AEA = E(zero-point corrected neutral) - E(zero-point corrected anion); and the vertical detachment energies were computed as the energy difference between the neutral species and the anion species both at the optimized anion geometry: VDE = E(neutral at optimized anion geometry) - E(optimized anion).

Results and discussion

The optimized structure of chlorpyrifos obtained at the B3PW91/6-31G(d,p) level of theory is shown in Fig. 1, and the numbering schemes are also depicted. According to the calculated results, the N–C bond lengths of ring are 1.318 and 1.320 Å, respectively. The C–C bond lengths of ring are 1.387–1.406 Å. The O–P bond lengths are 1.649, 1.604 and 1.597 Å, respectively. The S–P bond length is 1.922 Å. In addition, the dihedral angles are 81.5 and 7.4º for P-O2-C8-C9 and P-O3-C6-C7, respectively. This candidate structure was used to generate all the radicals and anions considered in the present investigation. These radicals were generated from chlorpyrifos by removing a hydrogen atom. And the corresponding anions were obtained starting from the optimized radical geometries.
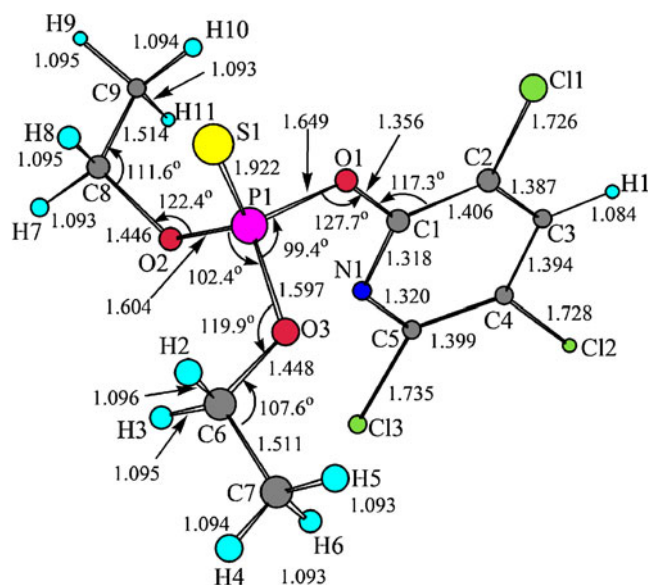
Fig. 1 Optimized structure of chlorpyrifos obtained at the B3PW91/6-31G(d,p) level of theory. The atoms are indicated with the following colors: C gray, Cl green, H blue, N navy blue, O red, S yellow, and P pink. And they are numbered respectively from the beginning of one. Bond lengths and major bond angles are also shown. All bond lengths are in angstrom, bond angles are in degree

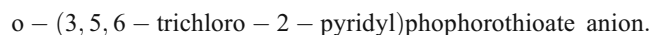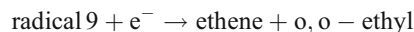Optimized structures and relative stabilities of the radicals and anions

The relative energies and optimized equilibrium geometries of radicals and anions derived from chlorpyrifos at the B3PW91/6-31G(d,p) level are shown in Table 1. The radicals are ordered with increasing energy and the corresponding anions are also followed at this theoretical level. Bond lengths and major bond angles of the most stable radical 1 and anion 2 are depicted in Figs. 2 and 3, respectively. The chlorpyrifos molecule contains eleven hydrogen atoms, but only eight of the possible radicals have unique structures. This is due to that the two optimized structures, by removing H4 or H6 bonded on the C7 atom, are equivalent, and the optimized structures by removing any hydrogen atom bonded on the C9 atom are equivalent.

As can be seen from Table 1, the radical 1 is the most stable structure. The radical 3 and 5 are higher in energy by only 0.3 and 0.4 kcal mol^{-1}, respectively. However, the radical 15 produced at the ring are found to be the highest in energy by more than 18.2 kcal mol^{-1}. According to the calculated energies, we find that the same chemical groups almost have the same stability order, and all the radicals have been classified as three groups; their stability order is methylene (radical 1, 3, 5, and 7) > methyl (radical 9, 11 and 13) > ring (15). That is to say, the hydrogen atoms on the methylene are easy to be dissociated.

