Supporting Information

Reactivity of Various Halogenating Agents Toward Different Substrates in Electrophilic Substitution Reactions: A Computational Study

Wenjie Huang, *Yong Dong Liu*,* *Rugang Zhong*

Beijing Key Laboratory of Environmental and Viral Oncology, College of Chemistry and Life Science, Beijing University of Technology, Beijing 100124, China

*Corresponding author: Phone: 86-10-6739-6211; fax: +86-10-6739-2001.

E-mail: ydliu@bjut.edu.cn;

Table S1. The E_{HOMO}/E_{LUMO} (in eV) and E_{LUMO}-E_{HOMO} (in eV) of substrates and electrophiles

Substrates	E_{HOMO}	$E_{LUMO-HOMO}$	Electrophiles	E_{LUMO}	$E_{LUMO-HOMO}$
Phenolate	-6.1	7.3	**ICl**	-2.5	6.1
Aniline(*C*)	-7.1	9.2	**BrCl**	-2.7	7.2
Phenol	-7.7	8.3	**BrOCl**	-2.7	7.0
Acetaminophen	-7.4	7.8	**Br_2O**	-2.8	6.6
Anisole	-7.6	8.8	**Cl_2O**	-2.0	7.7
Glycine	-7.0	10.9	**I_2**	-2.4	5.4
Morpholine	-7.8	11.3	**Br_2**	-2.9	6.7
Diethylamine	-7.7	11.5	**Cl_2**	-2.4	8.0
Ethylamine	-8.3	12.2	**HOI**	-1.3	6.8
Aniline(*N*)	-7.4	9.6	**HOBr**	-1.3	8.1
***N*-methyl acetamide**	-8.7	10.9	**HOCl**	-0.6	9.3
Alcohol	-9.3	13.2	**SO_3Cl^-**	-0.1	9.8
			CH_3COCl	0.1	10.3
			$(CH_3CO)_2O$	0.3	10.4
			NH_2Br	-0.3	8.6
			$NHBr_2$	-1.7	7.3
			NH_2Cl	0.5	9.7
			$NHCl_2$	-0.9	8.5

Table S2. The estimated rate constants of the ortho, [para] site of phenolate, aniline(*C*), phenol, acetaminophen, and anisole, the ortho, [meta] site of acetaminophen (k_{est}, in M^{-1} s^{-1}) and the experimental rates (k_{exp}, in M^{-1} s^{-1}) in brackets of electrophiles reacting with *C*–reactive substrates

Electrophiles	Phenolate	Aniline(*C*)	Phenol	Anisole	Acetaminophe
BrCl	-- [--]	6.9×10^{11} [--]	1.5×10^{8} $[1.0\times10^{8}]$	1.4×10^{7} $[1.6\times10^{7}]$ (9.0×10^{4})	5.6×10^{7} $[7.7\times10^{4}]$
Cl_2O	-- [--]	2.1×10^{10} $[6.5\times10^{9}]$	2.0×10^{6} $[1.0\times10^{6}]$ (9.0×10^{4})	4.4×10^{5} $[1.6\times10^{5}]$	3.7×10^{5} $[1.2\times10^{3}]$ (2.4×10^{5})
Br_2	-- [--]	4.7×10^{10} $[5.3\times10^{9}]$	3.8×10^{4} $[4.3\times10^{3}]$	2.2×10^{3} $[8.9\times10^{1}]$ (5.4×10^{2})	4.3×10^{3} [--]
Cl_2	6.9×10^{11} $[2.0\times10^{11}]$ (2.6×10^{9})	7.3×10^{8} $[2.1\times10^{8}]$	1.3×10^{5} $[1.0\times10^{5}]$ (8.9×10^{4})	1.9×10^{5} $[1.7\times10^{5}]$	2.9×10^{4} $[3.4\times10^{1}]$ (6.8×10^{4})
HOBr	5.4×10^{9} $[5.1\times10^{8}]$ (1.8×10^{8})	4.0×10^{4} $[1.7\times10^{8}]$	6.3×10^{-1} $[1.4\times10^{-2}]$ (5.0×10^{2})	1.3×10^{-4} $[8.8\times10^{-4}]$ (3.0×10^{-3})	6.9×10^{-4} [--]
HOCl	2.1×10^{6} $[5.2\times10^{4}]$ (2.19×10^{4})	1.3×10^{3} $[5.2\times10^{1}]$	1.0×10^{-4} $[7.1\times10^{-5}]$ (3.6×10^{-1})	3.9×10^{-6} $[9.4\times10^{-6}]$	1.2×10^{-3} $[6.4\times10^{-9}]$ (3.0×10^{-1})
SO_3Cl^-	2.7×10^{2} $[3.1\times10^{1}]$	9.4×10^{-2} [--]	3.2×10^{-5} [--]	1.7×10^{-7} $[1.7\times10^{-7}]$	1.4×10^{-5} $[1.2\times10^{-7}]$
NH_2Br	3.1×10^{-3} $[1.4\times10^{-5}]$	4.0×10^{-7} $[1.5\times10^{-9}]$	4.2×10^{-2} [--]	--/ [--]	7.1×10^{-2} [--]
NH_2Cl	6.1×10^{-10} $[2.0\times10^{-12}]$	2.2×10^{-13} $[7.1\times10^{-16}]$	-- [--]	2.9×10^{-19} $[1.3\times10^{-21}]$	-- [--]

Table S3. The estimated rate constants (k_{est}, in M^{-1} s^{-1}) and the experimental rates (k_{exp}, in M^{-1} s^{-1}) in brackets of electrophiles reacting with *C*–reactive substrates

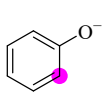
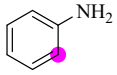
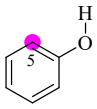
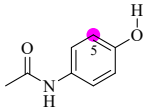
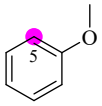
Electrophiles	 **Phenolate**	 **Aniline(*C*)**	 **Phenol**	 **Acetaminophen**	 **Anisole**
X–X'/OX'/OX					
ICl	--	--	4.2×10^{8}	2.7×10^{8}	--
BrCl	--	6.9×10^{11}	1.5×10^{8}	5.6×10^{7}	1.4×10^{7} (9.0×10^{4})
BrOCl	--	--	5.5×10^{7}	1.1×10^{8}	1.3×10^{2} (1.5×10^{3})
Br_2O	--	--	3.9×10^{7}	2.2×10^{5}	6.1×10^{2} (1.5×10^{1})
Cl_2O	--	2.1×10^{10}	2.0×10^{6} (9.0×10^{4})	3.7×10^{5} (2.4×10^{5})	6.1×10^{2}
X–X					
I_2	--	--	1.5×10^{2}	1.1×10^{0}	--
Br_2		4.7×10^{10}	3.8×10^{4}	4.3×10^{3}	2.2×10^{3} (5.4×10^{2})
Cl_2	6.9×10^{11} (2.6×10^{9})	7.3×10^{8}	1.3×10^{5} (8.9×10^{4})	2.9×10^{4} (6.8×10^{4})	1.2×10^{3}
X–OH					
HOI	3.9×10^{10}	3.7×10^{5}	7.4×10^{-2}	9.9×10^{-3}	--
HOBr	5.4×10^{9} (1.8×10^{8})	4.0×10^{4}	6.3×10^{-1} (5.0×10^{2})	6.9×10^{-4}	1.3×10^{-4} (3.0×10^{-3})
HOCl	2.1×10^{6} (2.19×10^{4})	1.3×10^{3}	1.0×10^{-4} (3.6×10^{-1})	1.2×10^{-3} (3.0×10^{-1})	3.9×10^{-6}
Sulfonylating/acylating agents					
SO_3Cl^-	2.7×10^{2}	9.4×10^{-2}	3.2×10^{-5}	1.4×10^{-5}	1.7×10^{-7}
CH_3COCl	5.5×10^{1}	2.6×10^{-3}	2.1×10^{-5}	4.2×10^{-7}	1.5×10^{-7}
$(CH_3CO)_2O$	1.0×10^{-6}	1.7×10^{-13}	1.7×10^{-13}	1.1×10^{-15}	4.8×10^{-16}
Halogenated amines					
NH_2Br	3.1×10^{-3}	4.0×10^{-7}	4.2×10^{-2}	7.1×10^{-2}	--
$NHBr_2$	6.1×10^{1}	2.2×10^{-7}	5.8×10^{-12}	3.7×10^{-11}	--
NH_2Cl	6.1×10^{-10}	2.2×10^{-13}	--	--	2.9×10^{-19}
$NHCl_2$	9.3×10^{-5}	3.8×10^{-11}	2.4×10^{-11}	3.7×10^{-9}	1.4×10^{-20}

Table S4. The estimated rate constants (k_{est}, in M^{-1} s^{-1}) and the experimental rates (k_{exp}, in M^{-1} s^{-1}) in brackets of electrophiles reacting with aliphatic amine-*N* substrates

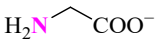
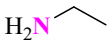
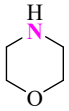
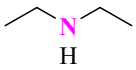
Electrophiles				
	Glycine	**Ethylamine**	**Morpholine**	**Diethylamine**
Chlorinating agents				
Cl_2	5.2×10^{8}	4.3×10^{9}	3.5×10^{10}	1.4×10^{9}
Cl_2O	2.9×10^{9}	8.1×10^{7}	8.2×10^{7}	1.4×10^{9}
HOCl	1.5×10^{8} (1.13×10^{8})	1.5×10^{8} (1.98×10^{8})	2.9×10^{8}	1.5×10^{9} (3.7×10^{7})
Brominating agents				
Br_2	1.9×10^{6}	2.3×10^{6}	5.4×10^{6}	2.7×10^{6}
BrCl	1.3×10^{5}	2.7×10^{6}	7.6×10^{6}	1.1×10^{6}
HOBr	7.2×10^{6} (3.8×10^{8})	1.1×10^{5}	5.7×10^{4}	4.7×10^{5} (3.0×10^{9})
Br_2O	5.7×10^{2}	2.4×10^{2}	1.4×10^{3}	1.2×10^{3}
BrOCl	7.6×10^{2}	2.0×10^{2}	1.6×10^{3}	2.6×10^{2}
Iodinating agents				
ICl	4.2×10^{1}	6.6×10^{0}	6.9×10^{1}	3.2×10^{1}
I_2	1.8×10^{1}	1.4×10^{0}	3.8×10^{0}	9.0×10^{0}
HOI	2.7×10^{-2}	2.4×10^{-1}	1.4×10^{-1}	2.7×10^{-1}
Sulfonylating/acylating agents				
SO_3Cl^-	1.2×10^{7}	6.9×10^{5}	5.3×10^{9}	5.0×10^{8}
CH_3COCl	1.4×10^{9}	2.0×10^{7}	--	4.2×10^{8}
$(CH_3CO)_2O$	1.4×10^{7}	6.5×10^{4}	--	--
Halogenated amines				
NH_2Br	2.0×10^{1}	8.7×10^{0}	8.0×10^{0}	6.0×10^{0}
$NHBr_2$	4.7×10^{1}	1.5×10^{0}	1.3×10^{0}	2.7×10^{0}
NH_2Cl	7.4×10^{-5}	6.9×10^{-5}	6.9×10^{-4}	2.9×10^{-4}
$NHCl_2$	3.7×10^{-3}	5.3×10^{-5}	2.3×10^{-4}	1.8×10^{-4}

Table S5. The estimated rate constants (k_{est}, in M^{-1} s^{-1}) of electrophiles reacting with amine-*N*, amid-*N*, and alcohol

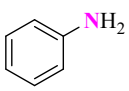
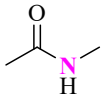
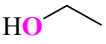
Electrophiles	 Aniline(*N*)	 *N*–methyl acetamide	 Alcohol
X–X'/OX'/OX			
ICl	1.0×10^{3}	7.1×10^{5}	9.0×10^{6}
BrCl	1.7×10^{7}	8.7×10^{5}	2.3×10^{4}
BrOCl	1.0×10^{4}	8.6×10^{2}	6.6×10^{2}
Br_2O	1.9×10^{2}	6.3×10^{2}	1.6×10^{3}
Cl_2O	1.7×10^{8}	1.4×10^{3}	1.4×10^{2}
X–X			
I_2	3.0×10^{1}	2.1×10^{-3}	6.7×10^{2}
Br_2	6.6×10^{5}	8.1×10^{3}	2.4×10^{2}
Cl_2	1.4×10^{10}	5.7×10^{6}	7.2×10^{1}
X–OH			
HOI	6.7×10^{-1}	1.4×10^{-3}	1.9×10^{-1}
HOBr	2.9×10^{0}	8.6×10^{-6}	1.6×10^{-3}
HOCl	3.9×10^{0}	3.0×10^{-10}	3.3×10^{-6}
Sulfonylating/acylating agents			
SO_3Cl^-	8.5×10^{5}	6.7×10^{1}	1.2×10^{3}
CH_3COCl	7.0×10^{5}	8.3×10^{-4}	1.6×10^{0}
$(CH_3CO)_2O$	3.1×10^{3}	5.2×10^{-11}	7.7×10^{-9}
Halogenated amines			
NH_2Br	1.3×10^{-3}	1.5×10^{-3}	1.1×10^{-2}
$NHBr_2$	5.6×10^{-6}	2.1×10^{-8}	4.3×10^{-6}
NH_2Cl	5.9×10^{-5}	1.4×10^{-10}	8.8×10^{-4}
$NHCl_2$	1.9×10^{-9}	5.1×10^{-14}	1.2×10^{-11}

Table S6. The estimated rate constants (k_{est}, in M^{-1} s^{-1}) of substrates reacting with halogenating agents Group A

Substrates	HOI	I_2	ICl	Br_2O	BrOCl	BrCl
***C*–reactive**						
Phenolate	3.9×10^{10}	--	--	--	--	--
Aniline(*C*)	3.7×10^{5}	--	--	--	--	6.9×10^{11}
Phenol	7.4×10^{-2}	1.5×10^{2}	4.2×10^{8}	3.9×10^{7}	5.5×10^{7}	1.5×10^{8}
Acetaminophen	9.9×10^{-3}	1.1×10^{0}	2.7×10^{8}	2.2×10^{5}	1.1×10^{8}	5.6×10^{7}
Anisole	--	--	--	6.1×10^{2}	1.3×10^{2}	1.4×10^{7}
***N*–reactive**						
Glycine	2.7×10^{-2}	1.8×10^{1}	4.2×10^{1}	5.7×10^{2}	7.6×10^{2}	1.3×10^{5}
Ethylamine	2.4×10^{-1}	1.4×10^{0}	6.6×10^{0}	2.4×10^{2}	2.0×10^{2}	2.7×10^{6}
Morpholine	1.4×10^{-1}	3.8×10^{0}	6.9×10^{1}	1.4×10^{3}	1.6×10^{3}	7.6×10^{6}
Diethylamine	2.7×10^{-1}	9.0×10^{0}	3.2×10^{1}	1.2×10^{3}	2.6×10^{2}	1.1×10^{6}
Aniline(*N*)	6.7×10^{-1}	3.0×10^{1}	1.0×10^{3}	1.9×10^{2}	1.0×10^{4}	1.7×10^{7}
N-methyl acetamide	1.4×10^{-3}	2.1×10^{-3}	7.1×10^{5}	6.3×10^{2}	8.6×10^{2}	8.7×10^{5}
***O*–reactive**						
Alcohol	1.9×10^{-1}	6.7×10^{2}	9.0×10^{6}	1.6×10^{3}	6.6×10^{2}	2.3×10^{4}

Table S7. The estimated rate constants (k_{est}, in M^{-1} s^{-1}) of substrates reacting with halogenating agents Group B

Substrates	Cl_2O	Br_2	Cl_2	HOBr	HOCl
***C*–reactive**					
Phenolate	--	--	6.9×10^{11}	5.4×10^{9}	2.1×10^{6}
Aniline(*C*)	2.1×10^{10}	4.7×10^{10}	7.3×10^{8}	4.0×10^{4}	1.3×10^{3}
Phenol	2.0×10^{6}	3.8×10^{4}	1.3×10^{5}	6.3×10^{-1}	9.9×10^{-5}
Acetaminophen	3.7×10^{5}	4.3×10^{3}	2.9×10^{4}	6.9×10^{-4}	1.2×10^{-3}
Anisole	6.1×10^{2}	2.2×10^{3}	1.2×10^{3}	1.3×10^{-4}	3.9×10^{-6}
***N*–reactive**					
Glycine	2.9×10^{9}	1.9×10^{6}	5.2×10^{8}	7.2×10^{6}	1.5×10^{8}
Ethylamine	8.1×10^{7}	2.3×10^{6}	4.3×10^{9}	1.1×10^{5}	1.5×10^{8}
Morpholine	8.2×10^{7}	5.4×10^{6}	3.5×10^{10}	5.7×10^{4}	2.9×10^{8}
Diethylamine	1.4×10^{9}	2.7×10^{6}	1.4×10^{9}	4.7×10^{5}	1.5×10^{9}
Aniline(*N*)	1.7×10^{8}	6.6×10^{5}	1.4×10^{10}	2.9×10^{0}	3.9×10^{0}
N-methyl acetamide	1.4×10^{3}	8.1×10^{3}	5.7×10^{6}	8.6×10^{-6}	3.0×10^{-10}
***O*–reactive**					
Alcohol	1.4×10^{2}	2.4×10^{2}	7.2×10^{1}	1.6×10^{-3}	3.3×10^{-6}

Table S8. The estimated rate constants (k_{est}, in M^{-1} s^{-1}) of substrates reacting with sulfonylating/acylating agents and halogenated amines

Substrates	SO_3Cl^-	CH_3COCl	$(CH_3CO)_2O$	NH_2Br	$NHBr_2$	NH_2Cl	$NHCl_2$
***C*–reactive**							
Phenolate	2.7×10^{2}	5.5×10^{1}	1.0×10^{-6}	3.1×10^{-3}	6.1×10^{1}	6.1×10^{-10}	9.3×10^{-5}
Aniline(C)	9.4×10^{-2}	2.6×10^{-3}	1.7×10^{-13}	4.0×10^{-7}	2.2×10^{-7}	2.2×10^{-13}	3.8×10^{-11}
Phenol	3.2×10^{-5}	2.1×10^{-5}	1.7×10^{-13}	4.2×10^{-2}	5.8×10^{-12}	--	2.4×10^{-11}
Acetaminophen	1.4×10^{-5}	4.2×10^{-7}	1.1×10^{-15}	7.1×10^{-2}	3.7×10^{-11}	--	3.7×10^{-9}
Anisole	1.7×10^{-7}	1.5×10^{-7}	4.8×10^{-16}	--	--	2.9×10^{-19}	1.4×10^{-20}
***N*–reactive**							
Glycine	1.2×10^{7}	1.4×10^{9}	1.4×10^{7}	2.0×10^{1}	4.7×10^{1}	7.4×10^{-5}	3.7×10^{-3}
Ethylamine	6.9×10^{5}	2.0×10^{7}	6.5×10^{4}	8.7×10^{0}	1.5×10^{0}	6.9×10^{-5}	5.3×10^{-5}
Morpholine	5.3×10^{9}	--	--	8.0×10^{0}	1.3×10^{0}	6.9×10^{-4}	2.3×10^{-4}
Diethylamine	5.0×10^{8}	4.2×10^{8}	--	6.0×10^{0}	2.7×10^{0}	2.9×10^{-4}	1.8×10^{-4}
Aniline(*N*)	8.5×10^{5}	7.0×10^{5}	3.1×10^{3}	1.3×10^{-3}	5.6×10^{-6}	5.9×10^{-5}	1.9×10^{-9}
N-methyl acetamide	6.7×10^{1}	8.3×10^{-4}	5.2×10^{-11}	1.5×10^{-3}	2.1×10^{-8}	1.4×10^{-10}	5.1×10^{-14}
***O*–reactive**							
Alcohol	1.2×10^{3}	1.6×10^{0}	7.7×10^{-9}	1.1×10^{-2}	4.3×10^{-6}	8.8×10^{-4}	1.2×10^{-11}

Table S9. The E_{LUMO} (in eV), $\Delta E_{LUMO\text{-}HOMO}$ (in eV) and APT charge of the electrophiles.

	E_{LUMO}	$E_{LUMO\text{-}HOMO}$	APT
ICl	-2.5	6.1	0.48
BrCl	-2.7	7.2	0.12
BrOCl	-2.7	7.0	0.13
Br_2O	-2.8	6.6	0.12
Cl_2O	-2.0	7.7	0.04
I_2	-2.4	5.4	0.00
Br_2	-2.9	6.7	0.00
Cl_2	-2.4	8.0	0.00
HOI	-1.3	6.8	0.39
HOBr	-1.3	8.1	0.15
HOCl	-0.6	9.3	0.08
SO_3Cl^-	-0.1	9.8	3.45
CH_3COCl	0.1	10.3	1.69
$(CH_3CO)_2O$	0.3	10.4	1.63
NH_2Br	-0.3	8.6	-0.11
$NHBr_2$	-1.7	7.3	-0.16
NH_2Cl	0.5	9.7	-0.17
$NHCl_2$	-0.9	8.5	-0.21

Table S10. The R^2 values of the lg*k* depending on E_{LUMO}, $\Delta E_{LUMO\text{-}HOMO}$ and APT charges for the reactions of various electrophiles with substrates.

***C*–reactive substrates**	**With halogenating agents and Sulfonylating/acylating agents** E_{LUMO}**/Functions/RMSE**
Phenolate	0.80/Y=-5.85X+0.81/2.6314
Aniline(*C*)	0.83/Y=-5.85X-3.69/3.1484
Phenol	0.87/Y=-5.13X-6.89/2.2496
Acetaminophen	0.82/Y=-5.23X-8.06/0.3935
Anisole	0.84/Y=-4.71X-8.76/2.4684
Aliphatic amine-*N* substrates	**With halogenating agents** $E_{LUMO\text{-}HOMO}(X_1)$**&**$E_{LUMO}(X_2)$**/Functions/RMSE**	**With Sulfonylating/acylating agents and halogenated amines APT/Functions/RMSE**
Glycine	0.71/Y=3.63X_1-2.58X_2-26.89/1.8295	0.66/Y=2.88X+0.31/2.8222
Morpholine	0.80/Y=3.90X_1-2.97X_2-29.90/1.5512	0.66/Y=2.67X-0.81/2.5154
Diethylamine	0.82/Y=4.01X_1-3.47X_2-31.36/1.4526	0.88/Y=3.11X-0.95/1.6974
Ethylamine	0.77/Y=3.72X_1-2.53X_2-27.32/1.6263	0.78/Y=3.25X-0.56/2.4111

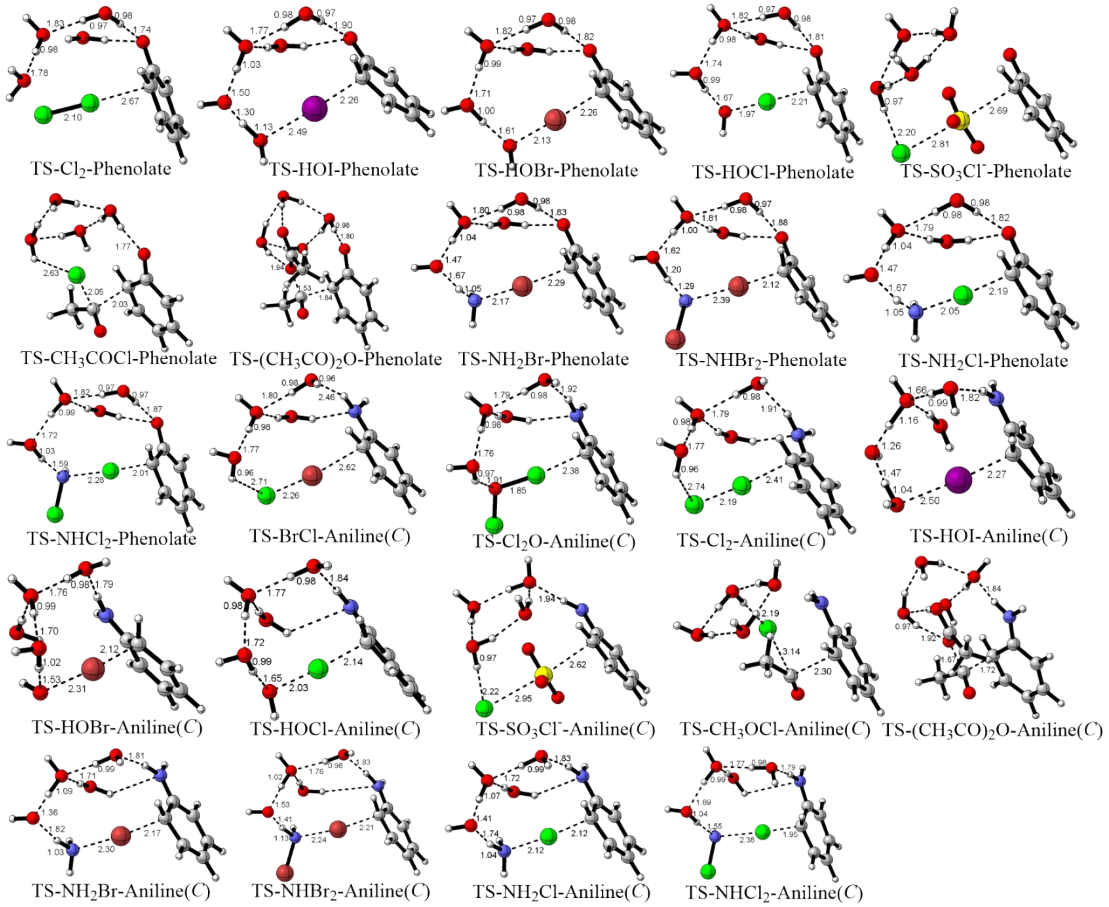


Figure S1. Structures of transition states of the electrophiles reacting with phenolate and aniline(*C*) (atoms in green color represent chlorine atom; atoms in red color represent bromine atom; atoms in purple color represent iodine atom; atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom; atoms in yellow represent sulfur atom; atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

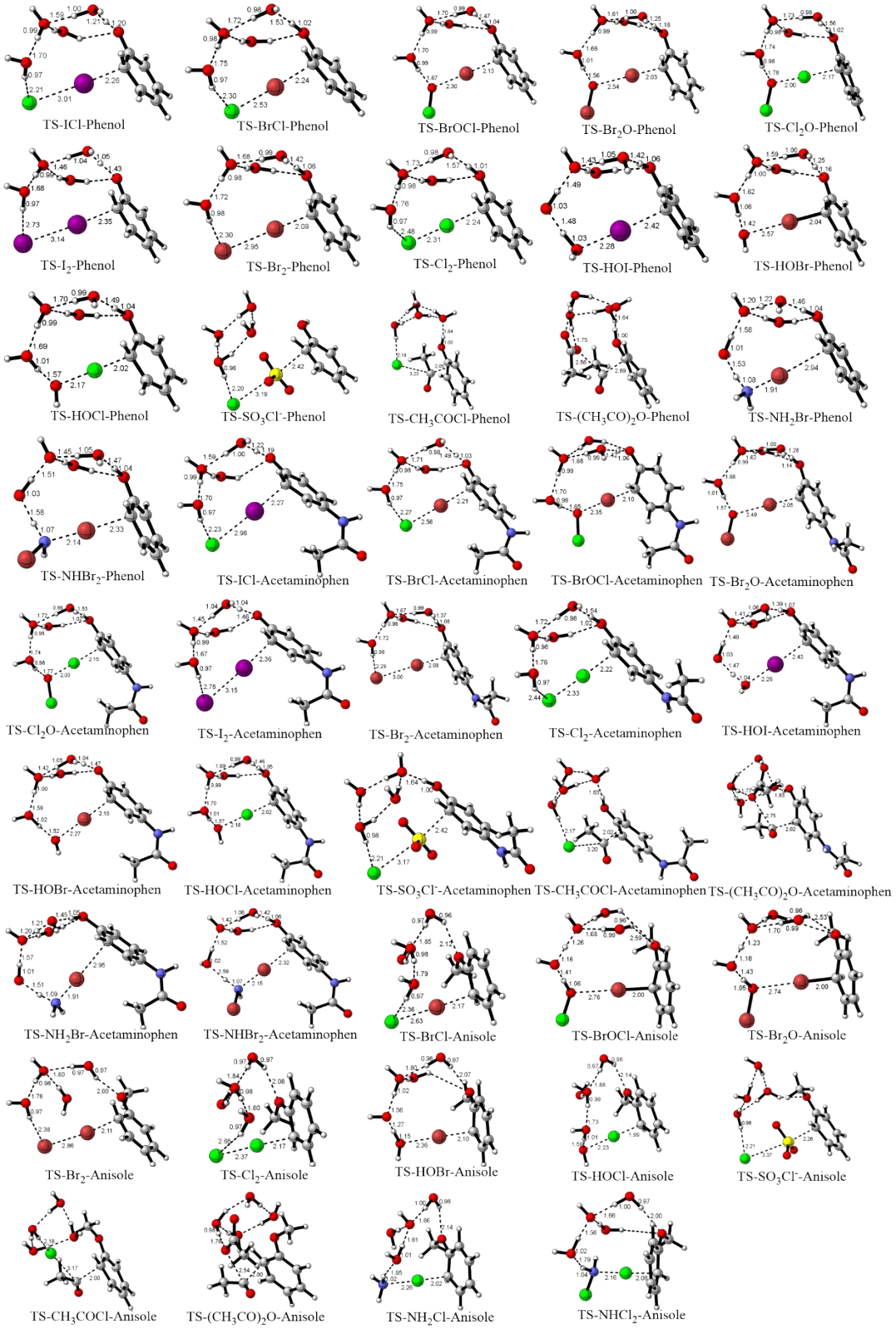


Figure S2. Structures of transition states of the electrophiles reacting with phenol, acetaminophen and anisole (atoms in green color represent chlorine atom; atoms in red color represent bromine atom; atoms in purple color represent iodine atom; atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom; atoms in yellow represent sulfur atom; atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

