Supporting Information

Insights into the reaction mechanisms and reaction sites of purine bases and nucleosides during chlorination: a computational study

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Text S1

Quantum Chemical Linear Free Energy Relationship (LFER) for Estimation of pK_a Values

Based on the proton theory of acids and bases, acid is a donor of protons, and the stronger the ability to provide protons, the stronger the acidity. Therefore, the bond dissociation energy (BDE) of R_1NH^+ releasing proton and R_1N, as shown in Eq. 1, can be as an indicator of acidity.

$$R_1NH^+ \rightarrow R_1N + H^+ \quad (1)$$

Thus, BDEs of nineteen Nitrogen-Containing Heterocycles were calculated at the M06-2X(D3)/cc-pvtz level with the SMD solvent model. Then the correlation between the BDEs and experimental pK_a values was established and illustrated in Figure S1 and Table S1, the squared correlation coefficient for the above system is $R^2 = 0.98$.

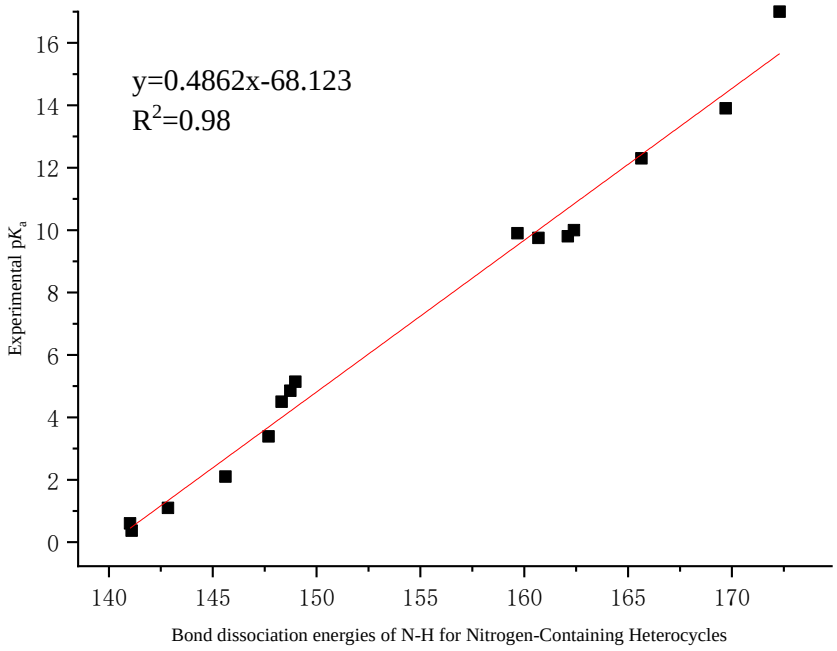

Figure S1. The correlation between BDEs and the experimental pK_a values of N-H bonds for Nitrogen-Containing Heterocycles.

Table S1. The calculated BDEs (in kcal/mol) and pK_a values of N−H bond in nitrogen-containing heterocycles along with the experimental known pK_a values.

Nitrogen-Containing Heterocycles	BDE (kcal/mol)	pK_a (exp.)	pK_a (calc.)
benzimidazole	165.6	12.3[1]	12.4
phthalimide	159.7	9.9[1]	9.5
indazole	169.8	13.9[1]	14.4
adenine	162.1	9.8[1]	10.7
indole	172.3	17.0[1]	16.5
cytosine	148.3	4.5[2]	4.0
quinoxaline	141.0	0.6[2]	0.4
3-Methyluracil	160.7	9.7[2]	10.0
1-Methyluracil	162.5	10.0[2]	10.8
pyridine	149.0	5.1[2]	4.4
phthalazine	147.7	3.4[2]	3.7
pyridazine	145.6	2.1[2]	2.7
pyrimidine	142.8	1.1[2]	1.3
quinoline	148.7	4.9[3]	4.2
pyrazine	141.1	0.4[4]	0.5

The correlation between the BDEs and experimental pK_a values of C-H bonds for nine organic compounds were established and illustrated in Figure S2 and Table S2. The squared correlation coefficient for the above system is $R^2 = 0.97$.

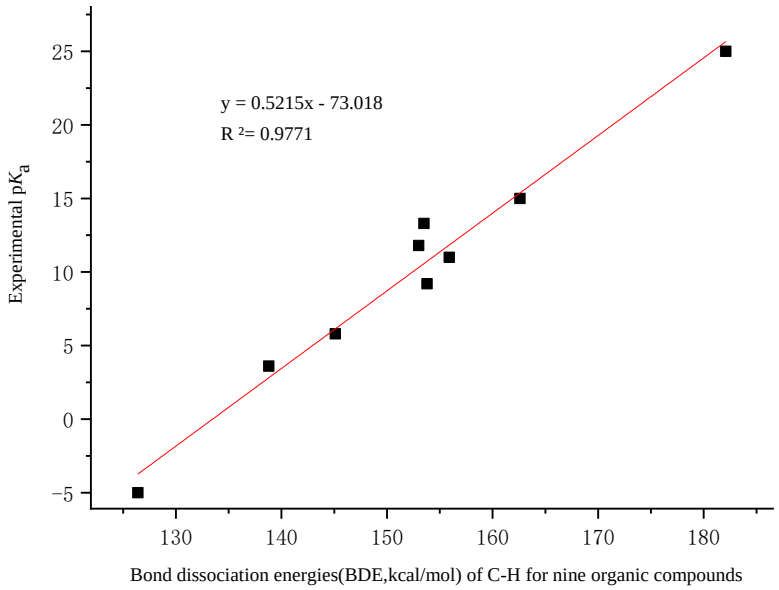

Figure S2. The correlation between BDEs and the experimental pK_a values of C-H bonds for nine organic compounds.

Table S2. The calculated BDEs (in kcal/mol) and pK_a values of C−H bond for nine organic compounds precursors along with the known experimental pK_a values.

Organic Compounds	BDE (kcal/mol)	pK_a (exp.)	pK_a (calc.)
$CH\text{-}(CN)_3$	126.4	-5.0[2]	-4.0
$CH_2\text{-}(COO\text{-}C_2H_5)_2$	153.5	13.3[2]	10.7
$C_2H_5\text{-}O_2C\text{-}CH_2\text{-}NO$	145.1	5.8[2]	6.1
HCN	153.8	9.2[2]	10.8
$CH_3COCH_2COOC_2H_5$	155.9	11.0[2]	11.9
$CH_3\text{-}CO\text{-}CHCl_2$	162.6	15.0[5]	15.6
$CH_3\text{-}CN$	182.1	25.0[5]	26.2
$CH_2\text{-}(NO_2)_2$	138.8	3.6[5]	2.7
$CH_2\text{-}(CN)_2$	153.0	11.8[5]	10.4

Table S3. The pK_a values of most stable isomers of guanine, adenine, and their chlorinated products.

Heterolytic reaction	BDE(kcal/mol)	pK_a (calc.)
G1		
G1 → C_8- **G1**$^-$ + H^+	200.3	31.4
G1 → NH- **G1**$^-$ + H^+	172.8	16.2
G1 → N_1- **G1**$^-$ + H^+	162.3	10.8
G1 → N_9- **G1**$^-$ + H^+	158.8	9.2
7-H- **G1**$^+$ →**G1** + H^+	144.7	2.2
3-H- **G1**$^+$ →**G1** + H^+	140.8	0.4
NH_3- **G1**$^+$→**G1** + H^+	128.9	-5.4
G2		
G2 → C_8- **G2**$^-$ + H^+	198.4	30.4
G2 → N_1- **G2**$^-$ + H^+	161.4	10.6
G2 → N_7- **G2**$^-$ + H^+	160.8	9.9
9-H- **G2**$^+$ →**G2** + H^+	145.8	2.8
3-H- **G2**$^+$ →**G2** + H^+	144.9	2.3
NH_3- **G2**$^+$→**G2** + H^+	130.5	-4.6
G2 → NH- **G2**$^-$ + H^+	174.7	16.8
G3		
1-H- **G3**$^+$ →**G3** + H^+	148.0	3.8
G3 → N_3- **G3**$^-$ + H^+	158.3	8.9
G3 → N_7- **G3**$^-$ + H^+	160.6	10.1
G3 → C_8- **G3**$^-$ + H^+	197.3	29.8
9-H- **G3**$^+$ →**G3** + H^+	140.8	0.3
NH_3- **G3**$^+$→**G3** + H^+	128.8	-5.4
G3 → NH- **G3**$^-$ + H^+	173.3	16.1
9-Cl-G1		
9-Cl-G1 → n1- **9-Cl-G1**$^-$ + H^+	161.4	10.3
9-Cl-G1 → nh- **9-Cl-G1**$^-$ + H^+	171.0	14.9
9-Cl-G1 → c8- **9-Cl-G1**$^-$ + H^+	192.8	27.5
3-H-**9-Cl-G1**$^+$ →**9-Cl-G1** + H^+	136.5	-1.7
7-H-**9-Cl-G1**$^+$ →**9-Cl-G1** + H^+	139.5	-0.2
Adenine isomer **A1**		
1-H- **A1**$^+$ →**A1** + H^+	147.7	3.7
A1 → C_2- **A1**$^-$ + H^+	215.3	39.2
3-H- **A1**$^+$ →**A1** + H^+	145.1	2.5
7-H- **A1**$^+$ →**A1** + H^+	143.7	1.8
A1 → C_8- **A1**$^-$ + H^+	199.1	30.8

A1 → N_9- **A1**$^-$ + H^+	160.2	9.8
NH_3- **A1**$^+$→**A1** + H^+	133.1	-3.3
A1 → NH- **A1**$^-$ + H^+	176.5	17.7
Adenine isomer **A2**		
1-H- **A2**$^+$ →**A2** + H^+	147.4	3.5
A2 → C_2- **A2**$^-$ + H^+	216.4	39.8
3-H- **A2**$^+$ →**A2** + H^+	148.6	4.2
A2 → N_7- **A2**$^-$ + H^+	160.5	9.9
A2 → C_8- **A2**$^-$ + H^+	198.1	30.3
9-H- **A2**$^+$ →**A2** + H^+	145.3	2.5
NH_3- **A2**$^+$→**A2** + H^+	132.6	-3.6
A2 → NH-**A2**$^-$ + H^+	174.5	16.7
9-Cl-A1		
7-H-**9-Cl-A1**$^+$ →**9-Cl-A1** + H^+	138.4	-0.7
1-H-**9-Cl-A1**$^+$ →**9-Cl-A1** + H^+	145.6	2.7
9-Cl-A1 → c8- **9-Cl-A1**$^-$ + H^+	191.6	26.9
9-Cl-A1 → c2- **9-Cl-A1**$^-$ + H^+	213.1	38.1
9-Cl-A1→ NH- **9-Cl-A1**$^-$ + H^+	174.4	16.5
3-H-**9-Cl-A1**$^+$ →**9-Cl-A1** + H^+	140.7	0.4
Gua 1		
Gua 1 → C_8-**Gua 1**$^-$ + H^+	192.1	27.2
Gua 1 → NH_2-**Gua 1**$^-$ + H^+	170.4	15.0
Gua 1 → N1- **Gua 1**$^-$ + H^+	162.3	10.8
7-H- **Gua 1**$^+$ →**Gua 1** + H^+	143.8	1.8
3-H- **Gua 1**$^+$ →**Gua 1** + H^+	140.0	-0.2
NH_3- **Gua 1**$^+$→**Gua 1** + H^+	128.4	-5.6
1-Cl-Gua 1		
3-H- **1-Cl-Gua 1**$^+$ →**1-Cl-Gua 1** + H^+	135.7	-2.1
7-H- **1-Cl-Gua 1**$^+$ →**1-Cl-Gua 1** + H^+	142.2	1.0
NH_3- **1-Cl-Gua 1**$^+$→**1-Cl-Gua 1** + H^+	124.2	-7.6
1-Cl-Gua 1 → NH- **1-Cl-Gua 1**$^-$ + H^+	167.6	13.3
1-Cl-Gua 1 → C_8- **1-Cl-Gua 1**$^-$ + H^+	196.0	29.1
Ado 1		
1-H- **Ado 1**$^+$ →**Ado 1** + H^+	147.3	3.5
3-H- **Ado 1**$^+$ →**Ado 1** + H^+	144.4	2.1
7-H- **Ado 1**$^+$ →**Ado 1** + H^+	143.5	1.6
NH_3- **Ado 1**$^+$→**Ado 1** + H^+	132.6	-3.6
Ado 1 → C_2- **Ado 1**$^-$ + H^+	214.5	38.8
Ado 1 → C_8- **Ado 1**$^-$ + H^+	195.4	28.8
Ado 1 → NH- **Ado 1**$^-$ + H^+	175.9	17.4

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Text S2

Calculation of proportion of neutral and anion forms

For the general acid (HA) and diprotic acid (H_2A) with $pK_{a1} << pK_{a2}$, as presented in eqs. (1)–(3), the fractions of the respective neutral and anion form can be calculated as follows.

$$HA \rightleftharpoons A^- + H^+ \qquad K_a = [HA^-][H^+]/[HA] \qquad (1)$$

$$H_2A \rightleftharpoons HA^- + H^+ \qquad K_{a1} = [HA^-][H^+]/[H_2A] \qquad (2)$$

$$HA^- \rightleftharpoons A^{2-} + H^+ \qquad K_{a2} = [A^{2-}][H^+]/[HA_1^-] \qquad (3)$$

$p(A)=1/(1+[H^+]/K_a)$ and $p(N) =1- p(A)$.

