

## Supporting Information

# **Initial Transformation Products Formation Mechanisms during Chlorination of the Indole Moiety: A Computational Study**

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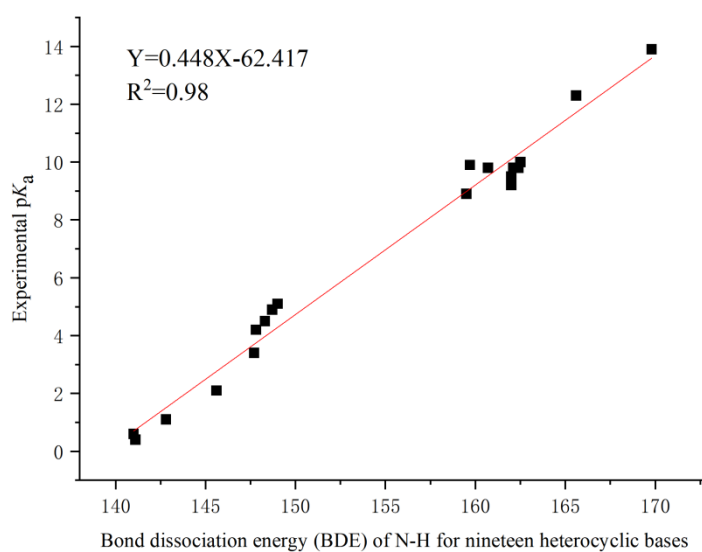
## Text S1

### Quantum Chemical LFER for Estimation of $pK_a$ Values

It is known that, based on the proton theory of acids and bases, acid is a donor of protons. Moreover, the stronger the ability to provide protons, the stronger the acidity. Therefore, the bond dissociation energy (BDE) of  $R_1NR_2(R_3)-H^+$  releasing proton and amine  $R_1NR_2(R_3)$ , as shown in Eq. 1, can be as an indicator of acidity.



Thus, the BDEs of N-H bonds in nineteen heterocyclic bases were calculated at the M06-2X/cc-pVTZ level with the SMD solvent model. Then the correlation between the BDEs and experimental  $pK_a$  values was established and illustrated in Figure S1 and Table S1, the squared correlation coefficient for the above system is  $R^2 = 0.98$ .

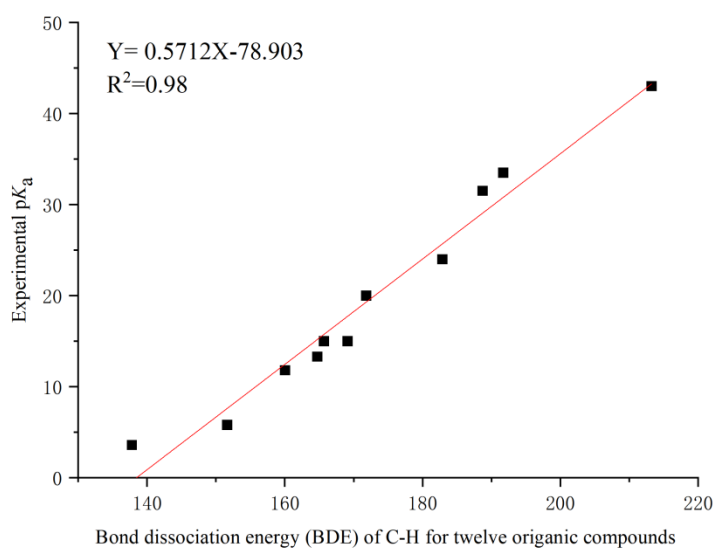


**Figure S1.** The correlation between the experimental  $pK_a$  values and BDEs for nineteen heterocyclic bases.


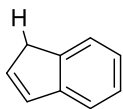
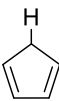
**Table S1.** The  $pK_a$  values and BDEs of nineteen heterocyclic bases.

Heterocyclic Bases	BDE (kcal/mol)	$pK_a$ (exp.)	$pK_a$ (calc.)
Quinoxaline	141.0	0.6 <sup>1</sup>	0.6
Pyrazine	141.1	0.4 <sup>2</sup>	0.6
Pyrimidine	142.8	1.1 <sup>1</sup>	1.4
Pyridazine	145.6	2.1 <sup>1</sup>	2.7
Phthalazine	147.7	3.4 <sup>1</sup>	3.7
Adenine	147.8	4.2 <sup>3</sup>	3.7
Cytosine	148.3	4.5 <sup>1</sup>	4.0
Quinoline	148.7	4.9 <sup>4</sup>	4.2
Pyridine	149.0	5.1 <sup>1</sup>	4.3
Purine	159.5	8.9 <sup>3</sup>	9.2
Phthalimide	159.7	9.9 <sup>3</sup>	9.3
3-Methyluracil	160.7	9.8 <sup>1</sup>	9.8
Uracil	162.0	9.5 <sup>1</sup>	10.4
Guanine	162.0	9.2 <sup>3</sup>	10.4
Adenine	162.1	9.8 <sup>3</sup>	10.5
Thymidine	162.4	9.8 <sup>1</sup>	10.6
1-Methyluracil	162.5	10.0 <sup>1</sup>	10.7
Benzimidazole	165.6	12.3 <sup>3</sup>	12.1
Indazole	169.8	13.9 <sup>3</sup>	14.1

Similarly, the BDEs of the C-H bonds in twelve compounds are related to their  $pK_a$  values. Then the correlation between the BDEs of carbon and experimental  $pK_a$  values was established and illustrated in Figure S2 and Table S2, the squared correlation coefficient for the above system is  $R^2 = 0.98$ . Based on the obtained quantum chemical linear free energy relationship (LFER), the calculated  $pK_a$  of indole and tryptophan, and their chlorinated products were listed in Table S3.

**Figure S2.** The correlation between the experimental  $pK_a$  values and BDE for twelve compounds.

**Table S2.** The  $pK_a$  values and BDEs of twelve compounds.

Compounds	BDE	$pK_a$ (exp.) <sup>5</sup>	$pK_a$ (calc.)
	219.8	46.0	46.7
PhH	213.2	43.0	42.9
Ph <sub>2</sub> C-H(H)	191.7	33.5	30.6
Ph <sub>3</sub> C-H	188.7	31.5	28.9
CH <sub>3</sub> -COOH	182.9	24.0	25.6
	171.8	20.0	19.2
	165.7	15.0	15.7
CH <sub>3</sub> -CO-C-H(Cl) <sub>2</sub>	169.1	15.0	17.7
C-H(H)-(COO-C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	164.7	13.3	15.2
CH <sub>2</sub> -(CN) <sub>2</sub>	160.0	11.8	12.5
C <sub>2</sub> H <sub>5</sub> -O <sub>2</sub> C-C-H(H)-NO	151.6	5.8	7.7
CH <sub>2</sub> -(NO <sub>2</sub> ) <sub>2</sub>	137.8	3.6	-0.2

**Table S3.** The  $pK_a$  values ( $pK_a$  (calc.)) of C, N, and O sites of indole, tryptophan and their chlorinated products by using LFER.

Compounds	Heterolytic Reaction	BDE	$pK_a$ (calc.)
Indole	Indole $\rightarrow$ N <sub>1</sub> -Indole <sup>-</sup> + H <sup>+</sup>	172.3	14.7
	Indole $\rightarrow$ C <sub>2</sub> -Indole <sup>-</sup> + H <sup>+</sup>	203.9	37.6
	Indole $\rightarrow$ C <sub>3</sub> -Indole <sup>-</sup> + H <sup>+</sup>	209.0	40.5
	Indole $\rightarrow$ C <sub>4</sub> -Indole <sup>-</sup> + H <sup>+</sup>	212.5	42.5
	Indole $\rightarrow$ C <sub>5</sub> -Indole <sup>-</sup> + H <sup>+</sup>	215.8	44.4
	Indole $\rightarrow$ C <sub>6</sub> -Indole <sup>-</sup> + H <sup>+</sup>	214.8	43.8
	Indole $\rightarrow$ C <sub>7</sub> -Indole <sup>-</sup> + H <sup>+</sup>	208.6	40.3
Isomer <b>T1</b>			
Tryptophan	Trp $\rightarrow$ N <sub>1</sub> -Trp <sup>-</sup> + H <sup>+</sup>	171.4	14.3
	Trp $\rightarrow$ C <sub>2</sub> -Trp <sup>-</sup> + H <sup>+</sup>	202.8	36.9
	Trp $\rightarrow$ C <sub>4</sub> -Trp <sup>-</sup> + H <sup>+</sup>	213.0	42.8
	Trp $\rightarrow$ C <sub>5</sub> -Trp <sup>-</sup> + H <sup>+</sup>	214.8	43.8
	Trp $\rightarrow$ C <sub>6</sub> -Trp <sup>-</sup> + H <sup>+</sup>	214.1	43.4
	Trp $\rightarrow$ C <sub>7</sub> -Trp <sup>-</sup> + H <sup>+</sup>	208.0	39.9
	S <sub>E</sub> Ar-1		
	2-Cl-Trp <sup>+</sup> $\rightarrow$ 2-Cl-Trp + H <sup>+</sup>	118.5	-11.2
	3-Cl-Trp <sup>+</sup> $\rightarrow$ 3-Cl-Trp + H <sup>+</sup>	139.3	-0.1
	4-Cl-Trp <sup>+</sup> $\rightarrow$ 4-Cl-Trp + H <sup>+</sup>	111.3	-15.3
	5-Cl-Trp <sup>+</sup> $\rightarrow$ 5-Cl-Trp + H <sup>+</sup>	109.9	-16.1

	$6\text{-Cl-Trp}^+ \rightarrow 6\text{-Cl-Trp} + \text{H}^+$	111.6	-15.1
	$7\text{-Cl-Trp}^+ \rightarrow 7\text{-Cl-Trp} + \text{H}^+$	107.3	-17.6
	<b>Isomer T2</b>		
	$\text{Trp} \rightarrow \text{N}_1\text{-Trp}^- + \text{H}^+$	171.3	14.3
	$\text{Trp} \rightarrow \text{C}_2\text{-Trp}^- + \text{H}^+$	211.7	42.0
	$\text{Trp} \rightarrow \text{C}_4\text{-Trp}^- + \text{H}^+$	211.2	41.7
	$\text{Trp} \rightarrow \text{C}_5\text{-Trp}^- + \text{H}^+$	215.2	44.0
	$\text{Trp} \rightarrow \text{C}_6\text{-Trp}^- + \text{H}^+$	214.2	43.4
	$\text{Trp} \rightarrow \text{C}_7\text{-Trp}^- + \text{H}^+$	208.4	40.1
	<b>Isomer T3</b>		
	$\text{Trp} \rightarrow \text{N}_1\text{-Trp}^- + \text{H}^+$	171.4	14.3
	$\text{Trp} \rightarrow \text{C}_2\text{-Trp}^- + \text{H}^+$	211.9	42.1
	$\text{Trp} \rightarrow \text{C}_4\text{-Trp}^- + \text{H}^+$	212.6	42.5
	$\text{Trp} \rightarrow \text{C}_5\text{-Trp}^- + \text{H}^+$	215.9	44.4
	$\text{Trp} \rightarrow \text{C}_6\text{-Trp}^- + \text{H}^+$	214.6	43.7
	$\text{Trp} \rightarrow \text{C}_7\text{-Trp}^- + \text{H}^+$	208.4	40.1
	<hr/>		
2-O-3-R-Indoline	$2\text{-O-3-R-Indoline} \rightarrow \text{N}_1\text{-2-O-3-R-Indoline}^- + \text{H}^+$	166.8	12.2
	$2\text{-O-3-R-Indoline} \rightarrow \text{C}_3\text{-2-O-3-R-Indoline}^- + \text{H}^+$	165.3	15.5
	$\text{N}_1\text{-2-O-3-R-Indoline}^- \rightarrow \text{N}_1\text{-2-O-3-R-Indoline}^{2-} + \text{H}^+$	179.6	23.7
2-OH-3-R-Indole	$2\text{-OH-3-R-Indole} \rightarrow \text{N}_1\text{-2-OH-3-R-Indole}^- + \text{H}^+$	168.3	12.9
	$2\text{-OH-3-R-Indole} \rightarrow \text{O-2-OH-3-R-Indole}^- + \text{H}^+$	161.0	10.4
	$\text{O-2-OH-3-R-Indole}^- \rightarrow \text{O-2-OH-3-R-Indole}^{2-} + \text{H}^+$	181.1	18.7
2-O-3-Cl-3-R-Indoline	$2\text{-O-3-Cl-3-R-Indoline} \rightarrow 2\text{-O-3-Cl-3-R-Indoline}^- + \text{H}^+$	162.7	10.4
2-OH-3-R-3H-Indole	$2\text{-OH-3-R-3H-Indole} \rightarrow \text{O-2-OH-3-R-3H-Indole}^- + \text{H}^+$	148.9	6.2
Int 3	$\text{Int 3} \rightarrow \text{Int 3}^- + \text{H}^+$	145.8	5.1
Int 3 <sup>-</sup> (X=O <sup>-</sup> )	$\text{Int 3}^- \rightarrow \text{Int 3}^{2-} + \text{H}^+$	169.9	13.6
Int 3 <sup>-</sup> (X=OCl)	$\text{Int 3}^- \rightarrow \text{Int 3}^{2-} + \text{H}^+$	150.3	4.9
2-OH-3-Cl-3-R-Indoline	$2\text{-OH-3-Cl-3-R-Indoline} \rightarrow 2\text{-OH-3-Cl-3-R-Indoline}^- + \text{H}^+$	177.7	17.1
2-OCl-3-Cl-3-R-Indoline	$2\text{-OCl-3-Cl-3-R-Indoline} \rightarrow 2\text{-OCl-3-Cl-3-R-Indoline}^- + \text{H}^+$	175.3	16.0
2-OH-3-OH-3-R-Indoline	$2\text{-OH-3-OH-3-R-Indoline} \rightarrow 2\text{-OH-3-OH-3-R-Indoline}^- + \text{H}^+$	181.9	19.0
2-OCl-3-OH-3-R-Indoline	$2\text{-OCl-3-OH-3-R-Indoline} \rightarrow 2\text{-OCl-3-OH-3-R-Indoline}^- + \text{H}^+$	175.9	16.3
2-OH-3-OCl-3-R-Indoline	$2\text{-OH-3-OCl-3-R-Indoline} \rightarrow 2\text{-OH-3-OCl-3-R-Indoline}^- + \text{H}^+$	176.8	16.7
2-OCl-3-OCl-3-R-Indoline	$2\text{-OCl-3-OCl-3-R-Indoline} \rightarrow 2\text{-OCl-3-OCl-3-R-Indoline}^- + \text{H}^+$	173.8	15.4
Int 6	$\text{Int 6} \rightarrow \text{Int 6}^- + \text{H}^+$	164.9	15.5

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## Text S2

### Different isomers and factions of different forms for each substrates

*Indole.* According to the different double bond positions in the pyrrole ring, three indole isomers were found as depicted in Figure S3, and Table S4 shows that isomer **I1** is more stable than isomer **I2** and **I3** with the relative free energy (RG) lower by 10–29 kcal/mol, leading to the Boltzmann distribution proportion  $f(\mathbf{I1})$  value of  $\sim 1$ . Thus, only isomer **I1** was investigated in chlorination of indole. The  $pK_a$  value of the N1–H moiety in indole is 16.97<sup>6</sup>, implying that the neutral indole form (NH) is predominant at pH 7 and the fraction of its anion form  $p(A)$  value is  $10^{-10}$ , which makes no or few contribution to the estimated apparent rate constant  $k_{\text{obs-est}}$  (see Table S7).

*Trp.* Due to zwitterion species being dominant for most amino acids, thus, the zwitterion form of the backbone in Trp was taken in chlorination of the indole moiety. According to the different structures of the backbone, nine Trp isomers were found as shown in Figure S3, and Table S4 shows that the RG values for isomers **T1–T3** are within 1 kcal/mol, leading to their Boltzmann distribution population  $f$  values being 0.52, 0.24, and 0.11, respectively. Due to their total percentage accounting for >85%, isomers **T1–T3** were chosen to represent Trp. So far no  $pK_a$  values of the N1–H moiety in isomers **T1–T3** have been reported, therefore, their  $pK_a$  values were calculated as described in Text S1. The calculated  $pK_a$  values of isomers **T1–T3** are very close to that of indole (14.3 vs. 14.7), and based upon the calculated results for indole, it infers that the neutral indole moiety (NH) is predominant at pH 7 and the fraction of the anion form  $p(A)$  is ignorable. Different from indole, there are two attack ways by HOCl on the indole moiety in Trp from the same and the opposite sides of the R group (Figure S4), but only the attack from the opposite side was discussed due to their relatively lower  $\Delta G^\ddagger$  values than the same side for almost all the sites (Table S10) probably ascribed to the steric hindrance effect.

*2-O-3-R-Indoline.* Three 2-O-3-R-Indoline isomers were found as depicted in Figure S3, and Table S4 displays that isomer **OT1** is the most stable one with the RG lower than isomers **OT2** and **OT3** by 4 and 12 kcal/mol, respectively, leading to the  $f$  values of above isomers of 0.9971, 0.0029, and  $10^{-9}$ , respectively. Considering tiny fraction of **OT3**, only isomers **OT1** and **OT2** were studied. The

calculated  $pK_{a1}$  and  $pK_{a1}'$  values of the N–H and C3–H moieties in **OT1** are 12.2 and 15.5, respectively, those of the O–H and N–H moieties in **OT2** are 10.4 and 12.9, respectively, and their  $pK_{a2}$  values are 23.7 and 18.7, respectively. This indicates that neutral forms of **OT1** and **OT2** are predominant at pH 7 with  $p(N)$  values of 0.9996–0.9999, while  $p(A^-)$  values are  $10^{-6}$ –0.0004 and  $p(A^{2-})$  are ignorable.

*2-X-3-Cl-3-R-Indoline* ( $X=OH/OCl$ ). The calculated  $pK_a$  of the N–H in 2-OH-3-Cl-3-R-Indoline is 17.1. This indicates that neutral form of 2-OH-3-OCl-3-R-Indoline is predominant at pH 7 with  $p(N)$  value of 0.9999, while  $p(A^-)$  value is  $10^{-10}$ , so anion form is ignored. The calculated  $pK_a$  of the N–H in 2-OCl-3-Cl-3-R-Indoline is 16.0. This indicates that neutral form of 2-OCl-3-OCl-3-R-Indoline is predominant at pH 7 with  $p(N)$  value of 0.9999, while  $p(A^-)$  value is  $10^{-9}$ , so anion form is also considered.

*2-O-3-Cl-3-R-Indoline*. Two isomers **OCIT1** and **OCIT2** were obtained as shown in Figure S3. Table S4 displays that isomer **OCIT1** is more stable than isomer **OCIT2** with the RG lower than by 14 kcal/mol, therefore, only the former is investigated. The calculated  $pK_a$  of the N–H in **OCIT1** is 10.4. This indicates that neutral form of **OCIT1** is predominant at pH 7 with  $p(N)$  value of 0.9996, while  $p(A^-)$  value is  $3.7 \times 10^{-4}$ , so both should be considered.

**Int 3** ( $X=O^-/OCl$ ). The calculated  $pK_{a1}$  of the O–H in **Int 3** ( $X=O^-$ ) is 5.1 and  $pK_{a2}$  of the N–H is 13.6. This indicates that the anion form with -1 charge ( $A^-$ ), and anion form with -2 charge ( $A^{2-}$ ) at pH 7 account for 0.9999 and  $10^{-7}$ , and anion form with -1 charge ( $A^{1-}$ ) of **Int 3** ( $X=O^-$ ) is predominant, while both two forms are considered. The calculated  $pK_a$  of the N–H in **Int 3** ( $X=OCl$ ) is 4.9. This indicates that the anion form with -1 charge ( $A^-$ ) is predominant at pH 7 with  $p(A^-)$  value of 0.9921, while  $p(N)$  value is  $7.9 \times 10^{-3}$ , so only anion form is considered.

*2-X-3-Y-3-R-Indoline* ( $X=OH/OCl$ ,  $Y=OH/OCl$ ). The calculated  $pK_a$  of the N–H in 2-OH-3-OH-3-R-Indoline is 19.0. This indicates that neutral form of 2-OH-3-OH-3-R-Indoline is predominant at pH 7 with  $p(N)$  value of 0.9999, while  $p(A^-)$  value is  $10^{-12}$ , so anion form is ignored. The calculated  $pK_a$  of the N–H in 2-OCl-3-OH-3-R-Indoline is 16.3. This indicates that neutral form of 2-OCl-3-



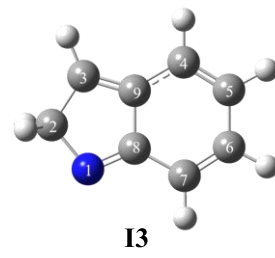
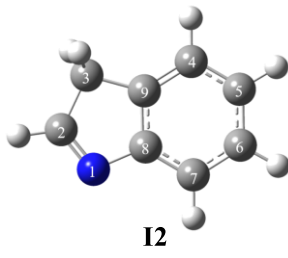
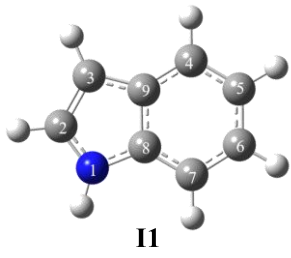
OH-3-R-Indoline is predominant at pH 7 with  $p(N)$  value of 0.9999, while  $p(A^-)$  value is  $10^{-10}$ , so anion form is considered. The calculated  $pK_a$  of the N–H in 2-OH-3-OCl-3-R-Indoline is 16.7. This indicates that neutral form of 2-OH-3-OCl-3-R-Indoline is predominant at pH 7 with  $p(N)$  value of 0.9999, while  $p(A^-)$  value is  $10^{-10}$ , so anion form is considered. The calculated  $pK_a$  of the N–H in 2-OCl-3-OCl-3-R-Indoline is 15.4. This indicates that neutral form of 2-OCl-3-OCl-3-R-Indoline is predominant at pH 7 with  $p(N)$  value of 0.9999, while  $p(A^-)$  value is  $10^{-9}$ , so anion form is also considered.