Compared to the structure of chlorpyrifos, the frameworks of these radicals have not been changed. Geometric distortions are only done on the relevant groups which remove a hydrogen atom. Detailed structure information for the most stable radical 1 is

presented in Fig. 2. When the H7 hydrogen atom bonded on the C8 atom is removed to form the radicals 1, the C8 atom contains an unpaired electron, and the C8-C9 and C8-O2 bond lengths are shorten by 0.036 and 0.056 Å, respectively. This is because the carbon atom goes from tetrahedral sp^3 hybridization to almost planar sp^2 hybridization, and its electron distribution is also affected. However, other bond lengths and major bond angles of radical 1 show very small difference with respect to neutral molecule, indicating that its other chemical groups are almost unaffected by radical production.

The anions generated from the radicals by adding an extra electron may be divided into two categories. Firstly, we report that some anions undergo a dissociation of one or more than one bonds. Secondly, other anions show only drastic geometrical distortions with respect to the original radicals. In the first category, taking the most stable anion 2 as an example, we observe its connectivity from the original radical 9, and prefer to know the energetics of the bond break at the B3PW91/6-31G(d,p) level of theory. The reaction of radical 9 with an electron leads to the loss of an ethene from the O2 position, and this reaction is also presented at the same theoretical level:

$$radical\ 9 + e^- \rightarrow ethene + o, o - ethyl$$

$$o - (3, 5, 6 - trichloro - 2 - pyridyl)phophorothioate\ anion.$$

Here, the energy change (ΔE) is found to be obviously negative: −77.6 kcal mol^{-1}. This indicates that the dissociation reaction is highly exothermic. The scheme of the decomposition reaction of the radical 9 is reported as follows:
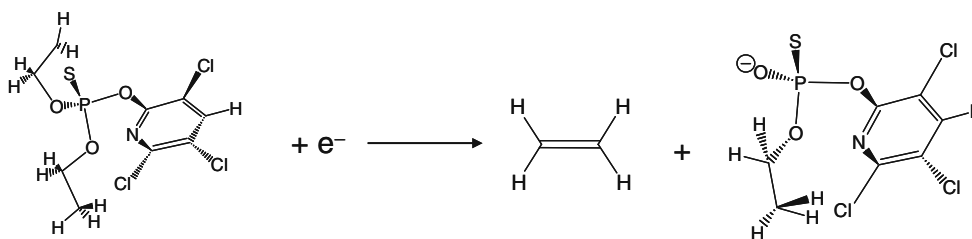
As can be seen from Fig. 3, the C8-O2 bond length of the most anion 2 is 2.218 Å. Similarly, the anions 4 and 6 are produced by adding an extra electron to the radicals 11 and 13, respectively. Their anions also undergo the loss of an ethene from the O2 position, and

the dissociation reactions are energetically favorable, being −77.7 and −77.8 kcal mol^{-1}. Meanwhile, we find that the anion 16 show minor rearrangements in the structure with respect to the original radical 15 (shown in Table 1). All the anions have the following relative

Table 1 The relative energies and optimized equilibrium geometries and of radicals and anions derived from chlorpyrifos at the B3PW91/6-31G(d, p) level of theory

No.[a]	Structure	Energy	No.[a]	Structure	Energy
1 radical C8-H7		−2748.86932 0.0	2 anion C9-H9[b]		−2748.99118 0.0
3 radical C6-H2		−2748.86881 0.3	4 anion C7-H4[c]		−2748.99040 0.5
5 radical C6-H3		−2748.86874 0.4	6 anion C7-H5		−2748.99029 0.6
7 radical C8-H8		−2748.86701 1.5	8 anion C6-H2		−2748.94976 26.0
9 radical C9-H9[b]		−2748.86033 5.6	10 anion C8-H8		−2748.94963 26.1
11 radical C7-H4[c]		−2748.85957 6.1	12 anion C6-H3		−2748.94884 26.6
13 radical C7-H5		−2748.85950 6.2	14 anion C8-H7		−2748.94550 28.7
15 radical C3-H1		−2748.84038 18.2	16 anion C3-H1		−2748.94245 30.6

