Persulfate–Based Advanced Oxidation Process for Chlorpyrifos Degradation: Mechanism, Kinetics, and Toxicity Assessment

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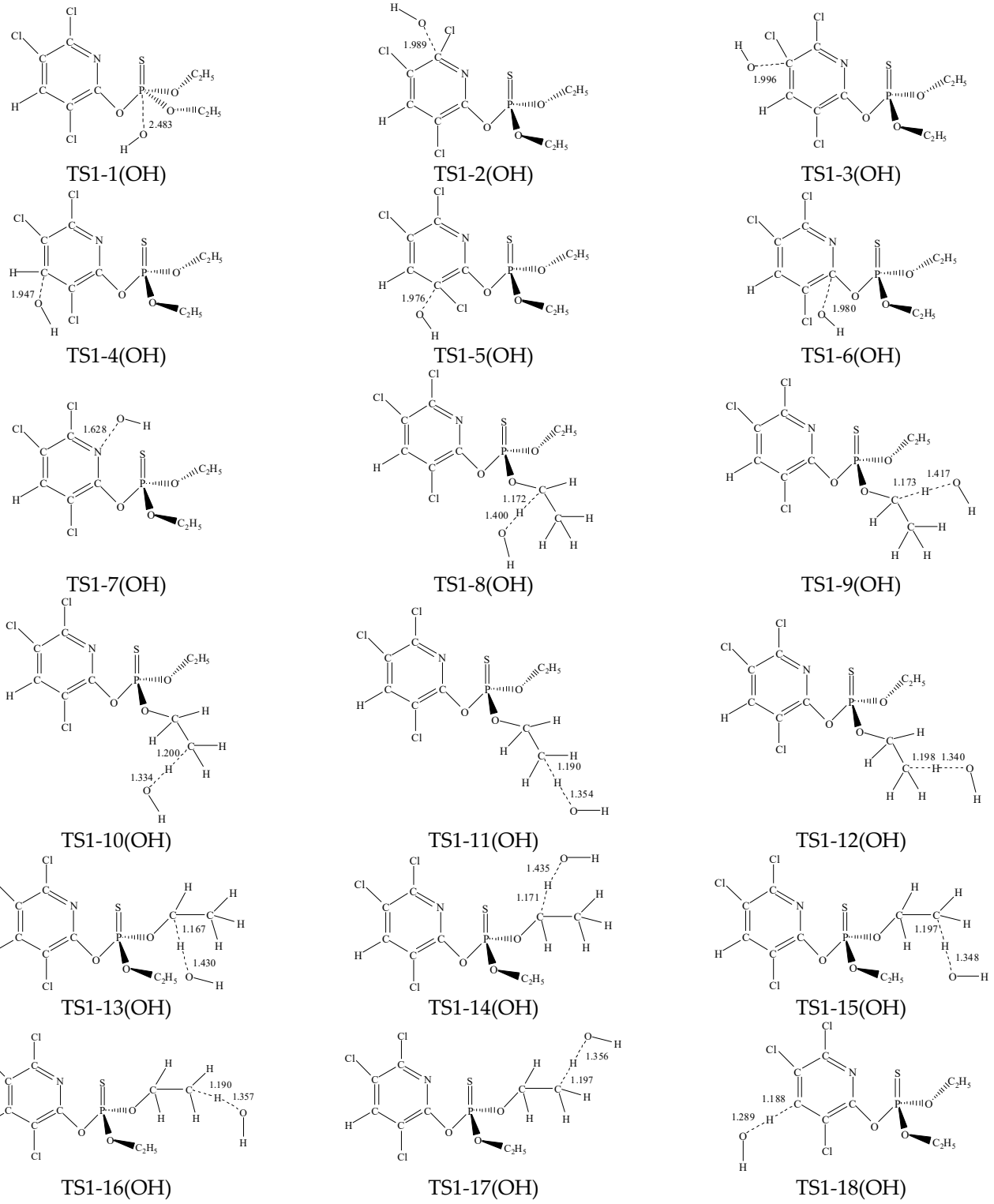
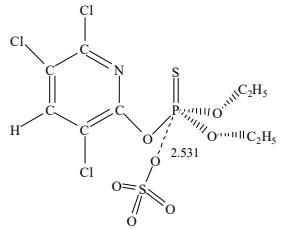


Figure S1. The optimized chemical conformations of TS for CPY with OH.