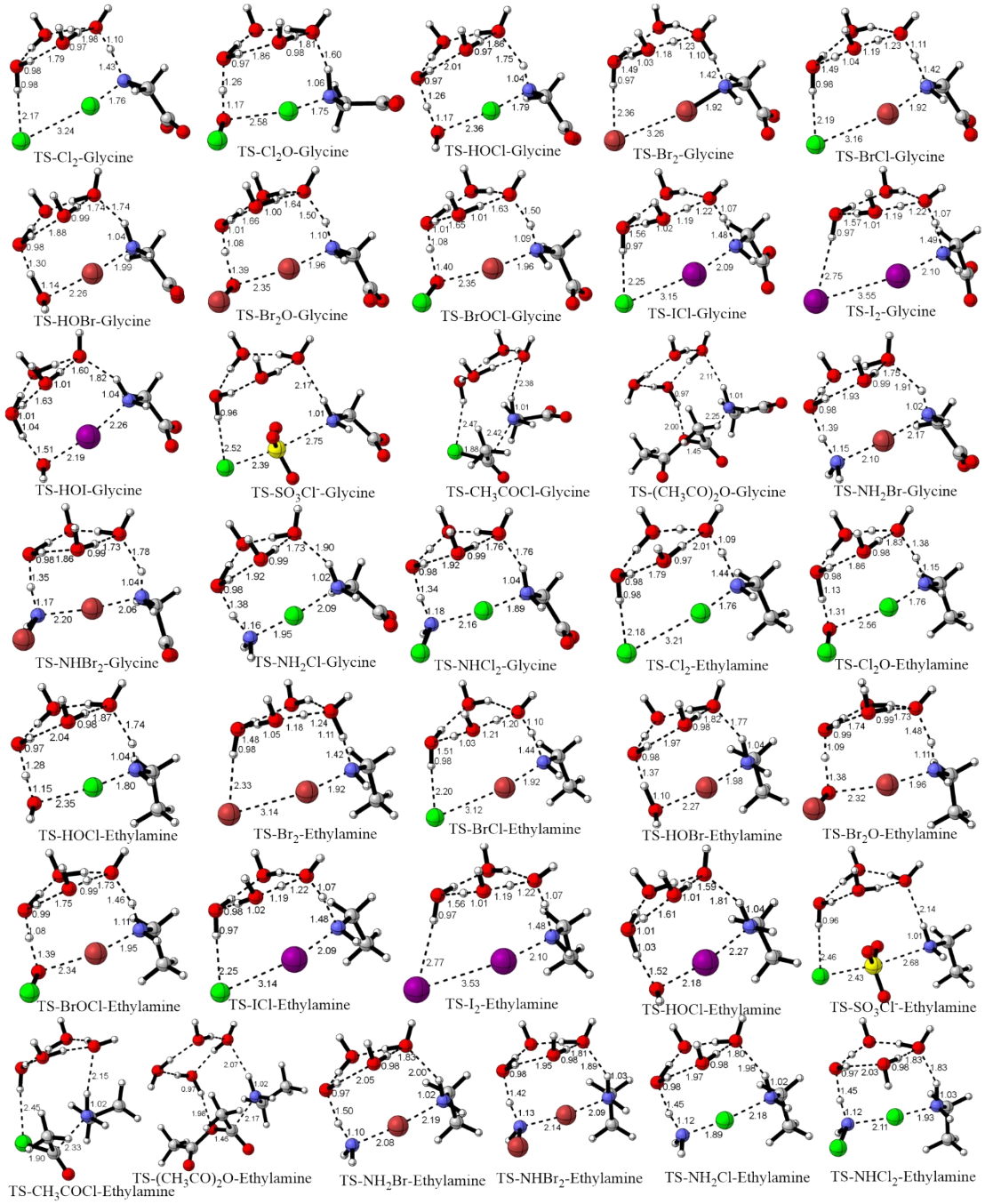


Figure S3. Structures of transition states of the electrophiles reacting with glycine and ethylamine (atoms in green color represent chlorine atom; atoms in red color represent bromine atom; atoms in purple color represent iodine atom; atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom; atoms in yellow represent sulfur atom; atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

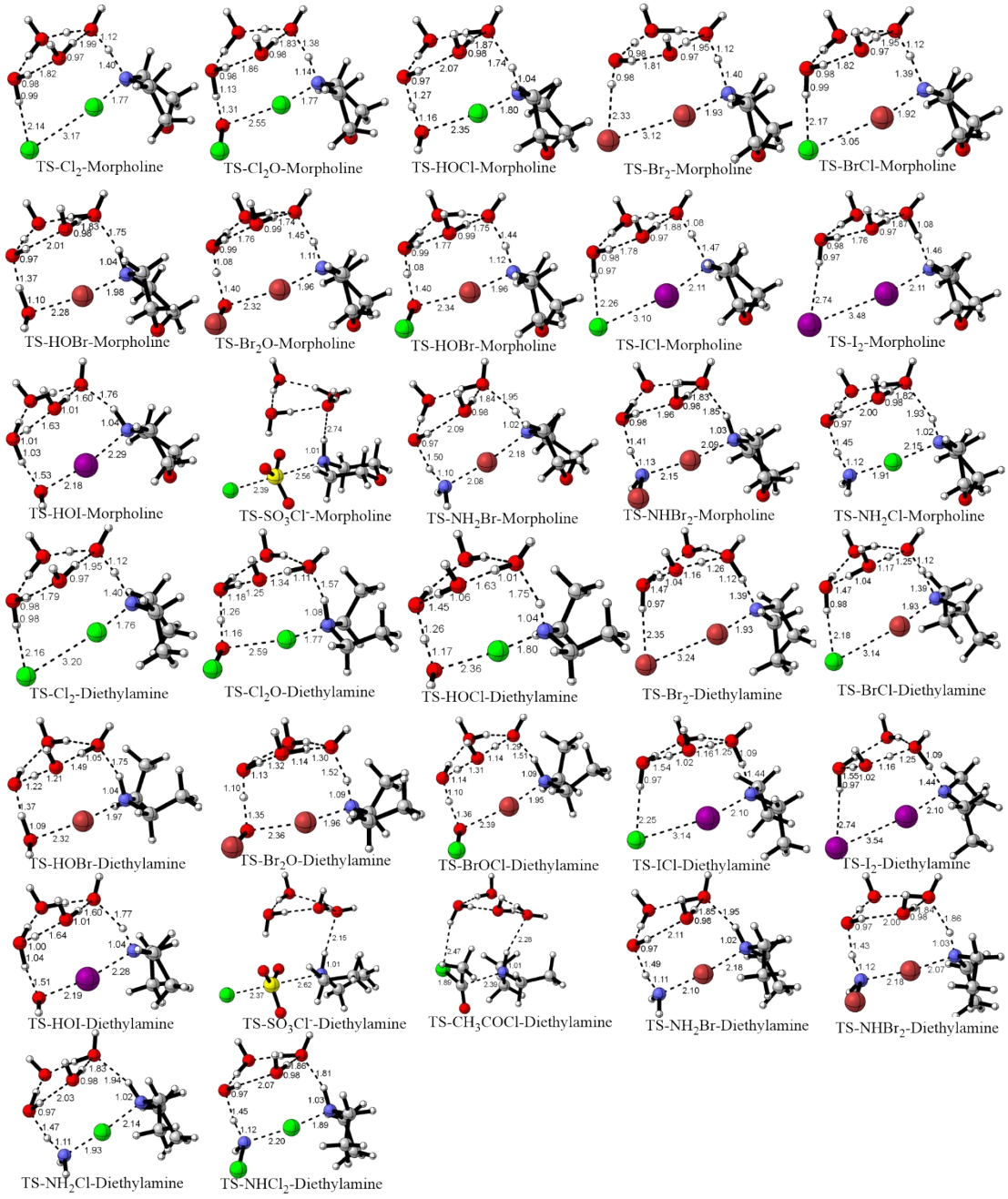


Figure S3. Structures of transition states of the electrophiles reacting with morpholine and diethylamine (atoms in green color represent chlorine atom; atoms in red color represent bromine atom; atoms in purple color represent iodine atom; atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom; atoms in yellow represent sulfur atom; atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

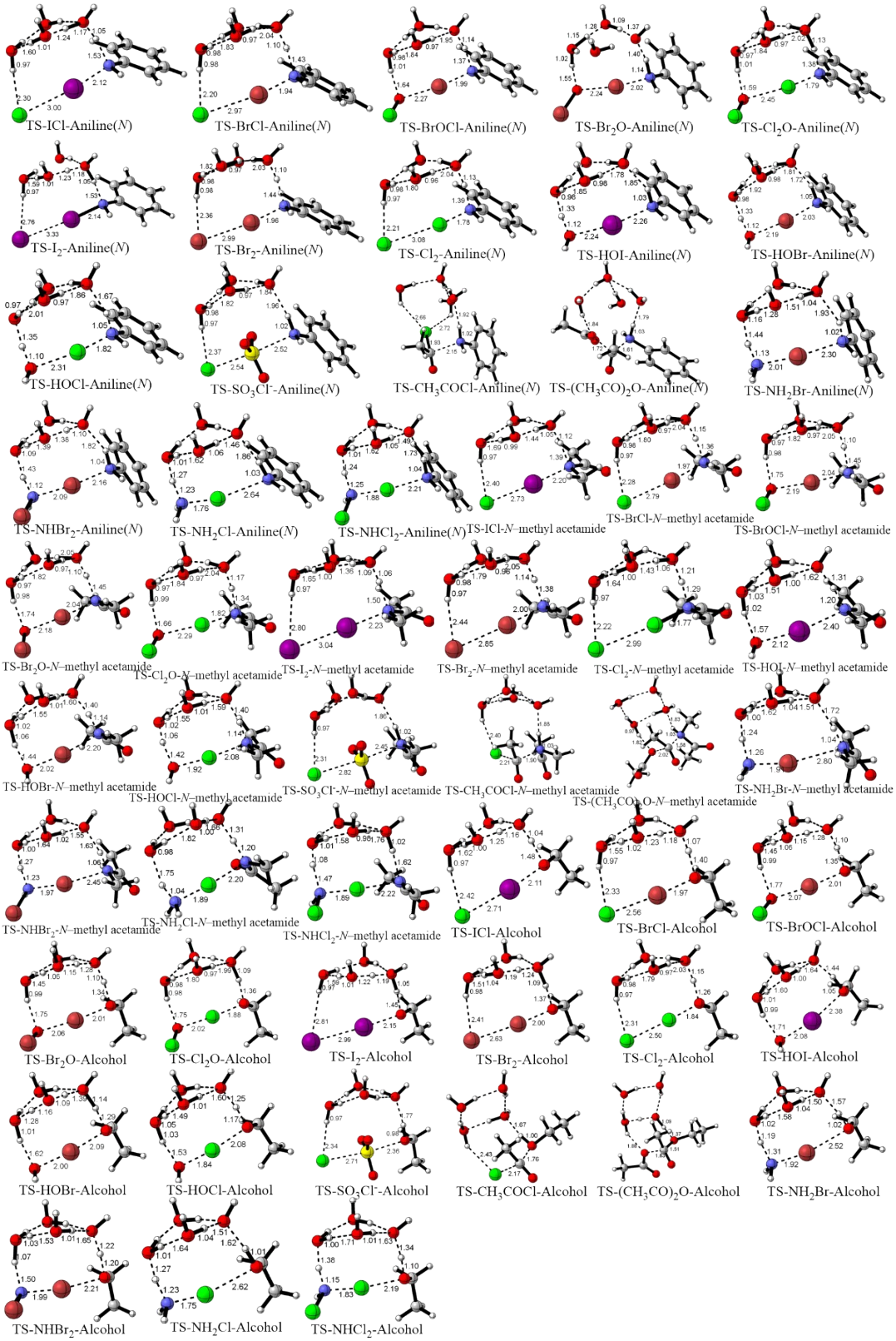


Figure S4. Structures of transition states of the electrophiles reacting with aniline(*N*), *N*–methyl acetamide and alcohol (atoms in green color represent chlorine atom; atoms in red color represent bromine atom; atoms in purple color represent iodine atom; atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom; atoms in yellow represent sulfur atom; atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

Standard orientation of TS-Cl_2-Phenolate

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

Standard orientation of transition state of TS-Cl_2-Phenolate
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -53.33 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.014342	0.661808	1.943934
2	17	0	-0.287736	-0.992241	-0.054008
3	8	0	-0.900522	2.604049	1.291404
4	1	0	-1.620433	2.131615	0.838491
5	1	0	-0.084131	2.420878	0.774442
6	8	0	-3.475638	-0.950757	1.566477
7	1	0	-3.774014	-1.741974	1.103674
8	1	0	-4.169229	-0.732188	2.199528
9	6	0	1.704191	0.253732	1.211743
10	6	0	2.874360	0.437059	-0.900180
11	6	0	3.370350	-1.401930	0.608884
12	6	0	3.575401	-0.716051	-0.599300
13	1	0	4.300275	-1.096346	-1.312725
14	6	0	1.919475	0.979191	0.003854
15	6	0	2.440104	-0.901870	1.505872
16	8	0	-0.898656	1.719420	-1.966901
17	1	0	-0.083301	1.821881	-1.435788
18	1	0	-1.587745	1.432405	-1.344421
19	8	0	-2.915477	1.196500	-0.060653
20	1	0	-3.738003	1.687544	-0.163012
21	1	0	-3.123215	0.401578	0.470886
22	1	0	3.047275	0.960218	-1.835833
23	8	0	1.262594	2.068869	-0.270285
24	1	0	2.261480	-1.411965	2.447435
25	1	0	3.931239	-2.301453	0.833551
26	17	0	-1.844983	-1.904197	-1.121623

Standard orientation of TS-HOI-Phenolate

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:
Standard orientation of transition state of TS-HOI-Phenolate
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -450.41 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.031935	0.650504	-1.764991
2	8	0	2.241827	-1.965922	1.021571
3	8	0	0.831626	2.440819	-1.632275
4	1	0	1.604451	2.004598	-1.224643
5	1	0	0.132091	2.425296	-0.961335
6	8	0	3.865145	-0.947724	-0.464483
7	1	0	3.028265	-1.521399	0.343125
8	1	0	4.718958	-0.942068	-0.020836
9	6	0	-1.524328	0.184137	-0.915470
10	6	0	-3.034490	0.801526	0.979212
11	6	0	-3.564990	-1.102803	-0.474337
12	6	0	-3.820455	-0.256753	0.666748
13	1	0	-4.684614	-0.475868	1.285475
14	6	0	-1.908437	1.158394	0.136166
15	6	0	-2.481783	-0.875519	-1.243789
16	8	0	1.323713	2.252134	1.655618
17	1	0	0.442210	2.133066	1.280344
18	1	0	1.944997	1.907837	0.985008
19	8	0	3.015209	1.431854	-0.330778
20	1	0	3.751184	2.043521	-0.431425
21	1	0	3.381085	0.471530	-0.401128
22	1	0	-3.257298	1.451925	1.817242
23	8	0	-1.278320	2.216762	0.300938
24	1	0	-2.260195	-1.497757	-2.103988
25	1	0	-4.250486	-1.910608	-0.697525
26	1	0	2.146095	-2.893791	0.780806
27	53	0	0.232990	-0.881586	0.034301

Standard orientation of TS-HOBr-Phenolate

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

Standard orientation of transition state of TS-HOBr-Phenolate
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -203.34 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.859657	0.479586	-1.843931
2	8	0	1.568500	-2.324808	0.928752
3	8	0	1.276882	2.354424	-1.658000
4	1	0	2.016422	1.916286	-1.201100
5	1	0	0.506715	2.281148	-1.063238
6	8	0	3.682134	-1.474337	-0.351778
7	1	0	2.888572	-1.840433	0.135672
8	1	0	4.461972	-1.739703	0.147309
9	6	0	-1.474470	0.184422	-1.000042
10	6	0	-2.716921	0.987747	0.972822
11	6	0	-3.592509	-0.852958	-0.378435
12	6	0	-3.657078	0.026078	0.747939
13	1	0	-4.491061	-0.069840	1.436238
14	6	0	-1.623872	1.177802	0.052890
15	6	0	-2.545661	-0.749784	-1.239510
16	8	0	1.549581	2.144330	1.707297
17	1	0	0.682108	2.104968	1.272030
18	1	0	2.186047	1.764051	1.076060
19	8	0	3.351334	1.192823	-0.205034
20	1	0	4.210592	1.626967	-0.232849
21	1	0	3.510519	0.222707	-0.267830
22	1	0	-2.798043	1.671438	1.810977
23	8	0	-0.818889	2.144557	0.171268
24	1	0	-2.470479	-1.401152	-2.103954
25	1	0	-4.376302	-1.583922	-0.534680
26	1	0	1.325431	-3.223846	0.676600
27	35	0	0.056968	-1.118400	0.029105

Standard orientation of TS-HOCl-Phenolate

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

Standard orientation of transition state of TS-HOCl-Phenolate
State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -354.33 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.672180	-0.298252	1.804277
2	8	0	1.455348	2.168287	-1.147743
3	17	0	0.090832	1.148020	-0.159534
4	8	0	1.323374	-2.207639	1.598500
5	1	0	2.039215	-1.723126	1.151206
6	1	0	0.544578	-2.148553	1.011617
7	8	0	3.444354	1.820966	0.579648
8	1	0	2.735005	2.041215	-0.074580
9	1	0	4.264369	2.191987	0.236624
10	6	0	-1.367617	-0.033795	1.015740
11	6	0	-2.721649	-0.804815	-0.881004
12	6	0	-3.446127	1.103217	0.461665
13	6	0	-3.605681	0.208790	-0.637413
14	1	0	-4.463243	0.331536	-1.291601
15	6	0	-1.592232	-1.022123	-0.017839
16	6	0	-2.367107	0.956147	1.282766
17	8	0	1.535296	-1.786543	-1.745709
18	1	0	0.681755	-1.835847	-1.282635
19	1	0	2.165610	-1.409992	-1.106941
20	8	0	3.335141	-0.862515	0.202773
21	1	0	4.210814	-1.263372	0.196096
22	1	0	3.452193	0.098087	0.372971
23	1	0	-2.873100	-1.497421	-1.702169
24	8	0	-0.807978	-2.008397	-0.181124
25	1	0	-2.220443	1.617876	2.130091
26	1	0	-4.181557	1.878928	0.636528
27	1	0	1.091027	3.062778	-1.163666

Standard orientation of TS-SO_3Cl^--Phenolate

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

Standard orientation of transition state of TS-SO_3Cl^--Phenolate
State=1-A Charge = -2 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -352.26 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.625676	-0.176156	-0.103578
2	1	0	-3.393547	0.221921	0.759056
3	1	0	-3.125676	-1.007840	-0.180982
4	8	0	-2.671739	1.765926	-1.761428
5	1	0	-3.052670	1.019518	-1.248949
6	1	0	-3.405665	2.343017	-1.998652
7	8	0	-2.903548	1.237866	2.161109
8	1	0	-2.323708	1.831438	1.638706
9	1	0	-3.649963	1.771762	2.453973
10	8	0	-1.361283	2.714738	0.457847
11	1	0	-1.760381	2.457456	-0.399151
12	1	0	-1.435703	3.672786	0.525132
13	6	0	3.541586	0.264535	-0.986645
14	6	0	4.106851	-0.439433	0.057645
15	6	0	3.568857	-0.387977	1.356611
16	6	0	2.438757	0.382172	1.570218
17	6	0	1.821624	1.070146	0.515419
18	6	0	2.386961	1.087301	-0.797472
19	1	0	3.982676	0.226157	-1.978509
20	1	0	4.990141	-1.043492	-0.129106
21	1	0	4.029374	-0.940826	2.166845
22	1	0	1.996682	0.436542	2.560858
23	1	0	0.980499	1.727674	0.712551
24	8	0	1.879338	1.785097	-1.754689
25	17	0	-1.924279	-2.825446	-0.471896
26	16	0	0.035562	-0.876360	0.021354
27	8	0	-0.563941	-0.606404	1.302748
28	8	0	1.045357	-1.891741	-0.103818
29	8	0	-0.408023	-0.144606	-1.135175

Standard orientation of TS-CH_3COCl-Phenolate

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

Standard orientation of transition state of TS-CH_3COCl-Phenolate
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -457.92 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.158454	-0.126458	1.211910
2	8	0	-1.864022	-2.023589	0.870683
3	1	0	-1.885226	-1.240629	1.453287
4	1	0	-1.003398	-2.003032	0.397855
5	8	0	-3.467990	1.402086	0.154725
6	1	0	-2.730127	1.715895	-0.383003
7	1	0	-3.694137	0.520621	-0.211992
8	8	0	-2.245290	0.293392	2.361376
9	1	0	-2.644126	0.817891	1.636810
10	1	0	-1.463259	0.771455	2.658746
11	6	0	1.131108	-0.123111	0.730184
12	6	0	2.819482	-1.422545	-0.487921
13	6	0	3.491500	0.415612	0.977344
14	6	0	3.783132	-0.588947	0.002355
15	1	0	3.068409	-2.229014	-1.169958
16	1	0	4.811227	-0.717188	-0.323027
17	1	0	1.948722	1.341587	2.115105
18	8	0	0.589823	-2.178188	-0.344728
19	6	0	1.453252	-1.306140	-0.046559
20	6	0	2.200151	0.592954	1.370630
21	8	0	-3.871602	-1.165845	-0.746853
22	1	0	-3.621457	-1.179645	-1.677243
23	1	0	-3.111652	-1.538555	-0.244357
24	1	0	4.295319	1.006662	1.399271
25	8	0	1.654442	1.456443	-1.440210
26	6	0	0.739880	1.276858	-0.679667
27	6	0	0.068536	2.356670	0.136616
28	1	0	-0.408114	3.049978	-0.559864
29	1	0	-0.675502	1.956495	0.820733
30	1	0	0.842275	2.890259	0.691206
31	17	0	-0.845444	0.322423	-1.569018

Standard orientation of TS-$(CH_3CO)_2O$-Phenolate

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

Standard orientation of transition state of TS-$(CH_3CO)_2O$-Phenolate
State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -377.21 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.170741	-1.454727	-0.364769
2	8	0	-1.919739	-0.937957	-2.161867
3	1	0	-1.874681	-1.677987	-1.526735
4	1	0	-1.138571	-0.372919	-1.998102
5	8	0	-2.996568	-0.800516	1.300282
6	1	0	-2.173466	-0.286889	1.334740
7	1	0	-3.507256	-0.383073	0.580758
8	8	0	-2.082269	-2.911851	-0.205349
9	1	0	-2.394908	-2.254652	0.450866
10	1	0	-1.241282	-3.252365	0.119349
11	6	0	1.104436	-0.910536	-0.241984
12	6	0	2.624747	0.656951	-1.414270
13	6	0	3.519534	-1.250120	-0.160757
14	6	0	3.681553	-0.022141	-0.893253
15	1	0	2.763871	1.538881	-2.030579
16	1	0	4.687944	0.343918	-1.072188
17	1	0	2.122703	-2.645070	0.620733
18	8	0	0.300162	0.693447	-1.800206
19	6	0	1.279782	0.168035	-1.218172
20	6	0	2.272483	-1.710741	0.089652
21	8	0	-3.826624	0.619745	-0.947680
22	1	0	-3.257167	1.322504	-0.594300
23	1	0	-3.225082	0.057645	-1.479539
24	1	0	4.398405	-1.799972	0.153630
25	8	0	1.686258	0.695667	1.751286
26	6	0	0.757015	-0.033966	1.341102
27	6	0	0.240528	-1.140652	2.250474
28	1	0	-0.205909	-0.669298	3.129950
29	1	0	-0.500793	-1.778703	1.770878
30	1	0	1.086193	-1.747556	2.573125
31	8	0	-0.537704	0.662649	0.921567
32	6	0	-0.683274	1.915034	0.503869
33	6	0	0.463204	2.881460	0.490803
34	1	0	0.701899	3.158930	1.519202
35	1	0	1.362359	2.459526	0.049361
36	1	0	0.148362	3.766468	-0.058169
37	8	0	-1.808942	2.273240	0.184093

Standard orientation of TS-NH_2Br-Phenolate

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

Standard orientation of transition state of TS-NH_2Br-Phenolate
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -212.49 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.972805	0.366796	-1.919710
2	8	0	1.226751	2.202056	-1.665382
3	1	0	1.899997	1.726197	-1.140418
4	1	0	0.404317	2.181061	-1.141533
5	8	0	3.963823	-1.296138	-0.590287
6	1	0	2.702650	-1.729335	0.411616
7	1	0	4.789509	-1.458602	-0.121864
8	6	0	-1.564273	0.082525	-1.055419
9	6	0	-2.823607	0.886382	0.899191
10	6	0	-3.557326	-1.104979	-0.314466
11	6	0	-3.680938	-0.166587	0.753918
12	1	0	-4.490732	-0.291079	1.466099
13	6	0	-1.761810	1.109016	-0.046264
14	6	0	-2.540995	-0.959101	-1.209473
15	8	0	1.306947	2.020434	1.706227
16	1	0	0.458345	2.028941	1.234147
17	1	0	1.944922	1.577219	1.113883
18	8	0	3.176752	1.039132	-0.079756
19	1	0	3.931898	1.637116	-0.087032
20	1	0	3.532953	0.084120	-0.301735
21	1	0	-2.948431	1.607464	1.699908
22	1	0	-2.426493	-1.650040	-2.038088
23	1	0	-4.273087	-1.912448	-0.407694
24	1	0	1.702123	-2.857123	1.218672
25	7	0	1.863017	-1.871104	1.033365
26	1	0	1.999487	-1.385377	1.915612
27	8	0	-1.007127	2.123918	0.024054
28	35	0	0.141164	-0.989312	0.044023

Standard orientation of TS-$NHBr_2$-Phenolate

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

Standard orientation of transition state of TS-$NHBr_2$-Phenolate
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -995.96 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.106085	0.217945	-1.778449
2	8	0	-1.641595	2.990555	-1.393504
3	1	0	-0.751901	3.079558	-1.004541
4	1	0	-2.138055	2.393581	-0.808411
5	8	0	2.980605	2.078614	-0.668421
6	1	0	2.641906	1.071965	-0.119076
7	1	0	3.728135	2.442727	-0.182725
8	6	0	-2.116091	-0.476735	-0.942670
9	6	0	-3.435482	-0.944591	1.127920
10	6	0	-2.902456	-2.743531	-0.455105
11	6	0	-3.462574	-2.255794	0.782604
12	1	0	-3.934206	-2.969886	1.450103
13	6	0	-2.862291	0.035199	0.229408
14	6	0	-2.284133	-1.886680	-1.293133
15	8	0	-0.933678	2.708024	1.925027
16	1	0	-1.626469	2.160201	1.528355
17	1	0	-0.284451	2.884694	1.218488
18	8	0	0.795691	3.416157	-0.127462
19	1	0	1.000460	4.356824	-0.094554
20	1	0	1.646947	2.933745	-0.342852
21	1	0	-3.891673	-0.585190	2.043378
22	1	0	-1.852703	-2.227216	-2.228185
23	1	0	-2.990159	-3.795957	-0.695270
24	7	0	2.135897	0.030719	0.459387
25	1	0	2.089173	0.144697	1.472240
26	8	0	-2.953261	1.259703	0.443175
27	35	0	-0.118389	-0.308803	-0.260208
28	35	0	3.258785	-1.471607	0.208811

Standard orientation of TS-NH_2Cl-Phenolate

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

Standard orientation of transition state of TS-NH_2Cl-Phenolate
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -376.23 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.842379	0.136270	-1.916137
2	17	0	0.120394	-1.038324	0.113268
3	8	0	1.372497	1.928605	-1.680673
4	1	0	2.038511	1.490705	-1.115436
5	1	0	0.545609	1.953440	-1.163454
6	8	0	3.711680	-1.631607	-0.639062
7	1	0	2.520397	-1.852431	0.506773
8	1	0	4.563585	-1.927919	-0.302467
9	6	0	-1.469012	-0.087653	-1.059723
10	6	0	-2.763968	0.822868	0.822755
11	6	0	-3.469214	-1.237989	-0.287531
12	6	0	-3.615189	-0.240554	0.723639
13	1	0	-4.436643	-0.328194	1.427865
14	6	0	-1.681582	0.990231	-0.110271
15	6	0	-2.439456	-1.137492	-1.174175
16	8	0	1.342138	1.727190	1.708928
17	1	0	0.528791	1.804910	1.184144
18	1	0	2.008847	1.325837	1.118626
19	8	0	3.267505	0.766088	-0.032454
20	1	0	4.073402	1.292211	-0.063293
21	1	0	3.512001	-0.211489	-0.299464
22	1	0	-2.903768	1.587224	1.579675
23	1	0	-2.308740	-1.873488	-1.960561
24	1	0	-4.180303	-2.052897	-0.345818
25	1	0	1.440656	-2.734467	1.518167
26	7	0	1.700019	-1.817742	1.166431
27	1	0	1.874412	-1.182008	1.939835
28	8	0	-0.912655	1.996165	-0.067639

Standard orientation of TS-$NHCl_2$-Phenolate

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

Standard orientation of transition state of TS-$NHCl_2$-Phenolate
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -282.8 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.367017	-0.849007	-1.744762
2	17	0	-0.033901	0.541878	-0.302236
3	8	0	-0.167686	-3.117848	-1.165062
4	1	0	-1.034755	-2.801209	-0.855749
5	1	0	0.497965	-2.722536	-0.576245
6	8	0	-3.838566	-0.017925	-0.987374
7	1	0	-3.212983	0.531942	-0.387108
8	1	0	-4.725628	0.057380	-0.619864
9	6	0	1.717795	-0.163925	-0.978771
10	6	0	3.176826	-0.131680	1.047448
11	6	0	3.392865	1.592638	-0.686043
12	6	0	3.738559	1.016129	0.590910
13	1	0	4.487640	1.517234	1.195556
14	6	0	2.204374	-0.839416	0.243764
15	6	0	2.451193	1.004508	-1.453619
16	8	0	-0.846478	-1.991815	1.975962
17	1	0	0.029823	-1.893189	1.575583
18	1	0	-1.480625	-2.011976	1.236475
19	8	0	-2.634493	-2.287769	-0.159295
20	1	0	-3.270027	-2.992721	0.005165
21	1	0	-3.136760	-1.514226	-0.505365
22	1	0	3.469515	-0.573342	1.993386
23	1	0	2.175386	1.414070	-2.419396
24	1	0	3.904940	2.488346	-1.015674
25	7	0	-2.071940	1.221837	0.475207
26	1	0	-1.953989	0.993935	1.463325
27	8	0	1.738754	-1.944699	0.588832
28	17	0	-2.125856	2.976555	0.462329

Standard orientation of TS-BrCl-Aniline(*C*)

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

Standard orientation of transition state of TS-BrCl-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -84.08 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.008677	0.858920	1.717017
2	8	0	-0.699529	2.927059	1.223619
3	1	0	-1.443811	2.385060	0.896525
4	1	0	-0.517360	2.629812	2.121738
5	8	0	-3.659578	-0.710097	1.599100
6	1	0	-3.655149	-1.511877	1.063347
7	1	0	-4.569349	-0.590892	1.895758
8	6	0	1.733059	0.364735	1.078474
9	6	0	3.170772	0.418954	-0.873168
10	6	0	3.462856	-1.312415	0.806352
11	6	0	3.826361	-0.704973	-0.404966
12	1	0	4.639676	-1.121478	-0.989535
13	6	0	2.116445	0.984319	-0.134250
14	6	0	2.430294	-0.765577	1.543802
15	8	0	-1.178334	1.812828	-2.041088
16	1	0	-0.280859	1.734905	-1.677462
17	1	0	-1.779780	1.584839	-1.309894
18	8	0	-2.833428	1.493114	0.184120
19	1	0	-3.617255	2.050569	0.121360
20	1	0	-3.102982	0.682667	0.663440
21	1	0	3.465252	0.881667	-1.809533
22	1	0	0.840859	2.568950	0.066120
23	1	0	2.136237	-1.204976	2.490682
24	1	0	3.989974	-2.190403	1.158904
25	17	0	-2.028979	-1.837283	-1.086153
26	7	0	1.427684	2.076162	-0.605746
27	1	0	1.917891	2.664172	-1.267293
28	35	0	-0.228713	-0.937564	-0.064567

Standard orientation of TS-Cl_2O-Aniline(*C*)