Total energies are in Hartree, ZPVE-corrected relative energies are in kcal mol^{-1}

[a] The Cn-Hn is indicated that the Hn atom bonded on the Cn atom is removed to form the radicals and the corresponding anions from chlorpyrifos

[b] In the radicals and anions from chlorpyrifos, the optimized equilibrium structures are H10=H11=H9

[c] In the radicals and anions from chlorpyrifos, the optimized equilibrium structure is H6=H4

energetic order: methyl (the carbon C7 and C9 atoms) > methylene (the carbon C6 and C8 atoms) > ring (the carbon C3 atom).

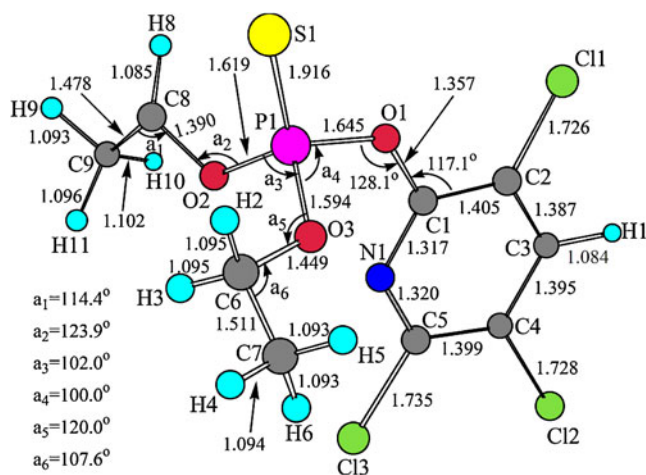Additionally, the previous studies [31, 32] show that the ring in the chlorpyrifos (CPF) molecule is easy to be dissociated. For comparison, we have reported the decomposition reaction by removing a ring from CPF molecule. And the reaction by removing a hydrogen atom to form the most radical **1** is also described as follows:
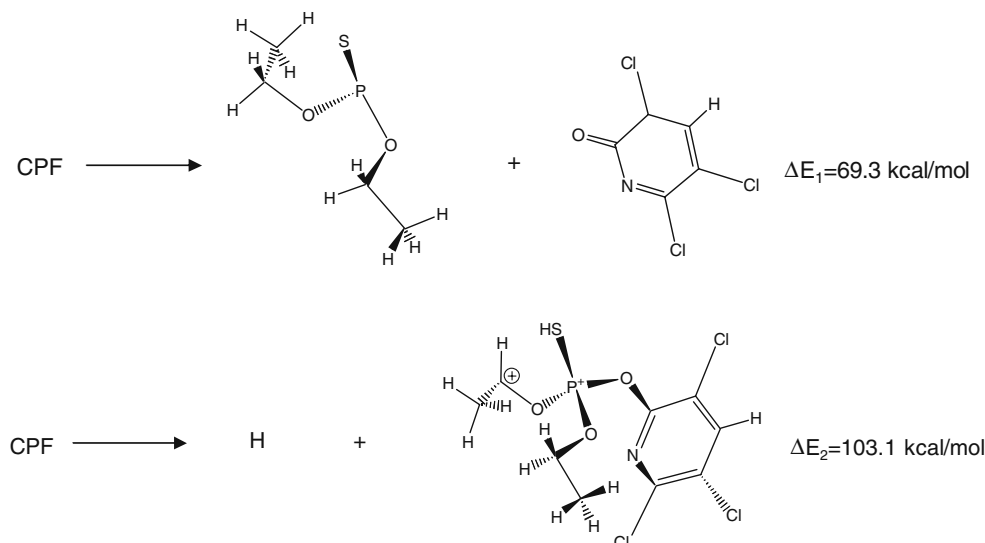
As can be seen from the above reactions, the dissociation energy ΔE_1 is 69.3 kcal mol^{-1} at the room temperature which is lower than the ΔE_2 value by 33.8 kcal mol^{-1}. Thus, it is deduced that the decomposition reaction which removes a ring from CPF molecule is easier than ones which remove a hydrogen atom. The result is consistent with the report obtained by Getzin [31] and Racke [32].