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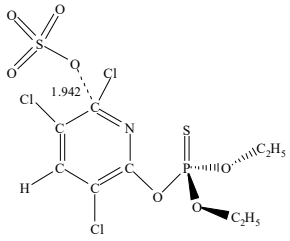

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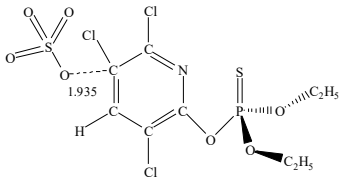

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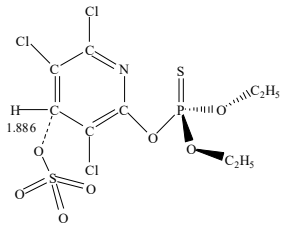

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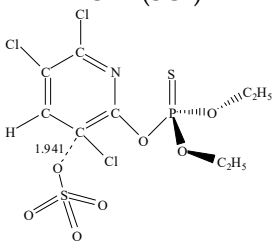

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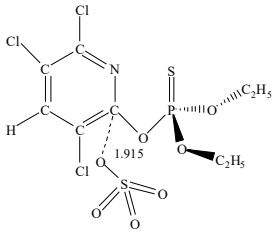

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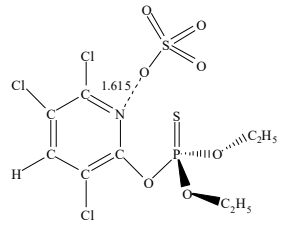

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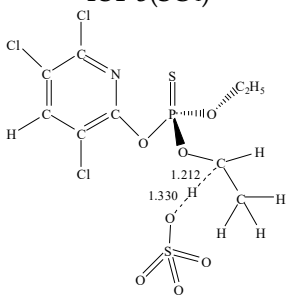

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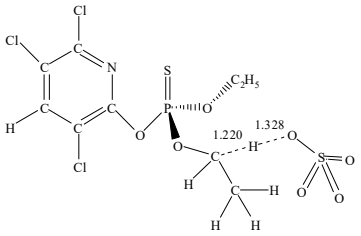

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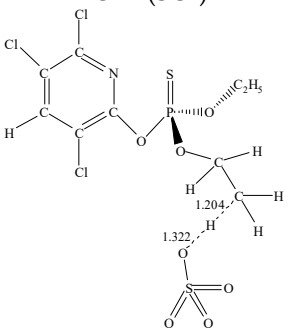

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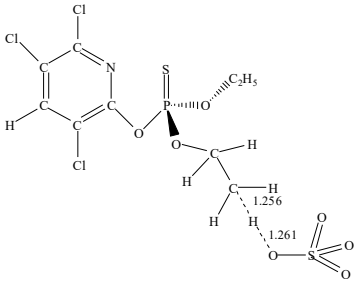

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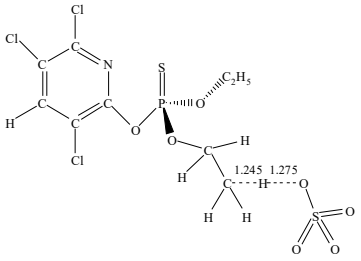

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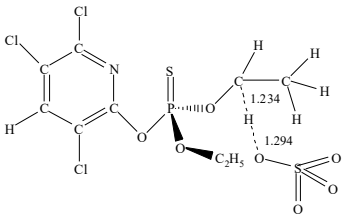

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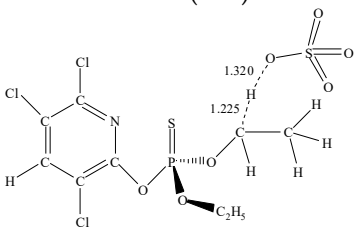

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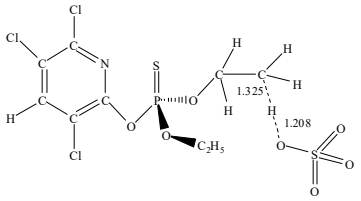

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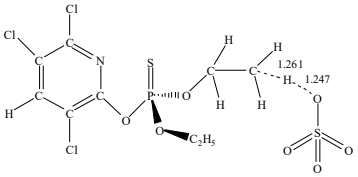

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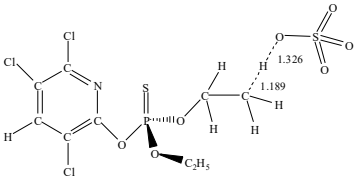

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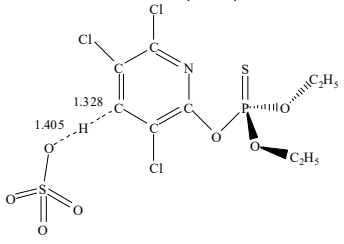


TS1-18(SO_4)

Figure S2. The optimized chemical conformations of TS for CPY with $SO_4^{\bullet-}$.

Table S1. The bond lengths of the calculated values and the experimental values of CPY.