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

Standard orientation of transition state of TS-Cl_2O-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -233.44 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.110043	-1.248221	-1.477717
2	8	0	-1.899651	1.280602	0.369228
3	17	0	-0.275869	0.612700	-0.216803
4	8	0	-0.119009	-3.469904	-0.548788
5	1	0	-0.954101	-2.964649	-0.510391
6	1	0	0.172229	-3.449846	-1.467004
7	8	0	-3.260037	0.053129	-1.737112
8	1	0	-3.010549	0.730336	-1.089172
9	1	0	-4.217657	0.105313	-1.833898
10	6	0	1.691568	-0.490179	-0.965190
11	6	0	3.053702	0.150532	0.947092
12	6	0	3.130800	1.457562	-1.105747
13	6	0	3.528505	1.224950	0.226915
14	1	0	4.232244	1.902923	0.697812
15	6	0	2.140698	-0.749767	0.357657
16	6	0	2.240854	0.590261	-1.694608
17	8	0	-1.194674	-1.580806	2.159259
18	1	0	-0.271642	-1.449141	1.895245
19	1	0	-1.690159	-1.706837	1.329493
20	8	0	-2.515174	-2.121882	-0.245240
21	1	0	-3.266560	-2.717799	-0.150410
22	1	0	-2.802888	-1.387452	-0.826850
23	1	0	3.381185	-0.024805	1.966312
24	1	0	1.152933	-2.535263	0.539508
25	1	0	1.919575	0.736729	-2.719838
26	1	0	3.529200	2.302264	-1.653779
27	17	0	-1.824348	2.917920	0.771366
28	7	0	1.641980	-1.803839	1.056027
29	1	0	2.117594	-2.076474	1.905441

Standard orientation of TS-Br_2-Aniline(*C*)

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

Standard orientation of transition state of TS-Br_2-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -115.57 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.502858	1.066100	1.525412
2	8	0	0.483686	3.500110	0.773440
3	1	0	-0.426228	3.177384	0.621378
4	1	0	0.698058	3.290496	1.689108
5	8	0	-3.124951	0.688576	1.866430
6	1	0	-3.125354	-0.135342	1.361201
7	1	0	-4.046686	0.871371	2.084161
8	6	0	2.027870	0.312919	0.948191
9	6	0	3.360530	-0.239635	-1.015897
10	6	0	3.407432	-1.684842	0.943671
11	6	0	3.802863	-1.374958	-0.374854
12	1	0	4.481358	-2.041610	-0.896306
13	6	0	2.489782	0.654243	-0.354852
14	6	0	2.547197	-0.836161	1.596537
15	8	0	-0.706190	2.070776	-2.161907
16	1	0	0.153708	1.715489	-1.894004
17	1	0	-1.222397	2.162570	-1.340517
18	8	0	-2.063023	2.597226	0.212786
19	1	0	-2.713113	3.302237	0.117704
20	1	0	-2.449975	1.929242	0.815581
21	1	0	3.692300	-0.002250	-2.020989
22	1	0	1.611757	2.505856	-0.380886
23	1	0	2.227541	-1.042777	2.611761
24	1	0	3.783403	-2.576599	1.429334
25	7	0	2.061720	1.791757	-0.955854
26	1	0	2.547800	2.102361	-1.786213
27	35	0	-0.105072	-0.704865	0.176895
28	35	0	-2.285707	-1.601127	-0.554853

Standard orientation of TS-Cl_2-Aniline(*C*)

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

Standard orientation of transition state of TS-Cl_2-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -266.95 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.683733	0.707352	1.620974
2	8	0	-0.851210	2.904438	1.184591
3	1	0	-1.550876	2.273807	0.923404
4	1	0	-0.605347	2.678832	2.088520
5	8	0	-2.848816	-1.137648	1.881278
6	1	0	-2.766340	-1.931562	1.339402
7	1	0	-3.689293	-1.218527	2.347162
8	6	0	1.439760	0.232633	1.005431
9	6	0	3.009460	0.376381	-0.848510
10	6	0	3.228923	-1.393180	0.807883
11	6	0	3.649064	-0.747752	-0.372515
12	1	0	4.501379	-1.138215	-0.918138
13	6	0	1.904611	0.911476	-0.152927
14	6	0	2.147787	-0.889555	1.493518
15	8	0	-1.398864	1.640174	-2.004459
16	1	0	-0.473318	1.616601	-1.717120
17	1	0	-1.918084	1.370628	-1.225271
18	8	0	-2.818139	1.145797	0.350436
19	1	0	-3.705899	1.516458	0.407255
20	1	0	-2.823750	0.311674	0.863561
21	1	0	3.355049	0.873759	-1.748673
22	1	0	0.615098	2.493169	0.030086
23	1	0	1.802110	-1.360618	2.406950
24	1	0	3.756198	-2.267898	1.167846
25	17	0	-1.901947	-1.964383	-1.259306
26	7	0	1.257430	2.019266	-0.605810
27	1	0	1.728779	2.591089	-1.293733
28	17	0	-0.254103	-0.977588	-0.207964

Standard orientation of TS-HOI-Aniline(*C*)

Cartesian coordinates of the transition state optimized at the M06-2X/ LANL08(d) level:

Standard orientation of transition state of TS-HOI-Aniline(*C*)

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -865.04 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.407029	0.045918	2.005322
2	8	0	-2.366780	-2.113696	-0.594573
3	8	0	-1.135925	1.537090	2.510097
4	1	0	-1.715431	1.579397	1.704433
5	1	0	-0.898456	0.608901	2.615328
6	8	0	-3.433556	0.085903	-1.166749
7	1	0	-2.851035	-1.229817	-0.847790
8	1	0	-3.100459	0.319940	-2.039281
9	6	0	1.637655	-0.045051	0.946902
10	6	0	2.398018	1.353155	-0.975480
11	6	0	3.508169	-0.773931	-0.463169
12	6	0	3.308047	0.392318	-1.280806
13	1	0	3.919705	0.513720	-2.167958
14	6	0	1.616572	1.228605	0.217442
15	6	0	2.723952	-0.970736	0.616526
16	8	0	-0.833531	1.880872	-1.949186
17	1	0	-0.409051	1.017372	-1.894061
18	1	0	-1.371268	1.943028	-1.129941
19	8	0	-2.459303	1.794773	0.238172
20	1	0	-3.040672	2.562046	0.243589
21	1	0	-2.964467	0.966603	-0.401391
22	1	0	2.284144	2.245474	-1.579651
23	1	0	0.238445	2.088004	1.447462
24	1	0	2.834187	-1.844963	1.247363
25	1	0	4.282115	-1.481967	-0.729022
26	7	0	0.874588	2.216234	0.648143
27	1	0	0.766007	3.043674	0.074066
28	1	0	-2.800233	-2.453439	0.196586
29	53	0	-0.226875	-1.094778	0.189573

Standard orientation of TS-HOBr-Aniline(*C*)

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

Standard orientation of transition state of TS-HOBr-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -172.20 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.887985	0.539068	-1.734202
2	6	0	-1.428282	0.091406	-0.904782
3	6	0	-3.048570	0.752796	0.873528
4	6	0	-3.474838	-1.206256	-0.541846
5	6	0	-3.802521	-0.331651	0.551620
6	1	0	-4.695549	-0.539353	1.131097
7	6	0	-1.888735	1.057130	0.097372
8	6	0	-2.354146	-0.982231	-1.259665
9	1	0	-3.329525	1.423528	1.677176
10	1	0	-0.379331	2.373024	-0.286650
11	1	0	-2.076063	-1.623183	-2.088389
12	1	0	-4.134614	-2.031889	-0.775803
13	35	0	0.147137	-0.882986	0.118041
14	7	0	-1.202082	2.157952	0.293169
15	1	0	-1.478330	2.804764	1.022051
16	8	0	1.967983	-1.797758	1.198060
17	1	0	2.200315	-1.065775	1.783089
18	8	0	1.014229	2.479985	-1.411124
19	1	0	1.781833	1.929746	-1.155753
20	1	0	0.786292	2.237498	-2.315402
21	8	0	1.991031	1.419794	1.932611
22	1	0	1.046857	1.267510	1.813672
23	1	0	2.406047	1.283574	1.058512
24	8	0	3.192862	1.075810	-0.544008
25	1	0	4.035837	1.533985	-0.632276
26	1	0	3.355675	0.119906	-0.729639
27	8	0	3.498339	-1.575405	-0.831867
28	1	0	2.906808	-1.727250	-0.010605
29	1	0	4.393504	-1.832894	-0.587202

Standard orientation of TS-HOCl-Aniline(*C*)

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

Standard orientation of transition state of TS-HOCl-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -368.95 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.675033	0.416131	-1.715367
2	8	0	1.538913	-1.986040	1.232251
3	17	0	0.080555	-1.037844	0.184759
4	8	0	1.304208	2.290732	-1.399837
5	1	0	2.059673	1.750773	-1.094665
6	1	0	1.061000	1.954230	-2.269469
7	8	0	3.319900	-1.853215	-0.708179
8	1	0	2.676246	-1.993448	0.036786
9	1	0	4.143807	-2.281219	-0.452266
10	6	0	-1.358126	0.059672	-0.952649
11	6	0	-2.896219	0.733421	0.854001
12	6	0	-3.420313	-1.181666	-0.575133
13	6	0	-3.700449	-0.320775	0.529785
14	1	0	-4.590443	-0.503136	1.122431
15	6	0	-1.733378	1.000947	0.075825
16	6	0	-2.299999	-0.968400	-1.313986
17	8	0	1.869582	1.343835	1.860099
18	1	0	1.017245	0.935713	1.666202
19	1	0	2.436852	1.152615	1.089416
20	8	0	3.398157	0.825587	-0.402596
21	1	0	4.289043	1.189821	-0.435399
22	1	0	3.462758	-0.142359	-0.568008
23	1	0	-3.140324	1.397913	1.675131
24	1	0	-0.137215	2.238234	-0.252796
25	1	0	-2.056678	-1.600708	-2.160343
26	1	0	-4.104107	-1.986193	-0.814205
27	7	0	-0.970156	2.057564	0.315796
28	1	0	-1.184011	2.672301	1.089656
29	1	0	1.167659	-2.866652	1.370452

Standard orientation of TS-SO_3Cl^--Aniline(*C*)

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

Standard orientation of transition state of TS-SO_3Cl^--Aniline(*C*)
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -285.92 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.385946	-0.081216	0.838568
2	1	0	-2.670046	0.338970	1.356237
3	1	0	-3.039119	-0.907448	0.456991
4	8	0	-3.195232	1.670859	-1.259099
5	1	0	-3.347950	1.020555	-0.539901
6	1	0	-4.003444	2.187950	-1.344034
7	8	0	-1.516378	1.512866	2.105740
8	1	0	-1.276006	2.079246	1.344888
9	1	0	-1.986243	2.079935	2.727293
10	8	0	-1.058409	2.987219	-0.185544
11	1	0	-1.828239	2.596094	-0.652797
12	1	0	-1.237027	3.928617	-0.084667
13	6	0	3.298962	0.419372	-1.123335
14	6	0	3.973062	-0.554510	-0.412542
15	6	0	3.614215	-0.878694	0.905893
16	6	0	2.554173	-0.211946	1.489368
17	6	0	1.819021	0.742423	0.766249
18	6	0	2.217785	1.107964	-0.537719
19	1	0	3.596757	0.670022	-2.136283
20	1	0	4.798360	-1.075525	-0.886150
21	1	0	4.160611	-1.637630	1.452302
22	1	0	2.249773	-0.444716	2.503997
23	1	0	1.040512	1.317414	1.259595
24	17	0	-2.324791	-2.657677	-0.711916
25	16	0	-0.024689	-0.950593	-0.001489
26	8	0	-0.346612	-1.250358	1.367253
27	8	0	0.850220	-1.822024	-0.735696
28	8	0	-0.701349	0.124042	-0.675958
29	7	0	1.582052	2.118557	-1.203257
30	1	0	0.660231	2.393348	-0.869797
31	1	0	1.690293	2.134482	-2.208091

Standard orientation of TS-CH_3COCl-Aniline(*C*)

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

Standard orientation of transition state of TS-CH_3COCl-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -228.5 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.790785	1.442076	0.675879
2	1	0	-3.181777	1.026109	-0.119046
3	1	0	-1.949948	1.848633	0.390364
4	8	0	-2.183363	-0.877112	1.926948
5	1	0	-2.468700	0.010965	1.613217
6	1	0	-2.594522	-1.031039	2.784595
7	8	0	-3.874667	-0.019275	-1.406746
8	1	0	-3.662259	-0.907134	-1.050964
9	1	0	-4.835240	0.054777	-1.411309
10	8	0	-3.082190	-2.355540	-0.196655
11	1	0	-2.754145	-1.931031	0.623076
12	1	0	-3.829521	-2.907660	0.058897
13	6	0	3.736548	0.151031	0.125769
14	6	0	3.691409	-1.139964	-0.447039
15	6	0	2.570114	-1.913762	-0.265928
16	6	0	1.456670	-1.390703	0.423987
17	6	0	1.549670	-0.149675	1.106195
18	6	0	2.706418	0.635947	0.897583
19	1	0	4.615280	0.768056	-0.027989
20	1	0	4.534883	-1.508183	-1.018080
21	1	0	2.500023	-2.904665	-0.699675
22	1	0	0.588488	-2.017407	0.604289
23	1	0	2.771375	1.611078	1.367063
24	17	0	-0.055313	2.702210	-0.298562
25	6	0	0.662311	-0.165362	-1.350837
26	8	0	1.511769	0.228794	-1.988034
27	6	0	-0.754100	-0.466603	-1.191767
28	1	0	-1.069606	-0.316136	-0.162232
29	1	0	-1.294358	0.192216	-1.874502
30	1	0	-0.874279	-1.516957	-1.472271
31	7	0	0.565091	0.266544	1.947021
32	1	0	-0.304341	-0.262072	1.962658

33	1	0	0.432984	1.270071	1.999396

Standard orientation of TS-$(CH_3CO)_2O$-Aniline(*C*)

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

Standard orientation of transition state of TS-$(CH_3CO)_2O$-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -217.28 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.309635	-1.425150	-0.457133
2	8	0	-1.929236	-0.801945	-2.069413
3	1	0	-1.873492	-1.626367	-1.539732
4	1	0	-2.018705	-1.061971	-2.993377
5	8	0	-2.967972	-0.967800	1.335331
6	1	0	-2.166681	-0.417568	1.313239
7	1	0	-3.557129	-0.550287	0.679488
8	8	0	-1.991196	-2.908866	-0.342476
9	1	0	-2.334352	-2.334392	0.374227
10	1	0	-1.141315	-3.252350	-0.044860
11	6	0	1.204064	-0.850727	-0.217321
12	6	0	2.789154	0.738667	-1.304665
13	6	0	3.625421	-1.206579	-0.060379
14	6	0	3.816581	0.050953	-0.741995
15	1	0	2.955544	1.633466	-1.893912
16	1	0	4.826617	0.431002	-0.852565
17	1	0	2.198830	-2.608620	0.647843
18	6	0	1.464268	0.216720	-1.188680
19	6	0	2.376829	-1.669911	0.135466
20	8	0	-3.980225	0.533048	-0.780691
21	1	0	-3.407780	1.224822	-0.404475
22	1	0	-3.385963	0.031566	-1.370298
23	1	0	4.493329	-1.764107	0.268725
24	8	0	1.640210	0.703563	1.735256
25	6	0	0.806049	-0.095580	1.274460
26	6	0	0.233969	-1.172291	2.183583
27	1	0	-0.279287	-0.683849	3.014044
28	1	0	-0.455525	-1.841781	1.671709

29	1	0	1.066062	-1.753496	2.583991
30	8	0	-0.626308	0.601889	0.783516
31	6	0	-0.843174	1.868218	0.529855
32	6	0	0.254251	2.890789	0.643141
33	1	0	0.480010	3.057623	1.697698
34	1	0	1.174793	2.569639	0.160441
35	1	0	-0.099603	3.819810	0.201100
36	8	0	-1.979620	2.226642	0.216451
37	7	0	0.476573	0.720807	-1.887939
38	1	0	0.639424	1.513184	-2.498534
39	1	0	-0.450134	0.279387	-1.886623

Standard orientation of TS-NH_2Br-Aniline(*C*)

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

Standard orientation of transition state of TS-NH_2Br-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -179.73 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.024674	0.440375	-1.853075
2	8	0	1.158733	2.196947	-1.549100
3	1	0	1.896274	1.727786	-1.091001
4	1	0	0.992604	1.723719	-2.371647
5	8	0	4.074943	-1.161534	-0.752377
6	1	0	2.762864	-1.665362	0.399226
7	1	0	4.909358	-1.294713	-0.290620
8	6	0	-1.553799	0.073592	-0.978509
9	6	0	-2.986011	0.870725	0.887730
10	6	0	-3.594985	-1.133741	-0.386330
11	6	0	-3.803881	-0.198381	0.680159
12	1	0	-4.654260	-0.341827	1.337924
13	6	0	-1.877348	1.088391	0.016990
14	6	0	-2.528923	-0.979741	-1.205241
15	8	0	1.679510	1.389606	2.010514
16	1	0	0.763585	1.204151	1.775841
17	1	0	2.213146	1.234736	1.197583
18	8	0	3.196729	1.066180	-0.207056

19	1	0	3.923982	1.697614	-0.189483
20	1	0	3.613779	0.088003	-0.455645
21	1	0	-3.177631	1.585964	1.679221
22	1	0	-0.299878	2.285862	-0.487504
23	1	0	-2.344294	-1.664693	-2.024877
24	1	0	-4.296832	-1.945727	-0.526948
25	7	0	-1.113415	2.155937	0.128434
26	1	0	-1.289843	2.830555	0.862600
27	1	0	1.856061	-2.779966	1.281315
28	7	0	1.964683	-1.799037	1.043744
29	1	0	2.119224	-1.263623	1.892959
30	35	0	0.093372	-0.931880	0.015835

Standard orientation of TS-NHBr$_2$-Aniline(*C*)

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

Standard orientation of transition state of TS-NHBr$_2$-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -689.7 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.258670	0.977613	-1.412433
2	8	0	-1.317350	3.364336	-0.352510
3	1	0	-0.349673	3.240279	-0.438128
4	1	0	-1.677543	3.366472	-1.246203
5	8	0	2.973569	1.475637	-1.490693
6	1	0	2.480624	0.515453	-0.578871
7	1	0	3.884047	1.677031	-1.249595
8	6	0	-2.358575	0.068097	-0.828562
9	6	0	-3.483506	-0.879806	1.161476
10	6	0	-3.310593	-2.177456	-0.908305
11	6	0	-3.690320	-2.033112	0.463118
12	1	0	-4.171693	-2.867715	0.961246
13	6	0	-2.871083	0.234692	0.518953
14	6	0	-2.698096	-1.144578	-1.539397
15	8	0	1.036927	1.963241	2.035767
16	1	0	0.107412	1.711813	2.085322
17	1	0	1.145255	2.460092	1.197477

18	8	0	1.410216	3.175543	-0.399706
19	1	0	1.834174	4.038854	-0.347859
20	1	0	2.057379	2.541466	-0.877086
21	1	0	-3.805228	-0.776831	2.191618
22	1	0	-2.246689	2.174436	0.677985
23	1	0	-2.404777	-1.216139	-2.580558
24	1	0	-3.524408	-3.102910	-1.427676
25	7	0	-2.721594	1.391297	1.139921
26	1	0	-3.010738	1.488114	2.104385
27	7	0	1.960343	-0.150892	0.177691
28	1	0	1.958790	0.300391	1.096060
29	35	0	-0.212740	-0.198571	-0.358007
30	35	0	2.868644	-1.785667	0.331564

Standard orientation of TS-NH_2Cl-Aniline(*C*)

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

Standard orientation of transition state of TS-NH_2Cl-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -361.72 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.856390	0.225682	-1.858282
2	17	0	0.090388	-1.011065	0.082429
3	8	0	1.324511	1.995633	-1.615793
4	1	0	2.024834	1.539533	-1.094214
5	1	0	1.112593	1.415897	-2.355625
6	8	0	3.731058	-1.526535	-0.769108
7	1	0	2.540530	-1.821526	0.468582
8	1	0	4.607573	-1.792533	-0.472962
9	6	0	-1.459123	-0.064132	-1.004654
10	6	0	-2.883026	0.799919	0.820195
11	6	0	-3.485930	-1.256661	-0.363624
12	6	0	-3.701261	-0.280195	0.657898
13	1	0	-4.552518	-0.396201	1.319979
14	6	0	-1.768498	0.977521	-0.047932
15	6	0	-2.417789	-1.126167	-1.191175
16	8	0	1.624163	1.228694	2.014918

17	1	0	0.717475	1.180533	1.689288
18	1	0	2.204600	1.085824	1.235509
19	8	0	3.250440	0.817232	-0.130634
20	1	0	4.050062	1.353448	-0.149749
21	1	0	3.510330	-0.178257	-0.419158
22	1	0	-3.077710	1.545750	1.582438
23	1	0	-0.162411	2.139303	-0.563883
24	1	0	-2.227395	-1.843017	-1.981713
25	1	0	-4.180546	-2.080014	-0.471022
26	7	0	-0.980560	2.037401	0.048124
27	1	0	-1.154192	2.734451	0.760857
28	1	0	1.515322	-2.739849	1.483392
29	7	0	1.742319	-1.813204	1.137349
30	1	0	1.911327	-1.172203	1.907661

Standard orientation of TS-$NHCl_2$-Aniline(*C*)

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

Standard orientation of transition state of TS-$NHCl_2$-Aniline(*C*)
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -161.56 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.500948	-0.677626	-1.792255
2	17	0	0.093300	0.571017	-0.279158
3	8	0	-0.301729	-2.829004	-1.325980
4	1	0	-1.177933	-2.657911	-0.925370
5	1	0	-0.239941	-2.253507	-2.096810
6	8	0	-3.988366	-0.081853	-0.631861
7	1	0	-3.262548	0.472410	-0.132695
8	1	0	-4.807622	0.000496	-0.132280
9	6	0	1.804545	-0.078109	-0.937482
10	6	0	3.324979	-0.354091	1.040713
11	6	0	3.566781	1.564400	-0.476219
12	6	0	3.917286	0.821396	0.711577
13	1	0	4.695871	1.215793	1.355278
14	6	0	2.310966	-0.890333	0.187092
15	6	0	2.583998	1.118690	-1.279608

16	8	0	-1.198315	-1.562413	2.005172
17	1	0	-0.602842	-0.912017	1.613528
18	1	0	-1.756288	-1.884568	1.271059
19	8	0	-2.738294	-2.388636	-0.143309
20	1	0	-3.337096	-3.132612	-0.019135
21	1	0	-3.284553	-1.595501	-0.367879
22	1	0	3.619496	-0.917969	1.918178
23	1	0	1.025892	-2.424840	-0.200023
24	1	0	2.293631	1.654449	-2.175986
25	1	0	4.108640	2.473114	-0.705902
26	7	0	1.776955	-2.061122	0.407367
27	1	0	2.060965	-2.604144	1.215136
28	7	0	-2.056611	1.217631	0.504679
29	1	0	-1.935471	1.175306	1.518382
30	17	0	-2.221610	2.945283	0.194678

Standard orientation of TS-ICl-Phenol

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d)level:

Standard orientation of transition state of TS-ICl-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1011.94 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.281522	0.694453	-1.767094
2	8	0	0.134022	2.894544	-0.998249
3	1	0	1.047120	2.541603	-0.778609
4	1	0	-0.053177	2.710374	-1.927296
5	8	0	3.510592	-0.104864	-1.483789
6	1	0	3.399962	-0.744877	-0.758543
7	1	0	4.458779	0.043491	-1.568706
8	6	0	-1.686027	0.122312	-0.935494
9	6	0	-3.204897	0.467676	1.011955
10	6	0	-3.557481	-1.407637	-0.535898
11	6	0	-3.882154	-0.654737	0.643338
12	1	0	-4.710624	-0.991426	1.257018
13	6	0	-2.142978	0.952505	0.194036
14	6	0	-2.518601	-1.024212	-1.306177

15	8	0	1.018591	2.046460	2.068113
16	1	0	0.171968	1.706176	1.759342
17	1	0	1.614530	1.971717	1.304225
18	8	0	2.488051	2.070544	-0.292287
19	1	0	3.135307	2.780951	-0.359800
20	1	0	2.859715	1.281063	-0.752783
21	1	0	-3.480242	1.045096	1.885609
22	8	0	-1.592076	2.066296	0.458053
23	1	0	-0.732583	2.441743	-0.284263
24	1	0	-2.240777	-1.568029	-2.201330
25	1	0	-4.154271	-2.272949	-0.792953
26	53	0	0.196613	-0.791272	-0.088818
27	17	0	2.766160	-1.895369	1.014544

Standard orientation of TS-BrCl-Phenol

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

Standard orientation of transition state of TS-BrCl-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -151.88 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.020084	0.631426	-1.838517
2	8	0	0.584043	2.720630	-1.243720
3	1	0	1.423263	2.318621	-0.923900
4	1	0	0.476803	2.477390	-2.170451
5	8	0	3.623089	-0.626728	-1.424123
6	1	0	3.334503	-1.299800	-0.788274
7	1	0	4.583737	-0.692697	-1.472293
8	6	0	-1.584945	0.161635	-1.040224
9	6	0	-2.999959	0.596945	0.925711
10	6	0	-3.484039	-1.286609	-0.562593
11	6	0	-3.745823	-0.510065	0.597449
12	1	0	-4.570141	-0.794651	1.241982
13	6	0	-1.949078	0.990785	0.081560
14	6	0	-2.447167	-0.943519	-1.375161
15	8	0	1.126076	1.952672	2.096479
16	1	0	0.211504	1.954001	1.786890

17	1	0	1.676281	1.707241	1.331791
18	8	0	2.789141	1.634594	-0.141538
19	1	0	3.525607	2.253527	-0.081140
20	1	0	3.120000	0.836568	-0.606408
21	1	0	-3.223930	1.197631	1.798474
22	8	0	-1.289531	2.090702	0.359715
23	1	0	-0.586572	2.339147	-0.336773
24	1	0	-2.219862	-1.509229	-2.271086
25	1	0	-4.113354	-2.136388	-0.793106
26	17	0	2.113923	-2.016531	1.024156
27	35	0	0.115688	-0.892336	-0.034937

Standard orientation of TS-BrOCl-Phenol

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

Standard orientation of transition state of TS-BrOCl-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -108.65 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.374479	0.361780	-1.847737
2	8	0	2.292584	-1.083330	0.779669
3	8	0	-0.482074	2.909412	-1.427113
4	1	0	0.441170	2.892264	-1.083066
5	1	0	-0.474454	2.565271	-2.327664
6	8	0	3.521189	0.783052	-0.655115
7	1	0	3.111899	0.062608	-0.111964
8	1	0	4.393426	0.951546	-0.282088
9	6	0	-1.672904	-0.211051	-0.973975
10	6	0	-3.161979	-0.049683	1.003545
11	6	0	-3.124279	-2.085225	-0.370989
12	6	0	-3.572689	-1.333433	0.758237
13	1	0	-4.278601	-1.794431	1.440426
14	6	0	-2.277503	0.569165	0.099103
15	6	0	-2.229256	-1.534973	-1.224181
16	8	0	0.215817	2.808306	2.009230
17	1	0	-0.642483	2.489642	1.704874
18	1	0	0.808423	2.787284	1.235857

19	8	0	1.903334	2.885245	-0.217493
20	1	0	2.400416	3.708094	-0.281837
21	1	0	2.530159	2.145060	-0.393610
22	1	0	-3.537723	0.523211	1.841906
23	8	0	-1.983578	1.821503	0.260990
24	1	0	-1.391132	2.230395	-0.484729
25	1	0	-1.861745	-2.075784	-2.088548
26	1	0	-3.507661	-3.084365	-0.531444
27	35	0	0.209839	-0.651210	-0.091365
28	17	0	2.854818	-2.593678	0.273861

Standard orientation of TS-Br_2O-Phenol

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

Standard orientation of transition state of TS-Br_2O-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -151.88 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.849556	-0.184078	-1.854793
2	8	0	2.311675	0.154580	0.768710
3	8	0	-2.011762	2.548163	-1.399109
4	1	0	-1.147491	2.907253	-1.045832
5	1	0	-1.884623	2.223045	-2.299294
6	8	0	2.480959	2.311348	-0.615500
7	1	0	2.470300	1.441894	-0.093155
8	1	0	3.170338	2.863290	-0.231134
9	6	0	-1.826851	-0.762344	-0.932521
10	6	0	-3.387564	-1.132931	0.997182
11	6	0	-2.523503	-3.033967	-0.310567
12	6	0	-3.275948	-2.472689	0.783824
13	1	0	-3.785945	-3.153642	1.456674
14	6	0	-2.764298	-0.232377	0.090845
15	6	0	-1.848085	-2.222730	-1.142959
16	8	0	-1.448251	2.776718	2.006517
17	1	0	-2.121973	2.169435	1.677054
18	1	0	-0.861046	2.967788	1.253196
19	8	0	0.118082	3.453398	-0.220718

20	1	0	0.236516	4.407714	-0.285786
21	1	0	1.003035	3.032210	-0.377063
22	1	0	-3.986842	-0.723878	1.800802
23	8	0	-2.986092	1.013323	0.177356
24	1	0	-2.512827	1.713119	-0.621528
25	1	0	-1.259544	-2.609809	-1.966598
26	1	0	-2.510926	-4.107940	-0.443528
27	35	0	-0.002837	-0.363101	-0.132544
28	35	0	3.462300	-1.118740	0.143347

Standard orientation of TS-Cl_2O-Phenol

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

Standard orientation of transition state of TS-Cl_2O-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -267.51 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.181837	0.662421	1.892615
2	8	0	-1.866933	-1.338311	-0.561132
3	17	0	-0.137432	-0.677307	0.194943
4	8	0	-0.274750	2.898150	1.257687
5	1	0	-1.127186	2.720031	0.801326
6	1	0	-0.311934	2.439376	2.104880
7	8	0	-3.474634	0.083074	1.137196
8	1	0	-3.000491	-0.539962	0.552592
9	1	0	-4.416341	-0.074542	1.007576
10	6	0	1.670742	0.127061	1.086899
11	6	0	2.993429	0.322670	-0.970213
12	6	0	3.286294	-1.597407	0.515828
13	6	0	3.584479	-0.883564	-0.672810
14	1	0	4.308087	-1.297550	-1.366351
15	6	0	2.065537	0.872397	-0.071342
16	6	0	2.372427	-1.086103	1.389896
17	8	0	-0.745997	2.047393	-2.199901
18	1	0	0.125278	2.021843	-1.782520
19	1	0	-1.389477	2.096123	-1.470561
20	8	0	-2.556216	2.323519	-0.084650

21	1	0	-3.208467	3.029927	-0.146942
22	1	0	-2.983022	1.562707	0.366604
23	1	0	3.242708	0.873486	-1.868916
24	8	0	1.538847	2.049032	-0.345666
25	1	0	0.875461	2.374141	0.350841
26	1	0	2.121277	-1.602651	2.308960
27	1	0	3.790390	-2.532905	0.722004
28	17	0	-1.980691	-3.014789	-0.475527