Calculated HOMO-LUMO gaps, adiabatic electron affinities, and vertical detachment energies

We report the calculated HOMO-LUMO gaps of the radicals and anions generated from chlorpyrifos by removing a hydrogen atom using the hybrid density functional B3PW91 method, and these energy gaps are listed in Table 2. As can be seen from Table 2, both radicals and

Fig. 2 Bond lengths and major bond angles of the most stable radical **1**, obtained at the B3PW91/6-31G(d,p) level of theory. All bond lengths are in angstrom, bond angles are in degree

Fig. 3 Bond lengths and major bond angles of the most stable anion **2**, obtained at the B3PW91/6-31G(d,p) level of theory. All bond lengths are in angstrom, bond angles are in degree

Table 2 The calculated HOMO-LUMO gaps (E_{gap}), dipole moments, the zero-point corrected adiabatic electron affinities (AEAs) of the radicals, and vertical detachment energies (VDEs) of the anions derived from chlorpyrifos at the B3PW91/6-31G(d,p) level of theory

Structure	Dipole	E_{gap}	AEA	Structure	Dipole	E_{gap}	VDE
1 C8-H7	2.40	3.53	2.07	2 C9-H9	10.07	3.58	4.28[a]
3 C6-H2	2.57	3.65	2.20	4 C7-H4	9.12	3.81	4.42
5 C6-H3	1.92	3.66	2.18	6 C7-H5	8.99	3.82	4.42
7 C8-H8	2.33	3.75	2.25	8 C6-H2	5.72	3.97	3.91
9 C9-H9	2.22	4.49	3.56	10 C8-H8	7.20	3.97	3.88
11 C7-H4	2.24	4.52	3.56	12 C6-H3	6.25	3.94	3.88
13 C7-H5	2.34	4.57	3.56	14 C8-H7	6.63	3.75	3.73
15 C3-H1	2.75	3.06	2.78	16 C3-H1	9.72	4.65	3.29

HOMO-LUMO gaps, the zero-point corrected adiabatic electron affinities, and vertical detachment energies are in eV, dipole moments are in Debye

anions have very large gaps (more than 3.0 eV). We also find that some radicals removed a hydrogen atom on the methyl group and have larger energy gaps (about 4.5 eV). But as for the anions, the anion which removed a hydrogen atom on the ring has the largest gap (4.65 eV). A large HOMO-LUMO gap can be associated with high-kinetic stability. This is due to that the molecules with a large gap are energetically unfavorable to add electrons to a high-lying LUMO or to extract electrons from a low-lying HOMO, and to form the activated complexes of any potential reaction [33–39]. Thus, these radicals and anions are predicted to be high-kinetic stable molecules. In addition, it is observed that the anions possess much larger dipole moments, which can be explained from the distorted anion structures.

The zero-point corrected adiabatic electron affinities (AEAs) and vertical detachment energies (VDEs) generated from chlorpyrifos are reported in Table 2. For the AEAs, their values are found to be large and spread over a range of 2.07–3.56 eV. In particular, radicals **9**, **11** and **13**, generated by removing a hydrogen atom from the methyl group, have the highest AEAs (3.56 eV), and this is easily understood because the methylene group has a high tendency to accommodate a negative charge. Radicals **1**, **3**, **5**, and **7** show smaller AEAs. For the VDEs, the larger values are found to be a range of 4.28–4.44 eV, which values are produced from anions **2**, **4**, and **6**. Moreover, these anions are also generated by removing a hydrogen atom from the methyl group as well as radicals **9**, **11**, and **13**. The smallest VDE is found for anion **16** (3.29 eV). In comparison with the AEAs, we may see that significant differences (more than 1 eV) between VDEs and the corresponding AEAs are found for anions **8**, **10**, **12**, and **14**. The previous studies have also reported the differences for some molecules [3, 40]. For the other anions, there is little difference between VDEs and the corresponding AEAs.