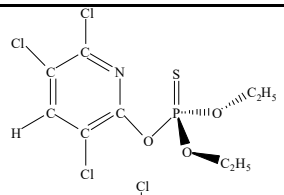
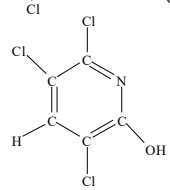
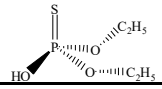
Bond	Calculated values (Å)	Experimental values (Å)	Relative errors
P1-O21	1.611	1.647	2.23%
P1-O23	1.562	1.593	1.98%
P1-O26	1.538	1.59	3.38%
P1=S22	1.898	1.921	1.21%
O23-O24	1.426	1.447	1.47%
C24-C25	1.44	1.512	5.00%
O26-C27	1.39	1.442	3.74%
C2-C3	1.37	1.394	1.75%
C3-C4	1.39	1.394	0.29%
C4-C5	1.37	1.384	1.02%
C5-C6	1.38	1.403	1.67%
C6-N7	1.308	1.319	0.84%
N7-C2	1.32	1.321	0.08%
C6-O21	1.364	1.347	1.25%

Table S2. The grading standards of the acute and chronic toxicity. The unit is $mg \cdot L^{-1}$.

Classification	Acute toxicity(1)	Chronic toxicity(2)
Very toxic	$LC_{50} \leq 1$ or $EC_{50} \leq 1$	$ChV \leq 0.1$
Toxic	$1 < LC_{50} \leq 10$ or $1 < EC_{50} \leq 10$	$0.1 < ChV \leq 1$
Harmful	$10 < LC_{50} \leq 100$ or $10 < EC_{50} \leq 100$	$1 < ChV \leq 10$
Not harmful	$LC_{50} > 100$ or $EC_{50} > 100$	$ChV > 10$

Criteria set by the Chinese hazard evaluation guidelines for new chemical substances (HJ/T 154–2004). Criteria set by the European Union (described in Annex VI of Directive 67/548/EEC).

Table S3. The toxicity value of the main transformation intermediates and products in the degradation of CPY. The unit is $mg \cdot L^{-1}$.

	Molecular Structure	ChV			LC_{50}		
		Fish	Daphnid	Algae	Fish	Daphnid	Algae
CPY		0.0065	0.000037	0.084	0.038	0.00019	0.176
P1		0.132	0.021	1.35	1.10	0.836	1.816
P2		0.359	0.00013	0.366	5.31	0.010	3.88

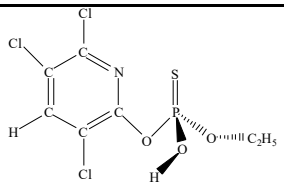
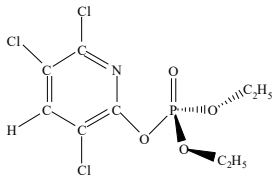
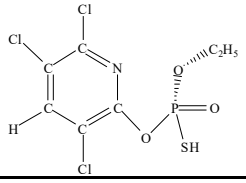
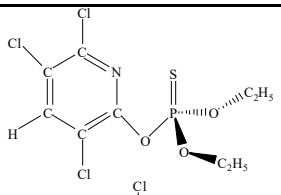
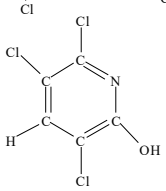
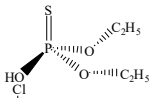
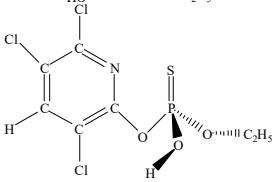
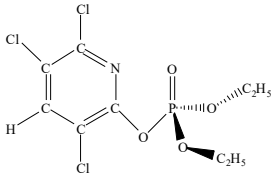
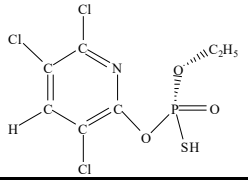
P3		0.015	0.000051	0.120	0.102	0.00044	0.338
P4	CH_3CH_2OH	245	83.1	81.9	3170	1480	486
P5		9.05	4.67	24.2	30.0	28.2	85.4
P6	CH_3CHO	12.1	0.242	4.20	29.0	32.6	15.1
P7/P8		1.34	6.66	6.42	19.5	44.1	20.0

Table S4. Estimated health effects of CPY and its transformation intermediates and products during the degradation process.

	Molecular Structure	Bioaccumulation factor	Developmental Toxicity	Mutagenicity
CPY		380.62	Developmental toxicant	Mutagenicity Negative
P1		73.23	Developmental NON-toxicant	Mutagenicity Negative
P2		2.66	Developmental NON-toxicant	Mutagenicity Negative
P3		143.97	Developmental toxicant	Mutagenicity Negative
P4	CH_3CH_2OH	1.26	Developmental NON-toxicant	Mutagenicity Negative
P5		109.09	Developmental toxicant	Mutagenicity Negative
P6	CH_3CHO	N/A	Developmental NON-toxicant	Mutagenicity Negative
P7/P8		N/A	Developmental toxicant	Mutagenicity Negative