However, for the diprotic acid (H_2A) possessing two close pK_{a1} values such as guanine, its pK_{a1} and pK_{a1}' values are 9.2 and 10.8 for **G1**, 9.9 and 10.6 for **G2**, as well as 8.9 and 10.1 for **G3**. Accordingly, the dissociation equilibriums of H_2A exist as follows.

$$H_2A \rightleftharpoons HA^{\vdash} + H^+ \qquad K_{a1}' = [HA^{\vdash}]\,[H^+]/[H_2A] \qquad (4)$$

$$HA^{\vdash} \rightleftharpoons A^{2-} + H^+ \qquad K_{a2}' = [A^{2-}][H^+]/[HA_2^-] \qquad (5)$$

Moreover, the calculated pK_{a2} and pK'_{a2} of above compounds are very high with the values of 14–15. This indicates that the secondary dissociations are very small, therefore, they can be ignored. Thus, the proportions of the neutral (H_2A) and the anion forms (HA^- and $HA^{\vdash}$) of guanine can be calculated from eqs. (6)–(8).

$$p(H_2A) = 1/ (1+ K_{a1}/[H^+] + K_{a1}'/[H^+]) \qquad (6)$$

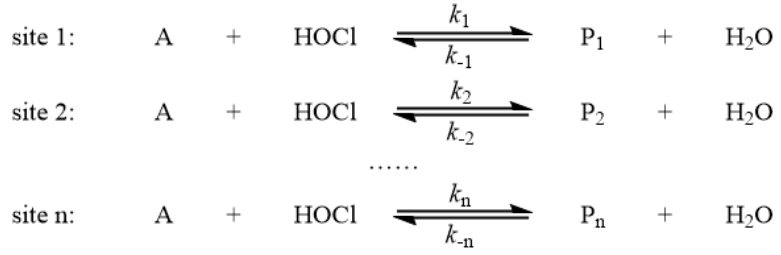
$$p(HA^-) = K_{a1}/ ([H^+]+ K_{a1} + K_{a1}') \qquad (7)$$

$$p(HA^{\vdash}) = K_{a1}' / ([H^+]+ K_{a1}+ K_{a1}') \qquad (8)$$

Text S3

Yield calculation of the chlorinated products based on numerical simulation methods

As it is known that there are several reactive sites in nucleobases/nucleosides during chlorination. These reactions as shown in Scheme S1 can be seen as parallel reactions, and in addition to the forward reactions, their reverse reactions should be considered.



Scheme S1. Parallel reactions for chlorination of all the potential reaction sites of A

The concentration changes of reactants and products in above reactions over time can be expressed as eqs. (1) and (2), respectively. The concentration of water in the dilute solution is 55.6 mol/L.

$$\frac{dc(\mathrm{A})}{dt} = \frac{dc(\mathrm{HOCl})}{dt} = -\sum k_n\, c(\mathrm{A})c(\mathrm{HOCl}) + \sum 55.6k_{-n}\, c(\mathrm{P}_n) \qquad (1)$$

$$\frac{dc(\mathrm{P}_n)}{dt} = k_n c(\mathrm{A})c(\mathrm{HOCl}) - 55.6k_{-n}c(\mathrm{P}_n) \qquad (2)$$

The numerical Euler method was used to obtain the concentrations of various products at reaction time ***t***. The idea behind Euler method is that d*t* in the equations can be replaced by a sufficiently small **Δ*t***, which is so small that the concentrations of reactants and products are approximately the same, which means the reaction rate ***v*** remains constant during **Δ*t***. Based upon this method, the concentration changes of reactants and products after a period of time **Δ*t*** can be calculated from the initial concentration of reactants and products at $\mathbf{t_0}$, and the concentrations of reactants and products at $\mathbf{t_0}$+**Δ*t*** are the sum of the concentration change and the concentration at time $\mathbf{t_0}$. Subsequently, let $\mathbf{t_0}$+**Δ*t*** to be the new time $\mathbf{t_0}$ and repeat the above process, and then the concentration of products after reaction time $\mathbf{t_0}$+**Δ*t*** can be obtained.

In this study, the rate constants *k* of forward reaction (k_n) is the estimated apparent rate constant ($k_{obs\text{-}est}$) calculated as described in the main text, the equilibrium constant K_{eq} can be obtained from eq. (3), and the rate constants *k* of reverse reaction (k_{-n}) can be calculated in eq. (4).

$$K_{eq} = e^{-\frac{\Delta G}{RT}} \qquad (3)$$

$$k_{-n} = k_n / K_{eq} \quad (4)$$

Following the general chlorination experimental conditions, the initial concentrations of nucleobase/nucleoside and HOCl were set to be 10^{-5} and 2×10^{-4} mol/L, respectively, and pH is 7, the same as calculating the estimated apparent rate constant $k_{obs\text{-}est}$. The step size of time $\boldsymbol{\Delta t}$ was set to be 10^{-6} s. In above conditions, it can be calculated that when the K_{eq} of a reaction site is less than 1, the yield of this reaction site is ~0.0004%. This means that the yield of the reaction with a positive ΔG value is so small that it can be ignored.

Table S4. Yields (%) of various chlorinated products at all possible reaction sites in guanine and adenine over time.

Time	15 min	30 min	1 h	2 h	6 h	12 h	1 d	3 d	7 d
guanine									
N1	3.20	3.20	3.19	3.19	3.17	3.15	3.10	2.92	2.63
N7	0.70	0.70	0.70	0.70	0.70	0.69	0.68	0.64	0.58
C8	$2*10^{-5}$	$4*10^{-5}$	$8*10^{-5}$	0.0002	0.0005	0.0010	0.0019	0.0056	0.012
N9	96.06	96.03	95.96	95.84	95.34	94.60	93.16	87.83	79.05
N^2	0.033	0.066	0.13	0.26	0.78	1.55	3.05	8.59	17.72
adenine									
N1	$8*10^{-6}$	$8*10^{-6}$	$8*10^{-6}$	$8*10^{-6}$	$8*10^{-6}$	$7*10^{-6}$	$7*10^{-6}$	$7*10^{-6}$	$7*10^{-6}$
N3	0.0053	0.0053	0.0053	0.0053	0.0053	0.0053	0.0053	0.0051	0.0049
N7	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.15	0.15
C8	$2*10^{-7}$	$3*10^{-7}$	$6*10^{-7}$	$1*10^{-6}$	$3*10^{-6}$	$7*10^{-6}$	$1*10^{-5}$	$4*10^{-5}$	$1*10^{-4}$
N9	99.78	99.76	99.73	99.68	99.45	99.11	98.44	95.79	90.72
N^6	0.014	0.029	0.057	0.11	0.34	0.68	1.36	4.01	9.09

Table S5. Yields (%) of various chlorinated products at all possible reaction sites in guanosine and adenosine over time.

Time	guanosine			adenosine		
	N1	C8	N^2	N1	C8	N^6
15 min	99.01	0.011	0.51	0.0028	0.0017	0.31
30 min	98.52%	0.021	1.00	0.0028	0.0033	0.61
1 h	97.55	0.042	1.95	0.0027	0.0067	1.22
2 h	95.63	0.082	3.84	0.0027	0.013	2.42
6 h	88.36	0.23	10.99	0.0026	0.039	7.07
12 h	78.52	0.44	20.67	0.0024	0.074	13.61
1 d	62.17	0.79	36.75	0.0020	0.14	25.29
3 d	25.72	1.61	72.55	0.0011	0.32	57.84
7 d	7.32	2.16	90.49	0.0004	0.47	86.07

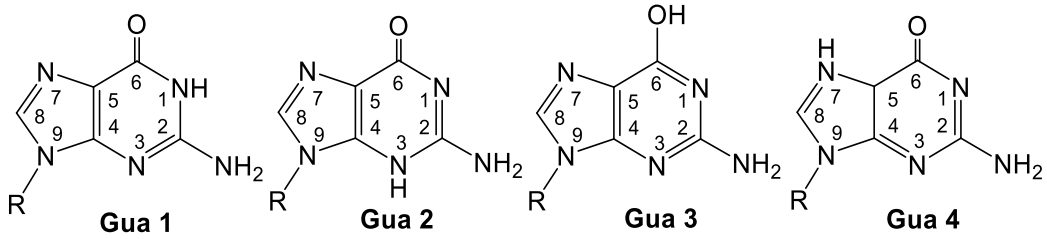
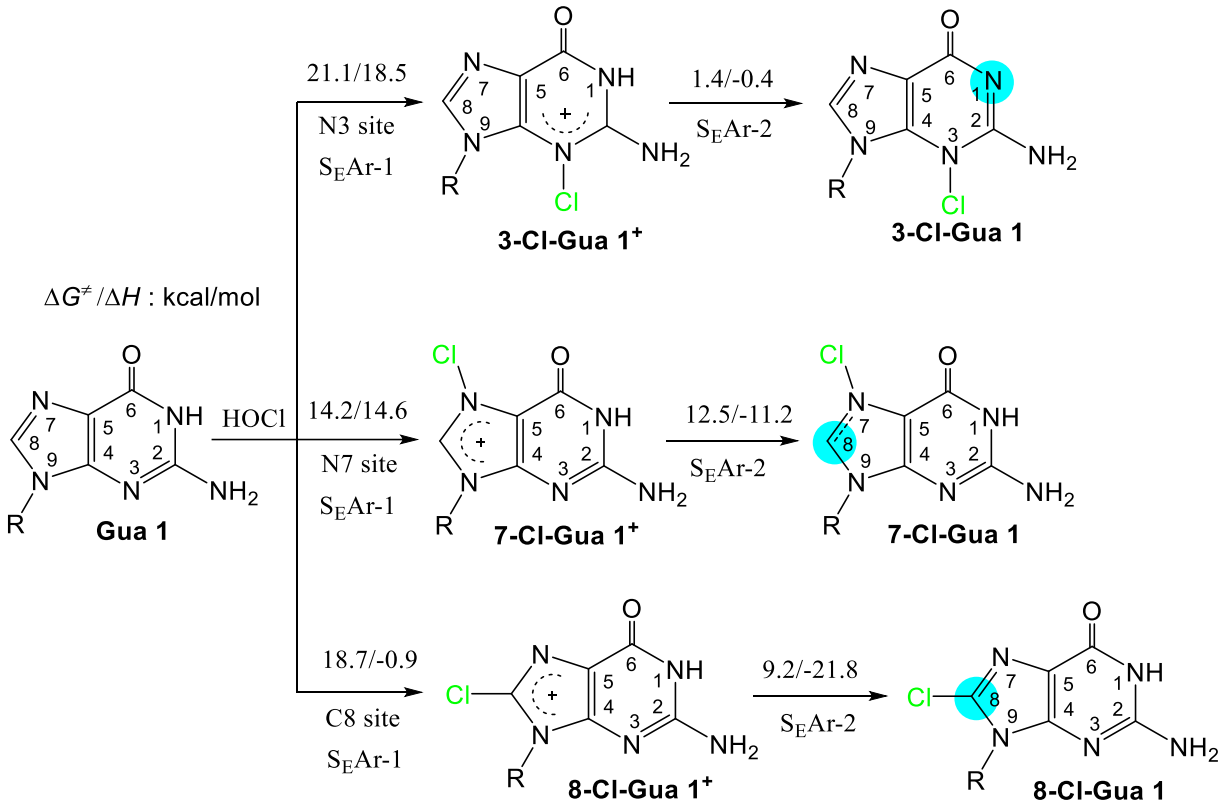


Figure S3. The structures of guanosine isomers.

Table S6. Relative energies (R*G*, in kcal/mol) and Boltzmann distribution populations *f* of various guanosine isomers.

Isomer	**Gua 1**	**Gua 2**	**Gua 3**	**Gua 4**
R*G*	0.0	7.3	8.1	10.4
f	0.99999	10^{-7}	10^{-7}	10^{-9}



Scheme S2. The classic S_EAr reaction mechanism of N3, N7, and C8 in guanosine during chlorination.

Table S7. $\Delta G^{\neq}$ and ΔH (in kcal/mol) in the chlorination of each site in the neutral and anion forms of **Gua 1** via concerted and classic S_EAr reaction mechanisms.

Reactive site	Neutral						Anion	
	Concerted		S_EAr-1		S_EAr-2		Concerted	
	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH
N1	27.9	-4.7	--	--	--	--	4.3	-0.3
N3	18.6	3.1	21.1	18.5	1.4	-0.4	7.6	1.3
N7	--	--	14.2	14.6	12.5	-11.2	10.3	-3.6
C8	38.1	-46.7	18.7	-0.9	9.2	-21.8	20.5	-15.4
N^2	25.6	-8.0	--	--	--	--	18.7	14.9

Table S8. The estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of each reactive site in the neutral and anion forms of isomer **Gua 1** and their contributions (c, %) the $k_{obs\text{-}est}$ of guanosine calculated at the M06-2X(D3)/aug-cc-pVTZ//M06-2X(D3)/6-311G(d) level with the SMD solvent model.