**Int 6.** The calculated  $pK_a$  of the N–H in **Int 6** is 15.5. This indicates that neutral form of **Int 6** is predominant at pH 7 with  $p(N)$  value of 0.9999, while  $p(A^-)$  value is  $10^{-9}$ , so both forms should be considered.

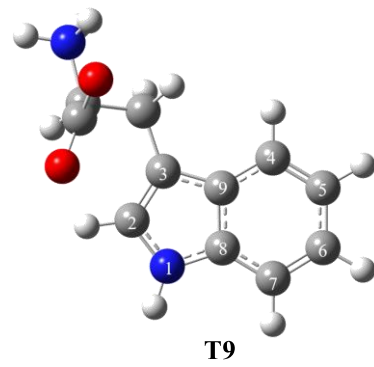
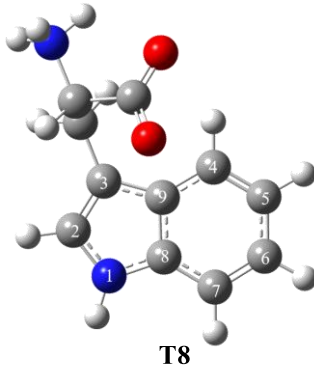
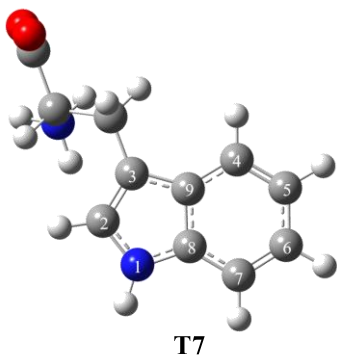
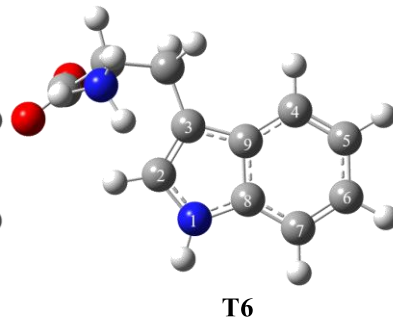
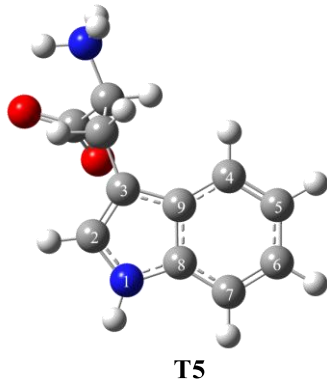
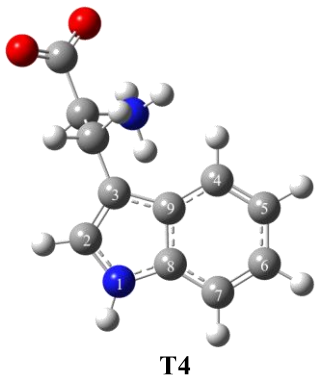
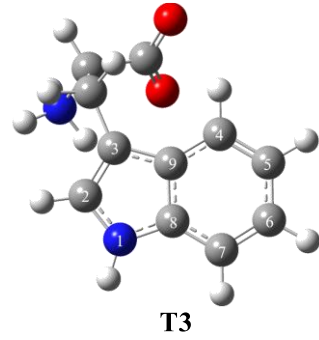
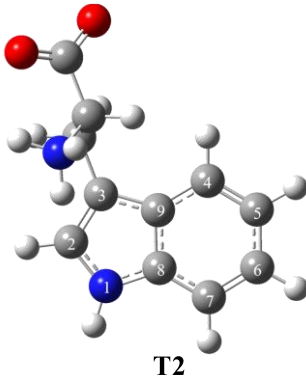
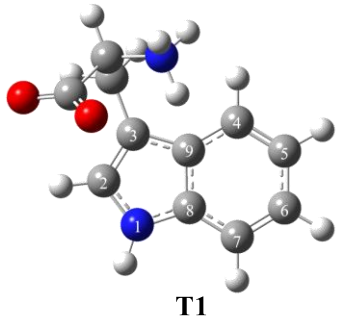
**Table S4.** Relative energies (RG, in kcal/mol) and  $f$  of indole, tryptophan, 2-O-3-R-Indoline and 2-O-3-Cl-3-R-Indoline isomers.

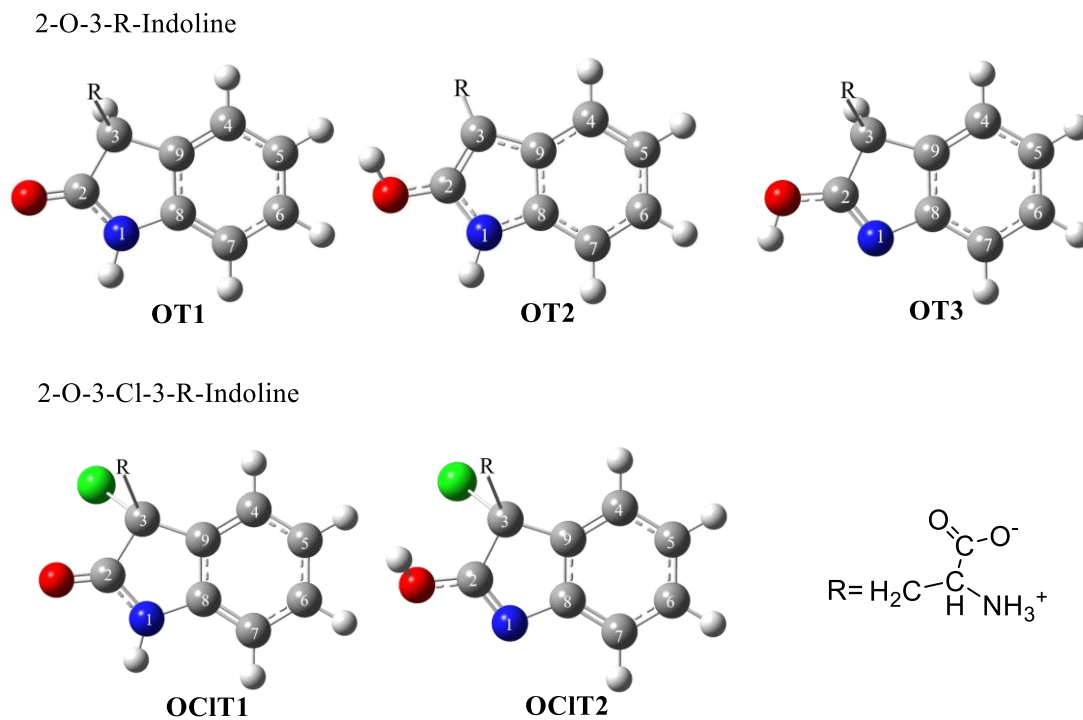
	Isomer	RG	$f$	Isomer	RG	$f$
Indole	<b>I1</b>	0.0	0.9999	<b>I3</b>	28.8	$10^{-22}$
	<b>I2</b>	10.0	$10^{-8}$			
Tryptophan	<b>T1</b>	0.0	0.5218	<b>T6</b>	1.9	0.0199
	<b>T2</b>	0.5	0.2434	<b>T7</b>	2.0	0.0182
	<b>T3</b>	1.0	0.1050	<b>T8</b>	2.9	0.0039
	<b>T4</b>	1.3	0.0543	<b>T9</b>	4.2	0.0004
	<b>T5</b>	1.6	0.0332			
2-O-3-R-Indoline	<b>OT1</b>	0.0	0.9971	<b>OT3</b>	12.0	$10^{-9}$
	<b>OT2</b>	3.5	0.0029			
2-O-3-Cl-3-R-Indoline	<b>OCIT1</b>	0.0	0.9999	<b>OCIT2</b>	13.8	$10^{-11}$

Indole



Tryptophan



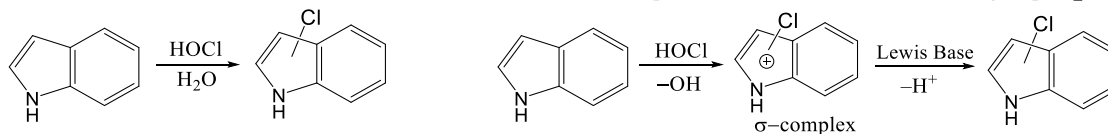


**Figure S3.** The spatial structure of indole, tryptophan, 2-O-3-R-Indoline and 2-O-3-Cl-3-R-Indoline isomers.

**Table S5.** The heterolytic bond dissociation energies (HEBDEs, in kcal/mol) of the H-N/C bond for Indole and Isomer **T1** and the chlorinated Trp cations (2/3/4/5/6/7-Cl-Trp<sup>+</sup>) calculated at the M06-2X/cc-pVTZ level.

Substance	N1	C2	C3	C4	C5	C6	C7
Indole	172.3	203.9	209.0	209.0	212.5	215.8	214.8
Isomer <b>T1</b>	171.4	202.8	--	213.0	214.8	214.1	208.0
2-Cl-Trp <sup>+</sup>	147.2	118.5	--	157.0	200.6	198.0	194.5
3-Cl-Trp <sup>+</sup>	139.3	171.0	--	201.2	205.0	204.5	194.9
4-Cl-Trp <sup>+</sup>	148.2	181.9	--	111.3	192.2	184.9	185.7
5-Cl-Trp <sup>+</sup>	149.0	189.9	--	188.9	109.9	192.4	191.6
6-Cl-Trp <sup>+</sup>	147.4	180.6	--	200.5	196.9	111.6	183.1
7-Cl-Trp <sup>+</sup>	148.4	190.8	--	191.2	182.0	188.6	107.3

(a) Concerted electrophilic substitution mechanism. (b) Classic electrophilic substitution on an aromatic group (S<sub>E</sub>Ar)



**Scheme S1.** Proposed chlorination mechanisms of indole ring in literature

**Table S6.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol) and reaction enthalpy changes ( $\Delta H$ , in kcal/mol) of HOCl attacking the indole via the  $S_{EAr}$  and concerted mechanisms.

Reactive site	Neutral						Anion	
	$S_{EAr-1}$		$S_{EAr-2}$		Concerted		$S_{EAr-1}$	
	$\Delta G^\ddagger$	$\Delta H$	$\Delta G^\ddagger$	$\Delta H$	$\Delta G^\ddagger$	$\Delta H$	$\Delta G^\ddagger$	$\Delta H$
N1	--	--	--	--	22.9	-15.6	--	--
C2	17.5	2.7	4.7	-19.2	21.0	-13.4	14.3	-20.1
C3	11.2	-6.7	5.8	-10.5	11.9	-31.9	5.5	-36.4
C4	22.9	4.8	2.0	-34.9	24.3	-10.9	10.6	-17.2
C5	22.1	6.6	1.5	-24.4	23.6	-11.5	11.1	-15.7
C6	21.4	4.9	3.2	-24.9	22.2	-13.5	15.6	-14.1
C7	21.5	6.9	1.2	-34.7	22.4	-11.2	13.2	-10.3

**Table S7.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol), estimated apparent rate constants ( $k_{obs-est}$ , in  $M^{-1} min^{-1}$ ), and the contribution ( $c$ , %) from neutral and anion forms to each reactive site and  $k_{obs-est}$  of indole  $S_{EAr}$  mechanism and concerted mechanism for N1 site.

Reactive site	Neutral form (NH)			Anion form (N <sup>-</sup> )			Indole
	$\Delta G^\ddagger$	$k_{obs-est}$	$c$	$\Delta G^\ddagger$	$k_{obs-est}$	$c$	$k_{obs-est}$
N1	22.9	$1.1 \times 10^{-4}$	100.0%	--	--	--	$1.1 \times 10^{-4}$
C2	17.5	$9.2 \times 10^{-1}$	100.0%	14.3	$2.2 \times 10^{-8}$	0.0%	$9.2 \times 10^{-1}$
C3	11.2	$4.3 \times 10^4$	100.0%	5.5	$6.3 \times 10^{-2}$	0.0%	$4.3 \times 10^4$
C4	22.9	$1.0 \times 10^{-4}$	90.0%	10.6	$1.2 \times 10^{-5}$	10.1%	$1.2 \times 10^{-4}$
C5	22.1	$4.5 \times 10^{-4}$	99.0%	11.1	$5.2 \times 10^{-6}$	1.2%	$4.5 \times 10^{-4}$
C6	21.4	$1.4 \times 10^{-3}$	100.0%	15.6	$2.4 \times 10^{-9}$	0.0%	$1.4 \times 10^{-3}$
C7	21.5	$1.1 \times 10^{-3}$	100.0%	13.2	$1.4 \times 10^{-7}$	0.0%	$1.1 \times 10^{-3}$

The fractions of neutral and anion form  $f(NH)$  and  $f(N^-)$  in indole **1** are 0.999 and  $1.1 \times 10^{-10}$ , respectively.

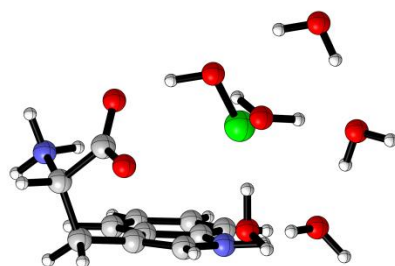
**Table S8.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol) for the chlorination of the indole C3 site concerted and  $S_{EAr}$  mechanisms by HOCl calculated with M06-2X(D3), M05-2X(D3), BMK(D3) and B3LYP(D3) functionals along with 6-31G(d), 6-31+G(d) and 6-311G(d) basis sets and the implicit SMD solvent model. To obtain more accurate energies, single point calculations were performed using the cc-pVTZ or aug-cc-pVTZ basis sets.

Basis set	M06-2X(D3)		M05-2X(D3)		BMK(D3)		B3LYP(D3)	
	Concerted	$S_{EAr}$	Concerted	$S_{EAr}$	Concerted	$S_{EAr}$	Concerted	$S_{EAr}$
6-31G(d)	12.5	10.9	9.9	9.5	8.4	6.1	2.0	2.7
6-31+G(d)	11.3	11.0	9.0	8.2	6.4	4.6	4.0	2.3
6-311G(d)	11.9	11.2	10.5	9.1	8.8	5.1	4.1	1.0

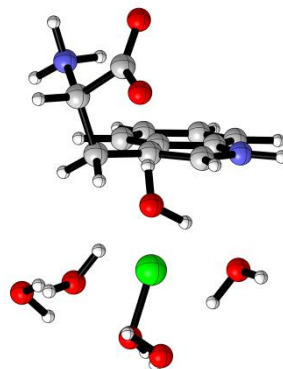
**Table S9.** The activation free energies ( $\Delta G^\ddagger$ , in kcal/mol) and estimated rate constants  $k_{\text{est}}$  (in  $\text{M}^{-1} \text{min}^{-1}$ ) in chlorination at C3 site of indole via  $\text{S}_{\text{E}}\text{Ar}$  mechanism assisted by 2-6 water molecules.

	2w	3w	4w	5w	6w
$\Delta G^\ddagger$	14.8	13.0	14.7	11.2	9.6
$k_{\text{est}}$	$5.7 \times 10^3$	$1.2 \times 10^5$	$6.7 \times 10^3$	$2.5 \times 10^6$	$3.6 \times 10^7$

(a) The same side attack



(b) The opposite side attack



**Figure S4.** Two ways for HOCl attacking the indole ring moiety in isomer **T1** of (a) The same side attack; (b) The opposite side attack.

**Table S10.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol) and reaction enthalpy changes ( $\Delta H$ , in kcal/mol) of opposite side and same side attack of seven reaction sites of three isomers of Trp with HOCl.

Mechanism	Site	Opposite side attack			Same side attack		
		<b>T1</b>	<b>T2</b>	<b>T3</b>	<b>T1</b>	<b>T2</b>	<b>T3</b>
Concerted	N1	23.0/-20.9	24.2/-16.7	22.8/-20.0	31.1/-5.5	22.4/-15.1	28.6/-8.0
	C2	18.4/-15.2	20.2/-17.2	20.1/-18.8	26.7/-11.6	21.1/-16.0	22.7/-14.2
	C3	13.8/-31.1	14.7/-29.8	13.9/-29.6	--	--	--
	C4	25.5/-10.3	25.1/-9.2	26.8/-11.4	25.2/-5.6	23.3/-6.6	30.0/0.3
	C5	24.6/-10.9	24.1/-10.3	24.8/-12.0	26.5/-6.9	24.3/-7.9	30.8/-4.6
	C6	23.8/-15.6	23.9/-12.4	24.0/-13.4	26.6/-8.4	25.4/-10.4	32.1/-5.6
	C7	23.6/-10.6	24.3/-10.4	24.1/-11.1	31.1/-1.8	25.3/-7.3	23.4/-10.2
$\text{S}_{\text{E}}\text{Ar}$	C2	17.9/1.8	18.0/0.2	17.8/2.4	24.5/3.6	15.0/0.3	30.5/16.3
	C3	12.8/-4.9	14.2/-0.4	13.6/-1.8	--	--	--
	C4	21.2/3.2	24.5/11.7	24.3/10.2	19.8/7.3	28.4/-2.3	35.2/18.5
	C5	21.9/8.8	22.2/8.1	22.1/8.3	27.5/16.9	22.7/9.3	29.3/13.8
	C6	21.6/5.5	21.7/6.7	21.5/6.0	22.4/6.0	23.4/7.4	34.1/22.2
	C7	22.4/7.8	23.0/8.0	21.9/7.1	33.7/19.6	24.0/7.1	34.4/19.6

**Table S11.** The estimated apparent rate constants ( $k_{\text{obs-est}}$ , in  $\text{M}^{-1} \text{s}^{-1}$ ) and contributions ( $c$ , %) to each reactive site of seven reaction sites of three isomers of Trp with HOCl.

	<b>T1</b>	<b>T2</b>	<b>T3</b>	<b>Trp</b>
N1	$4.5 \times 10^{-5}$ (72.4%)	$3.1 \times 10^{-6}$ (5.0%)	$1.4 \times 10^{-5}$ (22.6%)	$6.2 \times 10^{-5}$
C2	$2.6 \times 10^{-1}$ (60.4%)	$1.1 \times 10^{-1}$ (24.7%)	$6.5 \times 10^{-2}$ (15.0%)	$4.4 \times 10^{-1}$
C3	$1.5 \times 10^3$ (91.6%)	$6.3 \times 10^1$ (3.7%)	$7.9 \times 10^1$ (4.7%)	$1.7 \times 10^3$
C4	$1.1 \times 10^{-3}$ (99.7%)	$1.9 \times 10^{-6}$ (0.2%)	$1.0 \times 10^{-6}$ (0.1%)	$1.1 \times 10^{-3}$
C5	$3.3 \times 10^{-4}$ (72.6%)	$8.0 \times 10^{-5}$ (17.8%)	$4.3 \times 10^{-5}$ (9.7%)	$4.5 \times 10^{-4}$
C6	$5.2 \times 10^{-4}$ (61.4%)	$2.0 \times 10^{-4}$ (24.2%)	$1.2 \times 10^{-4}$ (14.4%)	$8.5 \times 10^{-4}$
C7	$1.3 \times 10^{-4}$ (61.1%)	$2.4 \times 10^{-5}$ (11.2%)	$5.9 \times 10^{-5}$ (27.7%)	$2.1 \times 10^{-4}$

**Table S12.** The APT charge of Trp, 3-Cl-Trp<sup>+</sup>, 2-OH-3-R-Indole, and 2-O-3-Cl-3-R-Indoline<sup>-</sup>.

	Trp	3-Cl-Trp <sup>+</sup>	2-OH-3-R-Indole	2-O-3-Cl-3-R-Indoline <sup>-</sup>
N1	-0.776	-0.500	-0.889	-1.575
C2	0.239	0.506	1.370	1.797
C3	-0.251	0.491	-0.614	0.513
C4	0.032	-0.061	-0.035	0.149
C5	-0.164	-0.042	-0.117	-0.365
C6	-0.117	-0.027	-0.194	0.146
C7	-0.006	-0.084	0.049	-0.317

**Table S13.** The activation free energies ( $\Delta G^\ddagger$ , in kcal/mol) of isomers **OT1** and **OT2** and their anion forms **OT1<sup>-</sup>** and **OT2<sup>-</sup>** of 2-O-3-R-Indoline reacting with HOCl.