Standard orientation of TS-I_2-Phenol

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-I_2-Phenol

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -84.33 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.271480	0.755202	-1.593655
2	8	0	-1.470229	3.183287	-0.522010
3	1	0	-0.447090	3.094927	-0.359138
4	1	0	-1.658532	3.066879	-1.463687
5	8	0	2.126900	1.669102	-2.083537
6	1	0	2.395569	0.839162	-1.662708
7	1	0	2.943142	2.120456	-2.326530
8	6	0	-2.434602	-0.049275	-0.882229
9	6	0	-3.595595	-0.604236	1.236006
10	6	0	-3.602998	-2.179540	-0.640710
11	6	0	-3.931401	-1.812633	0.705324
12	1	0	-4.478749	-2.522513	1.316339
13	6	0	-2.913103	0.372990	0.437181
14	6	0	-2.901510	-1.316655	-1.413646
15	8	0	-0.226322	2.017436	2.342533
16	1	0	-1.095780	1.748659	2.019014
17	1	0	0.295828	2.199941	1.546771
18	8	0	0.974207	2.947836	-0.046207
19	1	0	1.394617	3.806704	0.076498
20	1	0	1.435359	2.483996	-0.789001
21	1	0	-3.878884	-0.324785	2.243808

22	8	0	-2.711480	1.543431	0.872214
23	1	0	-2.005483	2.468701	0.038612
24	1	0	-2.636712	-1.561226	-2.435953
25	1	0	-3.923921	-3.139169	-1.025069
26	53	0	-0.185244	-0.480258	-0.341548
27	53	0	2.839258	-0.885584	0.403042

Standard orientation of TS-Br_2-Phenol

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-I_2-Phenol

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -53.29 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.723112	0.636564	-1.782370
2	8	0	-0.606829	3.034970	-1.087825
3	1	0	0.344445	2.947532	-0.836288
4	1	0	-0.698067	2.814728	-2.022200
5	8	0	3.431408	0.941902	-1.340632
6	1	0	3.268553	0.130867	-0.820528
7	1	0	4.365950	1.156471	-1.240761
8	6	0	-1.961082	-0.031991	-0.958522
9	6	0	-3.320996	-0.012560	1.129760
10	6	0	-3.540864	-1.845854	-0.496990
11	6	0	-3.854354	-1.213382	0.751045
12	1	0	-4.557151	-1.704233	1.415412
13	6	0	-2.442364	0.653423	0.250105
14	6	0	-2.650800	-1.269850	-1.331734
15	8	0	0.374816	2.376739	2.207105
16	1	0	-0.528550	2.157483	1.949224
17	1	0	0.891056	2.436233	1.383693
18	8	0	1.863617	2.788759	-0.136539
19	1	0	2.340342	3.624709	-0.085358
20	1	0	2.456585	2.141193	-0.579258
21	1	0	-3.595648	0.472643	2.057776
22	8	0	-2.042428	1.843600	0.537009
23	1	0	-1.454579	2.321245	-0.199635

24	1	0	-2.381115	-1.721766	-2.278932
25	1	0	-4.024666	-2.779294	-0.753299
26	35	0	-0.079033	-0.675500	-0.325643
27	35	0	2.586292	-1.615953	0.505574

Standard orientation of TS-Cl_2-Phenol

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-I_2-Phenol

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -256.58 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.828882	0.509182	-1.848393
2	17	0	0.147297	-0.957703	0.022151
3	8	0	0.808578	2.587517	-1.250192
4	1	0	1.584248	2.124856	-0.862366
5	1	0	0.710066	2.265343	-2.153514
6	8	0	3.276824	-0.947902	-1.598580
7	1	0	3.121887	-1.693673	-1.003942
8	1	0	4.187181	-1.028943	-1.905881
9	6	0	-1.483071	0.100252	-1.086856
10	6	0	-2.891390	0.550018	0.864907
11	6	0	-3.356700	-1.360505	-0.583282
12	6	0	-3.630657	-0.571155	0.558854
13	1	0	-4.452246	-0.851365	1.208708
14	6	0	-1.836046	0.929103	0.022649
15	6	0	-2.318787	-1.014293	-1.403290
16	8	0	1.127221	1.645985	2.126998
17	1	0	0.250229	1.765233	1.738409
18	1	0	1.715542	1.408632	1.388458
19	8	0	2.856030	1.276154	-0.054553
20	1	0	3.676633	1.779116	-0.006309
21	1	0	3.042622	0.468369	-0.577469
22	1	0	-3.118660	1.162881	1.728689
23	8	0	-1.161636	2.030932	0.308943
24	1	0	-0.439515	2.247356	-0.365178
25	1	0	-2.082952	-1.594827	-2.287473
26	1	0	-3.971815	-2.224114	-0.801756

27	17	0	1.879140	-2.035241	1.110155

Standard orientation of TS-HOI-Phenol

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-HOI-Phenol

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -107.22 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.338847	0.426728	-1.947391
2	8	0	2.009642	-2.242646	0.445965
3	8	0	0.894563	2.085430	-1.856923
4	1	0	1.752401	1.827250	-1.304059
5	1	0	0.714642	1.357559	-2.461576
6	8	0	3.707604	-0.444189	0.880193
7	1	0	2.744563	-1.542226	0.638649
8	1	0	3.621639	-0.170796	1.799649
9	6	0	-1.735076	0.223114	-0.958207
10	6	0	-2.521422	1.224055	1.138078
11	6	0	-3.586284	-0.791478	0.261808
12	6	0	-3.450272	0.216229	1.246144
13	1	0	-4.103211	0.197171	2.111785
14	6	0	-1.678462	1.280743	0.010765
15	6	0	-2.762832	-0.770805	-0.827713
16	8	0	1.396369	1.965170	1.706373
17	1	0	0.530598	2.192178	1.347446
18	1	0	1.966804	1.811940	0.912535
19	8	0	2.872746	1.512272	-0.469266
20	1	0	3.521027	2.222181	-0.507100
21	1	0	3.399201	0.353774	0.306600
22	1	0	-2.437753	2.003321	1.885862
23	8	0	-0.853907	2.290449	-0.112418
24	1	0	-0.161257	2.193675	-0.906600
25	1	0	-2.843625	-1.519296	-1.607392
26	1	0	-4.340952	-1.558963	0.373435
27	1	0	2.307131	-2.786446	-0.295177
28	53	0	0.167125	-1.068511	-0.194779

Standard orientation of TS-HOBr-Phenol

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

Standard orientation of transition state of TS-HOBr-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -762.11 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.917135	0.201172	-1.865247
2	8	0	2.137606	-2.325916	1.096065
3	8	0	0.932164	2.256807	-1.546490
4	1	0	1.756520	1.874228	-1.122546
5	1	0	0.815765	1.877613	-2.426858
6	8	0	3.600272	-1.186180	-0.550109
7	1	0	2.979908	-1.712196	0.135933
8	1	0	4.510220	-1.307230	-0.258697
9	6	0	-1.357600	-0.110546	-0.919665
10	6	0	-2.787305	0.963748	0.838410
11	6	0	-3.498960	-1.119735	-0.266677
12	6	0	-3.664907	-0.068771	0.705515
13	1	0	-4.537934	-0.098806	1.348506
14	6	0	-1.667847	1.038927	-0.033650
15	6	0	-2.411582	-1.132788	-1.057550
16	8	0	1.327577	2.228048	1.884839
17	1	0	0.440682	2.284632	1.508415
18	1	0	1.893144	1.844260	1.190619
19	8	0	2.951021	1.327086	-0.218370
20	1	0	3.757317	1.849294	-0.296936
21	1	0	3.201033	0.366770	-0.351582
22	1	0	-2.943217	1.766487	1.547981
23	8	0	-0.925123	2.068914	-0.027463
24	1	0	-0.062316	2.126830	-0.798669
25	1	0	-2.247003	-1.914241	-1.790197
26	1	0	-4.256093	-1.889313	-0.343585
27	1	0	1.860461	-3.201706	0.806982
28	35	0	0.168278	-1.041225	0.057423

Standard orientation of TS-HOCl-Phenol

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

Standard orientation of transition state of TS-HOCl-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -371.98 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.788701	-0.043750	-1.880038
2	8	0	-1.608547	2.226338	1.166175
3	17	0	-0.055333	1.150346	0.098783
4	8	0	-1.228579	-1.904933	-1.646495
5	1	0	-2.000958	-1.567928	-1.134134
6	1	0	-1.114242	-1.319846	-2.404541
7	8	0	-3.446656	1.648053	-0.540726
8	1	0	-2.744815	1.939835	0.126695
9	1	0	-4.290755	1.992418	-0.230327
10	6	0	1.347245	0.165095	-0.973114
11	6	0	2.654440	-0.969132	0.797550
12	6	0	3.487341	1.091528	-0.246146
13	6	0	3.585193	0.032827	0.707593
14	1	0	4.437121	0.015709	1.378627
15	6	0	1.559966	-0.967601	-0.088144
16	6	0	2.422333	1.137354	-1.081407
17	8	0	-1.492417	-1.767530	1.922282
18	1	0	-0.634841	-1.889294	1.495869
19	1	0	-2.096936	-1.453963	1.225246
20	8	0	-3.229677	-0.981949	-0.119974
21	1	0	-4.075804	-1.436308	-0.194243
22	1	0	-3.387926	-0.021598	-0.291378
23	1	0	2.755475	-1.783903	1.503548
24	8	0	0.721127	-1.959704	-0.055688
25	1	0	-0.041348	-1.909648	-0.754326
26	1	0	2.309128	1.926483	-1.815596
27	1	0	4.267944	1.839814	-0.292636
28	1	0	-1.291201	3.133462	1.085343

Standard orientation of TS-SO_3Cl^--Phenol

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

Standard orientation of transition state of TS-SO_3Cl^--Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -135.74 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.255724	-0.182520	1.007384
2	1	0	-2.508352	0.296560	1.416930
3	1	0	-2.907857	-0.994786	0.594101
4	8	0	-3.419664	1.396227	-1.222905
5	1	0	-3.450919	0.806431	-0.439003
6	1	0	-4.297362	1.780944	-1.319424
7	8	0	-1.364386	1.588860	2.009685
8	1	0	-1.322440	2.156791	1.212588
9	1	0	-1.813497	2.107474	2.686585
10	8	0	-1.472005	3.084025	-0.303243
11	1	0	-2.186914	2.554469	-0.715235
12	1	0	-1.844800	3.952567	-0.116973
13	6	0	3.293609	0.489660	-1.160910
14	6	0	3.989259	-0.508371	-0.500296
15	6	0	3.660164	-0.891930	0.810464
16	6	0	2.603350	-0.278653	1.444910
17	6	0	1.822478	0.685819	0.767204
18	6	0	2.231464	1.120471	-0.510574
19	1	0	3.569228	0.800362	-2.162964
20	1	0	4.813675	-0.996530	-1.007857
21	1	0	4.234956	-1.660444	1.311578
22	1	0	2.320178	-0.561572	2.452006
23	1	0	1.081640	1.273491	1.301098
24	17	0	-2.388197	-2.699972	-0.701958
25	16	0	0.099915	-0.839850	0.027986
26	8	0	-0.277762	-1.218925	1.366883
27	8	0	0.898239	-1.749989	-0.753374
28	8	0	-0.658556	0.182913	-0.649275
29	8	0	1.535075	2.126519	-1.063193
30	1	0	1.829497	2.302516	-1.968397

Standard orientation of TS-CH_3COCl-Phenol

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

Standard orientation of transition state of TS-CH_3COCl-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -296.05 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.214310	1.194479	0.176762
2	1	0	3.135732	0.527699	0.884716
3	1	0	2.340617	1.617095	0.063799
4	8	0	3.574037	-0.643574	-1.795198
5	1	0	3.514003	0.106371	-1.163097
6	1	0	4.501505	-0.899870	-1.839629
7	8	0	3.117771	-1.036078	1.865165
8	1	0	2.664198	-1.574047	1.190175
9	1	0	4.020657	-1.368589	1.919520
10	8	0	1.823396	-2.096063	-0.372382
11	1	0	2.535826	-1.742442	-0.954964
12	1	0	1.756855	-3.044503	-0.532713
13	6	0	-3.567827	0.088735	-1.009680
14	6	0	-3.884700	-0.679064	0.138383
15	6	0	-2.896309	-1.385520	0.763925
16	6	0	-1.549770	-1.261874	0.316015
17	6	0	-1.285904	-0.637977	-0.938403
18	6	0	-2.305983	0.098504	-1.561042
19	1	0	-4.353260	0.661130	-1.490813
20	1	0	-4.904257	-0.705117	0.501530
21	1	0	-3.096376	-1.977638	1.648977
22	1	0	-0.790822	-1.923065	0.721173
23	1	0	-2.086204	0.638522	-2.473950
24	8	0	-0.095769	-0.697075	-1.508895
25	17	0	0.499554	2.697173	-0.387665
26	6	0	-1.077725	0.459834	1.329459
27	8	0	-1.921584	1.230611	1.403436
28	6	0	0.277607	0.179757	1.823270
29	1	0	0.909806	-0.097982	0.982088
30	1	0	0.646748	1.079583	2.315436

31	1	0	0.207457	-0.661144	2.517324
32	1	0	0.551469	-1.280717	-1.021937

Standard orientation of TS-$(CH_3CO)_2O$-Phenol

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

Standard orientation of transition state of TS-$(CH_3CO)_2O$-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -295.95 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.485397	-1.656439	-0.354766
2	8	0	-1.685910	-1.241572	-1.939031
3	1	0	-1.683136	-1.975284	-1.283323
4	1	0	-1.578557	-1.632849	-2.813713
5	8	0	-3.056476	-0.912156	1.290497
6	1	0	-2.319348	-0.261168	1.279712
7	1	0	-3.606910	-0.634188	0.536992
8	8	0	-1.873588	-3.039108	0.060249
9	1	0	-2.285682	-2.361402	0.641088
10	1	0	-1.041131	-3.301213	0.469274
11	6	0	1.362335	-1.017436	-0.386855
12	6	0	2.457072	0.925339	-1.355234
13	6	0	3.783935	-0.845853	-0.316889
14	6	0	3.668422	0.427415	-0.912159
15	1	0	2.394934	1.871512	-1.879564
16	1	0	4.563583	1.019896	-1.066824
17	1	0	2.688603	-2.551737	0.378634
18	8	0	0.161297	0.614482	-1.692663
19	6	0	1.295145	0.171795	-1.169861
20	6	0	2.647318	-1.576774	-0.093759
21	8	0	-3.812062	0.356508	-1.090818
22	1	0	-3.277943	1.093746	-0.725207
23	1	0	-3.170109	-0.220098	-1.540460
24	1	0	4.757031	-1.231232	-0.041463
25	8	0	1.930295	0.672869	1.685650
26	6	0	1.275577	-0.250232	1.491511
27	6	0	0.486748	-1.242002	2.246514

28	1	0	0.310116	-0.825511	3.238716
29	1	0	-0.446464	-1.456499	1.737229
30	1	0	1.092558	-2.149589	2.308577
31	8	0	-0.991591	0.857281	1.066957
32	6	0	-1.148753	1.994691	0.537309
33	6	0	-0.022009	2.994685	0.700804
34	1	0	0.298768	3.035789	1.742783
35	1	0	0.835606	2.663638	0.108157
36	1	0	-0.318413	3.987075	0.365107
37	8	0	-2.168399	2.337608	-0.115433
38	1	0	-0.562184	-0.071513	-1.672494

Standard orientation of TS-NH_2Br-Phenol

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

Standard orientation of transition state of TS-NH_2Br-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1108.08 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.427408	0.703227	-2.022379
2	8	0	1.002523	2.063268	-1.780585
3	1	0	1.994009	1.712695	-1.167304
4	1	0	0.796911	1.404884	-2.451879
5	8	0	3.564238	-0.754027	0.769374
6	1	0	2.516351	-1.833847	0.482031
7	1	0	3.558080	-0.530794	1.707436
8	6	0	-1.919416	0.478253	-1.081471
9	6	0	-2.302709	0.984660	1.253493
10	6	0	-3.546830	-0.795611	0.181926
11	6	0	-3.252450	-0.025959	1.309505
12	1	0	-3.766516	-0.219172	2.244860
13	6	0	-1.628192	1.246590	0.055816
14	6	0	-2.879354	-0.535315	-1.008277
15	8	0	1.484466	1.881408	1.795033
16	1	0	0.612752	2.018794	1.390955
17	1	0	2.078177	1.703726	1.035451
18	8	0	2.936949	1.406846	-0.497643

19	1	0	3.645982	2.043032	-0.633497
20	1	0	3.356946	0.090581	0.263380
21	1	0	-2.065243	1.580915	2.128061
22	8	0	-0.708732	2.235105	0.035207
23	1	0	-0.059151	2.160902	-0.777784
24	1	0	-3.096330	-1.119841	-1.895804
25	1	0	-4.287439	-1.584689	0.234912
26	1	0	1.949165	-3.084596	-0.566768
27	35	0	0.225126	-1.353476	-0.266773
28	7	0	1.688767	-2.482286	0.217023
29	1	0	1.431104	-3.074667	1.009190

Standard orientation of TS-NHBr$_2$-Phenol

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

Standard orientation of transition state of TS-NHBr$_2$-Phenol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -159.18 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.819266	-0.240396	1.943907
2	8	0	1.282259	2.461853	1.894273
3	1	0	0.413343	2.795285	1.417482
4	1	0	1.028366	1.903559	2.636989
5	8	0	-2.393033	2.176881	-0.917301
6	1	0	-2.144692	0.620700	-0.920064
7	1	0	-2.198412	2.514888	-1.798727
8	6	0	2.122344	-0.694460	1.006372
9	6	0	3.458815	-0.461996	-1.032437
10	6	0	3.041991	-2.669130	-0.073330
11	6	0	3.591801	-1.831266	-1.072803
12	1	0	4.141850	-2.280602	-1.892289
13	6	0	2.764332	0.135962	0.033732
14	6	0	2.343951	-2.107181	0.958688
15	8	0	0.878324	3.050614	-1.524357
16	1	0	1.597534	2.473228	-1.236100
17	1	0	0.287948	3.154587	-0.737654
18	8	0	-0.717699	3.272225	0.638265

19	1	0	-0.915699	4.193528	0.833147
20	1	0	-1.741218	2.637063	-0.272563
21	1	0	3.901663	0.174766	-1.788699
22	8	0	2.695674	1.448721	0.092180
23	1	0	2.143575	1.814118	0.893388
24	1	0	1.916715	-2.718860	1.744862
25	1	0	3.184302	-3.740749	-0.128623
26	35	0	0.016109	-0.603126	0.008644
27	7	0	-1.945067	-0.426793	-0.836147
28	1	0	-1.943378	-0.862443	-1.759776
29	35	0	-3.324089	-1.195875	0.177982

Standard orientation of TS-BrCl-Anisole

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

Standard orientation of transition state of TS-BrCl-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -135.41 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.475441	0.028796	1.637986
2	8	0	2.460569	2.708226	1.181717
3	1	0	1.640933	2.270258	1.472776
4	8	0	-1.883242	-0.264414	2.446975
5	1	0	-2.503139	-0.149023	1.709123
6	1	0	-2.341118	0.056544	3.232738
7	6	0	1.971359	-0.745275	1.072925
8	6	0	0.925857	-1.491858	-1.041326
9	6	0	1.030198	-3.001538	0.878859
10	6	0	0.703212	-2.786064	-0.418338
11	1	0	0.222807	-3.549903	-1.018005
12	6	0	1.693515	-0.519139	-0.286909
13	6	0	1.650480	-1.957971	1.626553
14	8	0	0.067020	2.992629	-0.731081
15	1	0	0.993480	3.207452	-0.563338
16	1	0	-0.161504	2.364912	-0.024004
17	8	0	-0.098057	1.729127	1.779020
18	1	0	-0.511820	2.467358	2.242138

19	1	0	-0.636093	0.941024	1.997433
20	1	0	1.037299	-1.486981	-2.120330
21	8	0	2.109915	0.609626	-0.799594
22	1	0	2.814720	2.136678	0.489699
23	1	0	1.891110	-2.134402	2.669018
24	1	0	0.828471	-3.952457	1.354259
25	6	0	1.962975	0.879976	-2.206112
26	1	0	0.908907	0.899358	-2.477649
27	1	0	2.403099	1.861403	-2.352693
28	1	0	2.506847	0.130119	-2.779923
29	17	0	-3.355141	0.571305	-0.365724
30	35	0	-1.011636	-0.550676	-0.800632

Standard orientation of TS-BrOCl-Anisole

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

Standard orientation of transition state of TS-BrOCl-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -889.37 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.093633	1.126586	-1.645055
2	8	0	2.894189	-0.736638	0.568393
3	8	0	-0.621427	2.581667	-1.891421
4	1	0	0.290383	2.689846	-1.519747
5	8	0	3.384934	1.078579	-1.031401
6	1	0	3.110539	0.045101	-0.119705
7	1	0	4.274491	1.408415	-0.866013
8	6	0	-2.820018	0.173635	-1.210884
9	6	0	-1.843191	-1.129304	0.699001
10	6	0	-2.699254	-2.290852	-1.295017
11	6	0	-2.160546	-2.356600	-0.066670
12	1	0	-1.900300	-3.299280	0.400144
13	6	0	-2.334495	0.144785	0.107976
14	6	0	-3.003829	-1.008779	-1.871832
15	8	0	0.327361	3.514196	1.255268
16	1	0	-0.583038	3.517758	0.941100
17	1	0	0.896761	3.303803	0.472801

18	8	0	1.823024	2.916502	-0.869669
19	1	0	2.208806	3.706099	-1.262406
20	1	0	2.654036	1.973331	-0.955654
21	1	0	-2.084804	-1.221711	1.758080
22	8	0	-2.308420	1.257442	0.758049
23	1	0	-1.229717	2.646356	-1.147446
24	1	0	-3.415311	-0.982204	-2.874685
25	1	0	-2.907214	-3.187195	-1.863973
26	35	0	0.145813	-0.950486	0.620747
27	6	0	-2.010883	1.319351	2.175654
28	1	0	-0.988487	0.998499	2.360871
29	1	0	-2.131870	2.365060	2.436515
30	1	0	-2.730402	0.705107	2.715322
31	17	0	3.515429	-2.149175	-0.123495

Standard orientation of TS-Br_2O-Anisole

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

Standard orientation of transition state of TS-Br_2O-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1075.11 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.810290	0.529906	1.506405
2	8	0	-2.490218	0.268611	-0.489818
3	8	0	1.920285	2.628035	1.525124
4	1	0	0.992516	2.917251	1.349664
5	8	0	-2.634267	2.120227	1.164207
6	1	0	-2.580569	1.027126	0.236281
7	1	0	-3.378351	2.683532	0.926758
8	6	0	3.264610	-0.339618	1.164767
9	6	0	1.915772	-1.482646	-0.614549
10	6	0	2.442359	-2.645487	1.488924
11	6	0	1.881455	-2.670305	0.268586
12	1	0	1.351023	-3.537601	-0.106394
13	6	0	2.764049	-0.354673	-0.146921
14	6	0	3.115124	-1.457181	1.939106
15	8	0	0.440712	3.274933	-1.402911

16	1	0	1.105431	2.585390	-1.311927
17	1	0	0.007870	3.350617	-0.515016
18	8	0	-0.600218	3.413034	1.048679
19	1	0	-0.755691	4.318952	1.333748
20	1	0	-1.651363	2.779012	1.116246
21	1	0	2.090547	-1.739359	-1.659365
22	8	0	3.038837	0.654173	-0.904019
23	1	0	2.348339	2.515094	0.669564
24	1	0	3.540182	-1.454969	2.936665
25	1	0	2.395689	-3.504687	2.144594
26	35	0	0.066013	-0.720424	-0.551025
27	6	0	2.769105	0.642406	-2.327994
28	1	0	1.703341	0.528762	-2.516929
29	1	0	3.114428	1.607818	-2.680941
30	1	0	3.338697	-0.164206	-2.787011
31	35	0	-3.601678	-1.092996	0.013769

Standard orientation of TS-Cl_2O-Anisole

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

Standard orientation of transition state of TS-Cl_2O-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -275.38 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.709264	0.393836	1.361024
2	8	0	2.529530	-0.895213	-0.250537
3	8	0	-3.293215	-2.110630	0.712494
4	1	0	-2.429114	-1.965810	1.134028
5	8	0	1.663945	-0.692470	2.357466
6	1	0	2.114564	-0.797325	1.496508
7	1	0	2.126440	-1.260480	2.983764
8	6	0	-1.997191	1.081432	0.922158
9	6	0	-0.610466	1.750483	-0.997558
10	6	0	-0.584300	3.076082	1.047682
11	6	0	-0.182068	2.899668	-0.239326
12	1	0	0.511421	3.583085	-0.714789
13	6	0	-1.619888	0.906425	-0.419248

14	6	0	-1.488522	2.145406	1.626981
15	8	0	-0.655214	-2.870072	-0.972801
16	1	0	-1.590660	-2.780836	-1.187947
17	1	0	-0.561684	-2.495868	-0.077208
18	8	0	-0.650507	-1.994376	1.687667
19	1	0	-0.580888	-2.829088	2.165949
20	1	0	0.124641	-1.458914	1.962003
21	1	0	-0.534429	1.804026	-2.076538
22	8	0	-2.177685	-0.091143	-1.074870
23	1	0	-3.302635	-1.504716	-0.039150
24	1	0	-1.797656	2.284590	2.656892
25	1	0	-0.230622	3.915713	1.631848
26	6	0	-1.917726	-0.265358	-2.478299
27	1	0	-0.857989	-0.450934	-2.648825
28	1	0	-2.501039	-1.133527	-2.771029
29	1	0	-2.251639	0.616037	-3.025798
30	17	0	0.993747	0.414749	-0.625576
31	17	0	4.037823	-0.194360	-0.509743

Standard orientation of TS-Br_2-Anisole

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

Standard orientation of transition state of TS-Br_2-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -70.71 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.533162	0.673529	1.840358
2	8	0	-0.165600	2.944532	1.318521
3	1	0	-1.118348	2.874744	1.128622
4	1	0	0.289931	2.506357	0.588774
5	8	0	-3.524617	0.182754	1.750494
6	1	0	-3.278204	-0.437624	1.042459
7	1	0	-4.458767	0.037446	1.939184
8	6	0	1.928430	-0.009052	1.092330
9	6	0	3.466519	0.050438	-0.854883
10	6	0	3.664664	-1.712132	0.858250
11	6	0	4.052324	-1.098308	-0.363942

12	1	0	4.856562	-1.547755	-0.935985
13	6	0	2.449445	0.646727	-0.104139
14	6	0	2.653147	-1.171092	1.582528
15	8	0	-1.473943	1.723602	-1.621809
16	1	0	-1.543675	0.765044	-1.506898
17	1	0	-1.949346	2.109295	-0.863615
18	8	0	-2.829608	2.583179	0.669186
19	1	0	-3.544248	3.226288	0.614561
20	1	0	-3.182289	1.777632	1.101765
21	1	0	3.815226	0.493609	-1.777278
22	8	0	1.861749	1.773958	-0.400664
23	1	0	2.329632	-1.603822	2.521730
24	1	0	4.184671	-2.597657	1.198704
25	6	0	2.168450	2.449373	-1.636730
26	1	0	1.522739	3.321719	-1.648790
27	1	0	3.215803	2.747296	-1.640134
28	1	0	1.942515	1.792147	-2.475756
29	35	0	-2.368507	-1.589181	-0.836076
30	35	0	0.144019	-0.831910	0.313391

Standard orientation of TS-Cl_2-Anisole

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

Standard orientation of transition state of TS-Cl_2-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -258.79 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.189710	0.212420	1.661033
2	8	0	1.531945	2.831840	1.634528
3	1	0	0.800669	2.208278	1.791893
4	8	0	-1.608064	-1.403808	2.046878
5	1	0	-2.284755	-1.466005	1.359610
6	1	0	-2.072450	-1.497434	2.887130
7	6	0	1.873011	-0.545279	0.955022
8	6	0	1.122609	-1.140118	-1.307393
9	6	0	1.369013	-2.869208	0.388268
10	6	0	1.089302	-2.517077	-0.897348

11	1	0	0.790582	-3.253832	-1.633387
12	6	0	1.619909	-0.171775	-0.374855
13	6	0	1.750327	-1.865649	1.316486
14	8	0	-0.838602	2.853559	-0.419124
15	1	0	0.036270	3.233826	-0.273640
16	1	0	-0.906025	2.133687	0.234050
17	8	0	-0.754274	1.223244	1.865858
18	1	0	-1.375799	1.660991	2.459278
19	1	0	-0.978112	0.270905	1.889722
20	1	0	1.166693	-0.924432	-2.367165
21	8	0	1.805994	1.098506	-0.687493
22	1	0	1.984372	2.487446	0.854322
23	1	0	1.960465	-2.148681	2.341872
24	1	0	1.309123	-3.901690	0.707508
25	6	0	1.655773	1.529221	-2.049457
26	1	0	0.639970	1.346218	-2.398001
27	1	0	1.857653	2.596325	-2.036104
28	1	0	2.381404	1.015841	-2.680701
29	17	0	-0.960726	-0.601016	-1.000952
30	17	0	-3.243711	-0.064942	-0.675926

Standard orientation of TS-HOBr-Anisole

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

Standard orientation of transition state of TS-HOBr-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -258.79 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.389523	2.130673	1.835190
2	8	0	-1.713188	-2.617127	-0.574336
3	8	0	-1.414462	2.758404	1.354788
4	1	0	-1.974500	1.959417	1.325206
5	8	0	-2.733372	-1.925342	1.509616
6	1	0	-2.200307	-2.317953	0.423913
7	1	0	-3.594987	-2.348243	1.586521
8	6	0	1.811181	1.283859	1.309023
9	6	0	1.957983	-0.087299	-0.754678

10	6	0	3.301515	-0.667646	1.211507
11	6	0	2.964326	-0.901674	-0.076813
12	1	0	3.390905	-1.725057	-0.637543
13	6	0	1.494203	1.100244	-0.046342
14	6	0	2.699532	0.425416	1.904791
15	8	0	-2.907717	1.643909	-1.372815
16	1	0	-2.192323	2.280523	-1.270112
17	1	0	-3.003778	1.209324	-0.502293
18	8	0	-3.129708	0.594498	1.165376
19	1	0	-3.987071	0.809842	1.547855
20	1	0	-2.976040	-0.398147	1.315021
21	1	0	2.097733	0.022493	-1.826346
22	8	0	0.737649	2.004508	-0.609303
23	1	0	-0.784159	2.676936	0.628580
24	1	0	2.966706	0.592973	2.942274
25	1	0	4.020051	-1.293648	1.723762
26	1	0	-1.398815	-3.524990	-0.494562
27	35	0	0.224782	-1.276193	-0.639076
28	6	0	0.498885	1.994226	-2.033216
29	1	0	-0.054550	1.100866	-2.317401
30	1	0	-0.094861	2.882929	-2.223680
31	1	0	1.449719	2.055261	-2.560967