Reactive site	Neutral		Anion		Guanosine
	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$
N1	2.4×10^{-8}	0%	5.8×10^{5}	100%	5.8×10^{5}
N3	1.6×10^{-1}	0%	2.2×10^{3}	100%	2.2×10^{3}
N7	$2.6\times10^{2*}$	92%	2.4×10^{1}	8%	2.8×10^{2}
C8	$1.3\times10^{-1*}$	100%	7.9×10^{-7}	0%	1.3×10^{-1}
N^2	1.2×10^{-6}	7%	1.7×10^{-5}	93%	1.8×10^{-5}

* represents reaction via S_EAr mechanism.

The pK_a value of N1-H being 10.8, f(N(**1**))=0.99987 and f(A(1))=0.00013. $c = \frac{k\text{obs-est (N/A)}f(i)}{k\text{obs-est (Guanosine)}}\%$

Table S9. The apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) for the chlorination of the N1 site in **Gua 1** by HOCl calculated with M052X(D3), M062X(D3), and B3LYP(D3BJ) functionals along with 6-31+G(d), 6-311G(d), and 6-311+G(d) basis sets and two implicit CPCM and SMD solvent models.

Basis set	CPCM			SMD		
	M05-2X	M06-2X	B3LYP	M05-2X	M06-2X	B3LYP
6-31+G(d)	3.7×10^{6}	-	4.9×10^{8}	4.4×10^{6}	1.4×10^{4}	9.7×10^{8}
6-311G(d)	1.3×10^{7}	3.5×10^{5}	3.1×10^{9}	1.2×10^{7}	5.8×10^{5}	4.4×10^{9}
6-311+G(d)	8.7×10^{6}	-	3.7×10^{9}	2.2×10^{6}	2.0×10^{4}	6.9×10^{8}

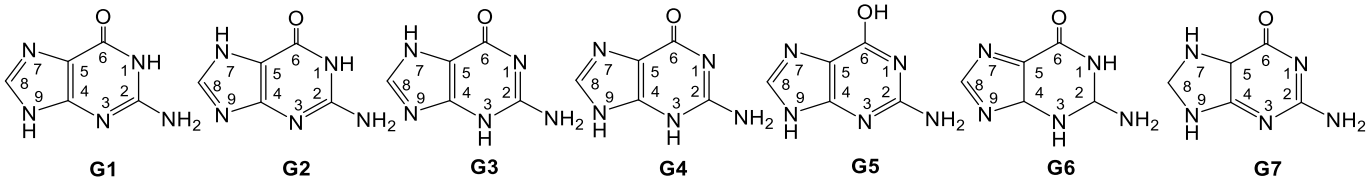
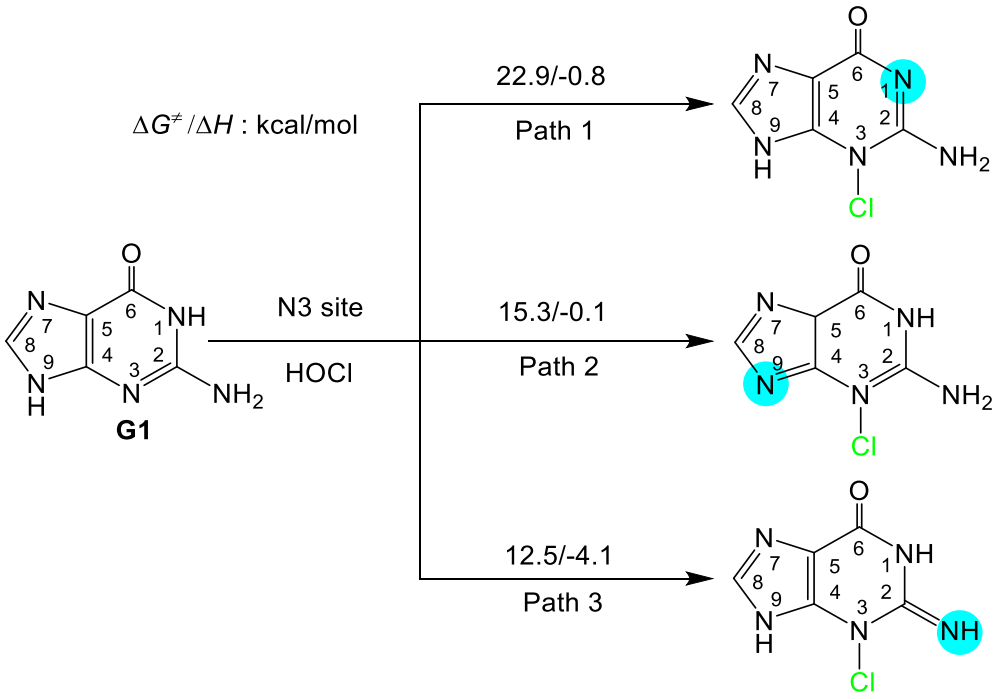


Figure S4. The structures of guanine isomers.

Table S10. Relative energies (R*G*, in kcal/mol) and Boltzmann distribution populations *f* of various guanine isomers.

Isomer	**G1**	**G2**	**G3**	**G4**	**G5**	**G6**	**G7**
R*G*	0.0	1.5	3.8	7.0	8.4	8.7	11.2
f	0.925	7.4×10^{-2}	1.4×10^{-3}	10^{-7}	10^{-8}	10^{-8}	10^{-9}



Scheme S3. Three concerted pathways for chlorination of the N3 site in guanine isomer **G1**.

Table S11. $\Delta G^{\neq}$ and ΔH (in kcal/mol) in chlorination of each site in guanine isomers **G1**, **G2,** and **G3** via concerted and classic S_EAr reaction mechanisms.

Reactive site	N (**G1**)				N (**G2**)				N (**G3**)			
	Concerted		S_EAr-1		Concerted		S_EAr-1		Concerted		S_EAr-1	
	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH
N1	19.5	-12.1	--	--	21.6	-8.4	--	--	8.2	-7.7	17.0	16.3
N3	12.5	-4.1	19.9	17.4	7.6	-7.2	14.5	12.1	16.5	-9.8	--	--
N7	13.8	11.6	14.7	13.4	17.5	-12.5	--	--	19.1	-12.1	--	--
C8	23.5	-19.6	24.8	5.9	33.5	-11.6	32.2	-21.0	32.2	-15.5	32.2	-22.2
N9	19.6	-12.7	--	--	10.2	6.6	10.6	8.5	16.6	12.8	16.9	14.7
N^2	21.3	-10.0	--	--	26.6	-11.0	--	--	25.9	-10.7	--	--

Reactive site	A^-(**G1/G2**)		$A^{\vdash}$(**G1**)		A^-(**G3**)/ $A^{\vdash}$(**G2**)		$A^{\vdash}$(**G3**)	
	Concerted		Concerted		Concerted		Concerted	
	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH
N1	23.3	-12.8	5.0	-0.2	4.2	-2.7	9.1	5.4
N3	5.1	1.6	6.0	0.5	5.4	-1.3	22.5	-12.3
N7	1.3	-1.8	6.1	4.8	20.8	-15.9	2.4	-1.3
C8	17.2	-8.3	16.1	-12.8	25.2	4.8	13.0	-9.7
N9	4.8	-0.7	23.8	-15.0	6.3	3.5	4.1	0.6
N^2	22.0	-12.4	10.8	7.2	10.1	6.0	22.6	16.4

Table S12. The estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of each reactive site in the neutral and anion forms of guanine isomers **G1**, **G2,** and **G3** and their contributions (c, %) in the parentheses to the $k_{obs\text{-}est}$ of guanine.

Reactive site	**G1**			**G2**			**G3**			Guanine
	N	A^-	A'^-	N	A^-	A'^-	N	A^-	A'^-	$k_{obs\text{-}est}$
N1	3.1×10^{-2} (0%)	3.2×10^{-7} (0%)	2.1×10^{5} (50%)	7.3×10^{-5} (0%)	5.2×10^{-9} (0%)	1.0×10^{5} (25%)	9.0×10^{3} (2%)	9.7×10^{4} (23%)	1.6 (0%)	4.2×10^{5}
N3	4.2×10^{3} (0%)	7.0×10^{6} (82%)	3.8×10^{4} (1%)	1.3×10^{6} (16%)	1.1×10^{5} (1%)	1.4×10^{4} (0%)	7.5×10^{-3} (0%)	1.3×10^{4} (0%)	2.4×10^{-10} (0%)	8.5×10^{6}
N7	4.7×10^{2} (0%)	4.5×10^{7} (98%)	3.3×10^{4} (0%)	7.3×10^{-2} (0%)	7.2×10^{5} (2%)	7.0×10^{-8} (0%)	9.3×10^{-5} (0%)	6.7×10^{-8} (0%)	3.5×10^{2} (0%)	4.5×10^{7}
C8	3.7×10^{-5} (0%)	9.5×10^{-3} (71%)	1.5×10^{-3} (12%)	1.4×10^{-13} (0%)	1.5×10^{-4} (1%)	4.2×10^{-11} (0%)	2.4×10^{-14} (0%)	4.0×10^{-11} (0%)	2.2×10^{-3} (16%)	1.3×10^{-2}
N9	2.6×10^{-2} (0%)	1.2×10^{7} (98%)	3.5×10^{-9} (0%)	1.6×10^{4} (0%)	1.9×10^{5} (2%)	3.0×10^{3} (0%)	6.3×10^{-3} (0%)	2.8×10^{3} (0%)	7.3×10^{3} (0%)	1.2×10^{7}
N^2	1.5×10^{-3} (0%)	2.9×10^{-6} (0%)	1.2×10^{1} (55%)	1.6×10^{-8} (0%)	4.7×10^{-8} (0%)	4.9 (23%)	9.7×10^{-10} (0%)	4.6 (22%)	2.0×10^{-10} (0%)	2.1×10^{1}

The pK_a of N9−H moiety and p$K_{a'}$ of N1−H moiety in **G1** are 9.2 and 10.8, respectively, with f(N(**G1**))=0.994, f(A^-(**G1**))=0.006, and f(A'^-(**G1**))=0.0002. pK_a of N7−H moiety and p$K_{a'}$ of N1−H moiety in **G2** are 9.9 and 10.6, respectively, with f(N(**G2**))=0.999, f(A^-(**G2**))=0.001, and f(A'^-(**G2**))=0.0003. pK_a of N3−H moiety and p$K_{a'}$ of N7−H moiety in **G3** are 8.9 and 10.1, respectively, with f(N(**G3**))=0.988, f(A^-(**G3**))=0.012, and f(A'^-(**G3**))=0.0008.

$$c = \frac{k\text{obs-est (N/A)}f(\boldsymbol{i})}{k\text{obs-est (Guanine)}}\%$$

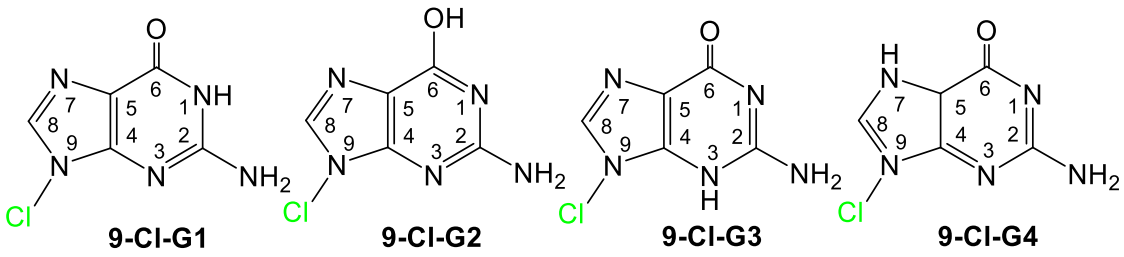


Figure S5. The structures of 9-Cl-guanine isomers.

Table S13. Relative energies (R*G*, in kcal/mol) and Boltzmann distribution populations *f* of various 9-Cl-guanine isomers.

Isomer	**9-Cl-G1**	**9-Cl-G2**	**9-Cl-G3**	**9-Cl-G4**
R*G*	0	7.2	8.5	13.3
f	1	10^{-6}	10^{-7}	10^{-10}

Scheme S4. Chlorination of all the potential reaction sites in 9-Cl-guanine by HOCl.