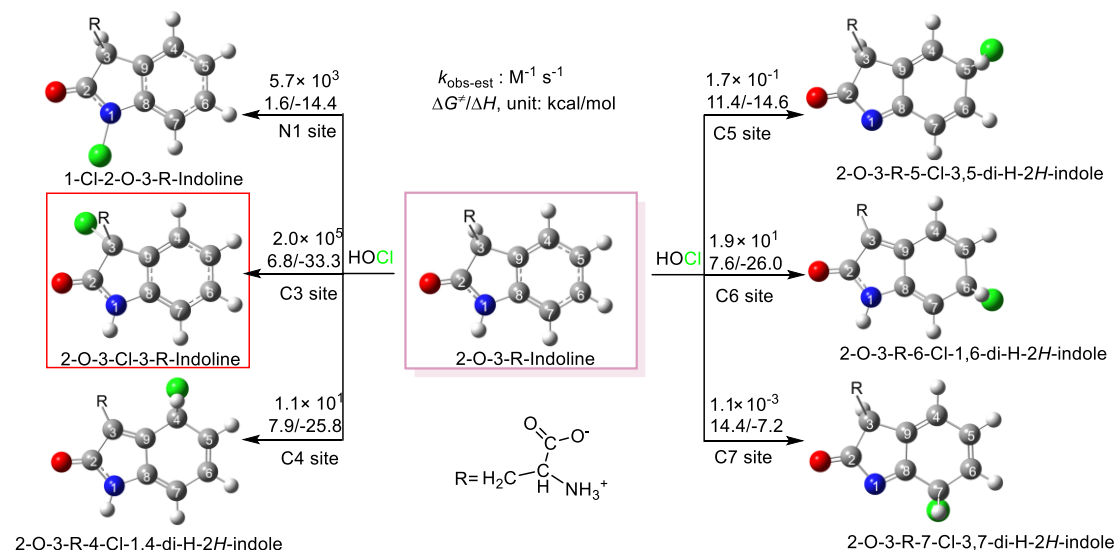
Reactive Site	<b>OT1</b>	<b>OT1<sup>-</sup></b>	<b>OT2</b>	<b>OT2<sup>-</sup></b>
N1	28.7	1.6	22.3	12.8
C2	--	--	23.4	--
C3	--	--	6.8	2.1
C4	38.6	30.9	17.4	7.9
C5	23.8	11.4	23.7	15.4
C6	35.8	29.5	16.1	7.6
C7	30.2	14.4	22.4	16.9

**Table S14.** The estimated apparent rate constants ( $k_{\text{obs-est}}$ , in  $\text{M}^{-1} \text{s}^{-1}$ ) and contributions ( $c$ , %) to seven reaction sites of two isomer and their anion forms of 2-O-3-R-Indoline with HOCl.

	OT1	OT1 <sup>-</sup>	OT2	OT2 <sup>-</sup>	2-O-3-R-Indoline
N1	$6.2 \times 10^{-9}$ (0.0%)	$5.7 \times 10^3$ (100.0%)	$8.6 \times 10^{-7}$ (0.0%)	$2.9 \times 10^{-3}$ (0.0%)	$5.7 \times 10^3$
C2	--	--	$1.3 \times 10^{-7}$ (100.0%)	--	$1.3 \times 10^{-7}$
C3	--	--	$2.0 \times 10^5$ (99.5%)	$1.1 \times 10^3$ (0.5%)	$2.0 \times 10^5$
C4	$3.4 \times 10^{-16}$ (0.0%)	$8.7 \times 10^{-16}$ (0.0%)	$3.4 \times 10^{-3}$ (0.0%)	$1.1 \times 10^1$ (100.0%)	$1.1 \times 10^1$
C5	$2.4 \times 10^{-5}$ (0.0%)	$1.7 \times 10^{-1}$ (100.0%)	$8.1 \times 10^{-8}$ (0.0%)	$3.6 \times 10^{-5}$ (0.0%)	$1.7 \times 10^{-1}$
C6	$3.9 \times 10^{-14}$ (0.0%)	$9.2 \times 10^{-15}$ (0.0%)	$3.0 \times 10^{-2}$ (0.2%)	$1.9 \times 10^1$ (99.8%)	$1.9 \times 10^1$
C7	$4.9 \times 10^{-10}$ (0.0%)	$1.1 \times 10^{-3}$ (99.7%)	$7.3 \times 10^{-7}$ (0.1%)	$2.9 \times 10^{-6}$ (0.3%)	$1.1 \times 10^{-3}$

**Table S15.** The reaction enthalpy changes ( $\Delta H^\ddagger$ , in kcal/mol) in chlorination of 2-O-3-R-Indoline.

Reactive site	N1	C2	C3	C4	C5	C6	C7
$\Delta H$	-14.4	7.0	-33.3	-25.8	-14.6	-26.0	-7.2



**Scheme S2.** Initial attack on the indole moiety of 2-O-3-R-Indoline by the  $\text{Cl}^+$  of HOCl.

**Table S16.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol), estimated apparent rate constants ( $k_{\text{obs-est}}$ , in  $\text{M}^{-1} \text{s}^{-1}$ ) and contributions (c, %) of 2-O-3-Cl-3-R-Indoline with HOCl.

	OCIT1	OCIT1 <sup>-</sup>	2-O-3-Cl-3-R-Indoline
N1	14.8/-21.1	2.7/-6.6	$3.8 \times 10^5$
	$9.4 \times 10^1$ (0.0%)	$3.7 \times 10^5$ (100.0%)	
C4	45.7/-45.0	36.1/21.8	$8.6 \times 10^{-18}$
	$2.0 \times 10^{-21}$ (0.0%)	$8.6 \times 10^{-18}$ (100.0%)	

**Table S17.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol), estimated apparent rate constants ( $k_{\text{obs-est}}$ , in  $\text{M}^{-1} \text{s}^{-1}$ ) and contributions (c, %) of 2-X-3-Cl-3-R-Indoline(X=OH/OCl) with HOCl.

	Neutral form (NH)		Anion form (N <sup>-</sup> )		$k_{\text{obs-est}}$
X=OH	12.1/-15.3	$9.0 \times 10^3$ (100.0%)	--	--	$9.0 \times 10^3$
X=OCl	15.9/-15.3	$1.5 \times 10^1$ (92.3%)	0.0/-21.0	$1.3 \times 10^0$ (7.7%)	$1.6 \times 10^1$

**Table S18.** The APT charge of 1,3-di-Cl-2-O-3-R-Indoline, **Int 3<sup>-</sup>** (X=O<sup>-</sup>/OCl), **Int 3<sup>2-</sup>**, **Int 6**, and **Int 6<sup>-</sup>**.

	1,3-di-Cl-2-O-3-R-Indoline	<b>Int 3<sup>-</sup></b> (X=O <sup>-</sup> )	<b>Int 3<sup>2-</sup></b> (X=O <sup>-</sup> )	<b>Int 3<sup>-</sup></b> (X=OCl)	<b>Int 6</b>	<b>Int 6<sup>-</sup></b>
N1	-0.860	-0.326	-0.602	-0.708	-1.219	-1.741
C2	1.576	1.707	1.823	1.805	1.693	1.943
C3	0.529	0.578	0.785	0.670	1.428	1.431
C4	0.060	-0.093	0.296	0.071	-0.005	0.105
C5	-0.207	-0.118	-0.704	-0.247	-0.208	-0.404
C6	0.070	0.003	0.378	0.064	0.124	0.247
C7	-0.215	-0.127	-0.393	-0.188	-0.272	-0.353

**Table S19.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol) and reaction enthalpy changes ( $\Delta H$ , in kcal/mol) in chlorination of 1,3-di-Cl-2-O-3-R-Indoline.

Reactive site	C4	C5	C6	C7
$\Delta G^\ddagger/\Delta H$	47.9/-43.3	30.4/19.3	42.7/-52.0	36.3/22.6

**Table S20.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol), estimated apparent rate constants ( $k_{\text{obs-est}}$ , in  $\text{M}^{-1} \text{s}^{-1}$ ) and contributions (c, %) of **Int 3** (X= O<sup>-</sup>/OCl) with HOCl.

	Anion form (N <sup>-</sup> )		Anion form (N <sup>2-</sup> )		<b>Int 3</b>	
X=O <sup>-</sup>	C5	20.5/1.3	$5.9 \times 10^{-3}$ (0.0%)	3.9/-30.7	$2.5 \times 10^2$ (100.0%)	$2.5 \times 10^2$
	C7	21.5/8.3	$1.1 \times 10^{-3}$ (0.0%)	3.5/-27.0	$2.5 \times 10^2$ (100.0%)	$2.5 \times 10^2$
X=OCl	C5	--	--	18.7/-15.3	$1.3 \times 10^{-1}$ (100.0%)	$1.3 \times 10^{-1}$
	C7	--	--	19.3/-11.2	$4.8 \times 10^{-2}$ (100.0%)	$4.8 \times 10^{-2}$

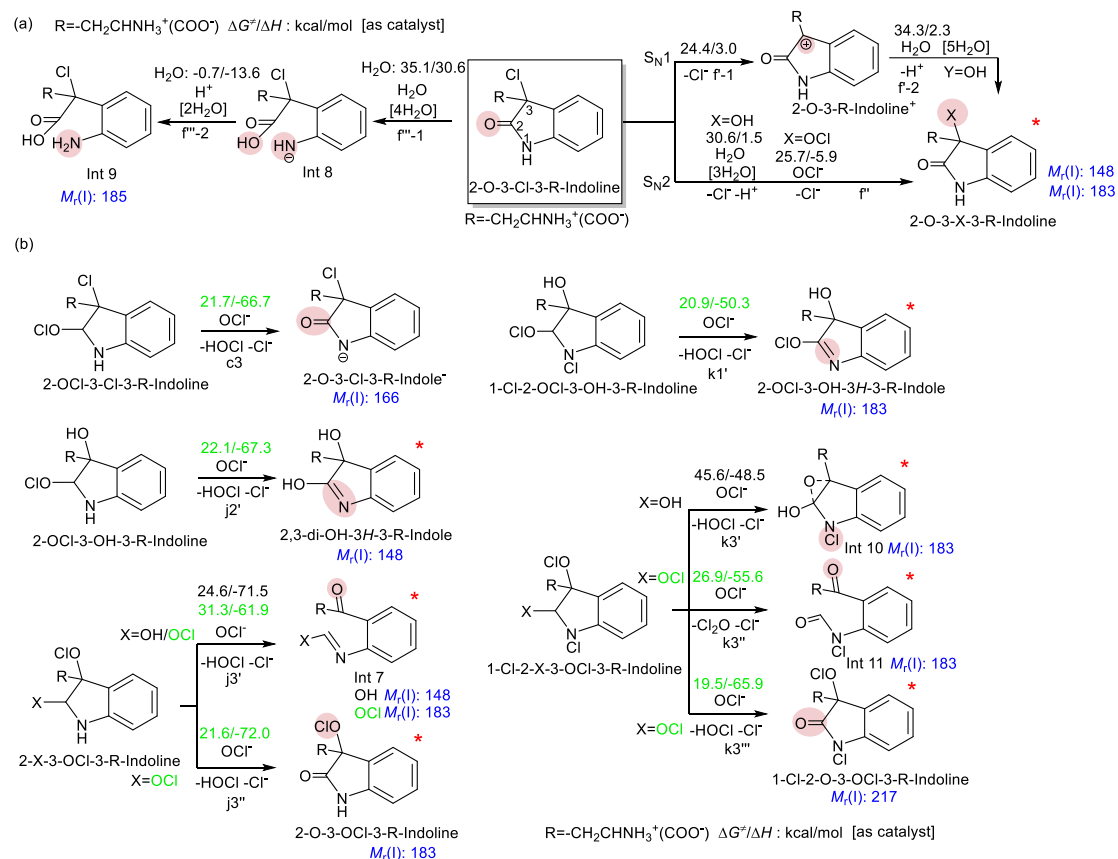


**Table S21.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol), estimated apparent rate constants ( $k_{\text{obs-est}}$ , in  $\text{M}^{-1} \text{s}^{-1}$ ) and contributions ( $c$ , %) of 2-X-3-Y-3-R-Indoline(X=OH/OCl, Y=OH/OCl) with HOCl.

	Neutral form (NH)		Anion form (N <sup>-</sup> )		$k_{\text{obs-est}}$
X=OH Y=OH	13.0/-17.5	$2.0 \times 10^3$ (100.0%)	--	--	$2.0 \times 10^3$
X=OCl Y=OH	16.4/-16.0	$6.3 \times 10^0$ (92.7%)	0.5/-22.1	$5.0 \times 10^{-1}$ (7.3%)	$6.8 \times 10^0$
X=OH Y=OCl	13.3/-16.3	$1.2 \times 10^3$ (100.0%)	0.5/-26.7	$1.9 \times 10^{-1}$ (0.0%)	$1.2 \times 10^3$
X=OCl Y=OCl	16.4/-15.8	$6.3 \times 10^0$ (60.8%)	-0.5/-24.8	$4.1 \times 10^0$ (39.2%)	$1.0 \times 10^1$

**Table S22.** The activation free energy ( $\Delta G^\ddagger$ , in kcal/mol), estimated apparent rate constants ( $k_{\text{obs-est}}$ , in  $\text{M}^{-1} \text{s}^{-1}$ ) and contributions ( $c$ , %) of **Int 6** with HOCl.

	Neutral form (NH)		Anion form (N <sup>-</sup> )		<b>Int 6</b>
C5	29.7/14.8	$1.2 \times 10^{-9}$ (42.6%)	17.9/-9.7	$1.6 \times 10^{-9}$ (57.4%)	$2.7 \times 10^{-9}$
C7	38.9/27.2	$2.3 \times 10^{-16}$ (0.0%)	22.0/-2.7	$1.5 \times 10^{-12}$ (100.0%)	$1.5 \times 10^{-12}$



**Scheme S3.** Formation of minor transformation products of (a) The nucleophilic substitution of 2-O-3-Cl-3-R-Indoline; (b) The elimination reactions of 2-O-3-Cl-3-R-Indoline, 2-O-3-OH-3-R-Indoline, 2-X-3-OCl-3-R-Indoline, 1-Cl-2-O-3-OH-3-R-Indoline, and 1-Cl-2-X-3-OCl-3-R-Indoline.

## Standard orientation of TS-T1-c-N1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-c-N1

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -151.1 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.878229	-0.754484	0.928646
2	8	0	3.364805	-0.006132	2.218114
3	1	0	3.297702	0.948740	2.100549
4	17	0	2.458220	-0.533408	-1.249718
5	8	0	1.183561	-0.998938	1.867081
6	1	0	1.211967	-1.961790	1.951076
7	1	0	2.197001	-0.560266	2.034276
8	8	0	4.215049	-0.916286	-1.830007
9	1	0	4.063693	-0.348789	1.587620
10	1	0	4.505804	-0.112175	-2.277646
11	8	0	5.221875	-0.926150	0.634565
12	1	0	4.918167	-0.936503	-0.305988
13	1	0	5.378076	-1.842995	0.883431
14	6	0	0.170852	1.186628	-0.283700
15	6	0	-1.204369	1.361408	-0.581767
16	6	0	-1.810780	2.604706	-0.340131
17	6	0	-1.038529	3.635525	0.172006
18	6	0	0.328421	3.449022	0.455093
19	6	0	0.946995	2.228027	0.234522
20	6	0	-0.582775	-0.740531	-1.064234
21	6	0	-1.671186	0.092112	-1.086440
22	1	0	-2.865273	2.758786	-0.552392
23	1	0	-1.491189	4.602632	0.360512
24	1	0	0.905177	4.275432	0.855200
25	1	0	1.998375	2.078700	0.458163
26	1	0	-0.534421	-1.782680	-1.355637
27	7	0	0.536918	-0.120408	-0.548128
28	6	0	-3.087623	-0.303071	-1.374708
29	1	0	-3.121790	-1.100096	-2.118807
30	1	0	-3.661428	0.540357	-1.770094
31	6	0	-3.788395	-0.843316	-0.121051

32	6	0	-2.992494	-2.021056	0.475113
33	8	0	-2.976383	-3.056203	-0.220530
34	8	0	-2.410918	-1.814956	1.564045
35	1	0	-4.807320	-1.150993	-0.351587
36	7	0	-3.879032	0.235377	0.910170
37	1	0	-4.275717	1.096646	0.527751
38	1	0	-4.451813	-0.065911	1.700271
39	1	0	-2.944767	0.431138	1.281198

## Standard orientation of TS-T1-s-C2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-s-C2

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -328.02 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	3.120945	-0.038275	-2.423166
2	1	0	3.586604	-0.476388	-1.673438
3	1	0	3.809030	0.348100	-2.975197
4	8	0	4.415398	-1.047038	-0.261244
5	1	0	4.219748	-0.319359	0.357517
6	1	0	3.833086	-1.788636	0.042671
7	8	0	2.657196	-2.732321	0.725799
8	1	0	2.407482	-3.603796	0.399705
9	17	0	1.159570	-1.487093	-0.171114
10	8	0	3.442682	0.941242	1.421329
11	1	0	3.027113	1.417556	0.663228
12	1	0	4.053233	1.550960	1.847758
13	8	0	2.464746	2.044653	-0.787210
14	1	0	2.584397	1.323273	-1.438336
15	1	0	1.548619	2.373985	-0.864973
16	8	0	2.193379	-1.095212	2.852247
17	1	0	2.286571	-1.812671	2.195170
18	1	0	2.568941	-0.315339	2.410197
19	6	0	-2.165809	-1.390046	-1.016630
20	6	0	-2.046268	-0.672408	0.215970
21	6	0	-3.030430	-0.837362	1.229731

22	6	0	-4.086229	-1.665372	0.977095
23	6	0	-4.191525	-2.360762	-0.265405
24	6	0	-3.254131	-2.248548	-1.260765
25	6	0	-0.212797	-0.287589	-1.091405
26	6	0	-0.870332	0.072577	0.142312
27	1	0	-2.929373	-0.324198	2.179967
28	1	0	-4.855003	-1.814059	1.724876
29	1	0	-5.045109	-3.010844	-0.419887
30	1	0	-3.337712	-2.791572	-2.193640
31	1	0	-0.905181	-1.532925	-2.687129
32	1	0	0.425370	0.389549	-1.645304
33	7	0	-1.108754	-1.097617	-1.797666
34	6	0	-0.307473	1.065357	1.102950
35	1	0	0.761590	1.174219	0.918210
36	1	0	-0.434702	0.725048	2.134080
37	6	0	-0.940226	2.457070	0.930289
38	6	0	-1.103820	2.816090	-0.562930
39	8	0	-0.041004	3.030841	-1.188686
40	8	0	-2.263283	2.814524	-1.012745
41	1	0	-0.317815	3.193697	1.433756
42	7	0	-2.289990	2.513815	1.565281
43	1	0	-2.308991	2.061984	2.482533
44	1	0	-2.587653	3.485365	1.679588
45	1	0	-2.977951	2.071890	0.946409

### Standard orientation of TS-T1-s-C3

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-s-C3

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -280.29 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-2.880462	1.136885	-2.329384
2	1	0	-3.041705	0.220994	-2.012350
3	1	0	-3.657669	1.383295	-2.841739
4	8	0	-3.531094	-1.287005	-1.259466
5	1	0	-3.595442	-0.943803	-0.347796

6	1	0	-2.920529	-2.051140	-1.216275
7	8	0	-1.809288	-3.298838	-0.650229
8	1	0	-1.286442	-3.951490	-1.129816
9	17	0	-0.486344	-1.817620	-0.197190
10	8	0	-3.577333	-0.087941	1.238964
11	1	0	-3.418530	0.823800	0.898354
12	1	0	-4.485291	-0.109516	1.560084
13	8	0	-3.161932	2.334043	0.132210
14	1	0	-3.008506	2.011742	-0.779256
15	1	0	-2.296958	2.594311	0.506911
16	8	0	-3.001666	-2.806270	1.742001
17	1	0	-2.585067	-3.145328	0.928315
18	1	0	-3.020574	-1.843859	1.639330
19	6	0	2.726085	-0.817205	0.860885
20	6	0	2.067363	-0.473406	-0.326595
21	6	0	2.737969	-0.588838	-1.542135
22	6	0	4.049229	-1.049663	-1.526996
23	6	0	4.683778	-1.398575	-0.326704
24	6	0	4.029130	-1.291077	0.894514
25	6	0	0.684623	-0.125069	1.459796
26	6	0	0.697782	-0.076837	0.026575
27	1	0	2.246112	-0.328253	-2.473620
28	1	0	4.592560	-1.143927	-2.459689
29	1	0	5.705642	-1.757578	-0.350235
30	1	0	4.510778	-1.556707	1.827732
31	1	0	2.021692	-0.790898	2.892386
32	1	0	-0.134650	0.122351	2.121385
33	7	0	1.829713	-0.591326	1.916885
34	6	0	-0.139683	0.893295	-0.769685
35	1	0	-1.176402	0.819967	-0.440510
36	1	0	-0.119014	0.605279	-1.823902
37	6	0	0.271697	2.359261	-0.626689
38	6	0	0.323563	2.756890	0.859332
39	8	0	-0.788797	2.866940	1.424711
40	8	0	1.452874	2.862280	1.373981
41	1	0	-0.441443	2.982789	-1.164485
42	7	0	1.616815	2.599965	-1.228357
43	1	0	1.723454	2.141161	-2.135996
44	1	0	1.780751	3.601122	-1.354830
45	1	0	2.341752	2.261342	-0.587556