Standard orientation of TS-HOCl-Anisole

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

Standard orientation of transition state of TS-HOCl-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -340.4 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.006817	-1.958816	1.791593
2	8	0	0.287060	3.147182	-1.071526
3	8	0	2.614761	-1.998549	1.327654
4	1	0	2.219153	-1.122721	1.474747
5	8	0	0.194410	2.863040	1.506168
6	1	0	0.213634	3.053955	0.516748
7	1	0	0.667841	3.579850	1.941691

8	6	0	-0.777422	-1.494398	1.207524
9	6	0	-1.588013	-0.628197	-0.971012
10	6	0	-3.026275	-0.524708	1.007064
11	6	0	-2.859007	-0.328567	-0.319937
12	1	0	-3.634262	0.113738	-0.934286
13	6	0	-0.601548	-1.349820	-0.179743
14	6	0	-1.961988	-1.096489	1.770338
15	8	0	2.957080	0.190691	-0.931624
16	1	0	3.081129	-0.762634	-0.856715
17	1	0	2.496672	0.449782	-0.111296
18	8	0	1.839715	0.711173	1.574280
19	1	0	2.596012	1.037391	2.076156
20	1	0	1.182178	1.445514	1.567548
21	1	0	-1.650314	-0.892693	-2.021624
22	8	0	0.500815	-1.819094	-0.695936
23	1	0	2.087655	-2.394949	0.623480
24	1	0	-2.102254	-1.233415	2.836918
25	1	0	-3.952034	-0.259490	1.500666
26	1	0	-0.426122	3.694047	-1.420865
27	6	0	0.708461	-1.820145	-2.123725
28	1	0	0.696947	-0.802082	-2.507669
29	1	0	1.688064	-2.266100	-2.264895
30	1	0	-0.058601	-2.430535	-2.599085
31	17	0	-0.684029	1.143973	-1.036959

Standard orientation of TS-SO_3Cl^--Anisole

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

Standard orientation of transition state of TS-SO_3Cl^--Anisole
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -131.79 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.296476	-0.822133	-0.743016
2	1	0	-3.315493	-0.411466	0.143630
3	1	0	-2.712218	-1.601236	-0.672251
4	8	0	-1.912377	1.359263	-1.730483
5	1	0	-2.334675	0.516631	-1.459510

6	1	0	-1.010719	1.329008	-1.384148
7	8	0	-3.284258	0.671221	1.595185
8	1	0	-3.353982	1.533663	1.137700
9	1	0	-4.070873	0.584796	2.144598
10	8	0	-3.364063	2.918777	-0.003544
11	1	0	-2.820180	2.465741	-0.682751
12	1	0	-4.252641	2.988791	-0.370147
13	6	0	2.570237	1.353390	-1.269930
14	6	0	3.726245	0.612776	-1.143537
15	6	0	4.055309	-0.061606	0.054112
16	6	0	3.183634	-0.015595	1.105589
17	6	0	1.925019	0.650607	0.977327
18	6	0	1.691308	1.440686	-0.184135
19	1	0	2.343068	1.902765	-2.175337
20	1	0	4.410484	0.563690	-1.983271
21	1	0	4.989477	-0.602993	0.130351
22	1	0	3.394801	-0.532471	2.034280
23	1	0	1.355528	0.850528	1.878689
24	8	0	0.622665	2.218382	-0.335073
25	6	0	-0.132337	2.621558	0.822843
26	1	0	0.542781	3.014617	1.583569
27	1	0	-0.793706	3.407208	0.469854
28	1	0	-0.713067	1.787121	1.212857
29	17	0	-1.581489	-3.489018	-0.499971
30	16	0	0.652074	-1.122218	0.377539
31	8	0	0.787640	-1.855123	1.619820
32	8	0	1.354000	-1.627630	-0.781288
33	8	0	-0.572499	-0.380068	0.163046

Standard orientation of TS-CH_3COCl-Anisole

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

Standard orientation of transition state of TS-CH_3COCl-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -281.97 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.268703	1.090543	-0.315869

2	1	0	-3.280700	0.323823	-0.921254
3	1	0	-2.423910	1.561709	-0.454735
4	8	0	-3.304197	-0.391373	1.976942
5	1	0	-3.323247	0.234260	1.220067
6	1	0	-4.211833	-0.685793	2.111462
7	8	0	-3.327746	-1.330610	-1.695950
8	1	0	-2.862832	-1.802350	-0.974923
9	1	0	-4.235765	-1.652861	-1.695690
10	8	0	-1.951031	-2.272874	0.492624
11	1	0	-2.395055	-1.679834	1.134195
12	1	0	-2.115146	-3.175446	0.787940
13	6	0	3.964455	-0.141381	0.294874
14	6	0	3.632871	-1.353559	-0.353792
15	6	0	2.337444	-1.784122	-0.324336
16	6	0	1.319013	-0.973978	0.280653
17	6	0	1.717623	0.132090	1.089499
18	6	0	3.042113	0.578808	1.025277
19	1	0	4.986993	0.216895	0.249486
20	1	0	4.400367	-1.922927	-0.861911
21	1	0	2.031537	-2.697185	-0.822313
22	1	0	0.345908	-1.422972	0.445063
23	1	0	3.325150	1.469952	1.572232
24	8	0	0.891829	0.803616	1.879907
25	6	0	-0.464028	0.354608	2.013413
26	1	0	-0.934007	1.057926	2.694583
27	1	0	-0.967167	0.385950	1.048464
28	1	0	-0.483217	-0.651372	2.434931
29	17	0	-0.565343	2.678717	-0.638662
30	6	0	0.963021	0.017404	-1.423058
31	8	0	1.829193	0.647299	-1.838987
32	6	0	-0.374395	-0.452946	-1.826000
33	1	0	-1.070641	-0.326688	-1.002531
34	1	0	-0.678261	0.114199	-2.705613
35	1	0	-0.280814	-1.519821	-2.050731

Standard orientation of TS-$(CH_3CO)_2O$-Anisole

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

Standard orientation of transition state of TS-$(CH_3CO)_2O$-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -308.52 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.177694	1.170142	0.168555
2	8	0	0.560717	2.334176	-2.073722
3	1	0	0.466785	2.844506	-1.244500
4	1	0	0.884837	2.950926	-2.739557
5	8	0	2.313169	1.733757	1.195028
6	1	0	1.950350	0.841475	1.395448
7	1	0	2.686669	1.638909	0.301038
8	8	0	0.432288	3.559446	0.423977
9	1	0	1.056638	2.927693	0.843395
10	1	0	-0.427618	3.424094	0.838855
11	6	0	-1.073592	0.600326	-0.044410
12	6	0	-2.075260	-1.107209	-1.460035
13	6	0	-3.485726	0.533089	-0.306964
14	6	0	-3.325270	-0.618286	-1.091291
15	1	0	-2.004667	-1.957282	-2.125236
16	1	0	-4.206642	-1.132814	-1.458127
17	1	0	-2.441402	2.051848	0.798137
18	8	0	0.307786	-0.758356	-1.331420
19	6	0	-0.938707	-0.457049	-0.989020
20	6	0	-2.363638	1.164259	0.178947
21	8	0	2.850679	0.846510	-1.430155
22	1	0	2.720183	-0.017269	-0.997147
23	1	0	1.973145	1.188126	-1.683352
24	1	0	-4.475301	0.914237	-0.091875
25	8	0	-1.683653	-1.367245	1.708434
26	6	0	-1.212620	-0.317427	1.729684
27	6	0	-0.806248	0.684298	2.737644
28	1	0	-0.412064	0.140357	3.595836
29	1	0	-0.080683	1.388761	2.344077
30	1	0	-1.723985	1.210791	3.017232
31	8	0	1.279630	-0.778724	1.576650
32	6	0	1.784951	-1.666044	0.828778
33	6	0	1.080889	-3.008253	0.790652
34	1	0	1.065668	-3.438372	1.794799
35	1	0	0.041007	-2.867541	0.483652
36	1	0	1.569646	-3.701191	0.107515
37	8	0	2.821248	-1.498348	0.136517
38	6	0	0.528185	-1.804282	-2.281892
39	1	0	1.606614	-1.868709	-2.399292

40	1	0	0.134547	-2.750975	-1.910127
41	1	0	0.061274	-1.547977	-3.234365

Standard orientation of TS-NH_2Cl-Anisole

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

Standard orientation of transition state of TS-NH_2Cl-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -297.3 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.721325	1.916668	1.614922
2	17	0	0.238524	-1.459640	-0.894540
3	8	0	-1.477708	3.156015	0.874793
4	1	0	-1.665315	2.203086	1.105173
5	1	0	-0.812285	3.121099	0.178327
6	8	0	-1.889831	-1.935430	1.874984
7	1	0	-1.904798	-2.663282	0.063564
8	1	0	-2.601673	-2.143547	2.489019
9	6	0	1.284938	1.113156	1.158293
10	6	0	1.833473	-0.227369	-0.851689
11	6	0	2.910945	-0.723569	1.286270
12	6	0	2.790048	-0.966139	-0.039279
13	1	0	3.352333	-1.751564	-0.530010
14	6	0	1.182071	0.913921	-0.228966
15	6	0	2.133583	0.315818	1.881992
16	8	0	-2.600362	0.502459	-1.132258
17	1	0	-1.948483	-0.068698	-1.551402
18	1	0	-2.375631	0.531934	-0.152012
19	8	0	-2.094054	0.635785	1.432271
20	1	0	-2.963591	0.789047	1.820885
21	1	0	-1.934592	-0.942711	1.712823
22	1	0	2.070527	-0.141846	-1.907001
23	1	0	2.226840	0.489556	2.948277
24	1	0	3.588734	-1.300860	1.901287
25	1	0	-1.334285	-3.766236	-1.065571
26	7	0	-1.577822	-2.796444	-0.895348
27	1	0	-2.279195	-2.493174	-1.562882

28	8	0	0.421381	1.738638	-0.896865
29	6	0	0.360109	1.694785	-2.336694
30	1	0	-0.346129	2.471744	-2.611018
31	1	0	1.346687	1.910394	-2.745955
32	1	0	0.002980	0.724035	-2.676772

Standard orientation of TS-$NHCl_2$-Anisole

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

Standard orientation of transition state of TS-$NHCl_2$-Anisole
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -297.3 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.980833	1.168684	1.213002
2	8	0	1.012518	3.399509	0.246826
3	1	0	0.214547	3.024470	0.709397
4	8	0	-2.103701	0.314943	2.507872
5	1	0	-2.496051	-0.341406	0.891242
6	1	0	-2.886435	0.537517	3.022780
7	6	0	2.692819	0.169423	0.910910
8	6	0	1.704765	-1.330008	-0.780861
9	6	0	2.502602	-2.236188	1.339841
10	6	0	1.976228	-2.441338	0.105445
11	1	0	1.696942	-3.430846	-0.236309
12	6	0	2.183664	-0.027879	-0.380920
13	6	0	2.847386	-0.915004	1.740078
14	8	0	-1.834333	2.059202	-1.082774
15	1	0	-1.007726	1.939674	-1.564931
16	1	0	-1.582206	2.254700	-0.124680
17	8	0	-1.174069	2.442850	1.405006
18	1	0	-1.624620	3.214314	1.765093
19	1	0	-1.735104	1.186222	2.132570
20	1	0	1.649836	-1.548259	-1.841384
21	8	0	2.095696	1.031192	-1.155703
22	1	0	1.424046	2.668609	-0.230466
23	1	0	3.256255	-0.758490	2.732032
24	1	0	2.668124	-3.061541	2.019823

25	6	0	1.681981	0.906971	-2.529907
26	1	0	0.671203	0.505677	-2.589460
27	1	0	1.708159	1.918112	-2.923974
28	1	0	2.386070	0.271242	-3.066256
29	17	0	-0.308830	-0.967477	-0.419302
30	7	0	-2.402892	-0.513666	-0.126712
31	1	0	-2.509860	0.367005	-0.651462
32	17	0	-3.544072	-1.682962	-0.649366

Standard orientation of TS-Cl_2-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Cl_2-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -700.7 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.674231	-0.459419	0.381349
2	1	0	-2.479435	-0.882704	-0.476484
3	1	0	-2.522026	0.500584	0.290163
4	8	0	-0.957698	-1.645047	1.820819
5	1	0	-1.702515	-1.132460	1.341395
6	1	0	-1.326825	-2.302106	2.417862
7	8	0	-1.699930	-1.920969	-1.715579
8	1	0	-0.910729	-2.329842	-1.337099
9	1	0	-2.170763	-2.587528	-2.220455
10	8	0	0.517570	-2.399102	0.071995
11	1	0	-0.170823	-2.098416	0.972849
12	1	0	0.996252	-3.222620	0.212894
13	17	0	0.562987	0.825581	-0.355788
14	6	0	2.995435	-0.045703	0.379871
15	1	0	1.188726	-1.582340	-0.208469
16	1	0	2.610362	-0.081515	1.396775
17	7	0	1.862171	-0.345137	-0.519201
18	1	0	3.679099	-0.884692	0.249242
19	17	0	-2.068577	2.618955	0.071881
20	6	0	3.688842	1.270811	0.085305
21	1	0	4.045264	1.300653	-0.944364

22	1	0	3.023869	2.115996	0.250769
23	1	0	4.548279	1.382739	0.744098
24	1	0	2.159740	-0.291251	-1.488091

Standard orientation of TS-Cl_2O-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Cl_2O-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1169.04 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.885009	-1.175640	-0.863835
2	8	0	-1.990051	1.293570	-0.749082
3	1	0	-1.895126	1.540297	0.193065
4	1	0	-1.987496	0.224189	-0.820558
5	8	0	0.053865	2.242136	-1.616496
6	1	0	-0.979015	1.775658	-1.267198
7	1	0	-0.057745	3.106152	-2.020424
8	7	0	1.979323	-0.223110	0.646659
9	1	0	1.827245	0.922264	0.612127
10	8	0	-1.057183	2.115657	1.673980
11	1	0	-0.130934	2.245374	1.386245
12	1	0	-1.337732	2.896538	2.155259
13	8	0	1.370279	2.188236	0.409151
14	1	0	0.746250	2.284108	-0.689641
15	1	0	2.028210	2.874982	0.536479
16	1	0	2.078594	-0.551286	1.603033
17	17	0	0.424157	-0.804249	0.050358
18	6	0	3.124324	-0.654655	-0.191816
19	1	0	2.931385	-0.276292	-1.192594
20	1	0	3.986450	-0.127731	0.214840
21	6	0	3.333504	-2.154517	-0.177766
22	1	0	4.214150	-2.396427	-0.769301
23	1	0	3.497385	-2.518195	0.836171
24	1	0	2.482696	-2.678697	-0.607535
25	17	0	-2.891319	-1.796681	0.343240

Standard orientation of TS-HOCl-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-HOCl-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -517.94 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.892252	2.604498	0.054541
2	1	0	-1.010229	3.132642	-0.738118
3	8	0	-2.677934	0.981002	0.342602
4	1	0	-2.708447	0.451462	-0.464490
5	1	0	-1.777817	1.879010	0.177508
6	8	0	-1.714635	-0.695635	1.927619
7	1	0	-2.151579	0.040220	1.308851
8	1	0	-2.393752	-1.078538	2.485918
9	7	0	1.602999	-0.619998	-0.552351
10	1	0	0.924696	-1.391357	-0.386473
11	8	0	-2.276575	-1.031362	-1.765788
12	1	0	-1.657822	-1.525344	-1.201895
13	1	0	-2.954307	-1.644400	-2.057825
14	8	0	-0.526902	-2.156161	0.133634
15	1	0	-0.967517	-1.684157	0.902307
16	1	0	-0.533375	-3.101850	0.297843
17	1	0	1.921428	-0.644656	-1.517474
18	17	0	0.597699	0.854776	-0.339829
19	6	0	2.744567	-0.701733	0.400383
20	1	0	2.313198	-0.648034	1.396161
21	1	0	3.173586	-1.691674	0.256931
22	6	0	3.764303	0.389330	0.155295
23	1	0	4.593710	0.255617	0.846341
24	1	0	4.159291	0.338774	-0.858847
25	1	0	3.340216	1.376759	0.321883

Standard orientation of TS-Br_2-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Br_2-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -856.25 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.502669	2.191517	0.480714
2	1	0	0.662734	2.553072	-0.721206
3	1	0	1.939329	1.325201	0.396812
4	8	0	-0.732515	2.197321	2.039787
5	1	0	0.848344	2.140624	1.205048
6	1	0	-0.940182	2.837706	2.723753
7	1	0	-2.282881	0.952442	-0.566440
8	8	0	-0.056514	2.750982	-1.427955
9	1	0	-1.135711	2.437898	-0.997643
10	1	0	-0.004390	3.665225	-1.722738
11	8	0	-2.140772	2.035385	-0.455341
12	1	0	-1.437508	2.223189	1.377928
13	1	0	-2.933437	2.523275	-0.700105
14	6	0	-3.046177	-1.096409	0.493407
15	1	0	-2.714847	-0.660626	1.433890
16	1	0	-4.064992	-0.752162	0.308041
17	6	0	-2.991613	-2.611848	0.529619
18	1	0	-1.989098	-2.967331	0.760093
19	1	0	-3.667206	-2.982249	1.299037
20	1	0	-3.302055	-3.035075	-0.425821
21	35	0	-0.354428	-0.792336	-0.365840
22	35	0	2.835113	-0.840738	0.077933
23	7	0	-2.239977	-0.481119	-0.578921
24	1	0	-2.478430	-0.887850	-1.477263

Standard orientation of TS-BrCl-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-BrCl-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -862.03 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.701269	0.767921	0.508259
2	1	0	2.175682	1.487092	-0.709354
3	1	0	2.622998	-0.201749	0.436320
4	8	0	0.768499	1.958334	2.027729
5	1	0	2.109199	1.075318	1.221623
6	1	0	0.899160	2.614709	2.715517
7	1	0	-1.173851	1.615531	-0.596630
8	8	0	1.667746	2.011315	-1.433689
9	1	0	0.566350	2.305437	-1.022271
10	1	0	2.185878	2.762309	-1.738275
11	8	0	-0.503491	2.480725	-0.501276
12	1	0	0.185775	2.337084	1.355389
13	1	0	-0.936550	3.296182	-0.773183
14	6	0	-2.871174	0.244601	0.478926
15	1	0	-2.370737	0.463628	1.419989
16	1	0	-3.575257	1.054027	0.279861
17	6	0	-3.588756	-1.090845	0.523839
18	1	0	-2.903281	-1.901416	0.763848
19	1	0	-4.362240	-1.063509	1.289703
20	1	0	-4.066025	-1.307252	-0.432012
21	35	0	-0.383857	-0.849420	-0.344965
22	7	0	-1.857799	0.355947	-0.588735
23	17	0	2.296001	-2.357467	0.155617
24	1	0	-2.262121	0.108709	-1.485862

Standard orientation of TS-HOBr-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-HOBr-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -961.74 cm^{-1}
Standard orientation:

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

1	8	0	1.038667	-2.478886	0.231981
2	1	0	1.169048	-3.074263	-0.510477
3	8	0	2.820566	-0.792162	0.417070
4	1	0	2.852573	-0.340015	-0.437857
5	1	0	1.881749	-1.800562	0.311947
6	8	0	1.913223	0.963681	1.823489
7	1	0	2.391810	0.070984	1.171277
8	1	0	2.600860	1.439783	2.292667
9	7	0	-1.593760	0.817797	-0.502740
10	1	0	-0.885952	1.565792	-0.366211
11	8	0	2.385047	1.065706	-1.757905
12	1	0	1.748486	1.568367	-1.217242
13	1	0	3.054658	1.681232	-2.063208
14	8	0	0.643564	2.271949	0.072768
15	1	0	1.144749	1.801603	0.847490
16	1	0	0.700677	3.222505	0.191521
17	1	0	-1.911757	0.821811	-1.467023
18	6	0	-2.729256	0.962584	0.444837
19	1	0	-2.306492	0.915168	1.444938
20	1	0	-3.131220	1.961953	0.285464
21	6	0	-3.786424	-0.098353	0.223202
22	1	0	-4.613313	0.073804	0.908919
23	1	0	-4.177117	-0.056541	-0.793239
24	1	0	-3.393563	-1.095739	0.408671
25	35	0	-0.493809	-0.797376	-0.222740

Standard orientation of TS-Br_2O-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Br_2O-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -695.66 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.623621	-0.326630	0.922209
2	8	0	1.089688	2.108967	0.789691
3	1	0	0.934249	2.308235	-0.166714
4	1	0	1.386178	1.101604	0.879318

5	8	0	-1.184139	2.432246	1.567532
6	1	0	0.058579	2.266070	1.246086
7	1	0	-1.366928	3.299924	1.935197
8	7	0	-2.337913	-0.602503	-0.696929
9	1	0	-2.481775	0.476665	-0.732089
10	8	0	0.046376	2.589366	-1.603966
11	1	0	-0.892422	2.403876	-1.351983
12	1	0	0.083423	3.444350	-2.037369
13	8	0	-2.328342	1.966674	-0.532764
14	1	0	-1.791854	2.255717	0.641613
15	1	0	-3.104585	2.494135	-0.730431
16	1	0	-2.334393	-0.997820	-1.631771
17	6	0	-3.344507	-1.260247	0.168445
18	1	0	-3.255169	-0.803932	1.151440
19	1	0	-4.316125	-0.992439	-0.245830
20	6	0	-3.167099	-2.763424	0.222270
21	1	0	-3.957996	-3.197895	0.830338
22	1	0	-3.228928	-3.199599	-0.774530
23	1	0	-2.210588	-3.033908	0.664936
24	35	0	-0.505090	-0.675357	-0.004012
25	35	0	3.017539	-0.742655	-0.175577

Standard orientation of TS-BrOCl-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-BrOCl-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -679.86 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.851568	-1.111426	0.804391
2	8	0	2.111659	1.375226	0.755157
3	1	0	2.008161	1.644151	-0.191496
4	1	0	2.072011	0.326155	0.812605
5	8	0	0.078753	2.385713	1.606771
6	1	0	1.195056	1.839728	1.245571
7	1	0	0.191077	3.255188	1.997729
8	7	0	-2.036255	-0.053885	-0.674498

9	1	0	-1.826402	1.017153	-0.684249
10	8	0	1.226493	2.237491	-1.592409
11	1	0	0.282777	2.354058	-1.318252
12	1	0	1.525757	3.046692	-2.011723
13	8	0	-1.200928	2.369421	-0.468316
14	1	0	-0.572358	2.439304	0.698992
15	1	0	-1.773804	3.120866	-0.632615
16	1	0	-2.179481	-0.402070	-1.617081
17	6	0	-3.181071	-0.380296	0.207247
18	1	0	-2.931196	0.000379	1.194771
19	1	0	-4.025884	0.191541	-0.175593
20	6	0	-3.488714	-1.863102	0.232671
21	1	0	-4.364089	-2.038793	0.854684
22	1	0	-3.705575	-2.234565	-0.768623
23	1	0	-2.658744	-2.432819	0.645695
24	35	0	-0.308698	-0.728613	-0.040790
25	17	0	2.899957	-1.814078	-0.316796

Standard orientation of TS-ICl-Ethylamine

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-ICl-Ethylamine

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -917.13 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.441383	1.416559	0.790098
2	1	0	1.853229	1.991064	-0.538111
3	1	0	2.578953	0.460955	0.664710
4	8	0	0.044933	1.941909	2.003480
5	1	0	1.644421	1.518638	1.352164
6	1	0	0.121742	2.735447	2.544113
7	7	0	-1.925710	0.150529	-0.653733
8	1	0	-1.433656	1.544725	-0.734751
9	8	0	1.344044	2.370913	-1.329792
10	1	0	0.199325	2.461070	-1.012243
11	1	0	1.702686	3.244992	-1.529380
12	8	0	-0.943564	2.486262	-0.597373

13	1	0	-0.401349	2.214404	1.184327
14	1	0	-1.465004	3.203026	-0.977321
15	1	0	-2.345982	-0.258046	-1.486256
16	6	0	-2.870392	0.065285	0.476795
17	1	0	-2.362664	0.476484	1.352224
18	1	0	-3.690637	0.745197	0.226403
19	6	0	-3.410736	-1.324987	0.753648
20	1	0	-4.154811	-1.285238	1.551637
21	1	0	-3.889605	-1.735443	-0.139032
22	1	0	-2.616377	-2.006386	1.064926
23	53	0	-0.111569	-0.847386	-0.338245
24	17	0	2.837957	-1.742357	0.274456

Standard orientation of TS-I_2-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-6X/LANL08(d) level:

Standard orientation of transition state of TS-I_2-Ethylamine

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -899.66 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.580051	2.509174	0.825785
2	1	0	-0.181582	2.760365	-0.517841
3	1	0	1.129257	1.721360	0.695841
4	8	0	-1.778702	1.843326	1.999243
5	1	0	-0.185212	2.231742	1.375251
6	1	0	-2.102838	2.558590	2.557263
7	7	0	-2.598848	-0.671197	-0.618981
8	1	0	-2.827458	0.785895	-0.717077
9	8	0	-0.797484	2.854542	-1.318047
10	1	0	-1.841759	2.379954	-1.014149
11	1	0	-0.906229	3.795224	-1.507964
12	8	0	-2.861038	1.849090	-0.600612
13	1	0	-2.297875	1.881032	1.178088
14	1	0	-3.659683	2.209782	-1.003224
15	1	0	-2.808360	-1.234279	-1.441160
16	6	0	-3.355036	-1.181654	0.540910
17	1	0	-3.065492	-0.580397	1.405199

18	1	0	-4.404759	-0.958587	0.325400
19	6	0	-3.181044	-2.663582	0.813784
20	1	0	-3.831720	-2.971224	1.634711
21	1	0	-3.445945	-3.250351	-0.069463
22	1	0	-2.151724	-2.899890	1.090905
23	53	0	-0.516216	-0.726298	-0.384242
24	53	0	2.947295	-0.275748	0.100505

Standard orientation of TS-HOI-Ethylamine

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-HOI-Ethylamine

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -419.79 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.203611	-2.286952	0.399442
2	1	0	1.455326	-2.787351	-0.385546
3	8	0	2.854169	-0.368531	0.656085
4	1	0	2.858975	0.056895	-0.256669
5	1	0	2.266332	-1.213794	0.593514
6	8	0	1.605348	1.432765	1.738198
7	1	0	2.311317	0.394101	1.234342
8	1	0	2.222914	2.068098	2.116265
9	7	0	-1.688103	0.911549	-0.660698
10	1	0	-0.959086	1.647596	-0.700284
11	8	0	2.553436	1.032628	-1.506182
12	1	0	1.804489	1.586496	-1.111941
13	1	0	3.306226	1.623006	-1.615529
14	8	0	0.657307	2.362963	-0.326515
15	1	0	1.156081	1.895025	0.846520
16	1	0	0.834537	3.307365	-0.382751
17	1	0	-2.126528	0.813847	-1.573867
18	6	0	-2.692021	1.247736	0.369578
19	1	0	-2.159587	1.320260	1.320257
20	1	0	-3.107577	2.233102	0.143961
21	6	0	-3.791052	0.206286	0.434341
22	1	0	-4.535140	0.491877	1.179412

23	1	0	-4.294873	0.116907	-0.531526
24	1	0	-3.391508	-0.772505	0.707110
25	53	0	-0.338070	-0.854130	-0.178681

Standard orientation of TS-SO_3Cl^--Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-SO_3Cl^--Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -151.64 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.016392	0.219987	0.284407
2	1	0	-2.862487	-0.299095	-0.528593
3	1	0	-2.479910	1.019335	0.222696
4	8	0	-2.022977	-1.693080	1.953078
5	1	0	-2.418845	-0.936092	1.472056
6	1	0	-2.731729	-2.174014	2.385215
7	7	0	1.911572	-1.165996	-0.719363
8	1	0	1.084306	-1.752185	-0.732831
9	8	0	-2.567586	-1.631573	-1.710840
10	1	0	-1.818952	-2.093961	-1.289117
11	1	0	-3.269218	-2.274366	-1.834740
12	8	0	-0.653583	-2.833835	-0.114907
13	1	0	-1.067554	-2.524693	0.717570
14	1	0	-0.574144	-3.789214	-0.071582
15	1	0	2.377347	-1.263271	-1.612648
16	6	0	2.801044	-1.576291	0.368873
17	1	0	2.232661	-1.495372	1.295159
18	1	0	3.124136	-2.618542	0.272225
19	6	0	4.014885	-0.663558	0.430607
20	1	0	4.675173	-0.944434	1.250983
21	1	0	4.588485	-0.720499	-0.496603
22	1	0	3.700237	0.369936	0.570278
23	17	0	-0.944394	2.937589	0.309327
24	16	0	0.530349	1.083474	-0.228238
25	8	0	0.574930	0.550949	1.116754
26	8	0	-0.369167	0.492234	-1.197187

27	8	0	1.646403	1.873185	-0.704825

Standard orientation of TS-CH_3COCl-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-CH_3COCl-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -156.74 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.195455	-1.512467	1.539702
2	1	0	1.188248	-1.960608	0.671285
3	1	0	0.305248	-1.180851	1.693789
4	8	0	3.181919	0.300077	1.198947
5	1	0	2.489790	-0.332797	1.482057
6	1	0	4.001148	0.072858	1.643103
7	1	0	0.593822	0.470293	-1.003918
8	8	0	1.328570	-2.422608	-1.034935
9	1	0	1.877386	-1.691499	-1.375702
10	1	0	1.735969	-3.254362	-1.284755
11	8	0	2.634029	-0.086855	-1.414784
12	1	0	3.014695	0.159603	-0.547216
13	1	0	3.089455	0.391070	-2.110155
14	8	0	-3.039948	0.804025	-0.650856
15	6	0	-2.319343	-0.103339	-0.425162
16	6	0	-1.954948	-1.277290	-1.269521
17	1	0	-1.927869	-0.953581	-2.307401
18	1	0	-1.000536	-1.698069	-0.977303
19	1	0	-2.741689	-2.023481	-1.144948
20	17	0	-2.024264	-0.498483	1.406295
21	7	0	-0.275466	0.945420	-0.781346
22	1	0	-0.581189	1.403825	-1.632368
23	6	0	-0.049522	1.945169	0.264902
24	1	0	-1.022890	2.334496	0.568692
25	1	0	0.369978	1.428440	1.127251
26	6	0	0.866367	3.086702	-0.160069
27	1	0	0.440364	3.628065	-1.006104
28	1	0	1.010330	3.794378	0.657072

29	1	0	1.842968	2.703659	-0.456471

Standard orientation of TS-$(CH_3CO)_2O$-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$(CH_3CO)_2O$-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -124.86 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.062306	-3.168037	-0.382238
2	1	0	-1.718531	-2.889640	0.287222
3	1	0	-0.292963	-3.518072	0.072179
4	8	0	-0.919749	-0.831634	-1.790825
5	1	0	-0.895913	-1.725557	-1.393610
6	1	0	-0.184376	-0.346419	-1.396025
7	8	0	-2.934864	-1.991227	1.207684
8	1	0	-3.149400	-1.195114	0.684678
9	1	0	-3.756159	-2.416549	1.462249
10	8	0	-3.041081	0.158988	-0.478643
11	1	0	-2.385689	-0.154744	-1.138557
12	1	0	-3.798041	0.532595	-0.934596
13	8	0	1.869289	1.394622	1.572345
14	6	0	1.128272	0.545718	1.158282
15	6	0	0.352248	-0.445524	1.966510
16	1	0	-0.056398	0.047674	2.844205
17	1	0	-0.444757	-0.895477	1.383976
18	1	0	1.046164	-1.223731	2.288568
19	8	0	1.342726	0.074693	-0.209705
20	6	0	2.431827	-0.706757	-0.405375
21	6	0	2.583180	-1.079123	-1.847701
22	1	0	2.422139	-0.211586	-2.483107
23	1	0	3.569687	-1.498137	-2.013360
24	1	0	1.829808	-1.825589	-2.100378
25	8	0	3.151249	-1.064641	0.490227
26	7	0	-0.602339	1.702524	0.550663
27	1	0	-1.494765	1.254203	0.362290
28	6	0	-0.224638	2.597354	-0.545972