Table 3 Natural population analysis charges of radicals and anions derived from chlorpyrifos at the B3PW91/6-31G(d,p) level of theory

Radicals		Anions		Δq[a]
Structure	Charge on Cn atom	Structure	Charge on Cn atom	
C3-H1(15)	0.23	C3-H1(16)	−0.22	0.45
C6-H2(3)	0.14	C6-H2(8)	−0.31	0.46
C6-H3(5)	0.14	C6-H3(12)	−0.31	0.45
C7-H4(11)	−0.35	C7-H4(4)	−0.49	0.14
C7-H5(13)	−0.35	C7-H5(6)	−0.48	0.14
C8-H7(1)	0.14	C8-H7(14)	−0.33	0.47
C8-H8(7)	0.16	C8-H8(10)	−0.28	0.44
C9-H9(9)	−0.34	C9-H9(2)	−0.48	0.14

For comparing the difference between the radical and anion charges on the Cn atom, we have listed their same structural order of radicals and anions. The stability order is in parentheses.

[a] Δq represent the difference between the radical and anion charges for each structure, $\Delta q = q_{radical} - q_{anion}$.

Natural population analyses

The natural population analysis (NPA) charges are computed and listed in Table 3. In Table 3 we show the charge on the Cn atoms for both the radicals and the anions in the same structural order. And we also compute the difference between the radical and anion charges to explore how the anion's excess charge will be redistributed in the molecule. For the stable radicals, we find that the charge is negative for C7 and C9 atoms (−0.35, −0.35 and −0.34, respectively) and positive for C3, C6, and C8 atoms. When adding an extra electron to the radicals, the charge on the C7 and C9 atoms is more negative, being −0.49, −0.48 and −0.48, respectively. However, there is the lowest Δq (0.14) for the C7 and C9 atoms. This is because when the radicals obtain an electron to form the corresponding anions, they undergo the decomposition reaction, which result in the excess charge is mostly on the O2 atom. In the meanwhile, the charge on the C3, C6, and C8 atoms has much higher Δq values, indicating these atoms are main sites for accommodating the electron. These charge-transfers may help us understand the molecular properties and the reaction mechanisms.

Conclusions

In this work, we have investigated the radicals and anions generated from chlorpyrifos by removing a hydrogen atom using the hybrid density functional B3PW91 method. Some molecular properties have been considered on the stable structures, including equilibrium structures, relative energies, the HOMO-LUMO gaps, zero-point corrected adiabatic electron affinities, vertical detachment energies, and natural population analysis charges. The results show that all the radicals have been classified as three groups and their stability order is methylene (radical **1**, **3**, **5**, and **7**) > methyl (radical **9**, **11**, and **13**) > ring (**15**). That is to say, the hydrogen atoms on the methylene are easy to be dissociated. The anions have the relative energetic order: methyl > methylene > ring. Some decomposition reactions are also reported. Moreover, it is found that the decomposition reaction by removing a ring from CPF molecule is easier than ones by removing a hydrogen atom. The large HOMO-LUMO gaps indicate that both radicals and anions are predicted to be high-kinetic stable molecules. We also see that radicals **9**, **11**, and **13** have the highest AEAs and anions **2**, **4**, and **6** have higher VDEs. Moreover, significant differences (more than 1 eV) between VDEs and the corresponding AEAs are found for anions **8**, **10**, **12**, and **14**. Additionally, natural population analysis charges show that there is the lowest Δq (0.14) for the C7 and C9 atoms. We hope that our theoretical results may provide a reference for further experiment and practical application.