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## Standard orientation of TS-T1-s-C4

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-s-C4

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -388.33 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-1.010882	-2.534543	0.546910
2	1	0	-1.650327	-2.339824	-0.185139
3	1	0	-1.124806	-3.468913	0.757465
4	8	0	-3.007588	-2.167111	-1.206876
5	1	0	-3.634053	-1.887668	-0.511913
6	1	0	-2.896245	-1.364333	-1.771828
7	8	0	-2.878021	0.202664	-2.388204
8	1	0	-2.357558	0.478017	-3.150825
9	17	0	-1.551662	0.667013	-0.786728
10	8	0	-4.510277	-1.057526	0.829754
11	1	0	-3.796644	-1.008619	1.501119
12	1	0	-5.235344	-1.557969	1.217253
13	8	0	-2.401476	-1.229969	2.504806
14	1	0	-1.816526	-1.688769	1.867390
15	1	0	-1.907372	-0.482580	2.856324
16	8	0	-4.920180	1.091831	-0.888415
17	1	0	-4.210964	0.890824	-1.531800
18	1	0	-4.843774	0.393638	-0.218105
19	6	0	1.552928	2.509832	0.129964
20	6	0	1.047147	1.181892	0.068667
21	6	0	-0.198334	0.880059	0.739618
22	6	0	-0.782427	1.945546	1.520915
23	6	0	-0.262337	3.212812	1.536824
24	6	0	0.930798	3.511204	0.837954
25	6	0	2.915202	1.317896	-1.147483
26	6	0	1.904166	0.436397	-0.754127
27	1	0	-0.329085	-0.123676	1.132105
28	1	0	-0.753591	3.997003	2.097652
29	1	0	1.345671	4.512958	0.860500
30	1	0	3.291109	3.351356	-0.774667
31	1	0	3.767314	1.126216	-1.783233

32	7	0	2.706105	2.539859	-0.625819
33	6	0	1.783148	-0.994958	-1.187654
34	1	0	2.243267	-1.113942	-2.168849
35	1	0	0.729235	-1.269105	-1.288425
36	6	0	2.473217	-1.987578	-0.250360
37	6	0	3.931448	-1.573690	0.026325
38	8	0	4.667818	-1.521883	-0.980862
39	8	0	4.225275	-1.304963	1.210486
40	1	0	2.447942	-2.983011	-0.693013
41	7	0	1.727974	-2.071221	1.037659
42	1	0	0.713138	-2.221318	0.870929
43	1	0	2.091389	-2.832022	1.612996
44	1	0	1.867824	-1.213371	1.577228
45	1	0	-1.687978	1.720959	2.073669

## Standard orientation of TS-T1-s-C5

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-s-C5

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -348.64 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	3.684311	2.789118	-0.047541
2	1	0	4.203597	2.072892	-0.481601
3	1	0	4.294521	3.523601	0.077390
4	8	0	5.182123	0.760764	-1.055361
5	1	0	5.115413	0.201700	-0.259181
6	1	0	4.575570	0.338531	-1.715891
7	8	0	3.437350	-0.556687	-2.515255
8	1	0	2.962198	-0.278559	-3.305171
9	17	0	2.039504	-0.011480	-0.954170
10	8	0	4.676364	-0.723750	1.259631
11	1	0	4.218787	0.022982	1.704959
12	1	0	5.483580	-0.895040	1.755784
13	8	0	3.616279	1.513734	2.327470
14	1	0	3.547357	2.047905	1.504691
15	1	0	2.748031	1.510708	2.742143

16	8	0	4.193323	-2.518166	-0.838783
17	1	0	3.874213	-1.942648	-1.560327
18	1	0	4.263898	-1.935474	-0.066671
19	6	0	-1.341977	-0.340180	0.042731
20	6	0	-0.409927	0.652987	-0.074731
21	6	0	0.854024	0.525473	0.609200
22	6	0	1.032486	-0.574956	1.548154
23	6	0	0.107384	-1.556067	1.693172
24	6	0	-1.081395	-1.440916	0.926905
25	6	0	-3.089232	-1.741880	-0.021566
26	6	0	-2.644442	-0.573177	-0.550529
27	1	0	1.353973	1.456122	0.858058
28	1	0	0.252816	-2.395182	2.361895
29	1	0	-2.237034	-3.121208	1.375011
30	1	0	-4.010544	-2.278572	-0.188836
31	7	0	-2.137505	-2.254176	0.861437
32	6	0	-3.366619	0.332380	-1.500682
33	1	0	-3.910492	-0.252617	-2.242044
34	1	0	-2.651152	0.960911	-2.036740
35	6	0	-4.397975	1.217951	-0.799071
36	6	0	-5.452612	0.372531	-0.054939
37	8	0	-6.108663	-0.406201	-0.775978
38	8	0	-5.529058	0.531811	1.181414
39	1	0	-4.889023	1.861526	-1.528109
40	7	0	-3.723659	2.117007	0.186256
41	1	0	-2.938262	2.621029	-0.231767
42	1	0	-4.386403	2.796281	0.563520
43	1	0	-3.382515	1.571930	0.982633
44	1	0	1.966245	-0.614888	2.096825
45	1	0	-0.572710	1.513536	-0.716157

## Standard orientation of TS-T1-s-C6

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-s-C6

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -374.57 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z



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1	8	0	-4.510863	-2.186918	0.813844
2	1	0	-4.878152	-1.385040	0.375893
3	1	0	-5.253414	-2.618516	1.249435
4	8	0	-5.506205	0.129191	-0.206826
5	1	0	-5.002330	0.705390	0.397365
6	1	0	-5.042585	0.202963	-1.077509
7	8	0	-3.961411	0.493765	-2.314578
8	1	0	-3.867546	-0.022045	-3.122486
9	17	0	-2.429537	-0.339066	-1.071566
10	8	0	-3.825760	1.566294	1.514410
11	1	0	-3.510285	0.760761	1.980109
12	1	0	-4.331433	2.080543	2.152344
13	8	0	-3.248285	-0.769950	2.728474
14	1	0	-3.643444	-1.377615	2.063734
15	1	0	-2.349463	-1.070947	2.893716
16	8	0	-3.534024	2.793107	-0.990941
17	1	0	-3.648552	2.058359	-1.623584
18	1	0	-3.525368	2.372319	-0.117238
19	6	0	1.055745	-1.463953	-1.075772
20	6	0	-0.165294	-1.939019	-0.725732
21	6	0	-1.048135	-1.212787	0.175508
22	6	0	-0.551301	-0.027868	0.827426
23	6	0	0.664947	0.446714	0.442647
24	6	0	1.503058	-0.235634	-0.500721
25	6	0	2.534198	1.616906	0.214547
26	6	0	2.676934	0.516211	-0.639708
27	1	0	-1.753109	-1.811006	0.743317
28	1	0	1.011669	2.269427	1.500581
29	1	0	3.231272	2.422922	0.396296
30	7	0	1.351705	1.578851	0.844152
31	6	0	3.893724	0.192618	-1.452756
32	1	0	4.338441	1.105709	-1.849596
33	1	0	3.623723	-0.439106	-2.302382
34	6	0	4.976096	-0.502811	-0.621322
35	6	0	5.357600	0.363451	0.596664
36	8	0	5.938705	1.432565	0.323779
37	8	0	5.003691	-0.061545	1.717395
38	1	0	5.852423	-0.701382	-1.235636
39	7	0	4.472652	-1.821228	-0.129494
40	1	0	4.035640	-2.369401	-0.874014
41	1	0	5.234199	-2.370332	0.273482
42	1	0	3.793935	-1.667904	0.622220
43	1	0	-1.169392	0.485697	1.555960

44	1	0	-0.538655	-2.865780	-1.145120
45	1	0	1.691823	-1.999306	-1.772020

## Standard orientation of TS-T1-s-C7

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-s-C7

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -355.47 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	4.366138	0.758673	1.825143
2	1	0	4.537427	0.126772	1.090849
3	1	0	5.165026	0.770215	2.362713
4	8	0	4.725714	-1.159124	-0.085427
5	1	0	3.912004	-1.640938	0.137610
6	1	0	4.527922	-0.679900	-0.928888
7	8	0	3.862741	0.090998	-2.264058
8	1	0	4.233170	0.892640	-2.648860
9	17	0	2.385117	0.829997	-0.891036
10	8	0	2.155357	-2.199263	0.700451
11	1	0	2.266924	-1.730978	1.562922
12	1	0	2.149497	-3.143444	0.894095
13	8	0	2.585032	-0.878595	3.000199
14	1	0	3.227354	-0.207096	2.675500
15	1	0	1.818799	-0.399338	3.332858
16	8	0	2.310569	-2.136012	-2.183193
17	1	0	2.828072	-1.342868	-2.413859
18	1	0	2.196114	-2.090317	-1.223594
19	6	0	-0.113449	0.437361	0.139261
20	6	0	-1.269990	1.054651	-0.412491
21	6	0	-1.327598	2.433727	-0.468594
22	6	0	-0.249127	3.219115	0.013096
23	6	0	0.863845	2.628913	0.545177
24	6	0	1.033014	1.191105	0.577199
25	6	0	-1.511978	-1.170255	-0.506335
26	6	0	-2.159195	-0.013624	-0.817062
27	1	0	-2.200214	2.926497	-0.887581

28	1	0	-0.320820	4.297759	-0.036880
29	1	0	1.680519	3.231398	0.925538
30	1	0	1.616084	0.779204	1.394354
31	1	0	0.455639	-1.560865	0.316732
32	1	0	-1.820228	-2.195897	-0.640319
33	7	0	-0.277288	-0.884165	0.072243
34	6	0	-3.533079	0.126576	-1.398524
35	1	0	-3.726322	-0.682357	-2.103107
36	1	0	-3.618298	1.067908	-1.947642
37	6	0	-4.636284	0.055694	-0.339561
38	6	0	-4.547483	-1.251537	0.474007
39	8	0	-4.694072	-2.298472	-0.188581
40	8	0	-4.314014	-1.135426	1.695654
41	1	0	-5.612359	0.130282	-0.817194
42	7	0	-4.527556	1.210766	0.602936
43	1	0	-4.470500	2.104601	0.109515
44	1	0	-5.331273	1.235130	1.232994
45	1	0	-3.699398	1.102844	1.195081

## Standard orientation of TS-T1-a1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-a1

State=1-A

Charge = 1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -946.48 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.476518	-2.014611	0.553086
2	8	0	-2.390114	-2.772248	0.546820
3	1	0	-3.200353	-2.198888	0.330229
4	1	0	-2.274423	-3.426062	-0.155266
5	8	0	-4.248991	-1.092345	0.038876
6	1	0	-5.041485	-1.226214	0.570194
7	1	0	-3.839708	-0.253285	0.346508
8	8	0	-3.049442	1.179986	0.932869
9	1	0	-3.679935	1.741426	1.397638
10	6	0	-0.733927	-0.058221	-0.522745
11	6	0	0.110720	1.014442	-0.250903

12	6	0	0.132371	2.119714	-1.081677
13	6	0	-0.705991	2.107017	-2.200282
14	6	0	-1.530798	1.014995	-2.471443
15	6	0	-1.561357	-0.097635	-1.627566
16	6	0	0.251726	-0.662053	1.361165
17	6	0	0.887018	0.666565	0.990334
18	1	0	0.775279	2.968128	-0.872531
19	1	0	-0.714664	2.959726	-2.868308
20	1	0	-2.166038	1.032095	-3.348794
21	1	0	-2.210034	-0.944357	-1.817203
22	1	0	0.490010	-1.224230	2.255074
23	7	0	-0.627380	-1.035465	0.512474
24	6	0	2.413738	0.629023	0.841214
25	1	0	2.837857	0.265016	1.777464
26	1	0	2.762597	1.654510	0.693741
27	6	0	2.967141	-0.259171	-0.274923
28	6	0	2.382042	-1.691144	-0.272508
29	8	0	2.544276	-2.315053	0.793887
30	8	0	1.790264	-2.056783	-1.308007
31	1	0	4.042403	-0.330287	-0.118242
32	7	0	2.781427	0.330153	-1.637738
33	1	0	2.849442	1.350171	-1.640992
34	1	0	3.492527	-0.036547	-2.273615
35	1	0	1.875775	0.041958	-2.021596
36	1	0	-2.748700	1.689166	0.170558
37	17	0	0.488448	1.802342	2.348197

## Standard orientation of TS-I-a1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-I-a1

State=1-A

Charge = 1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -932.98 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.327692	-1.738183	-0.765098
2	8	0	-3.962530	-0.475732	0.297115
3	1	0	-4.225613	0.188760	-0.348915

4	8	0	-2.429967	-2.201361	-0.842924
5	1	0	-2.469171	-3.041258	-0.367803
6	1	0	-3.074088	-1.556708	-0.404844
7	8	0	-2.328451	0.715684	2.118585
8	1	0	-3.396407	-0.019586	0.957576
9	1	0	-2.202930	1.630709	1.842016
10	6	0	0.004281	0.239665	-0.602484
11	6	0	1.355937	0.537570	-0.446818
12	6	0	1.774768	1.849553	-0.336863
13	6	0	0.799752	2.849528	-0.385971
14	6	0	-0.549236	2.536383	-0.550994
15	6	0	-0.974578	1.211858	-0.669158
16	6	0	0.965182	-1.753031	-0.590669
17	6	0	2.096575	-0.765790	-0.469654
18	1	0	2.822359	2.096598	-0.208970
19	1	0	1.097509	3.887227	-0.295690
20	1	0	-1.281632	3.333884	-0.589662
21	1	0	-2.020042	0.953476	-0.786974
22	1	0	1.080073	-2.829501	-0.611298
23	7	0	-0.172720	-1.175688	-0.676231
24	1	0	2.787353	-0.861323	-1.308663
25	1	0	-1.467090	0.295565	2.011986
26	17	0	3.048112	-1.097235	1.020200

### Standard orientation of TS-I-a1'

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-I-a1'

State=1-A

Charge = 1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1053.69 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.270130	0.045741	0.871847
2	8	0	-1.379795	1.038978	1.781765
3	1	0	-0.500064	1.492784	1.762431
4	1	0	-1.502769	0.638377	2.652100
5	8	0	0.887621	2.289247	1.239790
6	1	0	1.257971	2.936604	1.850170

7	1	0	1.607435	1.699889	0.983746
8	8	0	-1.267086	2.768807	-0.544970
9	1	0	-0.399706	2.720917	-0.113979
10	1	0	-1.865473	2.333935	0.072824
11	6	0	1.140202	-1.229280	0.318381
12	6	0	0.785863	0.409520	-1.421666
13	6	0	2.165146	0.562229	-1.478615
14	6	0	3.018799	-0.156987	-0.627153
15	6	0	2.519388	-1.068511	0.292782
16	6	0	-1.086377	-0.848077	-0.060807
17	6	0	0.271934	-0.502191	-0.504109
18	1	0	2.593966	1.256287	-2.191496
19	1	0	4.088744	-0.001282	-0.692584
20	1	0	3.165689	-1.632407	0.954108
21	17	0	-2.481040	-0.749187	-1.117818
22	1	0	0.130053	0.980614	-2.066586
23	1	0	-1.680878	-2.523815	1.343666
24	6	0	-0.918517	-1.942482	0.844789
25	7	0	0.359707	-2.088733	1.108945
26	1	0	0.730349	-2.711912	1.819757

## Standard orientation of TS-T1-a2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-a2

State=1-A

Charge = 1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -195.02 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-3.396108	-1.085040	1.957991
2	1	0	-3.278581	-0.147249	1.726013
3	1	0	-2.313318	-1.969463	0.984850
4	8	0	-1.601633	-2.307317	0.386936
5	8	0	-2.817460	1.532477	1.117741
6	1	0	-2.324964	1.969526	0.387039
7	1	0	-3.188124	2.224936	1.674456
8	8	0	-3.980713	-0.087780	-0.919445
9	1	0	-3.807040	0.594868	-0.252229

10	1	0	-4.322571	-1.294634	1.797686
11	1	0	-2.046562	-2.703585	-0.373553
12	1	0	-3.893055	-0.922386	-0.445056
13	6	0	0.958413	-0.237373	1.260003
14	6	0	1.503833	-0.823452	0.121603
15	6	0	2.846294	-1.150608	0.073549
16	6	0	3.627729	-0.857941	1.193841
17	6	0	3.070299	-0.246264	2.316311
18	6	0	1.712520	0.076757	2.372918
19	6	0	-0.809740	-0.495047	-0.127023
20	6	0	0.433469	-0.838885	-0.938332
21	1	0	3.278651	-1.608311	-0.809382
22	1	0	4.682775	-1.102433	1.187633
23	1	0	3.700419	-0.019717	3.167880
24	1	0	1.271116	0.551651	3.240163
25	1	0	-1.048725	0.520899	1.631504
26	1	0	-1.758733	-0.228340	-0.570581
27	7	0	-0.421461	-0.005901	1.023111
28	6	0	0.655545	0.254640	-2.019683
29	1	0	-0.227154	0.277021	-2.660006
30	1	0	1.497748	-0.080630	-2.629668
31	6	0	0.925851	1.700793	-1.587550
32	6	0	-0.113668	2.327228	-0.633572
33	8	0	-1.303337	2.228385	-1.021789
34	8	0	0.310180	2.841651	0.412420
35	1	0	0.912114	2.285834	-2.507188
36	7	0	2.289967	1.901635	-1.002432
37	1	0	3.001257	1.333142	-1.469064
38	1	0	2.559861	2.883884	-1.091955
39	1	0	2.301281	1.694132	0.000643
40	17	0	0.316081	-2.398081	-1.811598

## Standard orientation of TS-I-a2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-I-a2

State=1-A

Charge = 1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -232.71 cm<sup>-1</sup>

Standard orientation:

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Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	8	0	2.104544	-2.301281	0.687825
2	1	0	2.964485	-1.984601	0.343546
3	1	0	1.502180	-0.849158	1.357443
4	8	0	1.072177	0.040039	1.397610
5	8	0	4.349353	-1.103071	-0.246265
6	1	0	4.718907	-1.486463	-1.049770
7	1	0	5.056043	-1.108955	0.409512
8	8	0	3.448617	1.467242	-0.773135
9	1	0	3.807532	0.587294	-0.558935
10	6	0	-1.446077	-0.946470	-0.399632
11	6	0	-1.732230	0.411661	-0.282955
12	6	0	-3.018145	0.833545	-0.007831
13	6	0	-4.005961	-0.141238	0.154236
14	6	0	-3.704019	-1.495701	0.025335
15	6	0	-2.407215	-1.927164	-0.260476
16	6	0	0.569043	0.055241	-0.551220
17	6	0	-0.463852	1.156895	-0.588540
18	1	0	-3.252512	1.887602	0.088463
19	1	0	-5.021062	0.160453	0.381907
20	1	0	-4.488317	-2.232191	0.153102
21	1	0	-2.162413	-2.977518	-0.359694
22	1	0	0.438403	-1.977473	-0.678922
23	1	0	1.601959	0.187136	-0.843849
24	7	0	-0.059972	-1.090313	-0.672585
25	17	0	-0.116754	2.582734	0.414997
26	1	0	2.288057	-3.001868	1.321695
27	1	0	1.768371	0.679466	1.596114
28	1	0	3.113049	1.825008	0.054842
29	1	0	-0.476841	1.512935	-1.624074

### Standard orientation of TS-T1-a2'

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-a2'

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -37.28 cm<sup>-1</sup>

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	8	0	3.630860	-0.276474	0.689488
2	6	0	-0.411753	-1.216358	-0.781021
3	6	0	-0.973888	-0.887345	0.446158
4	6	0	-2.166477	-1.466775	0.838906
5	6	0	-2.772398	-2.367222	-0.040557
6	6	0	-2.194310	-2.672281	-1.272258
7	6	0	-0.985634	-2.098052	-1.670483
8	6	0	1.039332	0.267943	0.106880
9	6	0	-0.100446	0.151749	1.099475
10	1	0	-2.616260	-1.227129	1.796495
11	1	0	-3.706728	-2.837482	0.240275
12	1	0	-2.688114	-3.372946	-1.934284
13	1	0	-0.523838	-2.328538	-2.622193
14	1	0	1.454500	-0.585947	-1.692726
15	1	0	1.950416	0.833790	0.236845
16	7	0	0.813936	-0.493999	-0.905415
17	6	0	-0.786147	1.491146	1.420352
18	1	0	-0.021227	2.184679	1.769781
19	1	0	-1.480662	1.315242	2.245401
20	6	0	-1.523441	2.171169	0.264568
21	6	0	-0.698620	2.199526	-1.042996
22	8	0	0.422902	2.733855	-0.931918
23	8	0	-1.206247	1.655551	-2.042659
24	1	0	-1.716619	3.197744	0.571293
25	7	0	-2.858895	1.559446	-0.023575
26	1	0	-3.311225	1.178901	0.810944
27	1	0	-3.482841	2.260597	-0.428210
28	1	0	-2.757692	0.821569	-0.728605
29	17	0	0.633348	-0.476157	2.629257
30	17	0	4.065333	-0.420495	-0.964288