29	1	0	0.791182	2.942777	-0.350562
30	1	0	-0.191463	2.006849	-1.461053
31	1	0	-0.704179	2.230603	1.409513
32	6	0	-1.168971	3.779752	-0.719234
33	1	0	-1.194173	4.388883	0.185094
34	1	0	-0.846939	4.413251	-1.545858
35	1	0	-2.182485	3.435479	-0.927333

Standard orientation of TS-NH_2Br-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-NH_2Br-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -717.66 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.957214	-3.041057	-0.642177
2	8	0	2.935022	-0.774805	0.358606
3	1	0	2.932643	-0.301705	-0.483715
4	1	0	1.843901	-1.822724	0.247466
5	8	0	2.030919	0.907614	1.866537
6	1	0	2.494048	0.084814	1.179692
7	1	0	2.728712	1.367311	2.337053
8	7	0	-1.720460	0.898646	-0.515043
9	1	0	-1.005109	1.617873	-0.395603
10	8	0	2.357236	1.134556	-1.816510
11	1	0	1.732401	1.586603	-1.219236
12	1	0	2.996962	1.787476	-2.107864
13	8	0	0.715523	2.305516	0.122532
14	1	0	1.193782	1.812783	0.864337
15	1	0	0.840624	3.247378	0.257490
16	6	0	-2.801159	1.023945	0.476829
17	1	0	-2.350405	0.888563	1.458901
18	1	0	-3.214042	2.032681	0.433879
19	6	0	-3.884773	-0.008794	0.229344
20	1	0	-4.674483	0.092493	0.971464
21	1	0	-4.330061	0.125872	-0.756977
22	1	0	-3.482502	-1.018671	0.291814

23	7	0	0.920862	-2.396778	0.136725
24	1	0	0.676137	-2.901103	0.978702
25	35	0	-0.453225	-0.876272	-0.222562
26	1	0	-2.073769	0.923913	-1.463688

Standard orientation of TS-$NHBr_2$-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$NHBr_2$-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -927.18 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.251558	2.243243	0.743493
2	1	0	1.099178	2.423508	-0.196570
3	1	0	1.489452	0.864966	0.859165
4	8	0	-0.965246	2.629700	1.652013
5	1	0	0.193711	2.455258	1.236910
6	1	0	-1.068668	3.511585	2.014193
7	7	0	-2.441677	-0.675094	-0.703309
8	1	0	-2.628106	0.333969	-0.760690
9	8	0	0.035487	2.625981	-1.822921
10	1	0	-0.846238	2.437987	-1.447716
11	1	0	-0.014458	3.473636	-2.269445
12	8	0	-2.327286	2.121494	-0.434218
13	1	0	-1.848288	2.344401	0.450515
14	1	0	-3.040251	2.750621	-0.563880
15	6	0	-3.399882	-1.364493	0.184471
16	1	0	-3.284396	-0.926173	1.173654
17	1	0	-4.406057	-1.141810	-0.170208
18	6	0	-3.151565	-2.859719	0.207705
19	1	0	-3.877586	-3.341771	0.859277
20	1	0	-3.257358	-3.287286	-0.789433
21	1	0	-2.154440	-3.087226	0.580184
22	7	0	1.499329	-0.270779	0.848268
23	1	0	1.601841	-0.682957	1.768958
24	35	0	-0.479694	-0.621451	0.033272
25	1	0	-2.429599	-1.077263	-1.633762

26	35	0	2.948844	-0.865647	-0.192868

Standard orientation of TS-NH_2Cl-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-NH_2Cl-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -653.88 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.836234	3.043667	-0.794219
2	8	0	-2.724942	0.894423	0.430286
3	1	0	-2.819276	0.392648	-0.394835
4	1	0	-1.711849	1.839740	0.210612
5	8	0	-1.699178	-0.744317	1.906130
6	1	0	-2.282645	0.136928	1.175048
7	1	0	-2.321595	-1.193509	2.480779
8	7	0	1.797091	-0.700031	-0.663208
9	1	0	1.069351	-1.405499	-0.571235
10	8	0	-2.395716	-0.942866	-1.705319
11	1	0	-1.742418	-1.446865	-1.177952
12	1	0	-3.059975	-1.561561	-2.015329
13	8	0	-0.656065	-2.151942	0.048745
14	1	0	-1.043400	-1.645569	0.852317
15	1	0	-0.759514	-3.092954	0.204456
16	1	0	2.206263	-0.742736	-1.587178
17	17	0	0.481222	1.086850	-0.353364
18	6	0	2.805715	-0.811508	0.393977
19	1	0	2.289672	-0.678815	1.345222
20	1	0	3.252941	-1.808278	0.398089
21	6	0	3.879999	0.248001	0.220740
22	1	0	4.619471	0.176077	1.016760
23	1	0	4.397315	0.121404	-0.731338
24	1	0	3.443911	1.245855	0.243493
25	7	0	-0.760327	2.430986	0.008327
26	1	0	-0.447224	2.965004	0.809633

Standard orientation of TS-$NHCl_2$-Ethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$NHCl_2$-Ethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -592.72 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.242352	1.235735	-0.961609
2	1	0	-2.295232	1.455027	-0.022642
3	1	0	-1.893774	-0.209985	-0.963617
4	8	0	-0.206742	2.389856	-1.630969
5	1	0	-1.191445	1.852454	-1.362011
6	1	0	-0.397503	3.234706	-2.042286
7	7	0	2.081678	-0.112947	0.732410
8	1	0	1.872461	0.889153	0.872744
9	8	0	-1.473043	1.711658	1.874588
10	1	0	-0.591929	1.951437	1.534472
11	1	0	-1.411352	0.816951	2.216888
12	8	0	0.956015	2.398269	0.649121
13	1	0	0.555065	2.463216	-0.286002
14	1	0	1.345467	3.243721	0.882092
15	1	0	2.226542	-0.570703	1.626463
16	17	0	0.446220	-0.737873	0.022029
17	6	0	3.222512	-0.314035	-0.189594
18	1	0	2.939370	0.144301	-1.134200
19	1	0	4.063332	0.240793	0.224243
20	6	0	3.555612	-1.783173	-0.350211
21	1	0	4.410925	-1.887109	-1.014426
22	1	0	3.816898	-2.231367	0.608186
23	1	0	2.721583	-2.333754	-0.780063
24	7	0	-1.507539	-1.228257	-0.810941
25	1	0	-1.476159	-1.780914	-1.659447
26	17	0	-2.543455	-2.038032	0.309683

Standard orientation of TS-Cl_2-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Cl_2-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -980.26 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.070180	-0.416479	0.070516
2	1	0	2.657932	-0.799568	0.869558
3	1	0	2.886413	0.543647	0.055641
4	8	0	1.832752	-1.688876	-1.701458
5	1	0	2.417377	-1.134827	-1.048724
6	1	0	2.353184	-2.371773	-2.135140
7	8	0	1.594889	-1.813620	1.887750
8	1	0	0.968511	-2.264708	1.303804
9	1	0	1.932262	-2.452581	2.519245
10	8	0	-0.036501	-2.401748	-0.362648
11	1	0	0.890529	-2.108628	-1.099458
12	1	0	-0.460104	-3.236076	-0.586920
13	17	0	-0.234474	0.788491	-0.083134
14	6	0	-2.238279	-0.489789	1.192400
15	6	0	-2.381344	-0.222391	-1.308982
16	1	0	-0.779448	-1.566529	-0.277632
17	1	0	-3.155775	-1.034592	0.970148
18	1	0	-1.705442	-0.233024	-2.161645
19	7	0	-1.528699	-0.405469	-0.111673
20	1	0	-1.627440	-1.123179	1.834475
21	1	0	-2.986917	-1.127948	-1.359429
22	17	0	2.378923	2.636665	-0.052396
23	6	0	-2.537998	0.817239	1.910059
24	1	0	-3.156258	0.590089	2.777593
25	1	0	-1.624859	1.288324	2.265506
26	1	0	-3.075004	1.526903	1.288007
27	6	0	-3.261540	1.013877	-1.329775
28	1	0	-4.060265	0.954858	-0.593912
29	1	0	-2.681645	1.919515	-1.158201
30	1	0	-3.723378	1.092888	-2.312692

Standard orientation of TS-Cl_2O-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Cl_2O-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1076.98 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.652207	-0.584815	-1.067865
2	8	0	-2.385436	1.600917	-0.070155
3	1	0	-1.902466	1.464439	0.966454
4	1	0	-2.560910	0.495947	-0.593877
5	8	0	-0.050508	2.818750	-0.991331
6	1	0	-1.719383	2.094066	-0.580722
7	1	0	0.074463	3.765741	-1.081039
8	7	0	1.550305	-0.609747	-0.154058
9	1	0	1.508730	0.278513	0.437936
10	8	0	-1.235680	1.313006	2.046020
11	1	0	0.051452	1.468880	1.674045
12	1	0	-1.506216	1.936043	2.722918
13	8	0	1.044352	1.571604	1.206427
14	1	0	0.471843	2.515100	-0.224271
15	1	0	1.664985	1.981366	1.812955
16	17	0	-0.140988	-0.768731	-0.641916
17	6	0	2.458067	-0.407949	-1.338594
18	1	0	1.826564	-0.172795	-2.188000
19	1	0	2.951120	-1.357448	-1.529920
20	6	0	1.914093	-1.766693	0.720861
21	1	0	1.165002	-1.791705	1.507346
22	1	0	1.820308	-2.663691	0.113420
23	6	0	3.305999	-1.611961	1.302024
24	1	0	3.468980	-2.432522	1.997900
25	1	0	4.080946	-1.664315	0.541041
26	1	0	3.405328	-0.679381	1.855640
27	6	0	3.436434	0.724265	-1.081379
28	1	0	2.907348	1.665230	-0.942956
29	1	0	4.064045	0.543595	-0.212745
30	1	0	4.082745	0.822282	-1.951472
31	17	0	-3.456585	-1.547903	0.062593

Standard orientation of TS-HOCl-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-HOCl-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -669.11 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.374936	-2.043750	-0.974952
2	1	0	-2.560080	-2.765212	-0.369461
3	8	0	-3.300261	0.045965	-0.151203
4	1	0	-2.721093	0.201860	1.175269
5	1	0	-2.867407	-1.061682	-0.586214
6	8	0	-1.524963	2.181515	-1.138772
7	1	0	-2.869653	0.749760	-0.653558
8	1	0	-1.780203	3.101474	-1.234279
9	7	0	1.312938	-0.369842	-0.101864
10	1	0	0.973549	0.448506	0.441458
11	8	0	-2.211230	0.352032	2.083459
12	1	0	-0.871573	1.142160	1.656973
13	1	0	-2.798805	0.788170	2.703232
14	8	0	-0.089602	1.579006	1.205989
15	1	0	-0.968769	2.111773	-0.345053
16	1	0	0.267566	2.258975	1.781893
17	17	0	-0.240769	-1.192663	-0.506185
18	6	0	2.030834	0.099099	-1.335881
19	1	0	1.326935	0.032437	-2.158506
20	1	0	2.841745	-0.600541	-1.521872
21	6	0	2.114688	-1.257326	0.791167
22	1	0	1.457006	-1.527836	1.612627
23	1	0	2.343756	-2.151559	0.216781
24	6	0	3.367557	-0.571671	1.301727
25	1	0	3.854194	-1.242949	2.006645
26	1	0	4.076182	-0.358518	0.504715
27	1	0	3.130052	0.351642	1.828559
28	6	0	2.514831	1.529090	-1.172193
29	1	0	1.673444	2.204762	-1.026967
30	1	0	3.202360	1.641467	-0.337754
31	1	0	3.033780	1.826171	-2.081394

Standard orientation of TS-Br_2-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Br_2-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -853.33 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.318229	1.941302	-0.063332
2	1	0	1.368871	2.268794	-1.133647
3	1	0	2.547240	0.994614	-0.023888
4	8	0	0.514600	2.740103	1.799850
5	1	0	1.835857	2.179302	0.754648
6	1	0	0.583553	3.528234	2.342905
7	1	0	-1.745978	1.448956	-0.184135
8	8	0	0.570339	2.516019	-1.755315
9	1	0	-0.400335	2.554449	-1.120021
10	1	0	0.743718	3.330600	-2.237360
11	8	0	-1.358951	2.496057	-0.306749
12	1	0	-0.284235	2.813392	1.255524
13	1	0	-2.070174	3.114139	-0.500183
14	6	0	-2.710686	-0.068122	1.286423
15	1	0	-2.037175	0.358943	2.026801
16	1	0	-3.591113	0.575676	1.237630
17	6	0	-3.110190	-1.480689	1.673020
18	1	0	-2.264461	-2.164442	1.611123
19	1	0	-3.461227	-1.473001	2.703904
20	1	0	-3.919904	-1.856916	1.051708
21	35	0	-0.249408	-0.598845	0.011512
22	35	0	2.908663	-1.322986	0.056426
23	7	0	-2.046182	0.101706	-0.024745
24	6	0	-2.814630	-0.352825	-1.210050
25	1	0	-3.849836	-0.094574	-0.981669
26	1	0	-2.497042	0.274431	-2.042643
27	6	0	-2.700896	-1.816022	-1.610648
28	1	0	-3.419693	-2.007160	-2.406740
29	1	0	-1.709166	-2.040328	-1.996152
30	1	0	-2.914878	-2.494843	-0.790543

Standard orientation of TS-BrCl-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-BrCl-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -914.76 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.155997	0.572534	0.042699
2	1	0	2.463359	1.260846	-1.047424
3	1	0	2.994910	-0.390799	0.045924
4	8	0	1.693272	1.978344	1.852171
5	1	0	2.756125	0.959288	0.847505
6	1	0	2.033260	2.682361	2.408643
7	1	0	-0.783503	1.660727	-0.262698
8	8	0	1.854361	1.806823	-1.695896
9	1	0	0.929860	2.196099	-1.104886
10	1	0	2.350913	2.506952	-2.130846
11	8	0	-0.022604	2.489046	-0.343208
12	1	0	1.014232	2.352023	1.269905
13	1	0	-0.436775	3.333553	-0.544152
14	6	0	-2.282404	0.646196	1.191746
15	1	0	-1.657701	1.261987	1.838163
16	1	0	-3.177713	1.223269	0.955569
17	6	0	-2.645525	-0.639481	1.918970
18	1	0	-1.757813	-1.136250	2.303241
19	1	0	-3.277948	-0.382303	2.767977
20	1	0	-3.189165	-1.339135	1.291215
21	35	0	-0.153905	-0.782857	-0.051239
22	7	0	-1.561613	0.529559	-0.100919
23	17	0	2.467075	-2.506702	-0.012651
24	6	0	-2.405806	0.363519	-1.305194
25	1	0	-2.988542	1.284668	-1.365635
26	1	0	-1.725156	0.353489	-2.154087
27	6	0	-3.323249	-0.845459	-1.333832
28	1	0	-4.126854	-0.761101	-0.605692
29	1	0	-3.777959	-0.913785	-2.321013

30	1	0	-2.772153	-1.767524	-1.153112

Standard orientation of TS-HOBr-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-HOBr-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -925.47 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.491956	-1.909798	-0.556580
2	1	0	-2.735526	-2.548620	0.118171
3	8	0	-3.301261	0.357146	-0.017660
4	1	0	-2.747530	0.675228	1.042498
5	1	0	-2.925389	-0.948693	-0.320547
6	8	0	-1.479224	2.178788	-1.386881
7	1	0	-2.889587	0.939429	-0.670944
8	1	0	-1.670347	3.096893	-1.589780
9	7	0	1.437752	-0.231650	-0.004958
10	1	0	1.099329	0.656363	0.414054
11	8	0	-2.130533	1.001928	2.007835
12	1	0	-0.834208	1.559712	1.476404
13	1	0	-2.640971	1.621612	2.532321
14	8	0	0.004204	1.889617	0.972569
15	1	0	-0.886282	2.166361	-0.613911
16	1	0	0.351013	2.669031	1.412263
17	6	0	2.143799	0.049762	-1.297506
18	1	0	1.442657	-0.137081	-2.104091
19	1	0	2.956717	-0.667179	-1.384402
20	6	0	2.246870	-0.981994	0.996305
21	1	0	1.604031	-1.129078	1.860017
22	1	0	2.468935	-1.953419	0.560529
23	6	0	3.510803	-0.237818	1.387616
24	1	0	4.006242	-0.799865	2.177226
25	1	0	4.209184	-0.145820	0.558716
26	1	0	3.282357	0.754495	1.774571
27	6	0	2.628306	1.488748	-1.350295
28	1	0	1.785937	2.177227	-1.301683

29	1	0	3.315741	1.721355	-0.540627
30	1	0	3.145527	1.651854	-2.294030
31	35	0	-0.296875	-1.136911	-0.275515

Standard orientation of TS-Br_2O-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Br_2O-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -634.54 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.169579	-0.013451	-0.965119
2	8	0	-1.576717	2.232024	-0.077858
3	1	0	-1.102348	2.075070	0.934488
4	1	0	-1.899545	1.300668	-0.473659
5	8	0	0.801113	2.951324	-1.038646
6	1	0	-0.826545	2.572648	-0.624337
7	1	0	1.075697	3.864431	-1.144217
8	7	0	1.988175	-0.692855	-0.043308
9	1	0	2.092823	0.271683	0.430775
10	8	0	-0.375245	1.894737	2.005803
11	1	0	0.689689	1.793094	1.658473
12	1	0	-0.457939	2.606808	2.644073
13	8	0	1.852559	1.659828	1.053164
14	1	0	1.331005	2.545388	-0.307479
15	1	0	2.583512	2.029764	1.552078
16	6	0	2.869206	-0.801563	-1.247454
17	1	0	2.261297	-0.604574	-2.124417
18	1	0	3.219198	-1.829889	-1.307567
19	6	0	2.185535	-1.761594	0.971139
20	1	0	1.467293	-1.567641	1.763844
21	1	0	1.935492	-2.710951	0.501529
22	6	0	3.600202	-1.762617	1.524057
23	1	0	3.657339	-2.503593	2.319454
24	1	0	4.337634	-2.028166	0.769582
25	1	0	3.857137	-0.792440	1.947732
26	6	0	4.014331	0.195470	-1.176818

27	1	0	3.631823	1.214559	-1.161697
28	1	0	4.635464	0.045588	-0.296929
29	1	0	4.639826	0.077163	-2.059985
30	35	0	0.083006	-0.574442	-0.511846
31	35	0	-3.377828	-0.811943	0.141478

Standard orientation of TS-BrOCl-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-BrOCl-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -622.47 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.584594	-0.561597	-0.850962
2	8	0	-2.327003	1.781546	-0.047786
3	1	0	-1.798947	1.735437	0.948859
4	1	0	-2.508941	0.801875	-0.405816
5	8	0	-0.135178	2.832832	-1.125256
6	1	0	-1.659787	2.219741	-0.632339
7	1	0	-0.014667	3.774334	-1.264364
8	7	0	1.652307	-0.554260	-0.039111
9	1	0	1.620881	0.443081	0.376401
10	8	0	-1.013100	1.707546	1.993379
11	1	0	0.037161	1.765836	1.605730
12	1	0	-1.184660	2.417178	2.616500
13	8	0	1.187307	1.799884	0.951658
14	1	0	0.481132	2.538521	-0.407763
15	1	0	1.867602	2.300051	1.406747
16	6	0	2.516853	-0.611319	-1.258722
17	1	0	1.869557	-0.584270	-2.129167
18	1	0	3.029757	-1.570716	-1.254059
19	6	0	2.027536	-1.511497	1.034668
20	1	0	1.302025	-1.376104	1.832917
21	1	0	1.918143	-2.516964	0.633037
22	6	0	3.434846	-1.259666	1.547816
23	1	0	3.619709	-1.929099	2.386057
24	1	0	4.191640	-1.458149	0.791845

25	1	0	3.545811	-0.235795	1.903080
26	6	0	3.484215	0.560398	-1.294228
27	1	0	2.940704	1.502573	-1.341300
28	1	0	4.135744	0.579833	-0.423610
29	1	0	4.106124	0.478664	-2.184021
30	35	0	-0.258460	-0.746658	-0.456326
31	17	0	-3.518776	-1.436608	0.249471

Standard orientation of TS-ICl-Diethylamine

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d)level:

Standard orientation of transition state of TS-ICl-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -869.22 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.099559	1.048690	0.210908
2	1	0	2.339194	1.556728	-1.028868
3	1	0	3.043048	0.076761	0.226088
4	8	0	1.186341	2.210359	1.769011
5	1	0	2.485836	1.383896	0.899353
6	1	0	1.521482	3.026139	2.156087
7	7	0	-1.639935	0.505050	-0.132250
8	1	0	-0.929268	1.710160	-0.451934
9	8	0	1.741624	1.947746	-1.757792
10	1	0	0.749010	2.279155	-1.248004
11	1	0	2.190674	2.714545	-2.136554
12	8	0	-0.273751	2.572033	-0.596974
13	1	0	0.619746	2.471720	1.021793
14	1	0	-0.762088	3.314111	-0.971120
15	6	0	-2.247686	0.781083	1.187293
16	1	0	-1.430327	1.086991	1.844074
17	1	0	-2.883005	1.660782	1.036650
18	6	0	-3.055038	-0.336709	1.825743
19	1	0	-3.318266	-0.048281	2.845563
20	1	0	-3.982818	-0.525682	1.284452
21	1	0	-2.480633	-1.265093	1.875179
22	53	0	0.014803	-0.783861	-0.016008

23	17	0	2.835209	-2.157519	0.155634
24	6	0	-2.588962	0.202276	-1.226288
25	1	0	-3.451257	0.853196	-1.049223
26	1	0	-2.115514	0.537179	-2.153565
27	6	0	-3.045775	-1.240434	-1.395358
28	1	0	-3.818772	-1.273980	-2.166537
29	1	0	-2.223889	-1.878445	-1.724077
30	1	0	-3.462110	-1.660690	-0.480520

Standard orientation of TS-I_2-Diethylamine

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-I_2-Diethylamine

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -823.55 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.381565	2.648990	0.194432
2	1	0	0.454830	2.739505	-1.040980
3	1	0	1.789503	1.769467	0.183017
4	8	0	-0.793285	2.641832	1.823169
5	1	0	0.697931	2.632335	0.900056
6	1	0	-0.913476	3.490646	2.262363
7	7	0	-2.461958	-0.171695	-0.104900
8	1	0	-2.431260	1.239993	-0.393507
9	8	0	-0.273785	2.770612	-1.751767
10	1	0	-1.279854	2.567872	-1.209770
11	1	0	-0.281117	3.652293	-2.146117
12	8	0	-2.288041	2.310899	-0.518565
13	1	0	-1.435917	2.615025	1.092158
14	1	0	-3.092537	2.725628	-0.850133
15	6	0	-3.090898	-0.257942	1.230662
16	1	0	-2.505851	0.388578	1.888181
17	1	0	-4.075594	0.208877	1.117059
18	6	0	-3.241545	-1.642326	1.839376
19	1	0	-3.568142	-1.541312	2.876464
20	1	0	-3.988850	-2.237008	1.312668
21	1	0	-2.292784	-2.184563	1.835737

22	53	0	-0.388722	-0.528379	-0.051319
23	53	0	3.146478	-0.603526	0.045973
24	6	0	-3.178437	-0.863205	-1.199245
25	1	0	-4.241236	-0.700839	-0.992711
26	1	0	-2.941079	-0.322284	-2.119612
27	6	0	-2.905866	-2.346454	-1.409236
28	1	0	-3.587213	-2.720310	-2.176941
29	1	0	-1.887145	-2.514653	-1.761987
30	1	0	-3.058770	-2.935497	-0.505828

Standard orientation of TS-HOI-Diethylamine

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-HOI-Diethylamine

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -357.04 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.695532	-2.267246	0.247502
2	1	0	-1.673472	-2.637495	1.137583
3	8	0	-3.271491	-0.284193	0.211271
4	1	0	-2.893327	0.341364	0.899276
5	1	0	-2.717056	-1.158321	0.247697
6	8	0	-2.547563	1.003911	-1.735978
7	1	0	-3.006956	0.239565	-0.717217
8	1	0	-3.253398	1.593616	-2.022109
9	7	0	1.480558	0.827166	-0.179977
10	1	0	0.757892	1.527357	-0.438080
11	8	0	-2.081768	1.579161	1.603105
12	1	0	-1.563591	1.916083	0.804765
13	1	0	-2.706786	2.271860	1.841331
14	8	0	-0.826888	2.303250	-0.563354
15	1	0	-1.770479	1.618222	-1.266997
16	1	0	-0.917562	3.246149	-0.732924
17	6	0	2.486550	0.756769	-1.271129
18	1	0	1.979187	1.070834	-2.185363
19	1	0	3.260990	1.500156	-1.057246
20	6	0	3.108310	-0.614398	-1.485687

21	1	0	3.909162	-0.528160	-2.223168
22	1	0	3.534774	-1.026336	-0.570804
23	1	0	2.374449	-1.324041	-1.869877
24	53	0	0.003150	-0.898818	0.043527
25	6	0	2.014143	1.272037	1.129189
26	1	0	1.153857	1.360466	1.796611
27	1	0	2.433347	2.274602	0.994821
28	6	0	3.056113	0.342596	1.721262
29	1	0	3.977724	0.343734	1.136762
30	1	0	3.303311	0.678340	2.729912
31	1	0	2.682340	-0.681895	1.785763

Standard orientation of TS-SO_3Cl^--Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-SO_3Cl^--Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -146.63 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.494478	2.734303	-0.904484
2	1	0	-1.347855	2.406760	-1.245157
3	1	0	0.158074	2.028495	-1.023010
4	8	0	-1.079972	2.918657	1.724328
5	1	0	-0.775199	2.977606	0.792337
6	1	0	-1.331866	3.795862	2.019140
7	7	0	-0.698530	-1.154620	0.001974
8	1	0	-1.283013	-0.440720	0.423131
9	8	0	-2.981659	1.691562	-1.466533
10	1	0	-3.111777	1.339546	-0.565606
11	1	0	-3.721076	2.267181	-1.672063
12	8	0	-2.795745	0.917224	1.135438
13	1	0	-2.269621	1.636082	1.541656
14	1	0	-3.405478	0.565390	1.786734
15	17	0	4.011603	0.498269	-0.065915
16	16	0	1.769852	-0.282396	-0.043236
17	8	0	1.485498	0.091270	1.328839
18	8	0	1.302159	0.585637	-1.118262

19	8	0	2.075626	-1.662015	-0.365551
20	6	0	-1.119433	-1.373834	-1.378732
21	1	0	-1.048514	-0.414445	-1.890422
22	1	0	-0.385827	-2.035999	-1.844526
23	6	0	-0.690985	-2.350953	0.849155
24	1	0	0.205536	-2.331871	1.471816
25	1	0	-0.600876	-3.226753	0.204179
26	6	0	-1.913887	-2.477228	1.753248
27	1	0	-2.838018	-2.508312	1.177731
28	1	0	-1.852999	-3.382513	2.358551
29	1	0	-1.968910	-1.625394	2.432326
30	6	0	-2.524601	-1.944215	-1.558539
31	1	0	-2.610160	-2.944341	-1.133340
32	1	0	-3.262453	-1.301340	-1.077232
33	1	0	-2.773136	-2.010839	-2.618737

Standard orientation of TS-CH_3COCl-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-CH_3COCl-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -154.31 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.882837	-2.184252	-0.615300
2	1	0	1.754533	-1.512667	-1.312962
3	1	0	1.021020	-2.361079	-0.224687
4	8	0	3.562293	-0.845735	1.045811
5	1	0	3.019661	-1.464105	0.514511
6	1	0	4.480680	-1.114858	0.980779
7	1	0	0.323569	0.852921	0.035932
8	8	0	1.606118	-0.035592	-2.299648
9	1	0	2.007126	0.632294	-1.711843
10	1	0	2.019589	0.025894	-3.163094
11	8	0	2.537241	1.338935	-0.183528
12	1	0	3.021394	0.683139	0.358095
13	1	0	2.794852	2.222121	0.086761
14	8	0	-3.139773	-0.399608	0.033266

15	6	0	-2.130818	-0.847490	-0.384462
16	6	0	-1.636573	-0.958637	-1.787392
17	1	0	-2.165168	-0.232550	-2.399223
18	1	0	-0.566001	-0.797026	-1.844385
19	1	0	-1.873777	-1.963258	-2.138659
20	17	0	-1.251474	-2.108372	0.714928
21	7	0	-0.671807	0.947903	0.209537
22	6	0	0.274095	0.638190	2.468818
23	1	0	0.532398	-0.386750	2.205056
24	1	0	1.147770	1.264964	2.291151
25	1	0	0.039418	0.668368	3.532272
26	6	0	-1.203537	2.038689	-0.609962
27	1	0	-1.208184	1.714206	-1.650711
28	1	0	-2.243775	2.189737	-0.317325
29	6	0	-0.909254	1.123399	1.646645
30	1	0	-1.812823	0.568511	1.913290
31	1	0	-1.105950	2.172498	1.881232
32	6	0	-0.418104	3.343867	-0.506599
33	1	0	-0.894406	4.122921	-1.102297
34	1	0	-0.353873	3.700126	0.521143
35	1	0	0.595069	3.203500	-0.882677

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.882837	-2.184252	-0.615300
2	1	0	1.754533	-1.512667	-1.312962
3	1	0	1.021020	-2.361079	-0.224687
4	8	0	3.562293	-0.845735	1.045811
5	1	0	3.019661	-1.464105	0.514511
6	1	0	4.480680	-1.114858	0.980779
7	1	0	0.323569	0.852921	0.035932
8	8	0	1.606118	-0.035592	-2.299648
9	1	0	2.007126	0.632294	-1.711843
10	1	0	2.019589	0.025894	-3.163094
11	8	0	2.537241	1.338935	-0.183528
12	1	0	3.021394	0.683139	0.358095
13	1	0	2.794852	2.222121	0.086761
14	8	0	-3.139773	-0.399608	0.033266
15	6	0	-2.130818	-0.847490	-0.384462
16	6	0	-1.636573	-0.958637	-1.787392
17	1	0	-2.165168	-0.232550	-2.399223
18	1	0	-0.566001	-0.797026	-1.844385