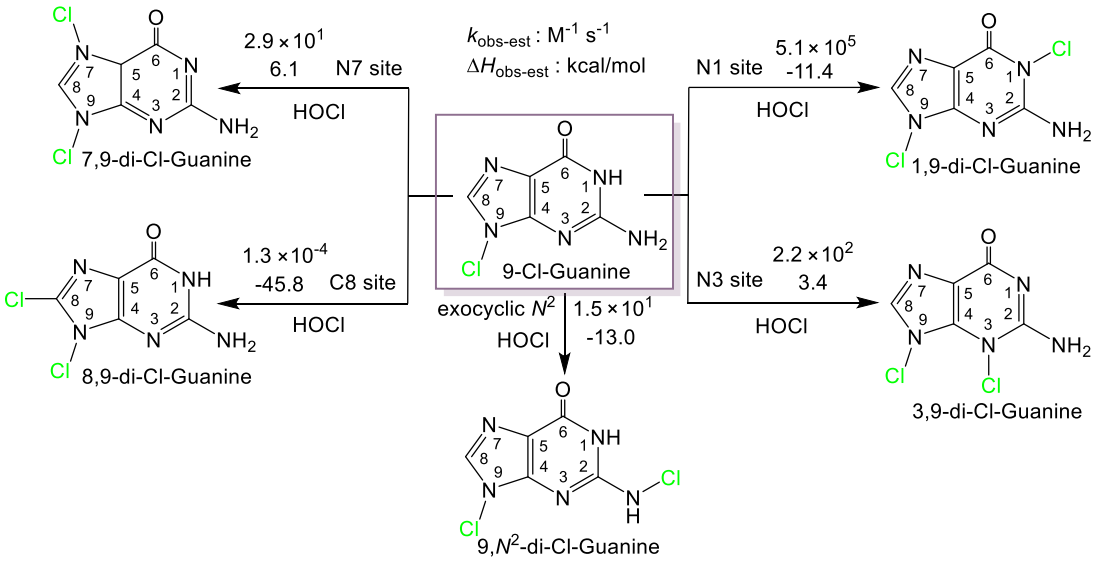


Table S14. $\Delta G^{\neq}$ and ΔH (in kcal/mol) in chlorination of each site in isomer **9-Cl-G1** via concerted and classic S_EAr reaction mechanisms.

Reactive site	Neutral				Anion	
	Concerted		S_EAr-1		Concerted	
	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH
N1	23.3	-4.1	--	--	5.2	-1.2
N3	19.8	2.8	--	--	9.8	7.3
N7	--	--	20.1	18.7	11.0	10.2
C8	--	--	27.7	7.6	18.3	-4.8
N^2	23.0	-8.8	--	--	11.4	8.4

Table S15. The estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of each reactive site in the neutral and anion forms of isomer **9-Cl-G1** to and their contributions (c, %) to the $k_{obs\text{-}est}$ of 9-Cl-guanine.

Reactive site	Neutral		Anion		9-Cl-Guanine
	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$
N1	5.6×10^{-5}	0%	5.1×10^{5}	100%	5.1×10^{5}
N3	2.0×10^{-2}	0%	2.2×10^{2}	100%	2.2×10^{2}
N7	1.2×10^{-2}	0%	2.9×10^{1}	100%	2.9×10^{1}
C8	3.3×10^{-8}	0%	1.3×10^{-4}	100%	1.3×10^{-4}
N^2	9.3×10^{-5}	0%	1.5×10^{1}	100%	1.5×10^{1}

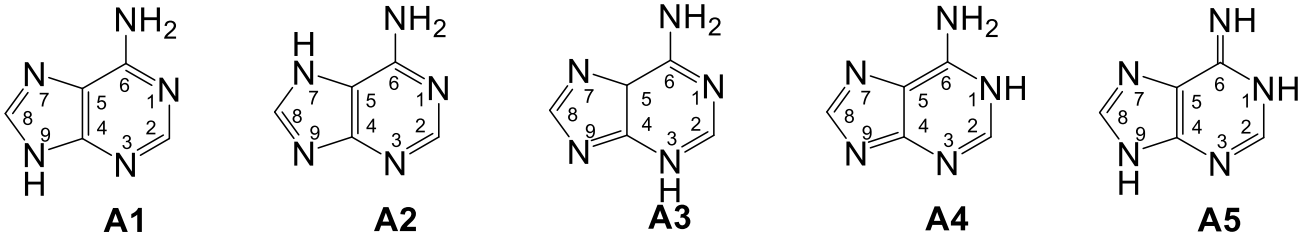


Figure S6. The structures of adenine isomers.

Table S16. Relative energies (RG, in kcal/mol) and Boltzmann distribution populations f of various adenine isomers.

Isomer	**1**	**A2**	**A3**	**A4**	**A5**
RG	0.0	1.8	5.0	6.3	12.5
f	0.956	0.044	10^{-4}	10^{-5}	10^{-10}

Table S17. $\Delta G^{\neq}$ and ΔH (in kcal/mol) in chlorination of each site in adenine isomers **A1** and **A2** via concerted and classic S_EAr reaction mechanisms.

Reactive site	Neutral (**A1**)				Neutral (**A2**)				Anion (**A1**/**A2**)	
	Concerted		S_EAr-1		Concerted		S_EAr-1		Concerted	
	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH
N1	10.3	-3.8	11.7	9.5	11.1	-4.6	10.8	8.8	2.0	0.2
C2	46.4	-84.2	47.6	34.4	44.7	-50.2	46.9	36.5	28.3	11.1
N3	11.8	-7.1	12.2	10.1	--	--	10.6	7.1	3.1	-0.4
N7	14.3	10.4	16.9	14.9	19.1	-8.9	--	--	1.3	-1.8
C8	31.1	-12.3	32.7	18.3	36.1	-10.0	37.0	-14.5	20.1	-4.9
N9	19.9	-10.8	--	--	12.4	7.2	12.2	9.3	2.9	-2.1
N^6	22.4	-15.9	--	--	21.6	-15.5	--	--	13.3	-17.8

Table 18. The estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of each reactive site in the neutral and anion forms of isomers **A1** and **A2** and their contributions (c, %) to the $k_{obs\text{-}est}$ of adenine.

Reactive site	**A1**		**A2**		Adenine
	N	A^-	N	A^-	$k_{obs\text{-}est}$
N1	1.8×10^{5}(7%)	2.2×10^{6}(89%)	2.1×10^{3}(0%)	9.9×10^{4}(4%)	~10^{6}
C2	6.3×10^{-22}(0%)	1.8×10^{-11}(96%)	5.1×10^{-22}(0%)	8.4×10^{-13}(4%)	1.9×10^{-11}
N3	1.4×10^{4}(0%)	2.2×10^{6}(96%)	$5.0\times10^{3*}$(0%)	9.9×10^{4}(4%)	~10^{6}
N7	2.1×10^{2}(0%)	2.2×10^{6}(96%)	2.9×10^{-3}(0%)	9.9×10^{4}(4%)	~10^{6}
C8	1.0×10^{-10}(0%)	1.9×10^{-5}(96%)	1.0×10^{-15}(0%)	8.6×10^{-7}(4%)	2.0×10^{-5}
N9	1.7×10^{-2}(0%)	2.2×10^{6}(96%)	2.4×10^{2}(0%)	9.9×10^{4}(4%)	~10^{6}
N^6	2.4×10^{-4}(0%)	1.8 (96%)	4.3×10^{-5}(0%)	8.2×10^{-2}(4%)	1.9

* represents reaction via S_EAr-1 mechanism.

The pK_a of N9−H moiety in **A1** and pK_a of N7−H moiety in **A2** are 9.8 and 9.9, respectively, with f(N(**A1**))=0.9984, f(A(**A1**))=0.016, f(N(**A2**))=0.999, and f(A(**A2**))=0.001. $c = \frac{k\text{obs}-\text{est (N/A)}f(i))}{k\text{obs}-\text{est (Adenine)}}$%

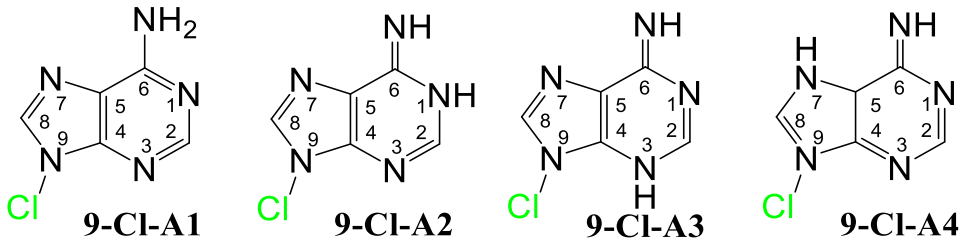


Figure S7. The structures of 9-Cl-adenine isomers.

Table S19. Relative energies (R*G*, in kcal/mol) and Boltzmann distribution populations *f* of various 9-Cl-adenine isomers.

Isomer	**9-Cl-A1**	**9-Cl-A2**	**9-Cl-A3**	**9-Cl-A4**
R*G*	0	11.5	20.9	28.0
f	0.999	10^{-9}	10^{-16}	10^{-21}

Scheme S5. Chlorination of all the potential reaction sites in 9-Cl-adenine by HOCl.

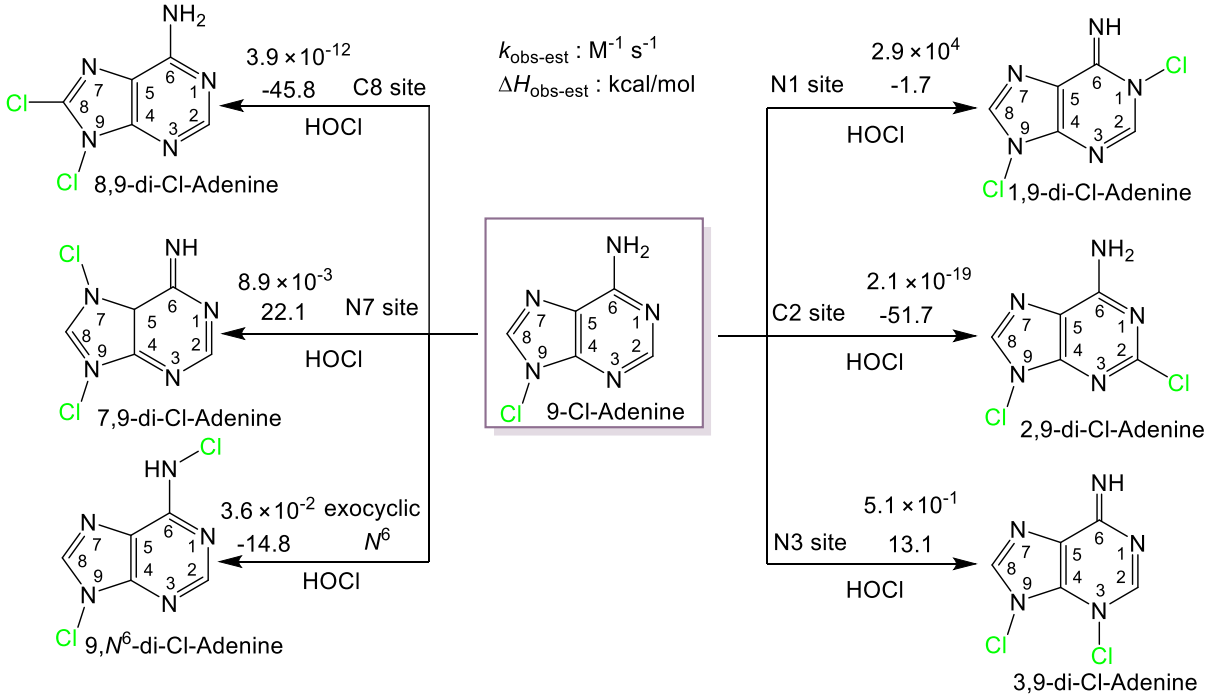


Table S20. $\Delta G^{\neq}$ and ΔH (in kcal/mol) in chlorination of each site in isomer **9-Cl-A1** via concerted and classic S_EAr reaction mechanisms.

Reactive site	Neutral				Anion	
	Concerted		S_EAr-1		Concerted	
	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH
N1	11.4	-14.0	14.0	11.9	2.3	-0.9
C2	43.0	-49.5	52.0	42.2	45.8	-51.4
N3	--	--	18.1	16.2	5.7	4.2
N7	--	--	20.3	17.4	9.8	9.7
C8	41.3	-39.8	33.2	40.3	20.1	-7.1
N^6	24.3	-12.3	--	--	6.5	-5.9

Table S21. The estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of each reactive site in the neutral and anion forms of isomer **9-Cl-A1** and their contributions (c, %) to the $k_{obs\text{-}est}$ of 9-Cl-adenine.

Reactive site	Neutral		Anion		9-Cl-Adenine
	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$
N1	2.9×10^{4}	100%	4.3×10^{1}	0%	2.9×10^{4}
C2	2.1×10^{-19}	100%	5.8×10^{-31}	0%	2.1×10^{-19}
N3	3.6×10^{-1}	72%	1.4×10^{-1}	28%	5.0×10^{-1}
N7	8.8×10^{-3}	98%	1.4×10^{-4}	2%	8.9×10^{-3}
C8	3.6×10^{-18}	0%	3.9×10^{-12}	100%	3.9×10^{-12}
N^6	1.0×10^{-5}	0%	3.6×10^{-2}	100%	3.6×10^{-2}

Table S22. $\Delta G^{\neq}$ and ΔH (in kcal/mol) in chlorination of each site in isomer **Gau 1** via concerted and classic S_EAr reaction mechanisms.