### Standard orientation of TS-T1-b1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-b1

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -441.33 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.972058	0.699057	0.321541
2	17	0	0.080899	1.533452	1.973202
3	8	0	-2.821000	1.304512	0.566215
4	8	0	1.220963	2.962971	-0.289451
5	6	0	2.482084	0.308990	-0.873439
6	6	0	1.761243	0.017192	0.292770
7	6	0	2.277619	-0.847870	1.243368
8	6	0	3.530670	-1.425916	1.021665
9	6	0	4.243500	-1.129682	-0.139273
10	6	0	3.729808	-0.258720	-1.101202
11	6	0	0.717319	1.792936	-0.892398
12	6	0	0.421214	0.678028	0.136320
13	1	0	1.722570	-1.059702	2.151047
14	1	0	3.952269	-2.099365	1.758499
15	1	0	5.218391	-1.577041	-0.298327
16	1	0	4.288567	-0.025028	-2.000896
17	1	0	2.282141	1.793216	-2.275145
18	1	0	-0.168546	2.029889	-1.482799
19	7	0	1.735335	1.138687	-1.724947
20	6	0	-0.710716	-0.130176	-0.242854
21	1	0	-1.067126	0.039442	-1.259998
22	6	0	-0.782146	-1.551767	0.203258
23	6	0	-2.229990	-2.070696	0.110639
24	8	0	-2.948865	-1.884398	1.113509
25	8	0	-2.559873	-2.592680	-0.981783
26	1	0	-0.414387	-1.681445	1.220269
27	7	0	0.063308	-2.469547	-0.674070
28	1	0	1.005266	-2.098812	-0.809560
29	1	0	0.135708	-3.411386	-0.284155
30	1	0	-0.411514	-2.546949	-1.576801
31	1	0	1.314600	3.627110	-0.983419
32	17	0	-3.860300	1.114188	-0.767801

## Standard orientation of TS-T1-b2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-b2

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) =  $-182.42 \text{ cm}^{-1}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	1.207531	3.313701	0.283207
2	8	0	-0.768839	-2.192633	-1.683222
3	8	0	-0.850956	1.882701	-1.914461
4	6	0	1.818130	-0.059904	-0.815851
5	6	0	1.221317	0.200026	0.451666
6	6	0	1.830193	-0.255755	1.646247
7	6	0	2.980614	-0.989877	1.544443
8	6	0	3.548307	-1.269218	0.268153
9	6	0	2.993544	-0.825904	-0.909050
10	6	0	-0.196078	0.852323	-1.252593
11	6	0	0.064085	0.946709	0.219496
12	1	0	1.380062	-0.030468	2.607712
13	1	0	3.472607	-1.367727	2.432069
14	1	0	4.458802	-1.857028	0.228381
15	1	0	3.440691	-1.047002	-1.870483
16	1	0	1.133184	0.114122	-2.740291
17	1	0	-0.779603	-0.095793	-1.324257
18	7	0	1.102534	0.520105	-1.810680
19	17	0	-0.101681	-2.945809	-0.308464
20	1	0	-1.795026	1.786774	-1.688899
21	6	0	-0.984408	1.355300	1.198630
22	1	0	-1.443470	2.283109	0.858637
23	1	0	-0.515888	1.547675	2.165382
24	6	0	-2.121571	0.347526	1.392656
25	6	0	-2.988260	0.030839	0.151583
26	8	0	-3.164173	0.969610	-0.660159
27	8	0	-3.473806	-1.115844	0.102346
28	1	0	-2.796691	0.773392	2.137503
29	7	0	-1.633699	-0.937507	1.976097
30	1	0	-1.116833	-0.781504	2.845122
31	1	0	-2.429830	-1.550566	2.168523
32	1	0	-1.022328	-1.450403	1.323733

### Standard orientation of TS-T1-*tautomerize1*

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-tautomerize1

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -752.83 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.390955	2.037988	0.289671
2	1	0	0.222549	2.802994	-2.274389
3	8	0	0.300116	2.817118	-1.309712
4	1	0	0.043634	1.804386	-0.907962
5	8	0	2.657558	2.675037	-0.412889
6	1	0	2.968963	3.469030	0.035673
7	1	0	1.289363	2.908164	-1.048846
8	8	0	1.461966	1.115518	1.458256
9	6	0	-1.898798	0.393425	0.945029
10	6	0	-1.410351	0.056859	-0.339447
11	6	0	-2.306291	-0.425930	-1.294461
12	6	0	-3.655021	-0.551939	-0.960513
13	6	0	-4.117311	-0.198862	0.309823
14	6	0	-3.238948	0.280054	1.283040
15	6	0	0.352692	0.767722	0.978595
16	6	0	0.014655	0.356140	-0.357513
17	1	0	-1.957836	-0.699530	-2.286341
18	1	0	-4.354760	-0.928354	-1.698386
19	1	0	-5.169967	-0.301434	0.547400
20	1	0	-3.588646	0.550055	2.273423
21	1	0	-0.868193	1.165059	2.654012
22	7	0	-0.820159	0.816510	1.707145
23	6	0	1.015639	-0.240545	-1.316331
24	1	0	0.586754	-0.267228	-2.322902
25	6	0	1.484772	-1.649696	-0.940430
26	1	0	2.086017	-2.075875	-1.742493
27	1	0	1.913382	0.380220	-1.375249
28	7	0	0.302414	-2.545200	-0.753935
29	1	0	-0.374008	-2.459678	-1.515198
30	1	0	0.594132	-3.521561	-0.685025
31	1	0	-0.156200	-2.309618	0.130883
32	6	0	2.299296	-1.648199	0.367751
33	8	0	1.741077	-2.133061	1.377499
34	8	0	3.433791	-1.135607	0.286845

## Standard orientation of TS-T1-tautomerize2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-tautomerize2

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -851.75 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.837073	-1.282913	0.262330
2	6	0	-1.473858	-0.223085	0.930766
3	6	0	-2.842856	-0.044949	0.839638
4	6	0	-3.585373	-0.921724	0.040225
5	6	0	-2.947290	-1.956196	-0.642290
6	6	0	-1.568797	-2.154368	-0.536582
7	6	0	0.836322	-0.293325	1.299973
8	6	0	-0.394121	0.561998	1.618662
9	1	0	-3.331538	0.773809	1.359809
10	1	0	-4.657783	-0.794361	-0.050458
11	1	0	-3.532325	-2.624942	-1.264241
12	1	0	-1.078265	-2.965411	-1.063726
13	7	0	0.542437	-1.319550	0.507064
14	6	0	-0.206099	2.012657	1.133709
15	1	0	0.743217	2.377799	1.530707
16	1	0	-0.990698	2.638458	1.567541
17	6	0	-0.177841	2.267865	-0.377283
18	6	0	0.801406	1.383105	-1.186955
19	8	0	2.003928	1.507798	-0.882621
20	8	0	0.299082	0.651144	-2.066787
21	1	0	0.117917	3.306025	-0.525839
22	7	0	-1.536889	2.138410	-0.999069
23	1	0	-2.279376	2.487691	-0.390167
24	1	0	-1.571482	2.653656	-1.880572
25	1	0	-1.718452	1.156444	-1.224765
26	8	0	1.973688	0.007917	1.750202
27	1	0	3.197145	-0.422662	0.932161
28	1	0	-0.524657	0.593738	2.704127
29	1	0	1.610083	-1.791910	-0.554566
30	8	0	2.421972	-1.910906	-1.187689

31	1	0	2.629285	-2.852248	-1.233988
32	1	0	3.291294	-1.326651	-0.519598
33	8	0	3.914985	-0.720616	0.267087
34	1	0	4.521041	-1.318531	0.722908

## Standard orientation of TS-T1-c1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-c1

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -220.85 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-3.457319	1.107631	-1.126842
2	8	0	-1.264431	-1.226398	0.915602
3	6	0	-0.010872	1.689251	-0.488097
4	6	0	1.242693	1.180743	0.000333
5	6	0	2.423881	1.959065	-0.063865
6	6	0	2.366815	3.198693	-0.642345
7	6	0	1.126496	3.696295	-1.151579
8	6	0	-0.039704	2.983077	-1.089119
9	6	0	-0.445014	-0.365135	0.145486
10	6	0	0.964788	-0.044516	0.637138
11	1	0	3.353109	1.574879	0.347675
12	1	0	3.253939	3.815850	-0.715586
13	1	0	1.115634	4.683457	-1.602094
14	1	0	-0.970715	3.383041	-1.475342
15	1	0	-2.465832	1.033412	-0.785679
16	1	0	-0.259954	-0.994644	-0.744813
17	7	0	-1.032662	0.857231	-0.315432
18	17	0	-3.884382	-0.485374	-1.505839
19	6	0	1.971666	-1.115721	0.956059
20	1	0	1.539043	-1.837016	1.648327
21	1	0	2.825430	-0.653098	1.455057
22	6	0	2.491815	-1.912845	-0.248358
23	6	0	1.416904	-2.734405	-0.987142
24	8	0	0.765936	-3.525123	-0.272932
25	8	0	1.296288	-2.538111	-2.216871

26	1	0	3.243012	-2.609694	0.124647
27	7	0	3.195098	-1.031188	-1.227495
28	1	0	3.944384	-0.497242	-0.779463
29	1	0	3.599597	-1.590955	-1.981084
30	1	0	2.545543	-0.371022	-1.664662
31	17	0	-2.401116	-0.473319	1.936370
32	17	0	0.600743	0.578089	2.873632

## Standard orientation of TS-T1-c2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-c2

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1150.40 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.298693	-1.850776	1.299715
2	8	0	1.588923	1.136889	1.162685
3	6	0	-1.825670	0.632834	0.521645
4	6	0	-1.365291	0.376311	-0.774735
5	6	0	-2.234268	-0.051016	-1.767610
6	6	0	-3.572844	-0.260780	-1.438886
7	6	0	-4.020960	-0.023653	-0.136540
8	6	0	-3.158166	0.426408	0.860366
9	6	0	0.438755	0.715527	0.661779
10	6	0	0.090653	0.732015	-0.834392
11	1	0	-1.878009	-0.222819	-2.779357
12	1	0	-4.267406	-0.608468	-2.194161
13	1	0	-5.063898	-0.193947	0.106581
14	1	0	-3.510278	0.607503	1.869629
15	1	0	-0.837447	0.836884	2.308886
16	1	0	0.543777	-0.499706	0.973678
17	7	0	-0.787148	1.107146	1.331260
18	17	0	-0.880669	-1.992467	2.502998
19	6	0	0.987709	-0.002979	-1.830954
20	1	0	1.947079	0.513407	-1.877010
21	1	0	0.519810	0.121668	-2.810683
22	6	0	1.329423	-1.484129	-1.664005

23	6	0	2.456526	-1.858801	-0.667353
24	8	0	3.258380	-0.961353	-0.342676
25	8	0	2.496458	-3.069095	-0.344355
26	1	0	1.712005	-1.805182	-2.635854
27	7	0	0.154695	-2.364402	-1.388125
28	1	0	-0.616774	-2.198377	-2.036219
29	1	0	0.447929	-3.340076	-1.468538
30	1	0	-0.157364	-2.227589	-0.403781
31	17	0	1.899547	3.045638	1.271722
32	17	0	0.139528	2.509284	-1.447305

## Standard orientation of TS-T1-2-OH-d

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-2-OH-d

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -928.50 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.924874	-0.498137	1.430463
2	8	0	4.027539	0.388177	2.194727
3	1	0	4.053948	1.338594	2.343189
4	17	0	2.078918	-1.069944	-0.466812
5	8	0	1.632089	-0.529825	2.833352
6	1	0	1.717631	-1.443456	3.126497
7	1	0	2.547655	-0.204272	2.627086
8	8	0	4.073971	-1.747327	-1.403647
9	1	0	4.419952	0.221731	1.268146
10	1	0	3.988622	-1.422474	-2.306075
11	8	0	5.101241	0.008996	-0.099463
12	1	0	4.607456	-0.909184	-0.787710
13	1	0	6.016794	-0.219354	0.086689
14	6	0	0.453398	1.019246	0.077530
15	6	0	-0.663634	1.195740	-0.723703
16	6	0	-1.000400	2.471754	-1.155853
17	6	0	-0.199297	3.536864	-0.751547
18	6	0	0.921494	3.332448	0.056808
19	6	0	1.272072	2.055481	0.485776



20	6	0	-0.714217	-1.021930	0.099394
21	6	0	-1.316650	-0.128601	-1.001905
22	1	0	-1.864964	2.633703	-1.790925
23	1	0	-0.447191	4.541273	-1.072539
24	1	0	1.529789	4.178110	0.353044
25	1	0	2.150362	1.866773	1.093394
26	7	0	0.641906	-0.375164	0.402831
27	6	0	-2.844613	-0.151022	-1.097894
28	1	0	-3.148078	-1.133305	-1.459964
29	1	0	-3.137009	0.578078	-1.857015
30	6	0	-3.666132	0.082781	0.168813
31	6	0	-3.553849	-1.025016	1.244900
32	8	0	-3.616724	-2.191473	0.815205
33	8	0	-3.417270	-0.636078	2.424171
34	1	0	-4.710314	0.108059	-0.146619
35	7	0	-3.413542	1.408827	0.812098
36	1	0	-3.557002	2.184543	0.161746
37	1	0	-4.049786	1.520767	1.604548
38	1	0	-2.466851	1.473346	1.195839
39	8	0	-0.629905	-2.342556	-0.228559
40	1	0	-0.712696	-2.880923	0.569096
41	17	0	-0.708457	-0.702128	-2.631838
42	1	0	-1.256154	-0.850081	1.033457

## Standard orientation of TS-T1-2-OCl-d

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-2-OCl-d

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -605.88 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.059084	-0.183936	-1.264182
2	8	0	-4.123186	0.751760	-1.845399
3	1	0	-3.830130	1.506467	-1.323991
4	17	0	-2.163433	-0.055238	0.763825
5	8	0	-1.855812	-0.396920	-2.554798
6	1	0	-2.007725	-1.335367	-2.711983

7	1	0	-2.741454	0.016343	-2.359105
8	8	0	-4.131874	-0.238229	1.863620
9	1	0	-4.556990	0.097401	-1.190200
10	1	0	-4.360784	0.683327	2.026729
11	8	0	-5.173216	-0.922299	-0.218935
12	1	0	-4.666667	-0.556631	0.909729
13	1	0	-4.700312	-1.730106	-0.445911
14	6	0	-0.170251	1.467550	-0.326026
15	6	0	0.996035	1.582231	0.414686
16	6	0	1.629588	2.812659	0.514617
17	6	0	1.066311	3.896553	-0.154340
18	6	0	-0.104503	3.754955	-0.902453
19	6	0	-0.750614	2.525533	-1.000094
20	6	0	0.522328	-0.701459	0.151509
21	6	0	1.367359	0.256178	1.018154
22	1	0	2.539465	2.924751	1.094608
23	1	0	1.546140	4.865741	-0.095577
24	1	0	-0.518195	4.613498	-1.416789
25	1	0	-1.659883	2.397832	-1.576274
26	7	0	-0.673810	0.112804	-0.293218
27	6	0	2.858795	-0.078226	1.112164
28	1	0	2.967963	-0.988326	1.701844
29	1	0	3.337469	0.729421	1.670790
30	6	0	3.637128	-0.335998	-0.176882
31	6	0	3.208041	-1.605013	-0.952670
32	8	0	3.053659	-2.623938	-0.256197
33	8	0	3.055709	-1.473093	-2.185822
34	1	0	4.677094	-0.480547	0.119250
35	7	0	3.647173	0.827503	-1.115712
36	1	0	3.993641	1.679445	-0.668278
37	1	0	4.249135	0.607268	-1.912271
38	1	0	2.719222	1.014026	-1.504650
39	8	0	0.185452	-1.849280	0.846144
40	17	0	0.734540	0.236177	2.734445
41	1	0	1.044406	-0.920422	-0.782623
42	17	0	-0.420168	-3.060710	-0.191769

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### Standard orientation of TS-T1-2-OCl-e(1,3-di-Cl-2-O-3-R-Indoline)

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-2-OCl-e(1,3-di-Cl-2-O-3-R-Indoline)

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1324.79 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.167347	-1.614670	-1.648882
2	8	0	-1.530202	1.002862	-1.001818
3	6	0	1.779386	0.752292	0.172473
4	6	0	1.145383	0.058593	1.208929
5	6	0	1.889157	-0.640144	2.145489
6	6	0	3.279074	-0.642634	2.021338
7	6	0	3.898537	0.064122	0.989738
8	6	0	3.157266	0.775864	0.046952
9	6	0	-0.430520	0.627154	-0.379518
10	6	0	-0.330902	0.318589	1.112735
11	1	0	1.402559	-1.175531	2.953960
12	1	0	3.881726	-1.193940	2.733158
13	1	0	4.979694	0.055703	0.911159
14	1	0	3.641931	1.303329	-0.765952
15	1	0	-0.186598	-0.492126	-1.016536
16	7	0	0.801867	1.393855	-0.632028
17	17	0	1.830512	-1.911689	-1.787750
18	6	0	-1.326789	-0.638998	1.774875
19	1	0	-2.243110	-0.084925	1.974297
20	1	0	-0.910182	-0.904305	2.749693
21	6	0	-1.806856	-1.913260	1.081039
22	6	0	-2.808265	-1.687378	-0.077251
23	8	0	-3.752540	-0.908553	0.176857
24	8	0	-2.622812	-2.338472	-1.127509
25	1	0	-2.363504	-2.461128	1.843533
26	7	0	-0.708556	-2.818562	0.638143
27	1	0	0.031588	-2.883251	1.340028
28	1	0	-1.072196	-3.757485	0.470533
29	1	0	-0.307248	-2.472032	-0.267315
30	17	0	-2.237924	2.731442	-0.627465
31	17	0	-0.569018	1.912653	2.101969
32	17	0	1.195548	1.530189	-2.318480

**Standard orientation of TS-T1-2-OH-e(1-Cl-2-OH-3-R-Indole)**

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-2-OH-e(1-Cl-2-OH-3-R-Indole)

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -702.45 cm<sup>-1</sup>

Standard orientation:

-----						
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)			
			X	Y	Z	
-----						
1	8	0	-1.228986	1.992938	0.160465	
2	8	0	-0.741588	-0.940058	2.158770	
3	6	0	1.859974	0.118592	0.069645	
4	6	0	1.017513	-0.475516	-0.912832	
5	6	0	1.443810	-0.548951	-2.261906	
6	6	0	2.661930	-0.003491	-2.587017	
7	6	0	3.467188	0.620014	-1.593344	
8	6	0	3.088938	0.701873	-0.267828	
9	6	0	-0.133278	-0.355217	1.068576	
10	6	0	-0.153799	-0.906538	-0.271948	
11	1	0	0.812797	-1.026466	-3.006555	
12	1	0	3.021671	-0.037474	-3.609750	
13	1	0	4.419711	1.047998	-1.891571	
14	1	0	3.713846	1.185466	0.475405	
15	1	0	-0.664698	0.705318	0.747716	
16	7	0	1.248427	0.015912	1.287199	
17	17	0	0.083233	3.009886	-0.185124	
18	6	0	-1.340118	-1.576762	-0.873811	
19	1	0	-1.698934	-2.346298	-0.184130	
20	1	0	-1.030951	-2.068233	-1.800392	
21	6	0	-2.527489	-0.653864	-1.183625	
22	6	0	-3.340643	-0.119810	0.021695	
23	8	0	-3.229583	-0.720626	1.124123	
24	8	0	-4.087577	0.851585	-0.229884	
25	1	0	-3.225982	-1.226258	-1.800085	
26	7	0	-2.106783	0.532438	-1.987790	
27	1	0	-1.469745	0.271583	-2.749052	
28	1	0	-2.930500	0.988058	-2.394277	
29	1	0	-1.647848	1.230218	-1.340201	
30	17	0	1.022631	-3.624891	0.425542	
31	1	0	-1.713289	-0.911970	1.976193	
32	17	0	1.627084	1.090118	2.555312	
-----						

## Standard orientation of TS-T1-2-OC1-e(1-Cl-2-OC1-3-R-Indole)

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-2-OC1-e(1-Cl-2-OC1-3-R-Indole)