19	1	0	-1.873777	-1.963258	-2.138659
20	17	0	-1.251474	-2.108372	0.714928
21	7	0	-0.671807	0.947903	0.209537
22	6	0	0.274095	0.638190	2.468818
23	1	0	0.532398	-0.386750	2.205056
24	1	0	1.147770	1.264964	2.291151
25	1	0	0.039418	0.668368	3.532272
26	6	0	-1.203537	2.038689	-0.609962
27	1	0	-1.208184	1.714206	-1.650711
28	1	0	-2.243775	2.189737	-0.317325
29	6	0	-0.909254	1.123399	1.646645
30	1	0	-1.812823	0.568511	1.913290
31	1	0	-1.105950	2.172498	1.881232
32	6	0	-0.418104	3.343867	-0.506599
33	1	0	-0.894406	4.122921	-1.102297
34	1	0	-0.353873	3.700126	0.521143
35	1	0	0.595069	3.203500	-0.882677

Standard orientation of TS-NH_2Br-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-NH_2Br-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -434.26 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.309201	-2.805777	1.379692
2	8	0	-3.325326	-0.522622	0.442391
3	1	0	-2.992847	0.158163	1.040578
4	1	0	-2.325451	-1.679186	0.513111
5	8	0	-2.853153	0.454576	-1.742363
6	1	0	-3.118018	-0.019906	-0.736038
7	1	0	-3.635359	0.855938	-2.125226
8	7	0	1.476794	0.644323	-0.418222
9	1	0	0.768170	1.242943	-0.845403
10	8	0	-1.867387	1.830466	1.600758
11	1	0	-1.465898	1.955752	0.721507
12	1	0	-2.304390	2.652329	1.833433

13	8	0	-0.932355	2.056240	-1.036997
14	1	0	-1.665322	1.463761	-1.395321
15	1	0	-1.020668	2.923094	-1.439234
16	6	0	2.426739	0.205815	-1.458268
17	1	0	1.836281	-0.269482	-2.240013
18	1	0	2.896284	1.094162	-1.888211
19	6	0	3.486858	-0.749278	-0.940842
20	1	0	4.085903	-1.105486	-1.777261
21	1	0	4.159909	-0.262571	-0.237010
22	1	0	3.033796	-1.612179	-0.454408
23	7	0	-1.461350	-2.339934	0.495140
24	1	0	-1.517451	-3.028661	-0.243312
25	6	0	2.080023	1.386014	0.715465
26	1	0	1.387785	2.185942	0.972303
27	1	0	2.998567	1.854394	0.355412
28	6	0	2.360557	0.543299	1.950815
29	1	0	2.959056	-0.334778	1.719690
30	1	0	2.907973	1.147358	2.673685
31	1	0	1.434983	0.213348	2.416957
32	35	0	0.070814	-0.960693	0.100094

Standard orientation of TS-NHBr$_2$-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-NHBr$_2$-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -973.87 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.925925	2.270200	-0.152887
2	1	0	-1.573320	2.246291	0.748362
3	1	0	-2.001411	0.912553	-0.596229
4	8	0	-0.068225	3.250118	-1.366887
5	1	0	-1.032816	2.788398	-0.791977
6	1	0	-0.178270	4.193004	-1.502687
7	7	0	2.330911	-0.178948	-0.001503
8	1	0	2.375964	0.848158	-0.021964
9	8	0	-0.156977	2.253233	2.149062

10	1	0	0.610667	2.340148	1.553436
11	1	0	-0.105706	2.964206	2.791296
12	8	0	1.820177	2.556371	0.195079
13	1	0	1.117437	2.878863	-0.481441
14	1	0	2.463870	3.255605	0.328144
15	6	0	3.166689	-0.713123	-1.102406
16	1	0	2.786350	-0.268116	-2.019477
17	1	0	4.179764	-0.340066	-0.942455
18	6	0	3.164314	-2.226293	-1.195204
19	1	0	3.714568	-2.522385	-2.086417
20	1	0	3.653048	-2.685362	-0.338147
21	1	0	2.151015	-2.616642	-1.277761
22	7	0	-1.854936	-0.164997	-0.877587
23	1	0	-2.067248	-0.357765	-1.850017
24	6	0	2.717269	-0.616768	1.369128
25	1	0	2.544467	0.236708	2.021372
26	1	0	3.791863	-0.802524	1.345850
27	6	0	1.970031	-1.828721	1.902076
28	1	0	2.005299	-2.672409	1.217981
29	1	0	2.434838	-2.132641	2.839010
30	1	0	0.928464	-1.591672	2.103732
31	35	0	0.298929	-0.328327	-0.431264
32	35	0	-3.001583	-1.231578	0.164879

Standard orientation of TS-NH_2Cl-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-NH_2Cl-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -935.80 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.035534	2.718270	-1.638717
2	8	0	-3.198449	0.681377	-0.569427
3	1	0	-2.884003	-0.076139	-1.081790
4	1	0	-2.166645	1.720125	-0.710367
5	8	0	-2.837627	-0.033983	1.720327
6	1	0	-3.069163	0.333035	0.603848

7	1	0	-3.636754	-0.358149	2.139474
8	7	0	1.441507	-0.474482	0.458154
9	1	0	0.714444	-1.011138	0.928868
10	8	0	-1.817004	-1.731721	-1.462978
11	1	0	-1.460544	-1.824086	-0.558632
12	1	0	-2.249862	-2.558091	-1.686986
13	8	0	-1.013806	-1.777888	1.200662
14	1	0	-1.726188	-1.116080	1.492382
15	1	0	-1.137929	-2.593668	1.690199
16	17	0	0.102829	1.061793	-0.212873
17	6	0	2.373127	0.078447	1.451071
18	1	0	1.770643	0.619800	2.179576
19	1	0	2.864306	-0.747493	1.973648
20	6	0	3.413811	1.001644	0.840879
21	1	0	4.013929	1.444303	1.634401
22	1	0	4.089550	0.464103	0.177305
23	1	0	2.940529	1.806329	0.279861
24	7	0	-1.251965	2.344479	-0.724014
25	1	0	-1.274981	3.094724	-0.045790
26	6	0	2.054889	-1.315002	-0.590617
27	1	0	1.394617	-2.166682	-0.746753
28	1	0	3.000227	-1.706681	-0.207160
29	6	0	2.276648	-0.598815	-1.915928
30	1	0	2.857884	0.312329	-1.791314
31	1	0	2.816963	-1.258557	-2.594368
32	1	0	1.327872	-0.336647	-2.378940

Standard orientation of TS-$NHCl_2$-Diethylamine

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$NHCl_2$-Diethylamine
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -265.92 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.990169	0.750682	-0.045331
2	1	0	-2.587925	0.918055	0.816311
3	1	0	-2.406266	-0.484731	-0.518727

4	8	0	-1.864528	2.420301	-1.455762
5	1	0	-2.415107	1.684566	-0.850320
6	1	0	-2.423963	3.181023	-1.622194
7	7	0	1.799499	0.473440	-0.140790
8	1	0	1.438096	1.435735	-0.220070
9	8	0	-1.150123	1.583555	2.152256
10	1	0	-0.610309	2.036893	1.481468
11	1	0	-1.361846	2.225059	2.833662
12	8	0	0.250218	2.742829	0.001788
13	1	0	-0.540295	2.695800	-0.623344
14	1	0	0.535542	3.656443	0.072562
15	17	0	0.204405	-0.461356	-0.489619
16	6	0	2.799491	0.238548	-1.213794
17	1	0	2.284700	0.432015	-2.151776
18	1	0	3.569282	0.999662	-1.084768
19	6	0	3.401036	-1.151918	-1.195512
20	1	0	4.041244	-1.260649	-2.068784
21	1	0	4.016014	-1.316923	-0.313332
22	1	0	2.630959	-1.919706	-1.244373
23	7	0	-1.790149	-1.360615	-0.832544
24	1	0	-1.972488	-1.665026	-1.781459
25	6	0	2.294450	0.300350	1.260012
26	1	0	1.784681	1.056273	1.852040
27	1	0	3.354868	0.549643	1.235872
28	6	0	2.067075	-1.073351	1.867931
29	1	0	2.444985	-1.875851	1.240608
30	1	0	2.595643	-1.109132	2.819301
31	1	0	1.012263	-1.250121	2.060454
32	17	0	-2.133289	-2.693910	0.215783

Standard orientation of TS-ICl-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-ICl-*N*–methyl acetamide

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -611.68 cm^{-1}

Standard orientation:

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

1	8	0	2.857018	1.567018	0.240867
2	1	0	1.884283	2.023158	-1.061660
3	1	0	2.971885	0.607181	0.201389
4	8	0	0.803371	2.131083	1.965608
5	1	0	2.197634	1.734938	0.945349
6	1	0	0.933372	2.959302	2.439937
7	7	0	-1.744288	0.001573	-0.471393
8	1	0	-1.334263	1.331285	-0.382172
9	8	0	1.194994	2.313213	-1.711266
10	1	0	-0.026294	2.386909	-0.960504
11	1	0	1.445920	3.190867	-2.020590
12	8	0	-0.871625	2.353307	-0.333446
13	1	0	0.126103	2.305025	1.293203
14	1	0	-1.508507	3.037503	-0.579820
15	6	0	-2.694068	-0.284507	0.528240
16	6	0	-2.277610	-0.004291	1.944471
17	1	0	-3.147103	0.351390	2.495665
18	1	0	-1.940585	-0.936782	2.404229
19	1	0	-1.466263	0.720304	2.006189
20	53	0	0.245934	-0.878578	-0.134090
21	17	0	2.799502	-1.789707	0.188439
22	6	0	-2.208059	-0.239472	-1.845226
23	1	0	-3.131782	0.313347	-2.020087
24	1	0	-1.441905	0.121237	-2.530381
25	1	0	-2.385757	-1.300628	-2.026525
26	8	0	-3.798051	-0.701717	0.242476

Standard orientation of TS-BrCl-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-BrCl-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -910.24 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.968712	0.987532	0.531149
2	1	0	2.728524	1.346703	-0.343465
3	1	0	2.959606	0.019814	0.460926

4	8	0	0.931849	1.932468	1.866375
5	1	0	1.774908	1.555955	1.485470
6	1	0	1.136455	2.636958	2.486488
7	8	0	1.838333	2.124825	-1.701179
8	1	0	0.960019	2.391234	-1.403268
9	1	0	2.200789	2.837951	-2.231561
10	8	0	-0.558107	2.327664	-0.039817
11	1	0	0.065554	2.242253	0.833152
12	1	0	-1.141907	3.093699	0.005627
13	6	0	-2.621517	-0.263737	0.467208
14	7	0	-1.618810	0.106375	-0.498751
15	1	0	-1.129106	1.345951	-0.237368
16	8	0	-3.739442	-0.500388	0.097083
17	6	0	-2.064554	0.031716	-1.900734
18	1	0	-1.246324	0.366784	-2.530076
19	1	0	-2.346859	-0.984872	-2.159963
20	1	0	-2.917780	0.692971	-2.023878
21	6	0	-2.182644	-0.269128	1.899794
22	1	0	-1.883897	-1.281410	2.172483
23	1	0	-1.337730	0.391080	2.079175
24	1	0	-3.029699	0.017488	2.515878
25	17	0	2.504201	-2.185477	0.119077
26	35	0	0.047121	-0.920971	-0.241976

Standard orientation of TS-BrOCl-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-BrOCl-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -495.74 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.097861	-1.041300	-0.931152
2	8	0	-2.415202	1.647984	-0.717366
3	1	0	-2.325119	1.772427	0.245277
4	1	0	-2.412307	0.679190	-0.882332
5	8	0	-0.146919	2.642029	-1.369435
6	1	0	-1.082628	2.272836	-1.220873

7	1	0	-0.190254	3.550967	-1.679402
8	8	0	-1.549083	2.063571	1.864105
9	1	0	-0.593413	2.157026	1.765038
10	1	0	-1.846467	2.721337	2.496681
11	8	0	1.123858	2.184742	0.637869
12	1	0	0.569838	2.459034	-0.318145
13	1	0	1.816888	2.814289	0.866008
14	6	0	2.812264	-0.598691	-0.303607
15	7	0	1.766657	-0.267643	0.575784
16	1	0	1.502191	1.156328	0.615896
17	8	0	3.793271	-1.193774	0.086833
18	6	0	1.913294	-0.792796	1.937027
19	1	0	1.075368	-0.436058	2.529315
20	1	0	1.925012	-1.881083	1.937075
21	1	0	2.842316	-0.424641	2.365730
22	6	0	2.651129	-0.137514	-1.724990
23	1	0	2.217422	-0.948059	-2.311102
24	1	0	1.996312	0.726100	-1.810038
25	1	0	3.633696	0.089887	-2.128331
26	17	0	-3.104956	-1.799405	0.192447
27	35	0	-0.075310	-0.728520	-0.165437

Standard orientation of TS-Br_2O-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Br_2O-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -634.54 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.848789	-0.313212	-1.003365
2	8	0	-1.496993	2.357521	-0.697699
3	1	0	-1.376246	2.434517	0.266531
4	1	0	-1.742420	1.423733	-0.883412
5	8	0	0.946124	2.746892	-1.349677
6	1	0	-0.052971	2.624685	-1.196895
7	1	0	1.132362	3.641577	-1.647995
8	8	0	-0.540330	2.510713	1.881856

9	1	0	0.407798	2.366244	1.771560
10	1	0	-0.659340	3.221713	2.515571
11	8	0	2.065954	1.956184	0.643013
12	1	0	1.597528	2.375059	-0.310862
13	1	0	2.898588	2.382869	0.873821
14	6	0	2.984775	-1.176469	-0.282650
15	7	0	2.049437	-0.577877	0.578449
16	1	0	2.164082	0.863788	0.617595
17	8	0	3.763056	-2.013061	0.122168
18	35	0	0.160557	-0.542046	-0.196929
19	6	0	2.979966	-0.689603	-1.704635
20	1	0	2.583692	0.318488	-1.797076
21	1	0	3.994656	-0.734915	-2.089581
22	1	0	2.354828	-1.353408	-2.302242
23	6	0	2.027037	-1.120797	1.940251
24	1	0	1.300112	-0.556478	2.517677
25	1	0	1.753281	-2.174131	1.936522
26	1	0	3.011366	-1.008285	2.388581
27	35	0	-3.154163	-0.938509	0.105583

Standard orientation of TS-Cl_2O-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Cl_2O-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1105.98 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.088284	-1.099555	-1.051227
2	8	0	-2.333022	1.518248	-0.743952
3	1	0	-2.259996	1.628239	0.219950
4	1	0	-2.311458	0.540259	-0.923976
5	8	0	-0.045613	2.523712	-1.367471
6	1	0	-0.981386	2.163411	-1.238465
7	1	0	-0.082394	3.422035	-1.705308
8	8	0	-1.547314	1.853927	1.898576
9	1	0	-0.598144	2.009635	1.818025
10	1	0	-1.890737	2.456021	2.562341

11	8	0	1.122753	2.036968	0.729791
12	1	0	0.657531	2.338875	-0.196676
13	1	0	1.830393	2.635791	0.992591
14	17	0	0.003786	-0.778532	-0.178944
15	6	0	2.707201	-0.705056	-0.354792
16	7	0	1.626535	-0.399363	0.552728
17	1	0	1.469189	0.921822	0.670228
18	8	0	3.677203	-1.278606	0.058100
19	6	0	1.746728	-1.013920	1.884460
20	1	0	0.902884	-0.679986	2.479774
21	1	0	1.746188	-2.097490	1.803645
22	1	0	2.674260	-0.676813	2.336913
23	6	0	2.529684	-0.218645	-1.759111
24	1	0	2.020237	-0.989834	-2.337207
25	1	0	1.926326	0.685041	-1.806198
26	1	0	3.511491	-0.050051	-2.190097
27	17	0	-3.073645	-1.828717	0.110208

Standard orientation of TS-I_2-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-I_2-*N*–methyl acetamide

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -102.68 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.190521	2.815275	0.216043
2	1	0	0.110455	2.856570	-1.028389
3	1	0	1.680822	1.987984	0.114702
4	8	0	-0.789634	2.352075	2.036188
5	1	0	0.560778	2.666222	0.952461
6	1	0	-1.007239	3.124143	2.569843
7	7	0	-2.354052	-0.559240	-0.452344
8	1	0	-2.501803	0.931195	-0.319749
9	8	0	-0.659465	2.822791	-1.659523
10	1	0	-1.706994	2.389864	-0.915260
11	1	0	-0.818402	3.720416	-1.973995
12	8	0	-2.469538	1.991736	-0.246831

13	1	0	-1.504126	2.259057	1.386765
14	1	0	-3.336849	2.375895	-0.434590
15	6	0	-3.073691	-1.207567	0.547314
16	6	0	-2.730292	-0.844682	1.966390
17	1	0	-3.641262	-0.874843	2.562803
18	1	0	-2.037392	-1.590047	2.365159
19	1	0	-2.259938	0.134888	2.044610
20	53	0	-0.137106	-0.579554	-0.189097
21	53	0	2.893754	-0.533078	0.060193
22	6	0	-2.726509	-0.929534	-1.821352
23	1	0	-3.797661	-0.778286	-1.964611
24	1	0	-2.183894	-0.284595	-2.511892
25	1	0	-2.484968	-1.972275	-2.038929
26	8	0	-3.960952	-2.003296	0.283528

Standard orientation of TS-Br_2-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Br_2-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -672.93 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.070103	2.139502	0.512814
2	1	0	1.705779	2.389181	-0.357650
3	1	0	2.409250	1.234778	0.437971
4	8	0	-0.142585	2.303921	1.884562
5	1	0	0.773671	2.246808	1.489920
6	1	0	-0.189510	3.034512	2.506678
7	8	0	0.595950	2.810114	-1.700718
8	1	0	-0.319066	2.758290	-1.399081
9	1	0	0.690585	3.607024	-2.227259
10	8	0	-1.696283	2.176296	0.001875
11	1	0	-1.063578	2.299363	0.873547
12	1	0	-2.506058	2.695928	0.063609
13	6	0	-2.766357	-0.976416	0.462598
14	7	0	-1.960253	-0.272325	-0.489479
15	1	0	-1.901463	1.078201	-0.202963

16	8	0	-3.738480	-1.581932	0.092552
17	6	0	-2.359550	-0.466922	-1.892139
18	1	0	-1.708612	0.139757	-2.513724
19	1	0	-2.279165	-1.513107	-2.175322
20	1	0	-3.388344	-0.135842	-2.006551
21	6	0	-2.346685	-0.855850	1.897079
22	1	0	-1.725982	-1.713923	2.155414
23	1	0	-1.771262	0.046358	2.088676
24	1	0	-3.238412	-0.878219	2.516517
25	35	0	-0.022789	-0.695638	-0.254670
26	35	0	2.775928	-1.143531	0.055889

Standard orientation of TS-Cl_2-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Cl_2-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1080.16 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.807583	0.992126	0.428856
2	1	0	2.122441	1.703402	-0.885325
3	1	0	2.859874	0.025618	0.330708
4	8	0	0.704269	1.771184	2.050879
5	1	0	2.169058	1.186902	1.138074
6	1	0	0.797685	2.292854	2.851438
7	8	0	1.506946	2.117748	-1.549564
8	1	0	0.210305	2.217350	-0.957782
9	1	0	1.894990	2.926940	-1.891129
10	8	0	-0.695961	2.158364	-0.418752
11	1	0	0.121700	2.248835	1.447659
12	1	0	-1.309904	2.850979	-0.687197
13	17	0	0.034184	-0.997553	-0.358257
14	6	0	-2.464466	-0.524253	0.536780
15	7	0	-1.526960	-0.188005	-0.548943
16	1	0	-1.178259	1.054172	-0.466401
17	8	0	-3.611790	-0.681711	0.247702
18	17	0	2.768357	-2.165110	-0.019671

19	6	0	-2.068900	-0.415520	-1.906493
20	1	0	-2.302576	-1.466593	-2.044031
21	1	0	-2.964247	0.187563	-2.011922
22	1	0	-1.316718	-0.092972	-2.618148
23	6	0	-1.884346	-0.575431	1.910157
24	1	0	-1.474891	-1.571122	2.083625
25	1	0	-1.079730	0.144536	2.042902
26	1	0	-2.686306	-0.397628	2.619282

Standard orientation of TS-HOI-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-HOI-*N*–methyl acetamide

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -723.24 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.017757	-1.957222	-0.486788
2	1	0	-2.299191	-2.488602	0.268132
3	8	0	-3.153728	0.351022	-0.400958
4	1	0	-2.893677	0.700926	0.535333
5	1	0	-2.832436	-0.615584	-0.472657
6	8	0	-1.506687	1.891811	-1.571035
7	1	0	-2.558185	0.929836	-1.006250
8	1	0	-1.907705	2.731839	-1.818897
9	8	0	-2.246299	1.374223	1.725453
10	1	0	-1.379162	1.723114	1.356697
11	1	0	-2.770125	2.139233	1.986915
12	8	0	-0.043071	2.188103	0.573662
13	1	0	-0.908456	2.068794	-0.781178
14	1	0	0.277997	3.074864	0.763175
15	6	0	2.635125	0.360445	-0.433624
16	7	0	1.684375	0.376274	0.571301
17	1	0	0.933222	1.307530	0.563737
18	8	0	3.765381	-0.071672	-0.259464
19	6	0	2.162364	0.025802	1.908965
20	1	0	1.332810	0.139532	2.606514
21	1	0	2.516158	-1.005495	1.944986

22	1	0	2.977240	0.686402	2.213542
23	6	0	2.192360	0.903244	-1.766431
24	1	0	2.191268	0.088998	-2.494374
25	1	0	1.200587	1.351488	-1.732402
26	1	0	2.922130	1.643988	-2.096911
27	53	0	-0.168206	-1.038827	-0.013885

Standard orientation of TS-HOBr-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-HOBr-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -253.15 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.688257	-2.184637	-0.490948
2	1	0	-1.812888	-2.876530	0.166703
3	8	0	-3.105974	-0.151538	-0.346528
4	1	0	-2.906174	0.259608	0.567273
5	1	0	-2.614363	-1.085616	-0.416006
6	8	0	-1.770436	1.612894	-1.597294
7	1	0	-2.661915	0.507497	-0.990254
8	1	0	-2.205350	2.389620	-1.955552
9	8	0	-2.289097	1.083370	1.722530
10	1	0	-1.477326	1.541800	1.333982
11	1	0	-2.846876	1.739318	2.146124
12	8	0	-0.262295	2.093648	0.452996
13	1	0	-1.138736	1.896766	-0.860561
14	1	0	0.000171	2.996964	0.641425
15	6	0	2.523726	0.293588	-0.423985
16	7	0	1.531579	0.313832	0.564569
17	1	0	0.805924	1.191595	0.509002
18	8	0	3.645210	-0.104877	-0.191061
19	35	0	-0.051341	-1.098313	-0.007534
20	6	0	2.086060	0.774853	-1.778617
21	1	0	1.141360	1.309384	-1.736353
22	1	0	2.864579	1.411627	-2.191950
23	1	0	1.973516	-0.088795	-2.434224

24	6	0	1.972758	0.007513	1.925476
25	1	0	1.109048	0.082232	2.580248
26	1	0	2.383079	-0.997379	1.975810
27	1	0	2.733362	0.719417	2.241230

Standard orientation of TS-HOCl-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-HOCl-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -328.69 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.452571	2.335489	-0.620336
2	1	0	1.523092	3.050819	0.020431
3	8	0	3.025171	0.440983	-0.395394
4	1	0	2.868023	0.074243	0.543903
5	1	0	2.452404	1.328225	-0.506637
6	8	0	1.801123	-1.458482	-1.555433
7	1	0	2.625594	-0.282339	-0.998254
8	1	0	2.281474	-2.222998	-1.880101
9	8	0	2.311001	-0.689545	1.770691
10	1	0	1.537201	-1.228231	1.407206
11	1	0	2.907881	-1.273908	2.242772
12	8	0	0.371798	-1.890042	0.547298
13	1	0	1.202964	-1.740670	-0.788699
14	1	0	0.129453	-2.784351	0.795328
15	17	0	-0.008911	1.217297	-0.072138
16	6	0	-2.452568	-0.182789	-0.401358
17	7	0	-1.447532	-0.136174	0.574451
18	1	0	-0.710174	-1.001165	0.559868
19	8	0	-3.579036	0.201572	-0.170888
20	6	0	-1.864685	0.254453	1.918729
21	1	0	-0.985469	0.237601	2.556697
22	1	0	-2.289804	1.254465	1.908566
23	1	0	-2.606364	-0.445524	2.299301
24	6	0	-2.011754	-0.703322	-1.739176
25	1	0	-1.831977	0.147592	-2.397107

26	1	0	-1.095814	-1.283079	-1.666314
27	1	0	-2.811251	-1.301366	-2.168449

Standard orientation of TS-SO_3Cl^--*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-SO_3Cl^--*N*–methyl acetamide
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -256.86 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.187649	0.619987	-0.174760
2	1	0	-2.850357	1.012313	0.651302
3	1	0	-2.972053	-0.324623	-0.169642
4	8	0	-1.706913	2.211419	-1.809116
5	1	0	-2.272568	1.560178	-1.340152
6	1	0	-2.260898	2.956356	-2.052166
7	8	0	-2.036643	2.135513	1.846285
8	1	0	-1.179238	2.254582	1.401793
9	1	0	-2.423328	3.007212	1.955053
10	8	0	0.141483	2.594571	0.120760
11	1	0	-0.450097	2.511258	-0.661850
12	1	0	0.472395	3.495756	0.148860
13	6	0	2.882621	0.113614	-0.437829
14	7	0	1.950888	0.401644	0.538981
15	1	0	1.407674	1.253143	0.389099
16	8	0	3.830781	-0.616088	-0.212703
17	6	0	2.308172	0.109124	1.925774
18	1	0	1.492238	0.436091	2.561391
19	1	0	2.452470	-0.960841	2.045934
20	1	0	3.225093	0.624082	2.206463
21	6	0	2.632236	0.723947	-1.789505
22	1	0	2.547090	-0.075689	-2.523003
23	1	0	1.733220	1.331264	-1.815046
24	1	0	3.496740	1.331077	-2.054033
25	17	0	-2.337947	-2.537193	-0.302785
26	16	0	0.011688	-1.031086	0.106821
27	8	0	-0.165770	-0.434772	-1.191161

28	8	0	0.802556	-2.226981	0.246858
29	8	0	-0.609680	-0.442912	1.265173

Standard orientation of TS-CH_3COCl-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-CH_3COCl-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -268.80 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.023043	-0.510673	-1.278169
2	1	0	-3.129303	-0.903672	-0.391683
3	1	0	-2.153942	-0.768043	-1.610865
4	8	0	-2.548439	2.029022	-0.476899
5	1	0	-2.841132	1.191965	-0.895663
6	1	0	-3.277256	2.652709	-0.484092
7	1	0	0.312268	0.460273	1.062194
8	8	0	-3.095143	-1.203564	1.384762
9	1	0	-2.578841	-0.457374	1.736731
10	1	0	-3.903178	-1.286934	1.895043
11	8	0	-1.392777	0.949585	1.684641
12	1	0	-1.824625	1.500452	0.993022
13	1	0	-1.337087	1.464531	2.493939
14	8	0	2.311758	-1.759931	-0.423593
15	6	0	1.220914	-1.421989	-0.157742
16	6	0	0.083012	-2.147888	0.483103
17	1	0	0.432317	-2.556321	1.430951
18	1	0	-0.773037	-1.505327	0.637630
19	1	0	-0.186476	-2.968409	-0.178058
20	17	0	0.217445	-0.592818	-1.942805
21	7	0	1.273070	0.215472	0.800676
22	6	0	1.864358	1.223467	-0.034685
23	8	0	3.047570	1.185727	-0.247183
24	6	0	0.941529	2.297490	-0.513444
25	1	0	-0.065466	1.935761	-0.689899
26	1	0	0.898987	3.057159	0.271685
27	1	0	1.349667	2.748429	-1.412760

28	6	0	2.091873	-0.109208	1.988130
29	1	0	1.548818	-0.823900	2.597892
30	1	0	3.032185	-0.535704	1.658722
31	1	0	2.278528	0.791466	2.567522

Standard orientation of TS-$(CH_3CO)_2O$-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$(CH_3CO)_2O$-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -149.84 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.939152	-0.676482	-0.467083
2	1	0	3.726788	0.271302	-0.564933
3	1	0	3.959542	-1.076094	-1.339016
4	8	0	2.066910	-1.283836	1.451212
5	1	0	2.768495	-1.224296	0.775458
6	1	0	1.222134	-1.397212	0.979125
7	8	0	3.029557	1.899760	-0.347397
8	1	0	2.537566	1.887174	0.492781
9	1	0	3.598773	2.672273	-0.356216
10	8	0	1.390545	1.238243	1.758981
11	1	0	1.728725	0.319015	1.888160
12	1	0	1.285353	1.668705	2.610852
13	8	0	-2.017277	0.043924	-1.584877
14	6	0	-0.891425	0.218731	-1.213796
15	6	0	0.356347	0.099477	-2.032605
16	1	0	0.338106	0.860008	-2.813715
17	1	0	1.252836	0.212663	-1.431016
18	1	0	0.337080	-0.885050	-2.488646
19	8	0	-0.361978	-1.223916	0.098574
20	6	0	-0.747136	-2.424663	-0.206511
21	6	0	-0.801585	-3.376923	0.972197
22	1	0	-1.423709	-2.951972	1.759159
23	1	0	-1.193678	-4.342741	0.668280
24	1	0	0.199257	-3.507195	1.384601
25	8	0	-1.042831	-2.798273	-1.338365

26	1	0	-0.020137	0.990754	0.614098
27	7	0	-0.749863	1.283240	-0.055256
28	6	0	-2.343154	0.292191	1.634989
29	1	0	-1.453206	0.022564	2.197815
30	1	0	-3.144929	0.614946	2.290975
31	1	0	-2.655308	-0.588169	1.074724
32	6	0	-0.342594	2.593821	-0.636761
33	1	0	0.670128	2.493617	-1.008862
34	1	0	-1.030147	2.857378	-1.432424
35	1	0	-0.376585	3.342092	0.147185
36	6	0	-2.062327	1.383285	0.664620
37	8	0	-2.764928	2.308335	0.409655

Standard orientation of TS-NH_2Br-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-NH_2Br-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1041.15 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.135395	-2.728347	0.391187
2	8	0	-3.215100	0.060875	-0.317653
3	1	0	-2.995872	0.481201	0.568313
4	1	0	-2.681140	-1.052164	-0.356246
5	8	0	-1.690720	1.680911	-1.661751
6	1	0	-2.749048	0.657949	-0.975929
7	1	0	-2.040659	2.484228	-2.051795
8	7	0	1.873224	0.473883	0.612717
9	1	0	1.092927	1.153042	0.522120
10	8	0	-2.247589	1.278555	1.758017
11	1	0	-1.423019	1.686394	1.282281
12	1	0	-2.731541	1.980490	2.197201
13	8	0	-0.292733	2.158171	0.405439
14	1	0	-1.074183	1.935457	-0.873310
15	1	0	-0.091115	3.085889	0.545455
16	7	0	-1.926224	-2.063036	-0.344695
17	1	0	-1.879145	-2.557369	-1.228653