Reactive site	Neutral				Anion	
	Concerted		S_EAr-1		Concerted	
	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH
N1	27.9	-4.7	--	--	6.3	-2.5
N3	18.6	3.1	21.1	18.5	8.3	6.5
N7	--	--	14.2	14.6	7.8	5.7
C8	--	--	18.7	-0.9	19.8	-16.3
N^2	25.6	-8.0	--	--	11.1	7.7

Table S23. The estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of each reactive site in the neutral and anion forms of isomer **Gau 1** and their contributions (c, %) to the $k_{obs\text{-}est}$ of guanosine calculated at the M06-2X(D3)/aug-cc-pVTZ//M06-2X(D3)/6-311+G(d) level with the SMD solvent model.

Reactive site	Neutral		Anion		Guanosine
	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$
N1	2.4×10^{-8}	0%	2.0×10^{4}	100%	2.0×10^{4}
N3	1.6×10^{-1}	0%	6.9×10^{2}	100%	6.9×10^{2}
N7	2.6×10^{2}	14%	1.6×10^{3}	86%	1.9×10^{3}
C8	1.3×10^{-1}	100%	2.6×10^{-6}	0%	0.13
N^2	1.2×10^{-6}	0%	6.1	100%	6.1

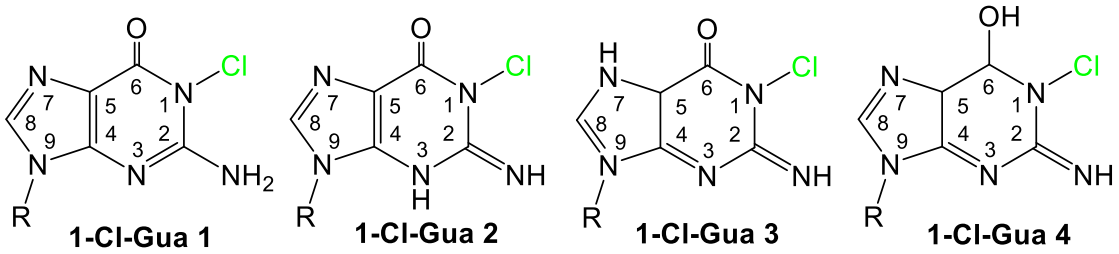


Figure S8. The structures of 1-Cl-guanosine isomers.

Table S24. Relative energies (RG, in kcal/mol) and Boltzmann distribution populations f of various 1-Cl-guanosine isomers.

Isomer	**1-Cl-Gua 1**	**1-Cl-Gua 2**	**1-Cl-Gua 3**	**1-Cl-Gua 4**
RG	0.0	14.2	19.7	27.0
f	0.999	10^{-11}	10^{-15}	10^{-20}

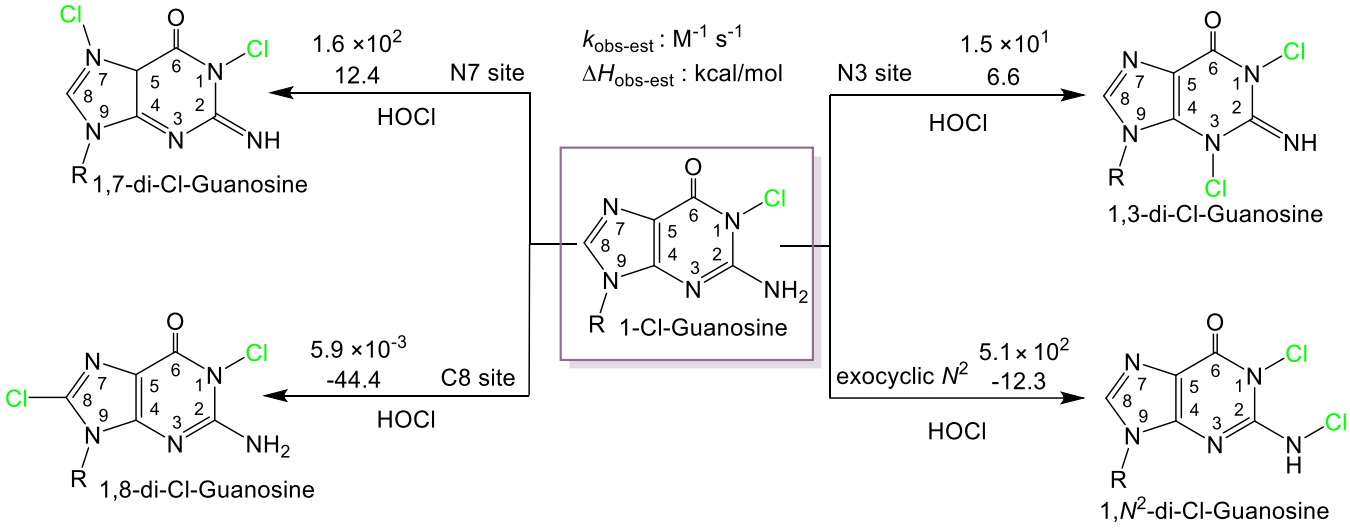
Table S25. $\Delta G^{\neq}$ and ΔH (in kcal/mol) in chlorination of each site in **1-Cl-Gua 1** via concerted and classic S_EAr reaction mechanisms.

Reactive site	Neutral				Anion	
	Concerted		S_EAr-1		Concerted	
	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH
N3	22.0	2.9	--	--	7.3	2.5
N7	--	--	14.5	13.4	9.5	8.7
C8	--	--	20.9	2.0	12.4	-15.9
N^2	27.9	-8.9	--	--	3.6	-9.5

Table S26. The estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of each reactive site in the neutral and anion forms of isomer **1-Cl-Gua 1** and their contributions (c, %) to the $k_{obs\text{-}est}$ of 1-Cl-guanosine.

Reactive site	Neutral		Anion		1-Cl-guanosine
	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$
N3	5.0×10^{-4}	0%	1.5×10^{1}	100%	1.5×10^{1}
N7	1.6×10^{2}	100%	3.6×10^{-1}	0%	1.6×10^{2}
C8	3.2×10^{-3}	54%	2.7×10^{-3}	46%	5.9×10^{-3}
N^2	2.4×10^{-8}	0%	5.1×10^{2}	100%	5.1×10^{2}

Scheme S6. Chlorination of all the potential reaction sites in 1-Cl-guanosine by HOCl.



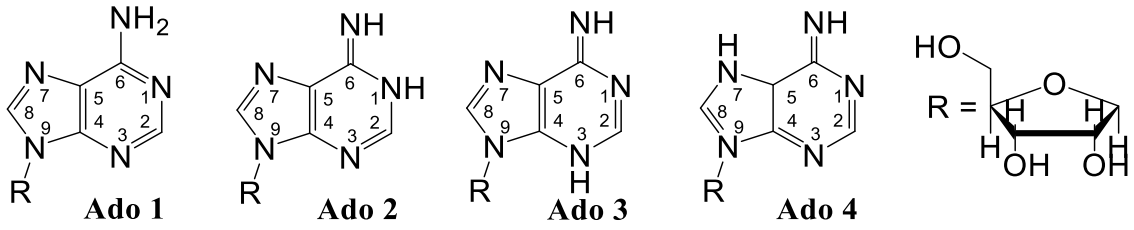


Figure S9. The structures of adenosine isomers.

Table S27. Relative energies (R*G*, in kcal/mol) and Boltzmann distribution populations *f* of various adenosine isomers.

Isomer	**Ado 1**	**Ado 2**	**Ado 3**	**Ado 4**
R*G*	0.0	11.1	19.5	24.9
f	0.999	10^{-9}	10^{-15}	10^{-19}

Table S28. $\Delta G^{\neq}$ and ΔH (in kcal/mol) in chlorination of each site in **Ado 1** via concerted and classic S_EAr reaction mechanisms.

Reactive site	Neutral				Anion	
	Concerted		S_EAr-1		Concerted	
	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH	$\Delta G^{\neq}$	ΔH
N1	9.0	6.7	--	--	2.6	-4.0
C2	42.9	-55.3	--	--	46.4	-52.4
N3	--	--	12.8	11.6	3.7	1.7
N7	--	--	11.8	11.1	5.6	5.1
C8	--	--	22.9	11.0	16.7	-7.7
N^6	20.1	-13.8	--	--	6.5	-7.6

Table S29. The estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of each reactive site in the neutral and anion forms of isomer **Ado 1** and their contributions (c, %) to the $k_{obs\text{-}est}$ of adenosine.

Reactive site	Neutral		Anion		Adenosine
	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$	c	$k_{obs\text{-}est}$
N1	1.7×10^{6}	100%	3.3	0%	1.7×10^{6}
C2	2.4×10^{-19}	100%	2.6×10^{-32}	0%	2.4×10^{-19}
N3	2.8×10^{3}	100%	5.1×10^{-1}	0%	2.8×10^{3}
N7	1.5×10^{4}	100%	2.1×10^{-2}	0%	1.5×10^{4}
C8	1.1×10^{-4}	100%	1.5×10^{-10}	0%	1.1×10^{-4}
N^6	1.2×10^{-2}	73%	4.5×10^{-3}	27%	1.7×10^{-2}

Table S30. The estimated reaction enthalpy changes ($\Delta H^{\neq}_{obs\text{-}est}$) of each reactive site in guanine, guanosine, and their chlorinated products.

Reactant	N1	N3	N7	C8	N9	N^2
G	-11.8	0.1	-10.3	-47.0	-13.3	-13.7
9-Cl-G	-11.4	3.4	6.1	-45.8	--	-13.0
Gua	-11.7	2.4	2.0	-44.5	--	-13.5
1-Cl-Gua	--	6.6	12.4	-44.4	--	-12.3

Table S31. The estimated reaction enthalpy changes ($\Delta H^{\neq}_{obs\text{-}est}$) of each reactive site in adenine, adenosine, and their chlorinated products.

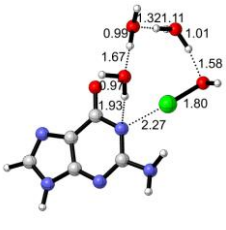
Reactant	N1	C2	N3	N7	C8	N9	N^6
A	-3.7	-52.4	-7.5	-9.7	-47.1	-13.1	-15.4
9-Cl-A	-1.7	-51.7	13.1	22.1	-45.8	--	-14.8
Ado	-2.4	-52.5	10.9	17.3	-45.5	--	-15.3

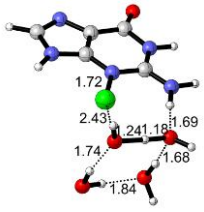
Table S32. The Mulliken charge, APT charge, FED^2(HOMO) and $lgk_{obs\text{-}est}$ of purine bases, purine nucleosides and their chlorinated products.

G	APT	Mulliken	FED^2	$lgk_{obs\text{-}est}$
N1	-1.012	-0.75	0.15	5.61
N3	-1.209	-0.618	16.31	6.92
N7	-0.577	-0.564	6.0	7.65
C8	0.311	0.218	15.6	-1.87
N9	-0.664	-0.7	0.65	7.07
9-Cl-G	APT	Mulliken	FED^2	$lgk_{obs\text{-}est}$
N1	-1.025	-0.755	0.12	5.70
N3	-1.262	-0.614	18.05	2.33
N7	-0.603	-0.552	5.09	1.45
C8	0.303	0.242	15.36	-3.89
Gua1	APT	Mulliken	FED^2	$lgk_{obs\text{-}est}$
N1	-1.022	-0.753	0.14	4.30
N3	-1.248	-0.623	16.27	2.83
N7	-0.629	-0.577	6.2	3.26
C8	0.295	0.207	15.68	-0.88
1-Cl-Gua1	APT	Mulliken	FED^2	$lgk_{obs\text{-}est}$
N3	-1.276	-0.619	15.97	1.16
N7	-0.644	-0.573	6.8	2.19
C8	0.295	0.214	15.68	-2.22
A1	APT	Mulliken	FED^2	$lgk_{obs\text{-}est}$
N1	-0.997	-0.577	3.84	6.35
C2	0.789	0.158	7.14	-10.71
N3	-0.887	-0.552	13.5	6.35
N7	-0.673	-0.571	7.36	6.35
C8	0.455	0.232	12.32	-4.70
N9	-0.703	-0.696	1.09	6.35
9-Cl-A1	APT	Mulliken	FED^2	$lgk_{obs\text{-}est}$
N1	-1.012	-0.578	5.48	4.46
C2	0.873	0.169	5.73	-18.68
N3	-0.942	-0.547	15.73	-0.30
N7	-0.704	-0.56	6.03	-2.04
C8	0.437	0.256	11.31	-11.40
Ado1	APT	Mulliken	FED^2	$lgk_{obs\text{-}est}$
N1	-1.01	-0.578	3.95	6.22
C2	0.815	0.161	7.02	-18.61
N3	-0.921	-0.556	13.61	3.43
N7	-0.736	-0.585	7.81	4.17
C8	0.44	0.219	12.19	-3.96

Table S33. The R^2 values of the $lgk_{obs\text{-}est}$ depending on APT, Mulliken charges, and FED^2 (HOMO).