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -842.25 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.642288	-2.047648	-0.952239
2	8	0	1.227184	0.321086	1.651085
3	6	0	-1.997328	0.041140	0.339575
4	6	0	-1.378130	0.894877	-0.618082
5	6	0	-2.146778	1.460316	-1.666993
6	6	0	-3.470232	1.124116	-1.746947
7	6	0	-4.054197	0.234701	-0.801797
8	6	0	-3.344505	-0.323998	0.236962
9	6	0	0.247389	0.005738	0.728305
10	6	0	-0.024151	0.993885	-0.302584
11	1	0	-1.685200	2.129833	-2.383472
12	1	0	-4.090037	1.527104	-2.537923
13	1	0	-5.105162	-0.010344	-0.905386
14	1	0	-3.806063	-1.001859	0.943712
15	1	0	0.509639	-0.967939	0.015683
16	7	0	-1.071568	-0.315870	1.273129
17	17	0	-0.896163	-2.658746	-1.337464
18	6	0	1.006650	1.808411	-1.000091
19	1	0	1.564174	2.374699	-0.252113
20	1	0	0.501969	2.521555	-1.652204
21	6	0	2.031217	1.011487	-1.821515
22	6	0	3.146688	0.332918	-0.991982
23	8	0	3.740647	1.078180	-0.186040
24	8	0	3.382303	-0.868623	-1.242855
25	1	0	2.526257	1.725001	-2.480773
26	7	0	1.372329	-0.000760	-2.698767
27	1	0	0.560268	0.394479	-3.179062
28	1	0	2.029246	-0.334480	-3.405520
29	1	0	1.075013	-0.836369	-2.135585
30	17	0	-0.478982	3.176016	1.707385

31	17	0	2.162230	-1.033580	2.148343
32	17	0	-1.270882	-1.758441	2.167818

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**Standard orientation of TS-T1-2-OH-e(2-OH-3-Cl-3-R-3H-Indole)**

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-2-OH-e(2-OH-3-Cl-3-R-3H-Indole)  
State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1203.65 cm<sup>-1</sup>

Standard orientation:

-----

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.522338	1.343346	-1.137017
2	8	0	0.339053	-1.834308	-1.644928
3	6	0	-1.595534	0.639858	-0.128319
4	6	0	-0.956563	0.208602	1.037662
5	6	0	-1.167594	0.861390	2.241777
6	6	0	-2.053775	1.939129	2.255333
7	6	0	-2.705926	2.352154	1.089037
8	6	0	-2.481022	1.708391	-0.123470
9	6	0	-0.071664	-0.791690	-0.844322
10	6	0	-0.108227	-0.980006	0.687199
11	1	0	-0.668238	0.539466	3.150140
12	1	0	-2.243587	2.462405	3.185299
13	1	0	-3.389913	3.191751	1.130025
14	1	0	-2.970222	2.027748	-1.036404
15	1	0	0.689583	0.212963	-1.014137
16	7	0	-1.186476	-0.091929	-1.278194
17	17	0	0.603885	2.612917	-1.768669
18	6	0	1.190638	-1.217984	1.465826
19	1	0	1.515705	-2.239331	1.265091
20	1	0	0.928476	-1.183449	2.526821
21	6	0	2.437834	-0.365897	1.263531
22	6	0	3.232215	-0.560070	-0.051382
23	8	0	2.923239	-1.528673	-0.785335
24	8	0	4.168220	0.245816	-0.227233
25	1	0	3.127435	-0.671676	2.053444
26	7	0	2.221708	1.098242	1.462870
27	1	0	1.669697	1.294118	2.299769

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28	1	0	3.125474	1.566558	1.551161
29	1	0	1.758395	1.484576	0.612331
30	17	0	-1.115340	-2.482911	1.078638
31	1	0	1.293829	-1.953918	-1.465001
32	17	0	-2.901977	-1.444600	-1.577757

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### Standard orientation of TS-T1-2-OCI-e(2-OCI-3-Cl-3-R-3H-Indole)

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-2-OCI-e(2-OCI-3-Cl-3-R-3H-Indole) State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1339.63 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.490673	-0.391605	1.598456
2	8	0	0.440661	2.139376	-0.481172
3	6	0	-1.713758	-0.407313	0.561393
4	6	0	-1.216308	-1.015276	-0.591911
5	6	0	-1.622334	-2.292093	-0.948014
6	6	0	-2.537495	-2.943464	-0.120268
7	6	0	-3.029149	-2.328085	1.034087
8	6	0	-2.620338	-1.046036	1.392760
9	6	0	-0.050827	0.897334	-0.091357
10	6	0	-0.254303	-0.067170	-1.257136
11	1	0	-1.242847	-2.773447	-1.843985
12	1	0	-2.871578	-3.942165	-0.376139
13	1	0	-3.737340	-2.857687	1.660498
14	1	0	-2.995188	-0.558429	2.285239
15	1	0	0.769924	0.264294	0.792032
16	7	0	-1.166315	0.901060	0.763612
17	17	0	0.699487	-0.473112	3.089767
18	6	0	0.939487	-0.683043	-1.998372
19	1	0	1.422907	0.104118	-2.576952
20	1	0	0.507785	-1.378124	-2.722749
21	6	0	2.077316	-1.412248	-1.282613
22	6	0	3.196819	-0.549107	-0.646145
23	8	0	3.258221	0.650830	-0.975438
24	8	0	3.986824	-1.177981	0.096629

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25	1	0	2.584547	-1.988132	-2.060164
26	7	0	1.641877	-2.418545	-0.267737
27	1	0	0.934285	-3.059230	-0.629763
28	1	0	2.456915	-2.961324	0.026573
29	1	0	1.292757	-1.927223	0.575637
30	17	0	-1.197897	0.781600	-2.629268
31	17	0	-2.672070	2.142993	0.080103
32	17	0	1.118904	3.019918	0.822709

### Standard orientation of TS-T1-f

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-f

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -26.56 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	4.017798	-2.005455	0.170164
2	1	0	3.526343	-2.514816	-0.484015
3	17	0	2.174838	1.443365	0.409757
4	8	0	2.229998	-1.513071	2.224806
5	1	0	1.605696	-0.853333	1.887995
6	1	0	2.861792	-1.672454	1.495873
7	8	0	3.718741	2.395218	0.195768
8	1	0	4.306249	-1.182374	-0.276979
9	1	0	3.508237	3.118251	-0.409822
10	8	0	4.910771	0.278310	-1.063295
11	1	0	4.601188	1.099367	-0.629095
12	1	0	5.873273	0.313182	-1.072801
13	6	0	0.108139	-0.780109	-0.311026
14	6	0	-1.205684	-1.255438	-0.185391
15	6	0	-1.676171	-2.293087	-0.969261
16	6	0	-0.816503	-2.849317	-1.921413
17	6	0	0.480829	-2.356754	-2.065693
18	6	0	0.964321	-1.319607	-1.264238
19	6	0	-0.698600	0.497497	1.336323
20	6	0	-1.876503	-0.405128	0.848241
21	1	0	-2.692166	-2.659554	-0.853973



22	1	0	-1.159485	-3.662660	-2.549677
23	1	0	1.134049	-2.791503	-2.814373
24	1	0	1.975277	-0.945388	-1.380228
25	7	0	0.396234	0.228158	0.616270
26	8	0	-0.816697	1.310829	2.254161
27	6	0	-3.093076	0.399233	0.378616
28	1	0	-3.930121	-0.290939	0.241320
29	1	0	-3.370205	1.091710	1.176253
30	6	0	-2.950684	1.226526	-0.905033
31	1	0	-3.867469	1.808306	-0.998063
32	7	0	-2.888310	0.372442	-2.133896
33	1	0	-3.517601	-0.431901	-2.075459
34	1	0	-3.148898	0.923256	-2.954669
35	1	0	-1.934377	0.036655	-2.294770
36	6	0	-1.769098	2.223445	-0.941215
37	8	0	-0.923337	2.065509	-1.849274
38	8	0	-1.791102	3.106883	-0.060294
39	17	0	-2.404159	-1.397444	2.274956

### Standard orientation of TS-T1-H<sub>2</sub>O-g-1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-H<sub>2</sub>O-g-1

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -887.18 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-3.282007	-1.422621	1.514937
2	1	0	-3.751154	-1.711137	2.305979
3	1	0	-2.942471	1.414673	0.498541
4	8	0	-2.596606	1.145494	1.390112
5	1	0	-2.827104	0.193795	1.513370
6	1	0	-1.396537	1.321269	1.574622
7	8	0	-4.713248	-0.908425	-0.787575
8	1	0	-4.437837	-1.475297	-1.514843
9	1	0	-4.216263	-1.205603	-0.002382
10	8	0	-3.746332	1.604567	-0.940064
11	1	0	-3.126287	1.711626	-1.668402

12	1	0	-4.124441	0.699842	-1.015220
13	17	0	1.575768	-0.800204	2.719551
14	17	0	-0.557542	2.639299	-0.818524
15	8	0	1.930775	1.985485	1.285749
16	6	0	0.208357	-0.945485	0.427121
17	6	0	-0.299008	-0.113848	-0.582430
18	6	0	-1.234004	-0.591662	-1.484676
19	6	0	-1.637951	-1.925314	-1.391679
20	6	0	-1.106787	-2.752761	-0.402860
21	6	0	-0.186891	-2.273529	0.533115
22	6	0	1.020491	1.204191	0.949777
23	6	0	0.464792	1.175594	-0.531289
24	1	0	-1.624519	0.051858	-2.266498
25	1	0	-2.353610	-2.323951	-2.100534
26	1	0	-1.420612	-3.788767	-0.346477
27	1	0	0.218766	-2.919375	1.302371
28	7	0	1.196701	-0.261957	1.140245
29	6	0	1.614025	1.263423	-1.554590
30	1	0	1.178212	1.565941	-2.509795
31	6	0	2.506205	0.050548	-1.847246
32	1	0	3.238610	0.415504	-2.568486
33	1	0	2.275177	2.070410	-1.232891
34	6	0	3.330922	-0.576084	-0.694208
35	8	0	3.219473	-1.811871	-0.544460
36	8	0	4.071134	0.216773	-0.083698
37	7	0	1.777106	-1.051700	-2.558869
38	1	0	1.051820	-0.703160	-3.188801
39	1	0	2.441038	-1.600026	-3.108993
40	1	0	1.362735	-1.703118	-1.886716
41	8	0	-0.271717	1.491962	1.874098
42	1	0	-0.148098	2.392407	2.202651
43	1	0	-2.496583	-1.977237	1.426415

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### Standard orientation of TS-T1-OCI-g-1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-OCI-g-1

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -159.95 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-3.968868	-0.605710	1.991590
2	1	0	-4.707158	-0.194596	2.454458
3	1	0	-3.061315	1.031182	-0.417874
4	8	0	-2.825332	1.329548	0.481084
5	1	0	-3.484516	0.118719	1.536177
6	1	0	-1.863338	1.533128	0.488911
7	8	0	-4.891304	-1.711153	-0.350904
8	1	0	-4.527055	-2.586300	-0.522069
9	1	0	-4.561452	-1.432126	0.529090
10	8	0	-3.818565	0.278329	-1.889933
11	1	0	-3.087287	-0.035266	-2.433293
12	1	0	-4.192146	-0.506419	-1.435889
13	17	0	1.985675	0.952576	2.483022
14	17	0	-0.529140	1.218930	-2.218420
15	8	0	2.100518	2.028465	-0.411614
16	6	0	0.352384	-0.622436	1.035574
17	6	0	-0.216940	-0.687583	-0.242328
18	6	0	-1.229453	-1.590149	-0.516063
19	6	0	-1.660281	-2.440483	0.505343
20	6	0	-1.085651	-2.365073	1.772905
21	6	0	-0.070199	-1.451340	2.062665
22	6	0	1.267642	1.185561	-0.111157
23	6	0	0.537654	0.252499	-1.134978
24	1	0	-1.664324	-1.647542	-1.509070
25	1	0	-2.443266	-3.164391	0.314252
26	1	0	-1.433780	-3.027738	2.556942
27	1	0	0.372701	-1.398215	3.049969
28	7	0	1.411778	0.298989	1.020202
29	6	0	1.558274	-0.446154	-2.059393
30	1	0	1.000852	-0.855020	-2.905945
31	6	0	2.438701	-1.584484	-1.526349
32	1	0	3.088216	-1.850798	-2.361931
33	1	0	2.228304	0.318433	-2.458077
34	6	0	3.387584	-1.304404	-0.337290
35	8	0	3.351575	-2.118279	0.612308
36	8	0	4.148279	-0.326404	-0.481682
37	7	0	1.655206	-2.830023	-1.234993
38	1	0	0.899226	-2.970133	-1.909893
39	1	0	2.272007	-3.644235	-1.271755
40	1	0	1.255022	-2.813437	-0.293262
41	8	0	-0.231837	2.072731	0.604476

42            17            0            -0.289099    3.686497    0.144612

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## Standard orientation of TS-T1-OH-g-2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OH-g-2

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -719.68 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-3.248738	1.664627	0.804377
2	1	0	-3.758294	2.377154	0.396705
3	1	0	-3.310930	-1.165084	0.256465
4	8	0	-3.621180	-0.431344	-0.293399
5	1	0	-2.306871	1.734691	0.489725
6	1	0	-3.559004	0.583217	0.318986
7	17	0	0.206786	2.696071	0.550742
8	17	0	-0.876032	-1.928684	-2.170720
9	8	0	0.390543	1.399407	-2.078432
10	6	0	-0.509633	0.162199	1.032151
11	6	0	-0.322151	-1.050185	0.368281
12	6	0	-0.411636	-2.251035	1.061808
13	6	0	-0.621362	-2.223023	2.437794
14	6	0	-0.737502	-1.001081	3.104746
15	6	0	-0.699020	0.203929	2.410392
16	6	0	-0.379788	0.712046	-1.352971
17	6	0	0.054324	-0.809867	-1.060646
18	1	0	-0.290401	-3.193830	0.537312
19	1	0	-0.683958	-3.150111	2.994555
20	1	0	-0.884330	-0.988561	4.178449
21	1	0	-0.825374	1.150596	2.923020
22	7	0	-0.632710	1.242093	0.132670
23	6	0	1.534399	-1.104850	-1.384864
24	1	0	1.621734	-2.174203	-1.589605
25	6	0	2.663456	-0.782775	-0.397329
26	1	0	3.574091	-1.097676	-0.907736
27	1	0	1.772693	-0.579721	-2.311165
28	6	0	2.904924	0.683637	0.034393

29	8	0	2.817866	0.915420	1.259249
30	8	0	3.219699	1.462184	-0.884782
31	7	0	2.603427	-1.618715	0.845930
32	1	0	2.284811	-2.572753	0.666167
33	1	0	3.531310	-1.665566	1.270971
34	1	0	1.993692	-1.177058	1.539117
35	8	0	-1.774781	0.724432	-1.787844
36	1	0	-2.942552	-0.260705	-0.997790
37	1	0	-1.757795	0.658613	-2.751611

## Standard orientation of TS-T1-OCl-g-2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OCl-g-2

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -679.58 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.474782	1.592142	1.961651
2	1	0	3.204871	1.064345	2.315156
3	1	0	1.991760	2.592762	-0.812563
4	8	0	2.786531	2.118114	-0.537404
5	1	0	1.612684	0.910773	1.677344
6	1	0	2.750659	1.961016	1.065956
7	17	0	-0.235710	-0.240757	2.766337
8	17	0	1.170024	-0.457393	-2.498855
9	8	0	0.495491	-2.098123	0.654692
10	6	0	-0.275367	1.269221	0.550590
11	6	0	-0.408128	0.957483	-0.796456
12	6	0	-0.898908	1.913596	-1.681028
13	6	0	-1.299807	3.148851	-1.185378
14	6	0	-1.202414	3.430399	0.179910
15	6	0	-0.672210	2.497870	1.063439
16	6	0	0.741314	-0.968875	0.228727
17	6	0	0.001258	-0.453341	-1.091338
18	1	0	-0.978572	1.686939	-2.739536
19	1	0	-1.691390	3.898403	-1.862315
20	1	0	-1.522614	4.395517	0.553667

21	1	0	-0.561263	2.720296	2.118499
22	7	0	0.463428	0.278226	1.264823
23	6	0	-1.141309	-1.390351	-1.537291
24	1	0	-1.289410	-1.238252	-2.608568
25	6	0	-2.538136	-1.313440	-0.909585
26	1	0	-3.109140	-2.105234	-1.393343
27	1	0	-0.792377	-2.415281	-1.403243
28	6	0	-2.683643	-1.529629	0.615285
29	8	0	-3.061614	-0.537545	1.274181
30	8	0	-2.450205	-2.686033	1.012790
31	7	0	-3.250346	-0.040033	-1.252446
32	1	0	-3.042397	0.291789	-2.196243
33	1	0	-4.259901	-0.181859	-1.180628
34	1	0	-3.012755	0.681606	-0.565444
35	8	0	2.220986	-0.613955	0.114896
36	1	0	2.626830	1.182156	-0.739019
37	17	0	3.190260	-1.930077	-0.313603

## Standard orientation of TS-T1-O-h1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-O<sup>-</sup>-h1

State=1-A

Charge = -2 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -267.18 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	4.243000	-2.299406	0.633689
2	1	0	4.257137	-3.263291	0.719100
3	8	0	3.419875	-0.468110	2.520578
4	1	0	3.784070	-1.212202	2.005693
5	1	0	4.104567	-0.205708	3.145728
6	8	0	5.820855	-0.092544	-0.113976
7	1	0	5.495432	-0.970980	0.137940
8	1	0	5.061929	0.506407	0.016937
9	8	0	3.520584	1.381561	0.474582

10	1	0	3.330248	0.785540	1.226914
11	17	0	2.887435	-1.912508	-0.535856
12	1	0	2.886886	1.162449	-0.222535
13	8	0	-2.743063	1.702621	1.554267
14	17	0	0.760162	3.719359	-0.573409
15	17	0	-0.439631	0.008148	2.257398
16	8	0	-2.857641	1.199763	-0.618875
17	6	0	0.324508	1.164326	-0.796949
18	6	0	-0.327618	-0.095297	-0.439729
19	6	0	0.074346	-1.252261	-1.060411
20	6	0	1.081240	-1.292879	-2.053626
21	6	0	1.616702	-0.063023	-2.486448
22	6	0	1.271138	1.119084	-1.881623
23	6	0	-2.385279	1.076430	0.544716
24	6	0	-1.365585	-0.100541	0.660916
25	1	0	-0.361206	-2.203094	-0.772649
26	1	0	1.235663	-2.197166	-2.628157
27	1	0	2.339040	-0.050247	-3.296955
28	1	0	1.721783	2.041846	-2.221540
29	7	0	-0.014234	2.215067	-0.071702
30	6	0	-2.192171	-1.399557	0.793141
31	1	0	-2.683768	-1.371975	1.765161
32	1	0	-1.517991	-2.254304	0.819345
33	6	0	-3.324247	-1.660475	-0.209864
34	6	0	-4.671539	-0.951371	0.094738
35	8	0	-4.942371	-0.744492	1.294148
36	8	0	-5.401024	-0.717441	-0.897927
37	1	0	-3.548559	-2.728850	-0.170377
38	7	0	-2.980632	-1.363649	-1.631108
39	1	0	-2.242115	-1.963986	-1.996279
40	1	0	-3.825973	-1.480422	-2.195401
41	1	0	-2.699201	-0.371146	-1.692572

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### Standard orientation of TS-T1-OCI-h1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-OCI-h1

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -425.50 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	5.394951	-1.117318	0.703008
2	1	0	5.798201	-1.993748	0.692884
3	8	0	3.886690	-0.115844	2.651944
4	1	0	4.511826	-0.554969	2.024885
5	1	0	4.421935	0.286023	3.344720
6	8	0	5.675602	1.471774	-0.146046
7	1	0	5.757926	0.526889	0.084900
8	1	0	4.781635	1.721069	0.149672
9	8	0	3.097021	1.859109	0.914475
10	1	0	3.264010	1.159401	1.581420
11	17	0	3.727499	-1.328983	-0.494029
12	1	0	2.514232	1.469246	0.252932
13	8	0	-2.203299	1.460420	1.123958
14	17	0	-0.946708	2.852998	-1.577254
15	17	0	0.039946	0.067352	2.119077
16	8	0	-2.611130	0.297801	-0.833193
17	6	0	0.327397	0.582694	-1.147589
18	6	0	0.192230	-0.655350	-0.437372
19	6	0	0.988191	-1.708880	-0.743890
20	6	0	2.023004	-1.558126	-1.733764
21	6	0	2.076570	-0.327363	-2.475390
22	6	0	1.276052	0.741532	-2.183251
23	6	0	-1.749318	0.653150	0.022862
24	6	0	-0.864096	-0.505022	0.623291
25	1	0	0.890282	-2.660006	-0.230116
26	1	0	2.367188	-2.454514	-2.235946
27	1	0	2.807407	-0.246607	-3.272318
28	1	0	1.352127	1.673141	-2.728815
29	7	0	-0.551992	1.468793	-0.665620
30	6	0	-1.615971	-1.765443	1.058814
31	1	0	-2.106535	-1.558277	2.009308
32	1	0	-0.859656	-2.527418	1.259378
33	6	0	-2.700096	-2.365545	0.162015
34	6	0	-4.109087	-1.738111	0.283238
35	8	0	-4.422580	-1.263419	1.393886
36	8	0	-4.838069	-1.841006	-0.730954
37	1	0	-2.817851	-3.407244	0.469786
38	7	0	-2.336784	-2.404160	-1.282379
39	1	0	-1.470002	-2.914880	-1.456383
40	1	0	-3.097013	-2.844426	-1.805183
41	1	0	-2.252297	-1.431806	-1.616293



