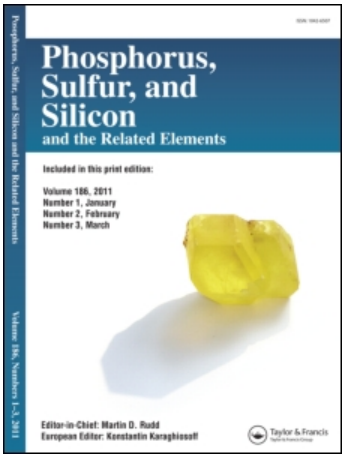

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Theory Study on Toxicity of the Organic Phosphorus Pesticide

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Theory Study on Toxicity of the Organic Phosphorus Pesticide

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Some organic phosphorus pesticides have been studied with ab initio method. Their total energies, atomic charges, dipole moments, multipole moments, molecular orbital compositions, orbital energies, etc. were obtained. The relationship between the total atomic charge of P and toxicity is basically in accordance with the experimental results.

Keywords *ab initio*; bond length; charge; organic phosphorus pesticide; toxicity

The organic phosphorus pesticide is a good insecticide. It has a very great function to ensure the agriculture bumper harvest. But it will also poison persons and animals. The main harm that the organic phosphorus pesticide causes to humans and animals is the surroundings mental derangement from the damage done to the pass neurotic. Between toxicity and structure of the organic phosphorus, pesticide has close inside contact. The *ab initio* ("from the beginning") calculation method would be a better method to solve this problem.

CALCULATION METHOD

Hartree-Fock method at the 6-31+G(d) level was employed to calculate the atomic charges, total energies, dipole moments, multipole moments, molecular orbital compositions, orbital energies, and so on of compounds of the organic phosphorus pesticide.

Molecular geometries of the organic phosphorus agrochemical are fully drawn with ChemDraw version 8.0.3 (ChemDraw is a tool that enables professional scientists, science students, and scientific authors

The auther thanks Guizhou University High Performance Computational Chemistry Laboratory.

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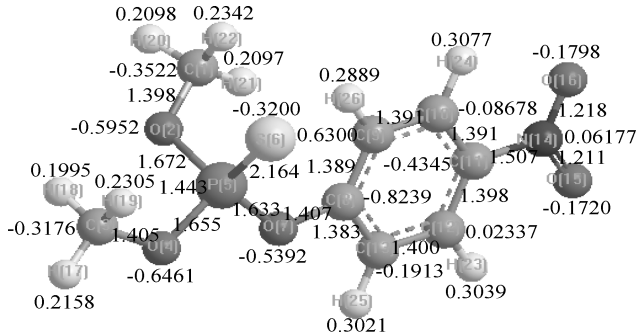


FIGURE 1 Bond lengths and total atomic charges of methyl parathion.

to communicate chemical structures). Geometry parameters are optimized with MOPAC (Molecular Orbital PACkage) of the Chem3D version 8.0.3 (Chem3D is an application that enables scientists to model chemicals). The input calculation files are directly created with Gaussian 98 (Gaussian 98 can serve as a powerful tool for exploring areas of chemical interest such as substituent effects, reaction mechanisms, potential energy surfaces, and excitation energies). All the calculations were carried out on the server of Guizhou University's high performance computation chemistry laboratory.

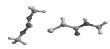
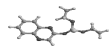
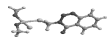
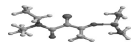
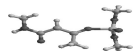
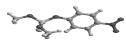
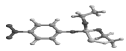
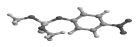
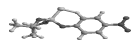
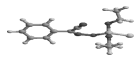
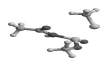
RESULTS AND DISCUSSION

Part of the calculated bond lengths and total atomic charges of methyl parathion are shown in Figure 1. Parts of the calculated bond lengths, the calculated total atomic charges, and the toxicity of phosphorus pesticides are listed in Table I.

Bond Length

7 sets of homologous organic phosphorus pesticides, which compare property with each other, are in the Table I. The bond length and toxicity of the phosphorus compound are positively related so that between the phosphorus atom and the atom of the main functional group connect with each other. Bond length is long and the toxicity is strong, the bond is short and the toxicity is small. This explains why the P-X bond splits easily, and why the organic phosphorus pesticide resolves easily.

TABLE I The Calculated Bond Lengths of P-X and Total Atomic Charges of a Phosphorous Atom

	Compound	Structure	Bond length P–X	Charge of P	Toxicity[1][2] LD50(mg/kg)
1	dimethoate		S 2.060739	0.157998	500~600
	folimat		S 2.516388	1.282291	30~60
2	quinalphos		O 1.601070	1.484277	62~137
	azinphose methyl		S 2.151919	0.112627	8.9
3	phosphamidon		O 1.853900	2.545263	28.3
	monocrotophos		O 1.874799	2.501057	13~23
4	methyl parathion		O 1.633240	1.442672	14
	parathion		O 1.676241	1.276033	13
5	methyl parathion		O 1.633240	1.442672	14
	parathion		O 1.690888	1.194937	13
6	phoxime		O 1.662674	1.247269	2170
	O,O-diethyl-O-penyl thiophosphate		O 1.663777	1.218846	800
7	methamidophos		N 2.454949	1.368161	30
	acephate		N 2.428593	1.482965	945

Charge

From the Table I, we can know that the charge of the phosphorus atom and toxicity of the phosphorus compound is negatively related, namely,

the charge of the phosphorus atom is positive, and the toxicity is small, and the charge is negative and the toxicity is strong.

In sum, the bond length between the phosphorus atom and the atom of the main functional group connected with each other is long and the toxicity is strong, the bond is short and the toxicity is small. The charge of the phosphorus atom is positive; the toxicity is small, the charge is negative, and the toxicity is strong.

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