APT	Mulliken	FED^2	APT+FED^2
0.72	0.65	0.04	0.71


TS-G1-n-N1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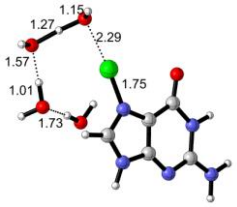
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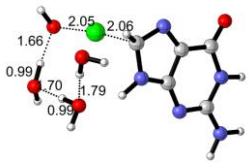
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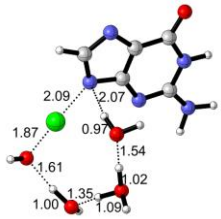
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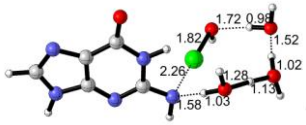
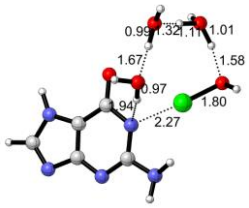

TS-G1-n-N^2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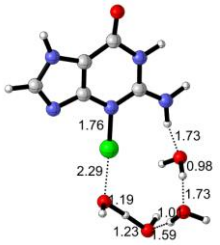
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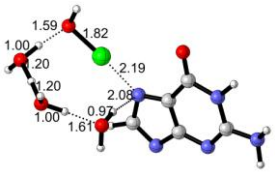
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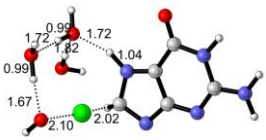
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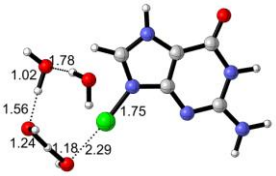
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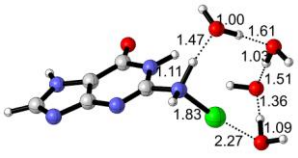
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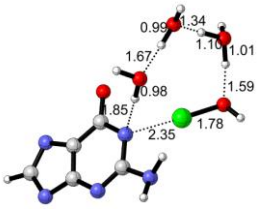
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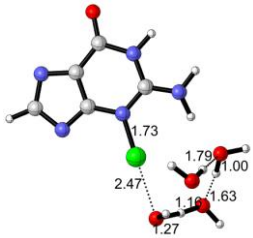
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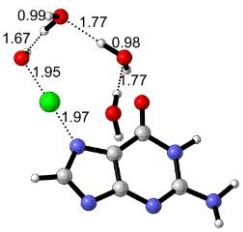
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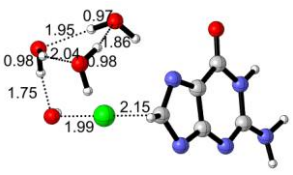
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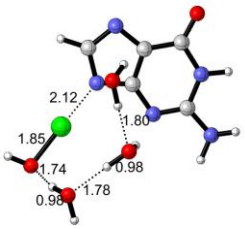
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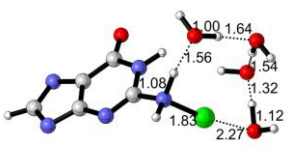
TS-G1-a-N^2

Figure S10. Structures of transition states and important geometric parameters calculated at the M06-2X(D3)/6-311+G(d) or M06-2X(D3)/6-311G(d) levels for chlorination of guanine (atoms in green color represent chlorine atom; atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom, atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

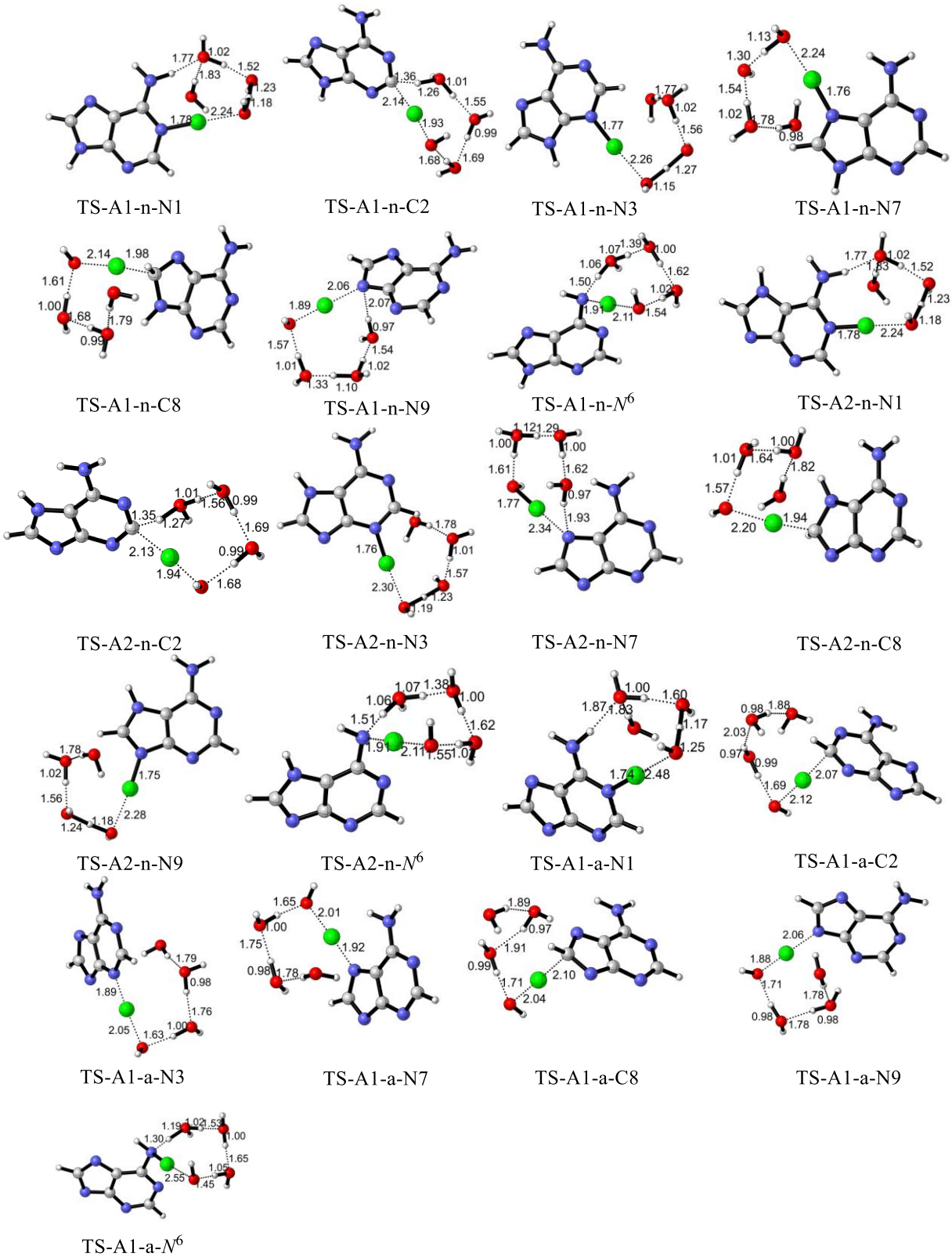

Figure S11. Structures of transition states and important geometric parameters calculated at the M06-2X(D3)/6-311+G(d) or M06-2X(D3)/6-311G(d) levels for chlorination of adenine (atoms in green color represent chlorine atom; atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom, atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

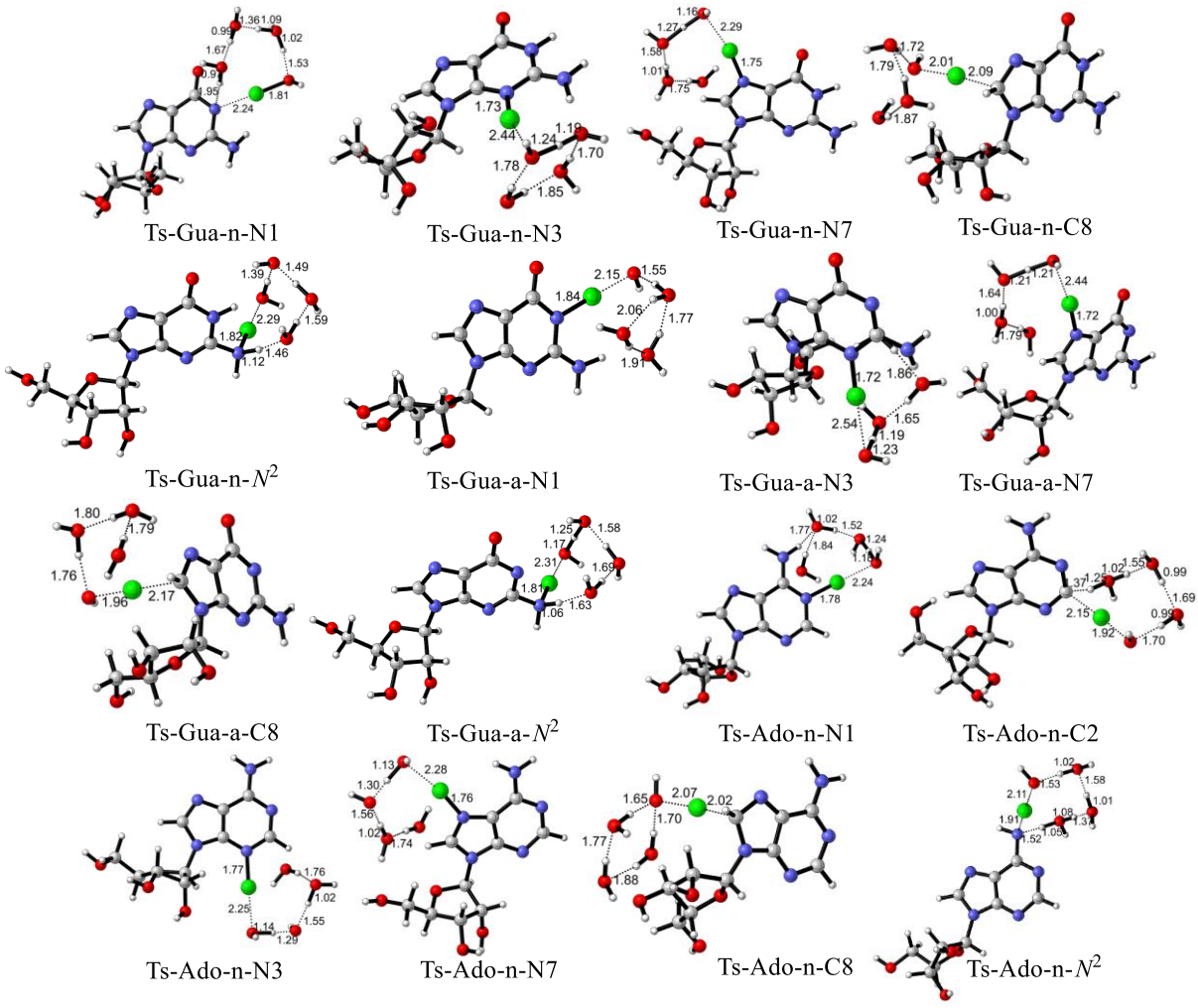

Figure S12. Structures of transition states and important geometric parameters calculated at the M06-2X(D3)/6-311+G(d) or M06-2X(D3)/6-311G(d) levels for chlorination of guanosine and adenosine (atoms in green color represent chlorine atom; atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom, atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

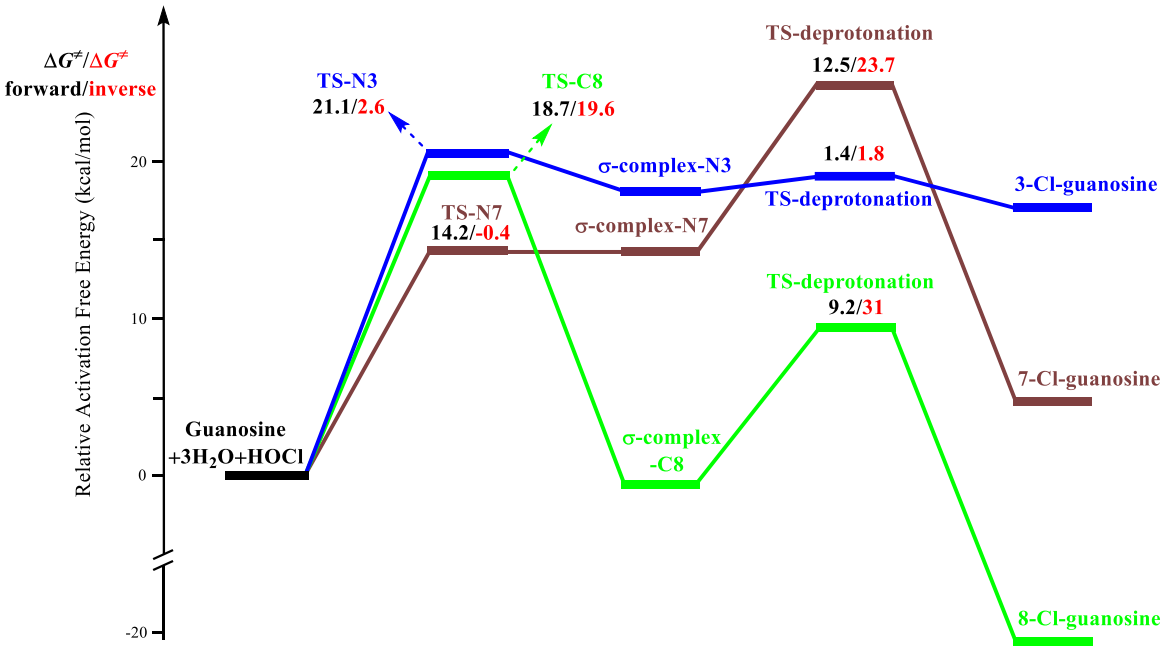

Figure S13. The activation free energy profile in chlorination of N3, N7, and C8 in guanosine by HOCl.