42            17            0            -3.558662    2.418769    0.771073

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## Standard orientation of TS-T1-OH-h2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-OH-h2

State=1-A

Charge = -2 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1286.34 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.054548	0.087291	2.917456
2	17	0	3.089250	2.225244	-0.154820
3	17	0	-1.275573	-2.110603	2.177315
4	8	0	-0.925333	1.118632	2.857446
5	6	0	1.863817	-0.164943	-0.047351
6	6	0	0.774937	-0.994778	0.317843
7	6	0	0.769172	-2.303589	-0.155601
8	6	0	1.774258	-2.794483	-0.985492
9	6	0	2.818016	-1.963168	-1.354238
10	6	0	2.864083	-0.654790	-0.879969
11	6	0	-0.065962	0.335763	2.408665
12	6	0	-0.392893	-0.392126	1.067223
13	1	0	-0.048325	-2.957158	0.117056
14	1	0	1.724377	-3.816174	-1.343028
15	1	0	3.607997	-2.321311	-2.004476
16	1	0	3.688669	-0.017115	-1.168448
17	7	0	1.824617	1.183822	0.415208
18	1	0	1.889152	1.200141	1.432827
19	6	0	-1.430530	0.216122	0.294624
20	1	0	-0.926060	1.415023	-0.067478
21	1	0	-2.228101	0.605653	0.928007
22	6	0	-2.007087	-0.401072	-0.958773
23	6	0	-1.063289	-0.753060	-2.129929
24	8	0	-0.281061	0.151610	-2.489606
25	8	0	-1.218904	-1.875946	-2.664233
26	1	0	-2.720947	0.313709	-1.375030
27	7	0	-2.842490	-1.612427	-0.628201
28	1	0	-3.260871	-2.000634	-1.475796

29	1	0	-2.276352	-2.347288	-0.197114
30	1	0	-3.582269	-1.368367	0.033366
31	8	0	-0.723217	2.635440	-0.411509
32	17	0	-2.250004	3.213493	-0.877046

## Standard orientation of TS-T1-OCI-h2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-OCI-h2

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1313.80 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-2.531210	-0.535377	-0.738742
2	17	0	-0.603356	0.215108	3.237523
3	17	0	-0.438262	-0.579361	-2.923992
4	8	0	-1.978828	1.653583	-0.876192
5	6	0	-0.431139	-1.424927	1.161774
6	6	0	0.039406	-1.304469	-0.152692
7	6	0	0.791234	-2.351189	-0.685999
8	6	0	1.080240	-3.480562	0.070132
9	6	0	0.601995	-3.592745	1.371140
10	6	0	-0.159684	-2.565104	1.910879
11	6	0	-1.651263	0.508377	-0.825497
12	6	0	-0.220163	-0.018805	-0.905544
13	1	0	1.157427	-2.288556	-1.702638
14	1	0	1.676734	-4.274363	-0.363966
15	1	0	0.814996	-4.476489	1.961018
16	1	0	-0.541157	-2.635826	2.923861
17	7	0	-1.226978	-0.341071	1.690801
18	1	0	-2.151348	-0.702172	1.925883
19	6	0	0.733529	1.052687	-0.796868
20	1	0	0.530792	1.717144	0.405053
21	1	0	0.444495	1.900683	-1.421358
22	6	0	2.219784	0.822843	-0.893564
23	6	0	2.886763	-0.178419	0.078617
24	8	0	2.613464	-0.029142	1.287761
25	8	0	3.689414	-0.999071	-0.421818

26	1	0	2.704923	1.782922	-0.698798
27	7	0	2.643410	0.472499	-2.301273
28	1	0	3.661226	0.498020	-2.386788
29	1	0	2.346035	-0.471555	-2.555511
30	1	0	2.238523	1.125793	-2.974528
31	8	0	0.443391	2.545632	1.314101
32	17	0	0.734291	4.041589	0.566492
33	17	0	-4.165126	-0.088320	-0.724381

### Standard orientation of TS-T1-OH-i-1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OH-i-1

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -162.71 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.005142	2.110444	1.106162
2	6	0	-1.776037	0.047923	1.039176
3	6	0	-1.168712	-0.391163	-0.179110
4	6	0	-1.847653	-1.291497	-1.041859
5	6	0	-3.073537	-1.753209	-0.656983
6	6	0	-3.650339	-1.331807	0.578620
7	6	0	-3.031821	-0.453734	1.433194
8	6	0	0.317235	0.911950	1.036525
9	6	0	0.042275	0.280126	-0.304068
10	1	0	-1.388670	-1.595984	-1.976249
11	1	0	-3.622550	-2.446639	-1.281183
12	1	0	-4.623417	-1.725423	0.850397
13	1	0	-3.487896	-0.143402	2.364812
14	1	0	-1.085638	1.148216	2.648351
15	1	0	0.883977	0.116802	1.562792
16	7	0	-0.991617	0.947290	1.659900
17	6	0	1.108247	0.096138	-1.328640
18	1	0	1.613379	1.048684	-1.483228
19	1	0	0.659611	-0.211444	-2.274269
20	6	0	2.192164	-0.908192	-0.923354
21	6	0	2.985412	-0.538564	0.352342

22	8	0	3.275624	0.674126	0.477118
23	8	0	3.271413	-1.478176	1.114434
24	1	0	2.904639	-0.968667	-1.747434
25	7	0	1.637941	-2.283734	-0.755717
26	1	0	1.223932	-2.637381	-1.621397
27	1	0	2.386451	-2.912648	-0.455260
28	1	0	0.922271	-2.314377	-0.023385
29	17	0	-0.932662	2.450264	-1.498640
30	1	0	1.944057	1.883914	0.966896

### Standard orientation of TS-T1-OCI-i-1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OCI-i-1

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -93.42 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.478625	-1.614182	0.240771
2	6	0	-1.651450	-0.805342	-0.944894
3	6	0	-1.466786	0.217358	0.043801
4	6	0	-2.561370	1.038143	0.444671
5	6	0	-3.760035	0.856020	-0.174373
6	6	0	-3.909920	-0.137007	-1.194352
7	6	0	-2.890584	-0.959916	-1.596367
8	6	0	0.554311	-0.808623	-0.434828
9	6	0	-0.160444	0.151917	0.483181
10	1	0	-2.423718	1.784137	1.220091
11	1	0	-4.616899	1.460508	0.093625
12	1	0	-4.880590	-0.241917	-1.665716
13	1	0	-3.024623	-1.710282	-2.364877
14	1	0	-0.356156	-2.061132	-1.942785
15	1	0	1.065440	-0.190553	-1.189684
16	7	0	-0.524455	-1.515839	-1.104610
17	6	0	0.555868	1.064817	1.416986
18	1	0	1.362904	0.519941	1.904557
19	1	0	-0.137510	1.413184	2.184037
20	6	0	1.199064	2.272248	0.715866

21	6	0	2.173302	1.840619	-0.400409
22	8	0	3.148371	1.170008	-0.016732
23	8	0	1.855332	2.159877	-1.566466
24	1	0	1.733678	2.846993	1.470073
25	7	0	0.163542	3.175525	0.134828
26	1	0	-0.239721	2.759600	-0.710028
27	1	0	-0.585637	3.382672	0.800385
28	1	0	0.590512	4.057965	-0.155495
29	17	0	-0.617864	-1.677016	2.482152
30	17	0	2.599532	-2.308040	-0.851092

### Standard orientation of TS-T1-OH-OH-i-2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OH-OH-i-2

State=1-A

Charge = 1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -308.50 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.776141	3.447338	0.861257
2	1	0	-0.718717	3.234452	-0.091823
3	1	0	-0.880086	4.402131	0.931341
4	8	0	-0.906252	2.495435	-1.714609
5	1	0	-1.817660	2.131074	-1.629201
6	1	0	-0.073010	1.072747	-2.132614
7	8	0	0.376211	0.201317	-2.241871
8	8	0	-3.280469	1.316679	-1.225366
9	1	0	-3.304769	1.489735	-0.257294
10	1	0	-4.035781	1.772953	-1.612250
11	8	0	-3.096002	2.134959	1.341925
12	1	0	-2.254197	2.633683	1.267775
13	1	0	-3.036593	1.594372	2.135794
14	8	0	-3.211053	-1.332715	-2.044397
15	1	0	-3.241348	-0.391927	-1.790996
16	1	0	-0.917139	3.139574	-2.431128
17	1	0	-0.258295	-0.409309	-2.638857
18	1	0	-2.332929	-1.485021	-2.408030
19	8	0	0.240930	-2.439141	-1.615922

20	6	0	2.857720	-0.496232	-0.442299
21	6	0	1.776560	0.286834	0.046193
22	6	0	1.991072	1.556598	0.625468
23	6	0	3.285407	1.990444	0.758749
24	6	0	4.360960	1.180349	0.310265
25	6	0	4.178541	-0.050787	-0.282382
26	6	0	1.016063	-1.804852	-0.651950
27	6	0	0.595239	-0.408911	-0.259944
28	1	0	1.147129	2.158352	0.948035
29	1	0	3.500167	2.952419	1.206503
30	1	0	5.372275	1.551093	0.435598
31	1	0	5.014774	-0.646797	-0.625791
32	1	0	3.002480	-2.447944	-1.076389
33	1	0	1.008556	-2.376667	0.291752
34	7	0	2.404948	-1.629879	-1.044560
35	6	0	-0.802373	-0.096092	0.159495
36	1	0	-1.478609	-0.454755	-0.613627
37	1	0	-0.931274	0.982940	0.252772
38	6	0	-1.270964	-0.767556	1.449991
39	6	0	-1.162116	-2.307597	1.466523
40	8	0	-1.559442	-2.879687	0.424172
41	8	0	-0.714052	-2.822222	2.504517
42	1	0	-2.326678	-0.518227	1.566630
43	7	0	-0.579008	-0.203258	2.643932
44	1	0	-0.795518	0.790504	2.758140
45	1	0	-0.873315	-0.713340	3.480346
46	1	0	0.437491	-0.306893	2.578435
47	1	0	-0.535027	-2.792077	-1.139027

## Standard orientation of TS-T1-OCI-OH-i-2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OCI-OH-i-2

State=1-A

Charge = 1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -262.56 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-3.282284	1.738165	0.386130

2	1	0	-3.004154	1.649840	-0.550311
3	1	0	-3.894841	2.478798	0.446718
4	8	0	-2.349165	1.027055	-2.088700
5	1	0	-2.783943	0.144949	-2.091003
6	1	0	-0.696291	0.258578	-2.259872
7	8	0	0.110349	-0.288042	-2.178289
8	8	0	-3.239374	-1.486806	-1.684801
9	1	0	-3.527085	-1.361515	-0.750072
10	1	0	-4.003326	-1.800764	-2.180451
11	8	0	-3.974333	-0.885382	0.827649
12	1	0	-3.847973	0.080786	0.750577
13	1	0	-4.920520	-1.034907	0.927727
14	8	0	-0.914124	-2.800205	-2.194827
15	1	0	-1.791703	-2.460793	-1.923527
16	1	0	-2.655621	1.506775	-2.865797
17	1	0	-0.180149	-1.225355	-2.252973
18	1	0	-0.519506	-3.212623	-1.418972
19	6	0	2.201870	1.541831	-0.516992
20	6	0	0.810713	1.482802	-0.208446
21	6	0	0.029451	2.666941	-0.165932
22	6	0	0.662244	3.863134	-0.359057
23	6	0	2.063283	3.906521	-0.605644
24	6	0	2.845140	2.778038	-0.684443
25	6	0	1.771274	-0.627581	-0.048833
26	6	0	0.469669	0.136559	-0.072363
27	1	0	-1.038508	2.615862	0.013193
28	1	0	0.104901	4.790250	-0.325988
29	1	0	2.531034	4.874583	-0.745702
30	1	0	3.907352	2.829797	-0.886673
31	1	0	3.721427	0.162825	-0.431521
32	7	0	2.733277	0.297573	-0.617915
33	6	0	-0.802651	-0.487165	0.396195
34	1	0	-0.798319	-1.542192	0.124846
35	1	0	-1.641816	-0.013127	-0.109596
36	6	0	-1.017325	-0.416762	1.917793
37	1	0	2.024966	-0.799432	1.006402
38	8	0	1.634431	-1.851293	-0.719223
39	17	0	2.885560	-2.934542	-0.310390
40	1	0	-1.868319	-1.051966	2.150738
41	7	0	-1.374400	0.963727	2.348433
42	1	0	-2.068361	1.392641	1.706015
43	1	0	-1.769669	0.944018	3.290587
44	1	0	-0.529420	1.539744	2.403276
45	6	0	0.236940	-0.896552	2.671703

46	8	0	0.892369	-0.022229	3.275696
47	8	0	0.504571	-2.105670	2.525302

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### Standard orientation of TS-T1-OH-OCI-i-2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OH-OCI-i-2

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -64.94 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.842285	1.132281	2.624040
2	1	0	1.714937	1.288120	1.647249
3	8	0	1.488893	1.621170	0.059887
4	1	0	2.433831	0.376988	2.692601
5	8	0	-0.917715	1.410138	-1.900203
6	6	0	1.273333	-1.161654	-1.312924
7	6	0	0.783576	-0.981441	0.029645
8	6	0	1.416492	-1.641855	1.125994
9	6	0	2.469800	-2.459315	0.858500
10	6	0	2.926603	-2.645799	-0.488692
11	6	0	2.354949	-2.033040	-1.570191
12	6	0	-0.587509	0.127480	-1.483906
13	6	0	-0.251258	-0.081353	-0.030361
14	1	0	1.042238	-1.495334	2.132475
15	1	0	2.975647	-2.988370	1.655923
16	1	0	3.767657	-3.310374	-0.651875
17	1	0	2.715295	-2.189368	-2.578773
18	1	0	0.584404	-0.561028	-3.170440
19	1	0	-1.422849	-0.570012	-1.681857
20	7	0	0.570546	-0.418516	-2.167745
21	6	0	-1.068848	0.493016	1.067833
22	1	0	-1.242228	1.547028	0.841520
23	1	0	-0.517619	0.431790	2.006717
24	6	0	-2.447106	-0.154016	1.219938
25	6	0	-3.336496	-0.077719	-0.041890
26	8	0	-3.334214	1.026905	-0.635300
27	8	0	-3.971197	-1.104937	-0.335066

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28	1	0	-2.969741	0.355392	2.030133
29	7	0	-2.325366	-1.582404	1.636297
30	1	0	-1.861628	-1.671100	2.543073
31	1	0	-3.256529	-2.002002	1.688471
32	1	0	-1.796849	-2.130187	0.951006
33	1	0	-1.841979	1.547899	-1.616186
34	17	0	1.758443	3.316865	0.028209

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### Standard orientation of TS-T1-OCI-OCI-i-2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OCI-OCI-i-2

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -64.40 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.890819	-0.176701	3.053494
2	1	0	1.831653	0.204896	2.141015
3	8	0	1.686049	0.997324	0.656156
4	1	0	2.416986	-0.977739	2.970914
5	8	0	-1.125866	1.702922	-1.509587
6	6	0	0.999170	-1.072909	-1.638982
7	6	0	0.615253	-1.161533	-0.257845
8	6	0	1.226695	-2.123998	0.597642
9	6	0	2.140173	-2.977607	0.056964
10	6	0	2.479446	-2.895785	-1.329316
11	6	0	1.929117	-1.975980	-2.185423
12	6	0	-0.702939	0.384466	-1.359598
13	6	0	-0.294494	-0.155383	-0.008625
14	1	0	0.950318	-2.168289	1.644368
15	1	0	2.620536	-3.730550	0.668332
16	1	0	3.209237	-3.596835	-1.718518
17	1	0	2.201909	-1.928217	-3.231718
18	1	0	0.236291	-0.024366	-3.250679
19	1	0	-1.622136	-0.172893	-1.615019
20	7	0	0.352697	-0.062097	-2.244230
21	6	0	-1.003638	0.192782	1.251308
22	1	0	-1.223092	1.262180	1.251734

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23	1	0	-0.351365	-0.026949	2.097603
24	6	0	-2.344971	-0.535739	1.435223
25	6	0	-3.296251	-0.306367	0.242813
26	8	0	-3.695259	0.863355	0.105059
27	8	0	-3.517367	-1.298122	-0.486841
28	1	0	-2.802872	-0.170039	2.351982
29	7	0	-2.127630	-2.002147	1.608843
30	1	0	-1.370181	-2.206322	2.265811
31	1	0	-2.979858	-2.448824	1.954727
32	1	0	-1.919117	-2.435303	0.704018
33	17	0	2.221134	2.533215	1.178230
34	17	0	0.063210	2.874259	-1.128706

### Standard orientation of TS-T1-OH-OH-j1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OH-OH-j1

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -663.60 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.104126	-0.561928	1.473271
2	8	0	3.936564	0.108341	2.193872
3	1	0	3.963627	1.068547	2.260058
4	17	0	2.058112	-0.794408	-0.789225
5	8	0	1.602595	-0.715324	2.484628
6	1	0	1.601888	-1.654041	2.713473
7	1	0	2.590206	-0.389235	2.391608
8	8	0	4.074428	-1.363274	-1.937730
9	1	0	4.397262	-0.156062	1.332244
10	1	0	4.054682	-0.612393	-2.539774
11	8	0	5.236482	-0.560190	0.079783
12	1	0	4.726510	-0.914246	-0.807772
13	1	0	5.852438	-1.247739	0.349991
14	6	0	0.390406	1.129348	0.070640
15	6	0	-0.771396	1.363018	-0.659024
16	6	0	-1.208303	2.662749	-0.863653
17	6	0	-0.453623	3.708460	-0.329775

18	6	0	0.714895	3.454882	0.389406
19	6	0	1.156114	2.150413	0.605294
20	6	0	-0.654255	-0.910999	-0.121947
21	6	0	-1.314264	0.039670	-1.145388
22	1	0	-2.113751	2.863425	-1.427243
23	1	0	-0.777719	4.731850	-0.476704
24	1	0	1.285270	4.282682	0.793503
25	1	0	2.062018	1.934947	1.162097
26	7	0	0.654799	-0.276439	0.222789
27	6	0	-2.832920	-0.103825	-1.279475
28	1	0	-3.013277	-1.020649	-1.843994
29	1	0	-3.190089	0.722672	-1.900082
30	6	0	-3.695541	-0.217318	-0.030898
31	6	0	-3.457690	-1.474504	0.840433
32	8	0	-3.158020	-2.522196	0.220737
33	8	0	-3.609939	-1.328714	2.067101
34	1	0	-4.736394	-0.263627	-0.357283
35	7	0	-3.613908	0.990469	0.849363
36	1	0	-3.871518	1.842906	0.346967
37	1	0	-4.239266	0.864958	1.648377
38	1	0	-2.672654	1.116897	1.232175
39	8	0	-0.500572	-2.211799	-0.578388
40	1	0	-1.346698	-2.656103	-0.378852
41	8	0	-0.740466	-0.185830	-2.427240
42	1	0	-0.723243	-1.144608	-2.564593
43	1	0	-1.196679	-0.880983	0.828499

## Standard orientation of TS-T1-OCl-OH-j1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OCl-OH-j1

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -430.42 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.124781	-0.400659	1.457225
2	8	0	3.952383	0.332486	2.197362
3	1	0	3.969236	1.288538	2.311683

4	17	0	2.095301	-0.516708	-0.869907
5	8	0	1.634396	-0.547854	2.441955
6	1	0	1.658845	-1.485660	2.673717
7	1	0	2.613447	-0.191253	2.357852
8	8	0	3.969104	-0.975605	-1.992591
9	1	0	4.408877	0.119675	1.328926
10	1	0	3.972523	-0.227383	-2.598962
11	8	0	5.268523	-0.229316	0.029240
12	1	0	4.741922	-0.536695	-0.812082
13	1	0	5.865397	-0.946080	0.264839
14	6	0	0.378215	1.333236	0.109958
15	6	0	-0.766312	1.613890	-0.627167
16	6	0	-1.173164	2.926830	-0.812932
17	6	0	-0.414253	3.943643	-0.234943
18	6	0	0.732866	3.646832	0.503839
19	6	0	1.148464	2.330673	0.688206
20	6	0	-0.654359	-0.685491	-0.225250
21	6	0	-1.342293	0.328815	-1.178246
22	1	0	-2.060392	3.157256	-1.393870
23	1	0	-0.715579	4.976457	-0.362344
24	1	0	1.309340	4.452400	0.942917
25	1	0	2.043316	2.085700	1.250153
26	7	0	0.640276	-0.071382	0.191697
27	6	0	-2.869741	0.233280	-1.249496
28	1	0	-3.116879	-0.670972	-1.810034
29	1	0	-3.209437	1.081299	-1.850299
30	6	0	-3.692402	0.154203	0.031479
31	6	0	-3.510093	-1.147559	0.847375
32	8	0	-3.563562	-2.201909	0.187670
33	8	0	-3.334423	-1.010184	2.077800
34	1	0	-4.742718	0.199236	-0.260016
35	7	0	-3.481162	1.325409	0.938446
36	1	0	-3.637623	2.214786	0.459224
37	1	0	-4.124218	1.258977	1.729899
38	1	0	-2.537906	1.330423	1.335772
39	8	0	-0.521030	-1.901418	-0.896876
40	8	0	-0.825714	0.206549	-2.494114
41	1	0	-1.216253	-0.805647	0.704003
42	17	0	-0.036542	-3.159436	0.146779
43	1	0	-1.118362	-0.636249	-2.866953