References

1. Chen ECM, Chen ES (2000) J Phys Chem B 104:7835–7844
2. Manojkumar TK, Choi HS, Tarakeshwar P, Kim KS (2003) J Chem Phys 118:8681–8686
3. Evangelista FA, Paul A, Schaefer HF III (2004) J Phys Chem A 108:3565–3571
4. Kumar A, Mishra PC, Suhai S (2005) J Phys Chem A 109:3971–3979
5. Wetmore SD, Boyd RJ, Eriksson LA (2000) Chem Phys Lett 322:129–135
6. Bondesson L, Mikkelsen KV, Luo Y, Garberg P, Agren H (2006) J Mol Struct Theochem 776:61–68
7. Li X, Sevilla MD, Sanche L (2003) J Am Chem Soc 125:8916–8920
8. Lacaze-Dufaure C, Najjar F, André-Barrès C (2007) J Mol Struct Theochem 803:17–21
9. O'Malley PJ (1997) Chem Phys Lett 274:251–254
10. Teberekidis VI, Sigalas MP (2007) J Mol Struct Theochem 803:29–38
11. Baranovski VI, Denisova AS, Kuklo LI (2006) J Mol Struct Theochem 759:111–115
12. Wolken JK, Turecek F (1999) J Phys Chem A 103:6268–6281
13. Rienstra-Kiracofe JC, Tschumper GS, Schaefer HF III, Nandi S, Ellison GB (2002) Chem Rev 102:231–282
14. Sarma RL, Karim M, Medhi C (2007) J Mol Struct Theochem 805:17–25
15. Ramírez-Arizmendi LE, Heidbrink JL, Guler LP, Kenttämaa HI (2003) J Am Chem Soc 125:2272–2281
16. Gao A, Gao J, Xu W (2007) J Mol Struct Theochem 815:45–53
17. Furuya K, Torii H, Furukawa Y, Tasumi M (1998) J Mol Struct Theochem 424:225–235
18. Dubbs MD, Gupta RB (1998) J Chem Eng Data 43:590–591
19. Mehta A, Verma RS, Srivastava N (2008) Environ Mol Mutagen 49:426–433
20. Eyer F, Roberts DM, Buckley NA, Eddleston M, Thiermann H, Worek F, Eyer P (2009) Biochem Pharmacol 78:531–537
21. Gordon CJ, Yang YL (2000) Pharmacol Toxicol 87:6–10
22. Smith JN, Campbell JA, Busby-Hjerpe AL, Lee S, Poet TS, Barr DB, Timchalk C (2009) Toxicol 261:47–58
23. Palanisami S, Prabaharan D, Uma L (2009) Pesticide Biochem Physiol 94:68–72
24. Saulsbury MD, Heyliger SO, Wang K, Johnson DJ (2009) Toxicol 259:1–9
25. Becke AD (1993) J Chem Phys 98:5648–5652
26. Perdew JP, Wang Y (1992) Phys Rev B 45:13244–13249
27. Su KH, Wei J, Hu XL, Yue H, Lü L (2000) Acta Phys Chim Sin 16:643–651
28. Su KH, Wei J, Hu XL, Yue H, Lü L (2000) Acta Phys Chim Sin 16:718–723
29. Reed AE, Curtiss LA, Weinhold F (1988) Chem Rev 88:899–926
30. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima HY, Kitao O, Nakai H, Vreven T, Montgomery JA, Peralta JE Jr, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ (2009) Gaussian 09, Revision A.02. Gaussian Inc, Wallingford, CT
31. Getzin LW (1981) J Econ Entomol 74:158–162

32. Racke KD (1993) Rev Environ Contam Toxicol 131:1–154
33. Manolopoulos DE, May JC, Down SE (1991) Chem Phys Lett 181:105–111
34. Li XJ (2009) J Mol Struct Theochem 896:25–29
35. Li XJ, Jiao GS (2009) J Mol Struct Theochem 893:26–30
36. Peng S, Li XJ (2009) Spectrochim Acta Part A 73:67–71
37. Yue Y, Li XJ (2009) Int J Quantum Chem. doi:10.1002/qua.22393
38. Sun Z, Li X, Tian M, Zhao G, Li J, Ma B (2009) J Mol Struct Theochem 913:265–269
39. Zhang Y, Peng S, Li XJ, Zhang DX (2009) J Mol Struct Theochem 906:41–45
40. Xu W, Gao A (2005) J Mol Struct Theochem 732:63–70