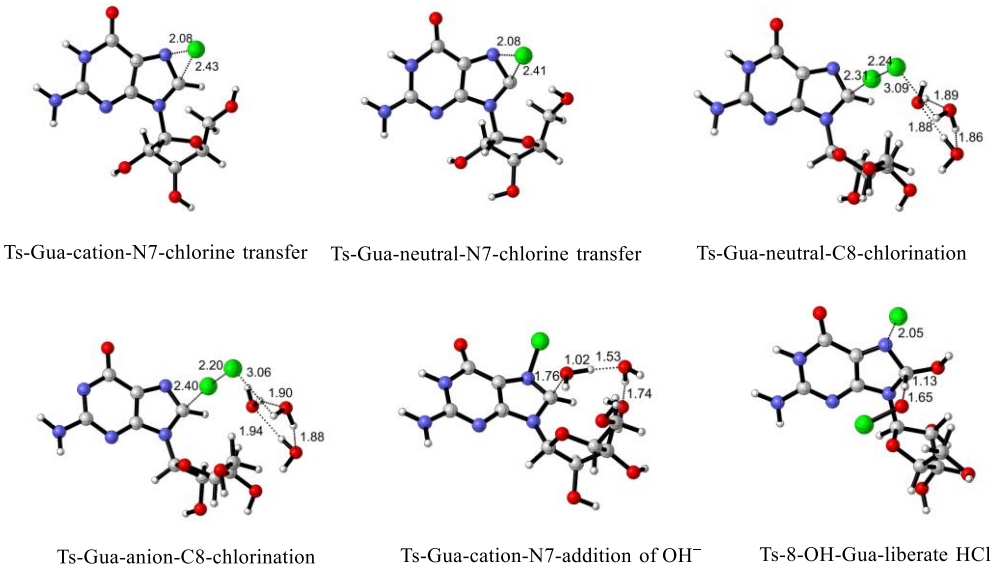

Figure S14. Structures of transition states and important geometric parameters for chlorine transfer, chlorination by Cl_2, and oxidation reactions in guanosine.

In addition to the standard orientation of transition states, their initial structures were also given due to the extreme sensitiveness of the structural optimization of the transition states to the initial structures.

Standard orientation of TS-G1-n-N1 and initial structure

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

Standard orientation of transition state of TS-G1-n-N1

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -89.37 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.915874	0.290938	-0.071550
2	6	0	2.138023	-0.837093	-0.266626
3	6	0	0.718072	-0.708885	-0.128494
4	6	0	1.180420	1.596443	0.344248
5	6	0	4.145967	-1.467732	-0.549415
6	1	0	5.042681	-2.036464	-0.740654
7	7	0	4.203170	-0.128489	-0.256453
8	1	0	-0.835672	0.083701	1.665300
9	8	0	-3.083162	-1.965823	1.041827
10	1	0	-3.748565	-2.189378	1.703114
11	17	0	-1.779499	1.045926	-0.592349
12	8	0	-1.418913	-0.338843	2.322013
13	1	0	-0.850757	-0.910949	2.849835
14	1	0	-2.441041	-1.341505	1.471750
15	8	0	-3.435375	1.311875	-1.249176
16	1	0	-3.680277	-1.499655	-0.035359
17	1	0	-3.876992	1.920688	-0.640581
18	8	0	-4.207225	-1.132586	-0.940630
19	1	0	-4.015789	-0.155621	-1.099303
20	1	0	-3.916814	-1.634186	-1.715062
21	8	0	-0.101056	-1.635166	-0.252996
22	7	0	0.626803	2.822420	0.603686
23	1	0	-0.293614	2.815450	1.018354
24	1	0	1.262600	3.498506	1.000676
25	7	0	0.303026	0.575781	0.180912
26	7	0	2.502485	1.534346	0.243284
27	7	0	2.928085	-1.936632	-0.565232
28	1	0	5.036438	0.439008	-0.188806

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.916749	0.291139	-0.071478
2	6	0	2.139513	-0.837269	-0.266478
3	6	0	0.719547	-0.709953	-0.127621
4	6	0	1.180801	1.595514	0.345713
5	6	0	4.147571	-1.466489	-0.550959
6	1	0	5.044524	-2.034566	-0.743094
7	7	0	4.204165	-0.127376	-0.257447

8	1	0	-0.836199	0.080783	1.665213
9	8	0	-3.087359	-1.964901	1.038146
10	1	0	-3.751767	-2.189908	1.699934
11	17	0	-1.777251	1.044763	-0.591417
12	8	0	-1.419513	-0.342957	2.321065
13	1	0	-0.851944	-0.919184	2.845038
14	1	0	-2.444935	-1.341402	1.468537
15	8	0	-3.432803	1.312997	-1.249549
16	1	0	-3.687372	-1.495548	-0.037751
17	1	0	-3.873461	1.924065	-0.642524
18	8	0	-4.215966	-1.125775	-0.939811
19	1	0	-4.018808	-0.149626	-1.099168
20	1	0	-3.932000	-1.629082	-1.715528
21	8	0	-0.099131	-1.636597	-0.251950
22	7	0	0.626656	2.821016	0.606032
23	1	0	-0.293495	2.813481	1.021266
24	1	0	1.262346	3.497447	1.002590
25	7	0	0.303836	0.574438	0.182143
26	7	0	2.502800	1.534131	0.244185
27	7	0	2.930016	-1.936177	-0.566134
28	1	0	5.037159	0.440563	-0.190147

Standard orientation of TS-G1-n-N3 and initial structure

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

Standard orientation of transition state of TS-G1-n-N3

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1038.89 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.486838	1.012898	-1.155033
2	1	0	3.492940	1.262981	-2.083550
3	8	0	3.660872	1.651772	1.450792
4	1	0	3.368692	0.766470	1.729729
5	1	0	3.675708	1.598417	0.476154
6	8	0	3.139180	-1.340580	-0.761915
7	1	0	3.388151	-0.216696	-1.027101
8	1	0	3.841970	-1.936356	-1.035475
9	8	0	2.981596	-1.020205	1.881030
10	1	0	3.087576	-1.193414	0.912702
11	1	0	3.787256	-1.339241	2.299982
12	1	0	-3.375348	3.380013	0.213116
13	6	0	-2.786696	0.261509	0.139552
14	6	0	-3.002112	2.370558	0.154147
15	1	0	-0.948477	2.821681	-0.244644
16	6	0	-1.540844	0.784414	-0.105886
17	7	0	-1.670402	2.125205	-0.098532
18	7	0	-3.699050	1.279663	0.301973
19	6	0	-2.962118	-1.160507	0.191361

20	6	0	-0.518067	-1.320104	-0.273267
21	7	0	-1.743594	-1.846798	-0.033907
22	7	0	-0.413718	0.031210	-0.310917
23	17	0	1.127034	0.728859	-0.651154
24	8	0	-3.976972	-1.791505	0.395036
25	1	0	-1.811729	-2.860973	0.000883
26	7	0	0.523265	-2.093390	-0.465311
27	1	0	0.378711	-3.094225	-0.413417
28	1	0	1.506369	-1.764763	-0.626623

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.501438	0.944170	-1.174269
2	1	0	3.489973	1.168853	-2.109359
3	8	0	3.608300	1.737944	1.383310
4	1	0	3.326359	0.860962	1.696070
5	1	0	3.640093	1.637572	0.412029
6	8	0	3.131379	-1.392844	-0.711654
7	1	0	3.389185	-0.280394	-1.010920
8	1	0	3.829586	-2.001983	-0.966511
9	8	0	3.006644	-0.939163	1.913951
10	1	0	3.092170	-1.161778	0.953688
11	1	0	3.843985	-1.185299	2.319616
12	1	0	-3.332043	3.399901	0.198051
13	6	0	-2.783341	0.274232	0.127875
14	6	0	-2.971387	2.385630	0.139975
15	1	0	-0.915250	2.811296	-0.269630
16	6	0	-1.532135	0.781042	-0.123613
17	7	0	-1.644680	2.123355	-0.119621
18	7	0	-3.681722	1.304151	0.293420
19	6	0	-2.974349	-1.145058	0.193205
20	6	0	-0.528432	-1.335518	-0.253223
21	7	0	-1.761483	-1.846763	-0.017923
22	7	0	-0.412899	0.013822	-0.319384
23	17	0	1.134588	0.691144	-0.664451
24	8	0	-3.996343	-1.762717	0.401192
25	1	0	-1.840051	-2.859369	0.036199
26	7	0	0.509484	-2.120372	-0.414967
27	1	0	0.357148	-3.118864	-0.345824
28	1	0	1.496472	-1.800777	-0.573973

Standard orientation of TS-G1-n-N7 and initial structure

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

Standard orientation of transition state of TS-G1-n-N7

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -691.57 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.746795	1.945616	-0.186520
2	1	0	4.112407	2.072200	-1.068192
3	8	0	0.544642	-1.381339	1.925473
4	1	0	1.375991	-1.537832	1.426471
5	1	0	0.489429	-0.431475	2.068441
6	8	0	4.646870	-0.131440	0.678385
7	1	0	4.212596	0.979570	0.232574
8	1	0	5.289644	-0.440663	0.032492
9	8	0	2.784089	-1.911528	0.492283
10	1	0	3.496518	-1.193283	0.573431
11	1	0	3.149573	-2.704879	0.897291
12	1	0	1.228008	-1.918939	-1.483408
13	6	0	-0.949340	0.212733	-0.390943
14	6	0	0.353158	-1.378311	-1.163549
15	1	0	-1.142573	-2.837395	-1.287218
16	6	0	-1.724907	-0.915350	-0.560481
17	7	0	-0.884310	-1.883603	-1.058421
18	7	0	0.333879	-0.113274	-0.792996
19	6	0	-1.531869	1.409240	0.130917
20	6	0	-3.583935	0.031263	0.184871
21	7	0	-2.888862	1.197174	0.390522
22	7	0	-3.028637	-1.065857	-0.301409
23	17	0	1.777902	0.854074	-0.580106
24	7	0	-4.879557	0.041267	0.497008
25	1	0	-5.324553	0.851937	0.899811
26	1	0	-5.414358	-0.805161	0.379467
27	1	0	-3.384326	1.998628	0.770237
28	8	0	-1.004761	2.486270	0.349453

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.609231	1.969479	-0.183050
2	1	0	3.949529	2.155917	-1.064124
3	8	0	0.433842	-1.297642	1.910543
4	1	0	1.261636	-1.461719	1.408475
5	1	0	0.395146	-0.349668	2.069427
6	8	0	4.553228	-0.141004	0.540658
7	1	0	4.096101	0.986162	0.165201
8	1	0	5.130248	-0.438852	-0.169640
9	8	0	2.652687	-1.887875	0.465074
10	1	0	3.381455	-1.182398	0.501839
11	1	0	3.010923	-2.673528	0.890908
12	1	0	1.304884	-1.981019	-1.312879
13	6	0	-0.894082	0.191763	-0.352306
14	6	0	0.422452	-1.425530	-1.041884
15	1	0	-1.075455	-2.879227	-1.178573
16	6	0	-1.671285	-0.935699	-0.519115

17	7	0	-0.820500	-1.921488	-0.961730
18	7	0	0.399093	-0.150723	-0.706172
19	6	0	-1.489885	1.410579	0.098222
20	6	0	-3.551195	0.045326	0.121282
21	7	0	-2.856447	1.213247	0.316513
22	7	0	-2.985503	-1.070287	-0.307387
23	17	0	1.841487	0.813261	-0.474502
24	7	0	-4.856868	0.073628	0.386738
25	1	0	-5.313038	0.905636	0.728269
26	1	0	-5.398392	-0.766414	0.257076
27	1	0	-3.360876	2.031020	0.646092
28	8	0	-0.966725	2.494463	0.290717