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**Standard orientation of TS-T1-OH-OCI-j1**

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OH-OCl-j1

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -611.17 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.277715	0.597252	1.688354
2	8	0	4.178968	1.384741	1.735660
3	1	0	4.237561	2.232020	1.281636
4	17	0	2.062348	-1.021751	-0.011233
5	8	0	1.850884	1.030339	2.568731
6	1	0	1.842357	0.403352	3.304405
7	1	0	2.833666	1.174439	2.256160
8	8	0	3.922903	-2.301877	-0.621323
9	1	0	4.545704	0.680812	1.115068
10	1	0	3.844967	-2.179124	-1.573102
11	8	0	5.266091	-0.369433	0.175556
12	1	0	4.699487	-1.201820	-0.164777
13	1	0	6.023637	-0.717386	0.655407
14	6	0	0.543262	1.160910	-0.430839
15	6	0	-0.641466	0.988118	-1.139754
16	6	0	-1.029105	1.917213	-2.094001
17	6	0	-0.205552	3.021474	-2.308479
18	6	0	0.983073	3.178395	-1.592783
19	6	0	1.377611	2.245629	-0.635659
20	6	0	-0.603076	-0.498369	0.662708
21	6	0	-1.265701	-0.326521	-0.728173
22	1	0	-1.947018	1.787299	-2.657827
23	1	0	-0.488150	3.765324	-3.043436
24	1	0	1.608708	4.042723	-1.780746
25	1	0	2.300683	2.350779	-0.075990
26	7	0	0.747738	0.115752	0.529124
27	6	0	-2.786022	-0.429927	-0.784937
28	1	0	-3.064801	-1.477919	-0.673056
29	1	0	-3.104077	-0.119981	-1.784210
30	6	0	-3.605849	0.301907	0.268315
31	6	0	-3.410872	-0.185031	1.725094
32	8	0	-3.205867	-1.413302	1.865661
33	8	0	-3.494979	0.684938	2.610066

34	1	0	-4.657321	0.137237	0.024931
35	7	0	-3.425527	1.787295	0.237907
36	1	0	-3.657556	2.181304	-0.676783
37	1	0	-4.027157	2.207378	0.950246
38	1	0	-2.466105	2.060682	0.469259
39	8	0	-0.527226	-1.774508	1.186580
40	1	0	-1.411352	-1.960354	1.555343
41	8	0	-0.673639	-1.198337	-1.720810
42	1	0	-1.108150	0.184401	1.358313
43	17	0	-1.074887	-2.863722	-1.615140

### Standard orientation of TS-T1-OCI-OCI-j1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-OCI-OCI-j1

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -207.75 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.386964	0.098146	-1.721697
2	8	0	-4.262677	0.841211	-1.945006
3	1	0	-4.315557	1.783999	-1.755004
4	17	0	-2.133449	-0.648006	0.655806
5	8	0	-1.972943	0.220588	-2.622880
6	1	0	-1.981837	-0.600001	-3.133753
7	1	0	-2.965150	0.474898	-2.346037
8	8	0	-3.817121	-1.407407	1.764320
9	1	0	-4.640492	0.347081	-1.157456
10	1	0	-3.822951	-0.802352	2.513962
11	8	0	-5.387558	-0.430746	0.022123
12	1	0	-4.768225	-0.824013	0.739268
13	1	0	-5.851562	-1.171239	-0.380783
14	6	0	-0.502694	1.437020	-0.002504
15	6	0	0.695448	1.568462	0.695217
16	6	0	1.109426	2.803615	1.173495
17	6	0	0.304814	3.910820	0.915687
18	6	0	-0.894626	3.771056	0.212312
19	6	0	-1.317973	2.530912	-0.257570

20	6	0	0.564767	-0.561330	-0.243122
21	6	0	1.312775	0.201108	0.882759
22	1	0	2.034813	2.903311	1.731602
23	1	0	0.608132	4.889090	1.268161
24	1	0	-1.507724	4.645083	0.026569
25	1	0	-2.252481	2.412970	-0.795413
26	7	0	-0.755337	0.096227	-0.404033
27	6	0	2.836499	0.117107	0.879492
28	1	0	3.133766	-0.890768	1.169852
29	1	0	3.196432	0.795069	1.658386
30	6	0	3.590181	0.381948	-0.420130
31	6	0	3.369715	-0.674293	-1.530467
32	8	0	3.467789	-1.858245	-1.160854
33	8	0	3.125057	-0.232788	-2.673998
34	1	0	4.652488	0.361596	-0.173357
35	7	0	3.340918	1.743673	-0.987779
36	1	0	3.532989	2.483342	-0.307979
37	1	0	3.939391	1.881859	-1.804790
38	1	0	2.377080	1.845967	-1.316450
39	8	0	0.498150	-1.922819	0.050437
40	8	0	0.793899	-0.122247	2.193014
41	1	0	1.084342	-0.389581	-1.190594
42	17	0	1.280098	-1.624712	2.867168
43	17	0	-0.036785	-2.829793	-1.295331

## Standard orientation of TS-T1-OCI-OH-j2

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-OCI-OH-j2

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1125.30 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.476063	-1.423234	1.519373
2	8	0	1.562137	1.567784	0.768362
3	6	0	-1.829053	0.756363	0.349935
4	6	0	-1.386799	0.307209	-0.898736
5	6	0	-2.256034	-0.319914	-1.775607

6	6	0	-3.576509	-0.537738	-1.373247
7	6	0	-4.001711	-0.112743	-0.114195
8	6	0	-3.137736	0.541940	0.764623
9	6	0	0.437164	0.984741	0.404098
10	6	0	0.056420	0.731177	-1.076078
11	1	0	-1.915097	-0.649649	-2.753417
12	1	0	-4.269236	-1.041175	-2.037151
13	1	0	-5.026001	-0.294630	0.192076
14	1	0	-3.474344	0.869625	1.741900
15	1	0	-0.814255	1.317778	2.045376
16	1	0	0.649953	-0.125687	0.933685
17	7	0	-0.796718	1.413779	1.034784
18	17	0	-0.617349	-1.365816	2.806501
19	6	0	0.955060	-0.194441	-1.903222
20	1	0	1.908707	0.318826	-2.039439
21	1	0	0.488268	-0.241224	-2.892901
22	6	0	1.299814	-1.623130	-1.488125
23	6	0	2.451890	-1.825936	-0.469491
24	8	0	3.210993	-0.863837	-0.244334
25	8	0	2.544478	-2.989373	-0.009571
26	1	0	1.642447	-2.130749	-2.392776
27	7	0	0.131892	-2.422075	-1.003486
28	1	0	-0.668999	-2.362488	-1.633577
29	1	0	0.414568	-3.400376	-0.919558
30	1	0	-0.128264	-2.100930	-0.048198
31	17	0	1.746278	3.503876	0.443339
32	8	0	0.077733	2.007920	-1.734723
33	1	0	-0.392028	1.912471	-2.574962

### Standard orientation of TS-T1-OH-OCl-j3

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-OH-OCl-j3

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -791.78 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.313734	-1.756274	1.344774



2	8	0	1.727456	-0.739175	-0.824442
3	6	0	-1.220357	-0.268325	-1.380697
4	6	0	-1.261396	-1.092615	-0.249682
5	6	0	-2.257414	-2.052729	-0.101717
6	6	0	-3.252998	-2.144490	-1.072656
7	6	0	-3.243146	-1.277544	-2.167656
8	6	0	-2.226897	-0.340081	-2.339578
9	6	0	0.867888	0.130525	-0.409399
10	6	0	-0.254349	-0.699493	0.804513
11	1	0	-2.278279	-2.688599	0.776819
12	1	0	-4.045001	-2.876783	-0.968839
13	1	0	-4.031922	-1.343839	-2.908741
14	1	0	-2.206832	0.310417	-3.206581
15	1	0	-0.307166	1.561771	-1.386570
16	1	0	1.252795	0.960409	0.199664
17	7	0	-0.098670	0.569046	-1.404583
18	6	0	-0.713484	0.284736	1.898687
19	1	0	0.175263	0.790796	2.286952
20	1	0	-1.099200	-0.325564	2.721770
21	6	0	-1.754478	1.369250	1.622431
22	6	0	-1.392427	2.433850	0.569508
23	8	0	-0.296588	3.008382	0.741331
24	8	0	-2.223020	2.639522	-0.344117
25	1	0	-1.896230	1.905166	2.562231
26	7	0	-3.099796	0.794662	1.289845
27	1	0	-3.291205	-0.055711	1.825165
28	1	0	-3.834643	1.474221	1.497407
29	1	0	-3.178455	0.578430	0.292197
30	1	0	3.096546	-0.426436	-0.350460
31	17	0	2.262386	-1.471235	1.986587
32	17	0	4.537749	0.781413	-1.501929
33	8	0	4.064126	-0.120176	-0.144991

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### Standard orientation of TS-T1-OCI-OCI-j3

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-OCI-OCI-j3

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -679.95 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	4.526455	0.195930	-0.993948
2	8	0	0.824591	1.522898	-1.192690
3	6	0	-1.015999	-1.454942	-1.366315
4	6	0	-1.350262	-1.207981	-0.027576
5	6	0	-2.263146	-2.019845	0.633655
6	6	0	-2.848693	-3.085080	-0.050405
7	6	0	-2.515408	-3.319922	-1.385633
8	6	0	-1.604432	-2.510450	-2.059570
9	6	0	-0.143388	0.678366	-1.104294
10	6	0	-0.557597	-0.062713	0.542485
11	1	0	-2.514840	-1.825588	1.672311
12	1	0	-3.560436	-3.728564	0.452889
13	1	0	-2.979044	-4.145306	-1.914661
14	1	0	-1.357399	-2.691464	-3.099832
15	1	0	-0.035771	-0.421799	-2.856036
16	1	0	-1.138125	1.142761	-1.207418
17	7	0	-0.066675	-0.561127	-1.850744
18	17	0	4.970453	-0.299543	0.562423
19	6	0	-1.229083	0.901451	1.509570
20	1	0	-0.464973	1.589785	1.873855
21	1	0	-1.537491	0.296955	2.372568
22	6	0	-2.416240	1.762070	1.082291
23	6	0	-2.104072	2.901229	0.085766
24	8	0	-1.103064	3.594346	0.356257
25	8	0	-2.901577	3.048950	-0.868491
26	1	0	-2.793848	2.249517	1.983101
27	7	0	-3.565769	0.959453	0.559813
28	1	0	-3.859735	0.245074	1.230041
29	1	0	-4.358061	1.576049	0.367125
30	1	0	-3.331464	0.494019	-0.321981
31	17	0	2.793034	0.773076	-1.066279
32	8	0	0.673019	-0.380856	0.900770
33	17	0	0.794915	-1.468413	2.604415

### Standard orientation of TS-T1-OCI-OH-k1

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-OCI-OH-k1

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1339.38 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-1.144745	1.127780	1.594723
2	8	0	-0.589328	-1.945334	0.843460
3	6	0	1.785088	0.547112	0.106173
4	6	0	1.011552	0.677780	-1.045015
5	6	0	1.253890	1.718155	-1.932383
6	6	0	2.275977	2.618867	-1.636869
7	6	0	3.045489	2.474200	-0.478950
8	6	0	2.808784	1.430829	0.411182
9	6	0	0.042885	-0.878879	0.370159
10	6	0	0.030598	-0.477151	-1.121971
11	1	0	0.665648	1.826404	-2.838751
12	1	0	2.478534	3.440783	-2.313674
13	1	0	3.834611	3.186799	-0.269104
14	1	0	3.397464	1.310433	1.313569
15	1	0	-0.582647	0.054164	1.022894
16	7	0	1.379687	-0.570090	0.919126
17	17	0	-0.057907	1.987871	2.565800
18	6	0	-1.317295	-0.205643	-1.800947
19	1	0	-1.806764	-1.173781	-1.921505
20	1	0	-1.061187	0.132456	-2.809364
21	6	0	-2.391383	0.732175	-1.257931
22	6	0	-3.306800	0.214516	-0.119300
23	8	0	-3.376834	-1.018086	0.051924
24	8	0	-3.961457	1.102157	0.477171
25	1	0	-3.074216	0.908785	-2.092489
26	7	0	-1.890213	2.082143	-0.860773
27	1	0	-1.300005	2.504327	-1.578413
28	1	0	-2.688885	2.695039	-0.686632
29	1	0	-1.376208	1.993209	0.039888
30	17	0	-0.174863	-3.652215	0.148659
31	8	0	0.574016	-1.504499	-1.967143
32	1	0	1.432121	-1.798646	-1.631730
33	17	0	2.598022	-1.916376	0.602651

**Standard orientation of TS-T1-OH-OH-k2**

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d)  
level:

Standard orientation of transition state of TS-T1-OH-OH-k2

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -462.00 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)			
			X	Y	Z	
-----						
1	17	0	-2.844207	2.237693	0.807379	
2	6	0	-1.675203	-0.397945	0.169857	
3	6	0	-0.990611	-0.274959	-1.048209	
4	6	0	-1.230769	-1.165908	-2.077889	
5	6	0	-2.198079	-2.153570	-1.874833	
6	6	0	-2.899785	-2.254202	-0.666466	
7	6	0	-2.647267	-1.375670	0.376997	
8	6	0	-0.045157	1.031199	0.616891	
9	6	0	-0.087688	0.933489	-0.951716	
10	1	0	-0.701255	-1.093795	-3.022204	
11	1	0	-2.418423	-2.852920	-2.673157	
12	1	0	-3.644303	-3.032129	-0.547347	
13	1	0	-3.169177	-1.446724	1.324138	
14	7	0	-1.242455	0.525721	1.126167	
15	6	0	1.220247	0.903274	-1.740943	
16	1	0	1.583410	1.931875	-1.774213	
17	1	0	0.951902	0.643894	-2.769943	
18	6	0	2.419817	0.062893	-1.333371	
19	6	0	3.193022	0.498072	-0.064338	
20	8	0	2.935700	1.625614	0.421584	
21	8	0	4.066319	-0.303158	0.326116	
22	1	0	3.142287	0.157883	-2.147248	
23	7	0	2.129357	-1.399108	-1.220751	
24	1	0	1.585503	-1.741654	-2.014134	
25	1	0	3.009269	-1.916931	-1.184952	
26	1	0	1.631822	-1.583453	-0.313863	
27	8	0	0.367566	2.224857	1.168502	
28	1	0	1.327828	2.278446	0.988845	
29	8	0	-0.747818	2.087350	-1.467152	
30	1	0	-1.568396	2.243773	-0.965201	
31	1	0	0.633224	0.128580	0.979548	
32	8	0	1.407969	-1.223890	1.334776	
33	17	0	0.305322	-2.104126	2.255875	

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### Standard orientation of TS-T1-OH-OCI-k3

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d)  
level:

Standard orientation of transition state of TS-T1-OH-OCI-k3

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1286.55 cm<sup>-1</sup>

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.251863	2.687426	-1.110609
2	8	0	-0.791210	1.023942	1.626492
3	6	0	2.158333	0.111520	-0.002800
4	6	0	1.284806	-0.692405	-0.737084
5	6	0	1.753567	-1.445708	-1.799725
6	6	0	3.122515	-1.411465	-2.076541
7	6	0	3.991501	-0.618402	-1.324046
8	6	0	3.517043	0.165606	-0.275685
9	6	0	0.153457	0.771361	0.646306
10	6	0	-0.122881	-0.479679	-0.225110
11	1	0	1.084150	-2.049548	-2.402294
12	1	0	3.515775	-2.006371	-2.892617
13	1	0	5.047734	-0.606152	-1.565946
14	1	0	4.177441	0.794357	0.309981
15	1	0	0.113965	1.717743	-0.212341
16	7	0	1.487005	0.864591	0.999262
17	17	0	-0.006155	4.165155	-0.322955
18	6	0	-1.124214	-0.317882	-1.369513
19	1	0	-1.169284	-1.265465	-1.913366
20	1	0	-0.718794	0.416116	-2.071477
21	6	0	-2.567937	0.062032	-1.035819
22	6	0	-3.293017	-0.943418	-0.116428
23	8	0	-3.501683	-2.066200	-0.622150
24	8	0	-3.622557	-0.546593	1.024039
25	1	0	-3.110453	0.090830	-1.980146
26	7	0	-2.668127	1.432602	-0.452731
27	1	0	-1.981124	2.081478	-0.879912
28	1	0	-3.612339	1.801976	-0.566152
29	1	0	-2.465035	1.390964	0.552858

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30	17	0	1.844781	-0.396761	2.766891
31	8	0	-0.556071	-1.480016	0.719568
32	17	0	-0.401595	-3.083673	0.168340
33	1	0	-0.495670	1.755641	2.186945

### Standard orientation of TS-T1-OCI-OCI-k3

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:

Standard orientation of transition state of TS-T1-OCI-OCI-k3

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1340.21 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.359347	2.145639	-1.664365
2	8	0	-1.027578	0.829554	1.274885
3	6	0	2.186901	0.200326	0.076929
4	6	0	1.507025	-0.785691	-0.638065
5	6	0	2.180681	-1.576046	-1.554102
6	6	0	3.556053	-1.382886	-1.702771
7	6	0	4.229872	-0.404889	-0.968914
8	6	0	3.548305	0.411134	-0.068667
9	6	0	0.056210	0.652648	0.414011
10	6	0	0.035043	-0.726546	-0.283585
11	1	0	1.662678	-2.325877	-2.141760
12	1	0	4.107667	-1.997931	-2.404128
13	1	0	5.296295	-0.272120	-1.108921
14	1	0	4.056313	1.181748	0.499283
15	1	0	-0.035565	1.512539	-0.635604
16	7	0	1.314704	0.957205	0.920884
17	17	0	-0.014377	3.785942	-1.451755
18	6	0	-0.862284	-0.879998	-1.511639
19	1	0	-0.724373	-1.894715	-1.895448
20	1	0	-0.494827	-0.210011	-2.292787
21	6	0	-2.371178	-0.682635	-1.357578
22	6	0	-3.026221	-1.600956	-0.300605
23	8	0	-3.028339	-2.816590	-0.580522
24	8	0	-3.505173	-1.049082	0.716434
25	1	0	-2.817940	-0.919974	-2.321986

26	7	0	-2.742693	0.736607	-1.059095
27	1	0	-2.048124	1.420163	-1.410861
28	1	0	-3.652030	0.957303	-1.467857
29	1	0	-2.839622	0.832480	-0.042707
30	17	0	1.596744	0.022666	2.778440
31	17	0	-1.244574	2.466637	1.742133
32	8	0	-0.336900	-1.661390	0.755150
33	17	0	0.091719	-3.279487	0.433977

### Standard orientation of TS-T1-tautomerize3

Cartesian coordinates of the transition state optimized at the M06-2X/6-311G(d) level:

Standard orientation of transition state of TS-T1-tautomerize3

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -706.40 cm<sup>-1</sup>

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.521367	2.018771	0.046665
2	1	0	4.188012	1.511573	-1.445025
3	8	0	3.767608	0.912660	-0.814218
4	1	0	3.043736	0.389112	-1.297326
5	8	0	2.306626	2.125553	0.665079
6	1	0	2.061826	1.545100	1.421962
7	1	0	3.168482	1.529311	-0.030763
8	8	0	1.775467	-0.394503	-1.785209
9	6	0	-0.998200	1.164998	-0.509190
10	6	0	-1.581806	-0.100549	-0.676832
11	6	0	-2.908962	-0.334669	-0.373742
12	6	0	-3.671757	0.720724	0.140576
13	6	0	-3.086304	1.969428	0.340674
14	6	0	-1.747410	2.210565	0.017853
15	6	0	0.672401	-0.012374	-1.320710
16	6	0	-0.487397	-1.020893	-1.143681
17	1	0	-3.345309	-1.319834	-0.513608
18	1	0	-4.715075	0.565896	0.388884
19	1	0	-3.683283	2.776729	0.750682
20	1	0	-1.304318	3.188966	0.168207
21	7	0	0.346952	1.207035	-0.915999

22	6	0	-0.125658	-2.119219	-0.127212
23	1	0	-0.936561	-2.855920	-0.146841
24	6	0	0.150500	-1.752553	1.333666
25	1	0	0.437854	-2.674223	1.839667
26	1	0	0.772797	-2.616852	-0.498722
27	7	0	-1.067274	-1.261982	2.056044
28	1	0	-1.900558	-1.802148	1.813214
29	1	0	-0.921899	-1.328679	3.065279
30	1	0	-1.239982	-0.275157	1.847199
31	6	0	1.293288	-0.739918	1.553535
32	8	0	1.000197	0.313851	2.176055
33	8	0	2.400608	-1.068642	1.100957
34	8	0	-0.713050	-1.631442	-2.403519
35	1	0	-1.456638	-2.241053	-2.312580

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