18	6	0	2.693449	0.270700	-0.437659
19	8	0	3.749179	-0.356278	-0.345790
20	35	0	-0.228338	-1.269556	0.006696
21	6	0	2.277069	0.063954	1.946866
22	1	0	1.454180	0.263478	2.627809
23	1	0	2.504617	-0.999698	1.966614
24	1	0	3.158704	0.611563	2.280038
25	6	0	2.221668	0.841526	-1.751814
26	1	0	1.261793	1.343649	-1.661934
27	1	0	2.969703	1.544350	-2.116151
28	1	0	2.144604	0.033450	-2.477972

Standard orientation of TS-$NHBr_2$-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$NHBr_2$-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -742.94 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.583528	2.294516	-0.472726
2	1	0	-1.318365	2.355965	0.489658
3	1	0	-1.787722	1.072445	-0.748043
4	8	0	0.819471	2.872498	-1.325086
5	1	0	-0.757253	2.587758	-0.952852
6	1	0	1.080697	3.773067	-1.526779
7	7	0	2.318957	-0.620632	0.671875
8	1	0	2.259428	0.430897	0.757537
9	8	0	-0.432624	2.350226	1.873222
10	1	0	0.530027	2.225312	1.549679
11	1	0	-0.470199	3.126717	2.434997
12	8	0	1.890245	2.013781	0.840045
13	1	0	1.328286	2.561926	-0.493452
14	1	0	2.588019	2.563942	1.202092
15	7	0	-1.766262	-0.143914	-0.894298
16	1	0	-1.848746	-0.460141	-1.855606
17	6	0	3.115438	-1.120394	-0.330627
18	8	0	3.575582	-2.250095	-0.290313

19	35	0	0.056573	-0.532117	-0.261621
20	35	0	-3.152488	-0.963653	0.086252
21	6	0	3.339365	-0.193072	-1.494931
22	1	0	2.910805	0.790546	-1.323391
23	1	0	4.409891	-0.106700	-1.671786
24	1	0	2.889810	-0.635099	-2.383601
25	6	0	2.210389	-1.376708	1.913872
26	1	0	1.526676	-0.847869	2.572146
27	1	0	1.820701	-2.371537	1.715127
28	1	0	3.181786	-1.469813	2.398161

Standard orientation of TS-NH_2Cl-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-NH_2Cl-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -768.91 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.447368	3.137664	0.698823
2	8	0	3.305585	0.542026	-0.238697
3	1	0	3.103529	0.027343	0.567026
4	1	0	2.279493	1.940509	-0.175812
5	8	0	1.955725	-1.176921	-1.898313
6	1	0	2.953961	-0.008105	-0.966009
7	1	0	2.376758	-1.917112	-2.339412
8	7	0	-1.446124	-0.342260	0.422847
9	1	0	-0.593249	-1.189129	0.216818
10	8	0	2.317679	-1.105287	1.726040
11	1	0	1.583442	-1.493229	1.179704
12	1	0	2.828842	-1.828639	2.093912
13	8	0	0.406349	-1.976411	0.101808
14	1	0	1.340277	-1.538634	-1.206569
15	1	0	0.134903	-2.895486	0.145625
16	17	0	0.025073	1.233153	0.117586
17	6	0	-2.391960	-0.190676	-0.569442
18	6	0	-3.766577	0.281551	-0.173983
19	1	0	-4.388176	0.344188	-1.060825

20	1	0	-4.222425	-0.397653	0.545491
21	1	0	-3.706242	1.263134	0.297264
22	7	0	1.418956	2.520661	-0.103692
23	1	0	1.256939	3.056139	-0.947833
24	6	0	-1.836121	-0.256535	1.826882
25	1	0	-0.937859	-0.391127	2.425213
26	1	0	-2.544507	-1.041727	2.091579
27	1	0	-2.268469	0.712727	2.070882
28	8	0	-2.099427	-0.408320	-1.737046

Standard orientation of TS-$NHCl_2$-*N*–methyl acetamide

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$NHCl_2$-*N*–methyl acetamide
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -169.46 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.608777	1.324720	-0.525084
2	1	0	-2.432793	1.446745	0.464236
3	1	0	-2.404484	0.297497	-0.772054
4	8	0	-0.600875	2.703208	-1.328777
5	1	0	-1.915525	1.905829	-0.977999
6	1	0	-0.650260	3.628774	-1.577671
7	7	0	1.881628	-0.269816	0.577568
8	1	0	1.262766	1.212063	0.801016
9	8	0	-1.742236	1.652898	1.864308
10	1	0	-0.794134	1.842063	1.695012
11	1	0	-2.086540	2.303799	2.479820
12	8	0	0.773264	2.102119	0.935017
13	1	0	0.009563	2.607707	-0.566190
14	1	0	1.374123	2.720346	1.358307
15	17	0	-0.106521	-0.746866	-0.284893
16	7	0	-1.856811	-1.063067	-0.925027
17	1	0	-1.751123	-1.472771	-1.846849

18	6	0	2.857245	-0.439868	-0.334524
19	8	0	3.847632	-1.169211	-0.176840
20	17	0	-2.688874	-2.238459	0.037157
21	6	0	2.006394	-1.060800	1.790069
22	1	0	1.153668	-0.847626	2.433322
23	1	0	2.023904	-2.131992	1.576327
24	1	0	2.921367	-0.812319	2.330650
25	6	0	2.687899	0.327875	-1.626800
26	1	0	2.472502	-0.377201	-2.430685
27	1	0	1.881275	1.054169	-1.574379
28	1	0	3.622385	0.830501	-1.870588

Standard orientation of TS-ICl-Alcohol

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-ICl-Alcohol

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -626.46 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.455235	1.442918	0.864002
2	1	0	1.897412	1.979207	-0.555105
3	1	0	2.562930	0.484756	0.777982
4	8	0	0.031884	2.031416	1.978427
5	1	0	1.633406	1.586380	1.380211
6	1	0	0.093558	2.847244	2.487073
7	1	0	-1.359591	1.520718	-0.801443
8	8	0	1.412591	2.321906	-1.363834
9	1	0	0.196767	2.409535	-1.065694
10	1	0	1.768654	3.193275	-1.577209
11	8	0	-0.904165	2.445982	-0.710204
12	1	0	-0.420928	2.261997	1.152632
13	1	0	-1.414247	3.121990	-1.174104
14	6	0	-2.777551	0.147440	0.414375
15	1	0	-2.261008	0.467109	1.326803
16	1	0	-3.516809	0.913576	0.161386
17	8	0	-1.850819	0.128113	-0.677958
18	6	0	-3.451732	-1.193338	0.609648

19	1	0	-2.728382	-1.962877	0.888428
20	1	0	-4.197445	-1.124989	1.404803
21	1	0	-3.954473	-1.503512	-0.308871
22	53	0	-0.027789	-0.851434	-0.283204
23	17	0	2.434755	-1.867981	0.237962

Standard orientation of TS-BrCl-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-BrCl-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -703.41 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.858533	-0.275582	0.496655
2	1	0	-2.444203	-1.065736	-0.772925
3	1	0	-2.583904	0.652348	0.458824
4	8	0	-1.195407	-1.837290	1.987387
5	1	0	-2.341080	-0.717691	1.198119
6	1	0	-1.457716	-2.470882	2.658878
7	1	0	0.816966	-1.747964	-0.590961
8	8	0	-2.019049	-1.648836	-1.488334
9	1	0	-0.963408	-2.123437	-1.066910
10	1	0	-2.647370	-2.302751	-1.809137
11	8	0	0.042083	-2.486751	-0.559687
12	1	0	-0.655586	-2.298821	1.332730
13	1	0	0.349444	-3.337371	-0.889854
14	6	0	2.688702	-0.743982	0.469397
15	1	0	2.211151	-0.711123	1.450062
16	1	0	3.136316	-1.729348	0.336691
17	8	0	1.678929	-0.652014	-0.550499
18	6	0	3.726220	0.344690	0.315961
19	1	0	3.284473	1.330019	0.456936
20	1	0	4.510022	0.214768	1.061920
21	1	0	4.178906	0.300495	-0.673513
22	35	0	0.410293	0.830294	-0.259052
23	17	0	-1.378118	2.620397	0.124684

Standard orientation of TS-BrOCl-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-BrOCl-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -822.55 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.866579	-0.923256	0.772103
2	8	0	1.933385	1.823106	0.718746
3	1	0	1.376143	2.127371	-0.631550
4	1	0	2.057583	0.856775	0.816585
5	8	0	-0.490851	2.580216	1.717618
6	1	0	1.186295	2.085061	1.291479
7	1	0	-0.714095	3.393244	2.175940
8	1	0	-1.773700	0.964453	-0.864145
9	8	0	0.829132	2.328209	-1.488253
10	1	0	-0.325185	2.207456	-1.270765
11	1	0	1.062160	3.188331	-1.851351
12	8	0	-1.494954	2.024390	-0.910891
13	1	0	-1.065609	2.502297	0.942305
14	1	0	-2.138177	2.539024	-1.407216
15	6	0	-2.958263	-0.696990	0.238244
16	1	0	-2.684851	-0.328381	1.230028
17	1	0	-3.847138	-0.156667	-0.090816
18	8	0	-1.921392	-0.366567	-0.692516
19	6	0	-3.215125	-2.188131	0.259331
20	1	0	-2.328837	-2.729811	0.587309
21	1	0	-4.029079	-2.418670	0.946649
22	1	0	-3.491063	-2.538924	-0.734298
23	35	0	-0.068710	-0.759292	0.005108
24	17	0	2.963854	-1.619670	-0.308167

Standard orientation of TS-Br_2O-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Br_2O-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -813.98 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.585516	-0.099984	0.865508
2	8	0	0.704585	2.490951	0.713564
3	1	0	0.094564	2.557174	-0.639620
4	1	0	1.161911	1.632909	0.834017
5	8	0	-1.847532	2.364534	1.671915
6	1	0	-0.093669	2.483294	1.277088
7	1	0	-2.352132	3.056001	2.105565
8	1	0	-2.434473	0.349099	-0.883938
9	8	0	-0.477889	2.545050	-1.505395
10	1	0	-1.513875	2.026182	-1.297054
11	1	0	-0.562289	3.430370	-1.873037
12	8	0	-2.550109	1.441820	-0.942638
13	1	0	-2.343317	2.070598	0.893522
14	1	0	-3.327792	1.689957	-1.451015
15	6	0	-2.976735	-1.618915	0.210537
16	1	0	-2.875902	-1.178254	1.205521
17	1	0	-3.992413	-1.431583	-0.141414
18	8	0	-2.104075	-0.940334	-0.698960
19	6	0	-2.684878	-3.103638	0.237235
20	1	0	-1.671262	-3.293016	0.588308
21	1	0	-3.378319	-3.610449	0.908342
22	1	0	-2.794216	-3.528889	-0.759651
23	35	0	-0.246699	-0.643590	0.046706
24	35	0	3.034382	-0.508820	-0.169141

Standard orientation of TS-Cl_2O-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Cl_2O-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -863.93 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.496744	-1.326550	-0.828009
2	8	0	-2.104968	1.313747	-0.914247
3	1	0	-2.111382	1.526060	0.038959
4	1	0	-1.996077	0.340538	-0.988532
5	8	0	0.074918	2.441790	-1.496359
6	1	0	-0.846385	1.994418	-1.365635
7	1	0	-0.023696	3.332491	-1.845680
8	1	0	1.619599	1.182875	0.672260
9	8	0	-1.473397	2.004062	1.651767
10	1	0	-0.520429	2.152822	1.578576
11	1	0	-1.842503	2.695184	2.205773
12	8	0	1.212954	2.191030	0.611321
13	1	0	0.699035	2.381253	-0.458517
14	1	0	1.862556	2.857087	0.856643
15	17	0	0.283597	-0.788907	-0.037133
16	6	0	3.015596	-0.480610	-0.204571
17	1	0	2.752961	-0.242009	-1.237415
18	1	0	3.834897	0.171687	0.099751
19	6	0	3.398558	-1.936262	-0.053088
20	1	0	4.261152	-2.161102	-0.680138
21	1	0	3.656952	-2.154540	0.982190
22	1	0	2.579349	-2.587090	-0.354813
23	17	0	-2.484829	-2.082573	0.311421
24	8	0	1.913485	-0.145739	0.647980

Standard orientation of TS-I_2-Alcohol

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d)level:

Standard orientation of transition state of TS-I_2-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -891.51 cm^{-1}
Standard orientation:

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

1	8	0	0.402769	2.678807	0.872526
2	1	0	-0.312371	2.783623	-0.544775
3	1	0	1.024866	1.940836	0.805712
4	8	0	-1.926867	1.803280	1.958159
5	1	0	-0.366578	2.347815	1.385905
6	1	0	-2.339514	2.488323	2.494993
7	1	0	-2.731448	0.563067	-0.767765
8	8	0	-0.894171	2.782827	-1.368225
9	1	0	-1.919413	2.196155	-1.078138
10	1	0	-1.089693	3.700461	-1.596518
11	8	0	-2.877561	1.596830	-0.700828
12	1	0	-2.429171	1.765736	1.128180
13	1	0	-3.678613	1.856324	-1.172264
14	6	0	-3.128161	-1.332750	0.465021
15	1	0	-2.843320	-0.786703	1.372113
16	1	0	-4.178703	-1.104277	0.256577
17	8	0	-2.384872	-0.836786	-0.650394
18	6	0	-2.943283	-2.824232	0.651664
19	1	0	-1.905428	-3.066043	0.891948
20	1	0	-3.573108	-3.182709	1.469010
21	1	0	-3.222697	-3.358937	-0.258799
22	53	0	-0.264052	-0.662989	-0.322967
23	53	0	2.668570	-0.231378	0.097001

Standard orientation of TS-Br_2-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Br_2-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -784.47 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.472482	2.360168	0.456955
2	1	0	0.610282	2.624019	-0.790075
3	1	0	1.936277	1.511437	0.411176
4	8	0	-0.761973	2.271787	2.005695
5	1	0	0.811611	2.307326	1.176322
6	1	0	-1.013516	2.905918	2.680709

7	1	0	-2.203271	0.843695	-0.553183
8	8	0	-0.113023	2.735597	-1.499717
9	1	0	-1.175141	2.358635	-1.055164
10	1	0	-0.124291	3.636513	-1.837118
11	8	0	-2.147593	1.915385	-0.504353
12	1	0	-1.474899	2.224939	1.354723
13	1	0	-2.969933	2.325426	-0.791241
14	6	0	-2.855382	-1.171805	0.489220
15	1	0	-2.456764	-0.886268	1.464461
16	1	0	-3.859139	-0.755462	0.394089
17	8	0	-2.082516	-0.538012	-0.542002
18	6	0	-2.877149	-2.673703	0.315297
19	1	0	-1.877119	-3.093180	0.415886
20	1	0	-3.512991	-3.125504	1.076451
21	1	0	-3.270857	-2.936157	-0.665601
22	35	0	-0.118133	-0.755349	-0.284658
23	35	0	2.519159	-0.868299	0.072053

Standard orientation of TS-Cl_2-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-Cl_2-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -560.71cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.820639	0.106197	0.446464
2	1	0	-2.708794	-0.305511	-0.430990
3	1	0	-2.420525	0.986823	0.404576
4	8	0	-1.336451	-1.586304	1.803040
5	1	0	-1.962303	-0.912991	1.422974
6	1	0	-1.820695	-2.205668	2.354498
7	1	0	0.837505	-1.602728	-0.297949
8	8	0	-2.140627	-1.329136	-1.790637
9	1	0	-1.418791	-1.895473	-1.491284
10	1	0	-2.721270	-1.854391	-2.345557
11	8	0	0.000926	-2.374475	-0.114706
12	1	0	-0.559715	-2.128031	0.753337

13	1	0	0.317721	-3.284121	-0.093914
14	17	0	0.554528	0.838726	-0.244176
15	6	0	2.776425	-0.631543	0.398331
16	1	0	2.430570	-0.444070	1.414102
17	1	0	3.169507	-1.645461	0.338757
18	6	0	3.793999	0.384089	-0.059181
19	1	0	4.671526	0.331119	0.584153
20	1	0	4.101771	0.179973	-1.083135
21	1	0	3.393279	1.394564	-0.003076
22	8	0	1.628214	-0.636849	-0.483902
23	17	0	-0.988865	2.775111	0.100443

Standard orientation of TS-HOI-Alcohol

Cartesian coordinates of the transition state optimized at the M06-2X/LANL08(d) level:

Standard orientation of transition state of TS-HOI-Alcohol

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -502.35 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.296965	-2.229857	0.420989
2	1	0	1.629278	-2.692511	-0.357819
3	8	0	2.820472	-0.049363	0.759965
4	1	0	2.810936	0.332616	-0.175057
5	1	0	2.381592	-0.941069	0.719321
6	8	0	1.312219	1.607912	1.686396
7	1	0	2.130070	0.682806	1.284039
8	1	0	1.815701	2.333863	2.071996
9	1	0	-0.915431	1.544956	-0.691252
10	8	0	2.461221	1.208060	-1.466687
11	1	0	1.627294	1.672572	-1.168238
12	1	0	3.134947	1.887940	-1.573615
13	8	0	0.285314	2.311344	-0.468450
14	1	0	0.844290	1.965792	0.803888
15	1	0	0.194003	3.262468	-0.576876
16	6	0	-2.581060	1.175209	0.364322
17	1	0	-2.027269	1.155354	1.310589
18	1	0	-2.934510	2.197862	0.202519

19	6	0	-3.740051	0.205847	0.393808
20	1	0	-4.432439	0.467672	1.196219
21	1	0	-4.283566	0.232881	-0.553052
22	1	0	-3.388490	-0.814504	0.563536
23	53	0	-0.236272	-0.963471	-0.177470
24	8	0	-1.693354	0.838020	-0.707100

Standard orientation of TS-HOBr-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-HOBr-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -444.77 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.959516	-2.402638	0.303580
2	1	0	0.996975	-3.040419	-0.415425
3	8	0	2.794519	-0.521590	0.508238
4	1	0	2.602009	0.211771	-0.578747
5	1	0	2.223987	-1.336633	0.463048
6	8	0	1.549098	1.465804	1.845957
7	1	0	2.436220	0.062292	1.210262
8	1	0	1.971574	2.172944	2.338000
9	1	0	-0.571524	1.547294	-0.658829
10	8	0	2.335134	0.905849	-1.410515
11	1	0	1.473433	1.494006	-1.129212
12	1	0	3.076077	1.463987	-1.666908
13	8	0	0.370539	2.143173	-0.599442
14	1	0	1.045910	1.861617	1.112198
15	1	0	0.237157	3.040125	-0.915310
16	6	0	-2.501804	0.985963	0.390864
17	1	0	-2.009218	0.894577	1.364946
18	1	0	-2.806788	2.028897	0.272328
19	8	0	-1.574925	0.686640	-0.644910
20	6	0	-3.710174	0.073799	0.319644
21	1	0	-3.411849	-0.967012	0.442887
22	1	0	-4.424227	0.320807	1.105885
23	1	0	-4.206928	0.179337	-0.644562

24	35	0	-0.366628	-0.986002	-0.188197

Standard orientation of TS-HOCl-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-HOCl-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -743.70 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.823743	2.449943	0.145886
2	1	0	-0.887227	3.046800	-0.607342
3	8	0	-2.622343	0.689126	0.521309
4	1	0	-2.626672	0.148528	-0.362125
5	1	0	-2.019383	1.502771	0.397223
6	8	0	-1.374267	-1.080245	1.820708
7	1	0	-2.177110	0.044480	1.188095
8	1	0	-1.845283	-1.725504	2.352498
9	1	0	0.731867	-1.305593	-0.568952
10	8	0	-2.339805	-0.815063	-1.468550
11	1	0	-1.551617	-1.357260	-1.163008
12	1	0	-3.047599	-1.405615	-1.735892
13	8	0	-0.287116	-1.994628	-0.379856
14	1	0	-0.909754	-1.546921	1.067035
15	1	0	-0.124853	-2.929233	-0.520597
16	17	0	0.388752	1.128230	-0.290107
17	6	0	2.551513	-0.694369	0.362023
18	1	0	2.069654	-0.519005	1.329371
19	1	0	2.890312	-1.733092	0.343471
20	8	0	1.599108	-0.522395	-0.680821
21	6	0	3.720335	0.248950	0.168560
22	1	0	3.382502	1.284642	0.188925
23	1	0	4.457380	0.112787	0.960179
24	1	0	4.203251	0.060920	-0.789972

Standard orientation of TS-SO_3Cl^--Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-SO_3Cl^--Alcohol
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -230.44 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.889096	-0.300593	0.577050
2	1	0	-2.767894	-0.741561	-0.284323
3	1	0	-2.569056	0.608435	0.487041
4	8	0	-1.289150	-2.080473	1.873203
5	1	0	-1.860291	-1.357008	1.535807
6	1	0	-1.860895	-2.751073	2.253044
7	1	0	1.329742	-1.475359	-0.704691
8	8	0	-2.331222	-1.930000	-1.594326
9	1	0	-1.413746	-2.135516	-1.346846
10	1	0	-2.808851	-2.761761	-1.628161
11	8	0	0.094389	-2.689392	-0.356903
12	1	0	-0.329756	-2.549361	0.521331
13	1	0	0.331221	-3.616774	-0.433906
14	6	0	2.918905	-0.990280	0.355278
15	1	0	2.401081	-1.067478	1.312702
16	1	0	3.397772	-1.946056	0.140188
17	6	0	3.934604	0.128010	0.377990
18	1	0	4.690680	-0.071250	1.136599
19	1	0	4.428692	0.213451	-0.589259
20	1	0	3.456586	1.078430	0.608197
21	17	0	-1.631919	2.738254	0.241823
22	16	0	0.383285	0.985164	-0.249328
23	8	0	0.395003	0.598364	1.138689
24	8	0	-0.454934	0.289689	-1.192977
25	8	0	1.277910	2.014519	-0.711899
26	8	0	1.955065	-0.722919	-0.673971

Standard orientation of TS-CH_3COCl-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-CH_3COCl-Alcohol

State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -167.00 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.432349	-1.101605	-1.130077
2	1	0	-2.877474	-0.823679	-0.304534
3	1	0	-1.835857	-1.831969	-0.927697
4	8	0	-0.771067	0.894296	-1.618142
5	1	0	-1.425501	0.149579	-1.587642
6	1	0	-0.695542	1.209963	-2.522565
7	1	0	0.632870	0.451159	-0.865102
8	8	0	-3.354983	0.080674	1.137173
9	1	0	-2.901087	0.942235	1.069524
10	1	0	-4.278291	0.236514	1.345355
11	8	0	-1.733435	2.219112	0.611042
12	1	0	-1.409956	2.016459	-0.282301
13	1	0	-1.957926	3.151176	0.650926
14	6	0	1.769388	1.615533	0.346295
15	1	0	0.893139	1.957613	0.893350
16	1	0	2.570867	1.385043	1.041916
17	17	0	0.582093	-2.335977	-0.747646
18	8	0	2.418498	-1.294015	1.174456
19	6	0	1.339277	-0.985709	0.837385
20	6	0	0.092094	-0.725774	1.615514
21	1	0	0.318774	0.033921	2.363684
22	1	0	-0.719249	-0.395291	0.980255
23	1	0	-0.183215	-1.650830	2.115577
24	8	0	1.445989	0.348421	-0.297080
25	6	0	2.206288	2.612251	-0.701145
26	1	0	1.398669	2.824058	-1.400623
27	1	0	2.485168	3.545849	-0.214235
28	1	0	3.065511	2.236927	-1.253182

Standard orientation of TS-$(CH_3CO)_2O$-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$(CH_3CO)_2O$-Alcohol
State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -371.15 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.189566	-2.091920	-0.611695
2	1	0	-2.025359	-2.144114	-0.086933
3	1	0	-0.423864	-2.069088	-0.009775
4	8	0	-1.018565	0.153823	-1.551631
5	1	0	-1.115224	-0.888964	-1.217484
6	1	0	-0.769774	0.208333	-2.481129
7	1	0	-0.285770	0.687241	-0.887214
8	8	0	-3.453198	-1.758738	0.719595
9	1	0	-3.663849	-0.844042	0.452247
10	1	0	-4.242775	-2.296850	0.634749
11	8	0	-3.456099	0.808852	-0.199373
12	1	0	-2.794477	0.841460	-0.901285
13	1	0	-4.173884	1.401521	-0.432656
14	6	0	0.638083	2.674077	0.081301
15	1	0	0.051052	2.982116	0.946689
16	1	0	1.680588	2.923636	0.254546
17	8	0	1.897452	0.870446	1.788948
18	6	0	0.896880	0.483376	1.201653
19	6	0	-0.385863	0.175005	1.942480
20	1	0	-0.724545	1.092808	2.422693
21	1	0	-1.174765	-0.185722	1.288925
22	1	0	-0.180549	-0.566817	2.710384
23	8	0	0.551216	1.241237	-0.050822
24	6	0	0.115052	3.303984	-1.189400
25	1	0	-0.939057	3.074071	-1.341138
26	1	0	0.217622	4.386208	-1.126911
27	1	0	0.681569	2.957949	-2.053334
28	8	0	1.095402	-1.033328	0.415876
29	6	0	2.155409	-1.278600	-0.326779
30	6	0	2.227825	-2.724426	-0.764157
31	1	0	2.074588	-3.386299	0.085902
32	1	0	1.433155	-2.919607	-1.485282
33	1	0	3.186876	-2.926721	-1.230537
34	8	0	2.986372	-0.456324	-0.662528

Standard orientation of TS-NH_2Br-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-NH_2Br-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1153.99 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.572201	-2.792685	-0.507186
2	8	0	2.795704	-0.207433	0.663454
3	1	0	2.755822	0.299000	-0.222572
4	1	0	2.198081	-1.227878	0.511951
5	8	0	1.145700	1.436381	1.858099
6	1	0	2.236678	0.382827	1.267679
7	1	0	1.552362	2.187505	2.308997
8	1	0	-1.061511	1.333928	-0.743786
9	8	0	2.349192	1.200439	-1.460826
10	1	0	1.479052	1.659005	-1.112495
11	1	0	2.989359	1.900258	-1.643052
12	8	0	0.238538	2.162172	-0.436887
13	1	0	0.728540	1.797371	0.988942
14	1	0	0.121438	3.113692	-0.548783
15	6	0	-2.660554	0.913800	0.336814
16	1	0	-2.040484	0.850143	1.238445
17	1	0	-3.087808	1.920882	0.294142
18	8	0	-1.848173	0.691629	-0.814417
19	6	0	-3.764138	-0.124783	0.375280
20	1	0	-3.337265	-1.129106	0.421424
21	1	0	-4.398925	0.023295	1.251186
22	1	0	-4.384573	-0.052286	-0.520263
23	35	0	-0.188899	-1.121681	-0.247749
24	7	0	1.330913	-2.179325	0.267313
25	1	0	1.072571	-2.751455	1.067431

Standard orientation of TS-$NHBr_2$-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$NHBr_2$-Alcohol
State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -799.72 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.872694	2.320348	0.830862
2	1	0	0.653243	2.475873	-0.161006
3	1	0	1.251415	1.358157	0.942604
4	8	0	-1.558412	2.387784	1.548520
5	1	0	-0.046558	2.374602	1.279518
6	1	0	-1.952656	3.197422	1.880438
7	1	0	-2.441888	0.445678	-0.859620
8	8	0	-0.044495	2.586578	-1.509991
9	1	0	-0.973974	2.247092	-1.388233
10	1	0	-0.076104	3.448759	-1.930492
11	8	0	-2.412539	1.629559	-0.836002
12	1	0	-2.011948	2.126483	0.700850
13	1	0	-3.208010	2.003292	-1.220436
14	6	0	-3.250382	-1.305028	0.155501
15	1	0	-3.038983	-0.889140	1.148393
16	1	0	-4.260559	-0.986301	-0.120050
17	8	0	-2.334005	-0.785481	-0.791209
18	6	0	-3.176656	-2.819215	0.199094
19	1	0	-2.175880	-3.143240	0.485318
20	1	0	-3.887525	-3.222240	0.921418
21	1	0	-3.405583	-3.236802	-0.781373
22	35	0	-0.252610	-0.654128	0.063520
23	7	0	1.505010	-0.193466	0.874748
24	1	0	1.602015	-0.749468	1.717548
25	35	0	2.990158	-0.673321	-0.200752

Standard orientation of TS-NH_2Cl-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-NH_2Cl-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -912.77 cm^{-1}
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	1	0	-1.401356	2.980526	-0.662843
2	8	0	-2.734175	0.501136	0.561907
3	1	0	-2.729663	-0.037714	-0.284696
4	1	0	-2.042241	1.513675	0.367333
5	8	0	-1.210699	-1.166290	1.854405
6	1	0	-2.247887	-0.084011	1.213250
7	1	0	-1.560440	-1.866011	2.409090
8	1	0	1.091559	-1.190348	-0.669826
9	8	0	-2.292401	-1.042172	-1.476555
10	1	0	-1.455677	-1.504297	-1.092446
11	1	0	-2.917334	-1.713300	-1.757105
12	8	0	-0.242705	-2.031079	-0.342652
13	1	0	-0.773675	-1.584995	1.025275
14	1	0	-0.138726	-2.981588	-0.417583
15	17	0	0.205579	1.375176	-0.355706
16	6	0	2.694102	-0.642827	0.362622
17	1	0	2.091573	-0.426726	1.251103
18	1	0	3.106665	-1.649095	0.480562
19	6	0	3.811252	0.369925	0.230277
20	1	0	4.458370	0.349376	1.107142
21	1	0	4.416678	0.154418	-0.650082
22	1	0	3.400914	1.374763	0.127589
23	7	0	-1.160008	2.366581	0.107593
24	1	0	-0.899396	2.934297	0.906690
25	8	0	1.879195	-0.583549	-0.799229

Standard orientation of TS-$NHCl_2$-Alcohol

Cartesian coordinates of the transition state optimized at the M05-2X/6-311+G(d) level:

Standard orientation of transition state of TS-$NHCl_2$-Alcohol
State=1-A Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -232.95 cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.035015	1.449501	0.851426
2	1	0	1.896379	1.755786	-0.077410

3	1	0	1.931009	0.040953	0.846262
4	8	0	-0.358637	2.321037	1.653833
5	1	0	1.247128	1.802715	1.330077
6	1	0	-0.513910	3.198951	2.007345
7	1	0	-1.809852	0.716418	-0.820776
8	8	0	1.122079	2.189499	-1.541618
9	1	0	0.144197	2.150146	-1.325693
10	1	0	1.310388	3.039368	-1.944097
11	8	0	-1.369714	1.994081	-0.747458
12	1	0	-0.827401	2.246392	0.772052
13	1	0	-2.003150	2.632229	-1.080327
14	6	0	-3.027331	-0.605084	0.200841
15	1	0	-2.657471	-0.288651	1.181500
16	1	0	-3.907563	-0.001190	-0.032041
17	8	0	-2.032645	-0.355288	-0.786402
18	6	0	-3.379727	-2.077246	0.212968
19	1	0	-2.501131	-2.678485	0.446208
20	1	0	-4.144205	-2.282257	0.962370
21	1	0	-3.759269	-2.383895	-0.761281
22	7	0	1.630194	-1.038271	0.699097
23	1	0	1.571179	-1.559846	1.569249
24	17	0	-0.055584	-0.860523	-0.007504
25	17	0	2.754753	-1.834618	-0.338862