Standard orientation of TS-G1-n-C8 and initial structure

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

Standard orientation of transition state of TS-G1-n-C8

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -432.16 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.088617	0.512057	0.421934
2	6	0	-1.487936	-0.869485	0.454678
3	6	0	-2.835021	-1.214868	0.014929
4	6	0	-3.040803	1.208935	-0.387181
5	6	0	0.559040	-0.824204	1.069983
6	1	0	1.231938	-1.028169	1.891455
7	7	0	0.156743	0.518047	0.879097
8	8	0	2.466932	1.954354	0.542092
9	1	0	2.694207	2.873400	0.715375
10	17	0	1.847743	-1.203955	-0.490028
11	8	0	3.091698	0.347363	2.691635
12	1	0	2.323140	0.488523	3.253368
13	1	0	2.944849	0.911784	1.909482
14	8	0	3.191755	-1.353999	-2.032626
15	1	0	2.902509	1.692466	-0.306013
16	1	0	3.926692	-1.804999	-1.599184
17	8	0	3.633433	1.247915	-1.770923
18	1	0	3.512564	0.269857	-1.902133
19	1	0	3.108216	1.676731	-2.454159
20	1	0	0.844371	1.285301	0.819698
21	7	0	-3.533215	-0.077907	-0.376182
22	7	0	-1.816014	1.545526	0.003358
23	7	0	-0.529725	-1.649452	0.878665
24	8	0	-3.332486	-2.318522	-0.022137
25	1	0	-4.484917	-0.232749	-0.696517
26	7	0	-3.865803	2.149107	-0.819518
27	1	0	-4.804670	1.940437	-1.127983
28	1	0	-3.545070	3.105907	-0.841241

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.088805	0.508200	0.427459
2	6	0	-1.487647	-0.873739	0.448174
3	6	0	-2.834570	-1.215785	0.005349
4	6	0	-3.040828	1.211151	-0.376847
5	6	0	0.559146	-0.833011	1.064566
6	1	0	1.231820	-1.043472	1.884616
7	7	0	0.156361	0.510736	0.885126
8	8	0	2.465760	1.951138	0.558639
9	1	0	2.691459	2.869111	0.739501
10	17	0	1.849091	-1.198831	-0.497502
11	8	0	3.096912	0.316027	2.685368
12	1	0	2.335080	0.456098	3.256409
13	1	0	2.946708	0.890750	1.911469
14	8	0	3.197757	-1.333801	-2.039198
15	1	0	2.897091	1.698754	-0.294463
16	1	0	3.934235	-1.782441	-1.605942
17	8	0	3.621380	1.269682	-1.767838
18	1	0	3.508112	0.291057	-1.902251
19	1	0	3.082001	1.696181	-2.441473
20	1	0	0.843736	1.278711	0.832264
21	7	0	-3.533070	-0.075786	-0.376253
22	7	0	-1.816331	1.544867	0.017106
23	7	0	-0.529277	-1.656969	0.865698
24	8	0	-3.331717	-2.319230	-0.041042
25	1	0	-4.484565	-0.228325	-0.698328
26	7	0	-3.865625	2.154619	-0.802308
27	1	0	-4.804277	1.948459	-1.113135
28	1	0	-3.544853	3.111552	-0.816375

Standard orientation of TS-G1-n-N9 and initial structure

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

Standard orientation of transition state of TS-G1-n-N9

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -87.31 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.917341	-0.376706	-0.347585
2	6	0	-2.109686	-0.961636	0.075738
3	6	0	-3.289068	-0.168286	0.134125
4	6	0	-1.811990	1.639790	-0.668844
5	6	0	-0.627090	-2.458288	0.145316

6	1	0	-0.103951	-3.394794	0.281299
7	7	0	0.028950	-1.347927	-0.302141
8	1	0	0.743984	-0.691370	1.525248
9	8	0	2.410346	1.856087	1.606886
10	1	0	2.863405	2.170708	2.401075
11	17	0	2.067870	-1.173880	-0.756879
12	8	0	0.981632	-0.150353	2.293482
13	1	0	0.149579	0.177364	2.655212
14	1	0	1.845937	1.045491	1.855220
15	8	0	3.884850	-0.952789	-1.128212
16	1	0	3.147305	1.637719	0.839799
17	1	0	4.343363	-1.577729	-0.552350
18	8	0	4.101298	1.447080	-0.109730
19	1	0	4.084353	0.533068	-0.511394
20	1	0	3.964062	2.078880	-0.824698
21	7	0	-1.910818	-2.290401	0.387623
22	7	0	-3.030237	1.147557	-0.270983
23	7	0	-0.723028	0.920182	-0.721024
24	8	0	-4.426166	-0.492598	0.477356
25	1	0	-3.830168	1.771562	-0.267292
26	7	0	-1.801026	2.940752	-1.074062
27	1	0	-0.880942	3.353910	-1.125617
28	1	0	-2.512252	3.551354	-0.696209

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.931849	-0.365151	-0.347296
2	6	0	-2.111608	-0.961684	0.094240
3	6	0	-3.301094	-0.183704	0.156745
4	6	0	-1.857069	1.635147	-0.680737
5	6	0	-0.609851	-2.439033	0.161622
6	1	0	-0.073136	-3.367444	0.300157
7	7	0	0.026984	-1.324280	-0.302858
8	1	0	0.753850	-0.664295	1.515632
9	8	0	2.479212	1.848603	1.613446
10	1	0	2.922297	2.155614	2.416139
11	17	0	2.052780	-1.151778	-0.781151
12	8	0	0.992193	-0.123536	2.283678
13	1	0	0.162008	0.224003	2.630861
14	1	0	1.891879	1.052938	1.852639
15	8	0	3.871600	-0.944743	-1.174091
16	1	0	3.229527	1.610581	0.858939
17	1	0	4.326131	-1.621258	-0.656389
18	8	0	4.191120	1.392606	-0.064809
19	1	0	4.131833	0.489896	-0.491994
20	1	0	4.105273	2.047521	-0.767075
21	7	0	-1.892566	-2.284770	0.416280
22	7	0	-3.064399	1.130960	-0.264916
23	7	0	-0.758593	0.930075	-0.735413
24	8	0	-4.429878	-0.520205	0.515010
25	1	0	-3.872555	1.744350	-0.260271
26	7	0	-1.868476	2.930923	-1.101362

27	1	0	-0.955148	3.356424	-1.169351
28	1	0	-2.584990	3.536287	-0.725165

Standard orientation of TS-G1-n-N^2 and initial structure

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

Standard orientation of transition state of TS-G1-n-N^2

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -265.40 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.247014	-0.767730	1.689244
2	8	0	3.463294	-0.820538	-2.082781
3	1	0	4.278194	-1.152037	-1.688647
4	17	0	1.904736	-1.245927	-0.488041
5	8	0	2.099397	0.096777	2.457054
6	1	0	2.837817	0.471422	1.884623
7	1	0	-5.742626	-0.216330	-0.745845
8	1	0	1.600140	0.839191	2.815745
9	8	0	3.260463	1.525952	-1.406179
10	1	0	3.407016	0.247084	-1.841019
11	1	0	2.309026	1.661389	-1.342519
12	8	0	4.027209	0.966348	0.947953
13	1	0	3.705203	1.221570	0.003283
14	1	0	4.596249	0.196947	0.839527
15	7	0	-3.926036	-1.197072	-0.203060
16	7	0	-4.027512	1.015017	-0.488285
17	6	0	-4.695104	-0.112029	-0.511687
18	6	0	-2.673296	-0.729489	0.034874
19	6	0	-2.752528	0.640243	-0.144705
20	6	0	-1.577466	1.442107	0.037387
21	6	0	-0.539013	-0.717336	0.533437
22	7	0	-0.481883	0.630744	0.396762
23	7	0	-1.574573	-1.460414	0.368556
24	8	0	-1.444600	2.647394	-0.074420
25	7	0	0.702163	-1.335313	0.885789
26	1	0	0.545730	-2.314549	1.135048
27	1	0	0.397116	1.117078	0.564042
28	1	0	-4.228158	-2.162461	-0.163974

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.247014	-0.767730	1.689244
2	8	0	3.463294	-0.820538	-2.082781
3	1	0	4.278194	-1.152037	-1.688647

4	17	0	1.904736	-1.245927	-0.488041
5	8	0	2.099397	0.096777	2.457054
6	1	0	2.837817	0.471422	1.884623
7	1	0	-5.742626	-0.216330	-0.745845
8	1	0	1.600140	0.839191	2.815745
9	8	0	3.260463	1.525952	-1.406179
10	1	0	3.407016	0.247084	-1.841019
11	1	0	2.309026	1.661389	-1.342519
12	8	0	4.027209	0.966348	0.947953
13	1	0	3.705203	1.221570	0.003283
14	1	0	4.596249	0.196947	0.839527
15	7	0	-3.926036	-1.197072	-0.203060
16	7	0	-4.027512	1.015017	-0.488285
17	6	0	-4.695104	-0.112029	-0.511687
18	6	0	-2.673296	-0.729489	0.034874
19	6	0	-2.752528	0.640243	-0.144705
20	6	0	-1.577466	1.442107	0.037387
21	6	0	-0.539013	-0.717336	0.533437
22	7	0	-0.481883	0.630744	0.396762
23	7	0	-1.574573	-1.460414	0.368556
24	8	0	-1.444600	2.647394	-0.074420
25	7	0	0.702163	-1.335313	0.885789
26	1	0	0.545730	-2.314549	1.135048
27	1	0	0.397116	1.117078	0.564042
28	1	0	-4.228158	-2.162461	-0.163974

Standard orientation of TS-G2-n-N1 and initial structure

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

Standard orientation of transition state of TS-G2-n-N1

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -85.88 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.958447	0.317241	-0.071774
2	6	0	2.139094	-0.781233	-0.257008
3	6	0	0.721637	-0.681267	-0.131954
4	6	0	1.189320	1.618256	0.334924
5	6	0	4.234467	-1.327791	-0.514399
6	1	0	5.096704	-1.947001	-0.707798
7	7	0	4.275792	-0.036811	-0.236417
8	1	0	-0.826636	0.090275	1.670637
9	8	0	-3.061111	-1.983509	1.044457
10	1	0	-3.722842	-2.212185	1.707647
11	17	0	-1.782863	1.048652	-0.589601
12	8	0	-1.403381	-0.345479	2.323672
13	1	0	-0.827071	-0.912672	2.847946
14	1	0	-2.422005	-1.356289	1.473539
15	8	0	-3.444331	1.299741	-1.238190

16	1	0	-3.668881	-1.513703	-0.031978
17	1	0	-3.887669	1.907089	-0.629360
18	8	0	-4.201036	-1.146326	-0.929940
19	1	0	-4.013768	-0.167449	-1.087055
20	1	0	-3.914889	-1.645076	-1.707808
21	8	0	-0.077419	-1.625701	-0.265914
22	7	0	0.621738	2.845786	0.587384
23	1	0	-0.288737	2.822207	1.023874
24	1	0	1.256289	3.515609	0.997561
25	7	0	0.305030	0.595748	0.172923
26	7	0	2.504916	1.559708	0.239079
27	7	0	2.984760	-1.832757	-0.540021
28	1	0	2.722953	-2.790650	-0.726036

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.958859	0.317252	-0.070842
2	6	0	2.139223	-0.780526	-0.259323
3	6	0	0.721741	-0.680258	-0.136138
4	6	0	1.189569	1.618412	0.334856
5	6	0	4.234789	-1.327947	-0.513171
6	1	0	5.097081	-1.947389	-0.705685
7	7	0	4.276348	-0.037367	-0.233339
8	1	0	-0.823476	0.088374	1.669124
9	8	0	-3.063388	-1.981286	1.047811
10	1	0	-3.724704	-2.207161	1.712372
11	17	0	-1.783978	1.048962	-0.589600
12	8	0	-1.396153	-0.350398	2.323735
13	1	0	-0.817115	-0.924198	2.837780
14	1	0	-2.422175	-1.354829	1.474825
15	8	0	-3.446409	1.299368	-1.235979
16	1	0	-3.671479	-1.512852	-0.029051
17	1	0	-3.889485	1.905845	-0.626080
18	8	0	-4.203869	-1.146112	-0.927073
19	1	0	-4.015752	-0.167487	-1.084900
20	1	0	-3.918577	-1.645796	-1.704659
21	8	0	-0.077359	-1.624319	-0.272574
22	7	0	0.622067	2.845870	0.588002
23	1	0	-0.289150	2.822154	1.022937
24	1	0	1.256185	3.514899	1.000151
25	7	0	0.305096	0.596465	0.170103
26	7	0	2.505273	1.559478	0.241054
27	7	0	2.984881	-1.832156	-0.541961
28	1	0	2.722968	-2.789567	-0.730293

Standard orientation of TS-G2-n-N3 and initial structure

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

Standard orientation of transition state of TS-G2-n-N3

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1059.53 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.998660	1.880693	-0.258047
2	1	0	-3.002454	2.236443	0.637158
3	8	0	-3.007506	-1.739123	-0.605633
4	1	0	-3.383756	-1.409263	0.240689
5	1	0	-3.183040	-1.047841	-1.253266
6	8	0	-5.132481	0.758007	-0.380454
7	1	0	-4.040689	1.313912	-0.375326
8	1	0	-5.143802	0.118068	-1.098671
9	8	0	-4.186193	-0.642069	1.573441
10	1	0	-4.660371	-0.081432	0.885828
11	1	0	-4.825331	-1.287021	1.892188
12	1	0	3.479966	3.404773	0.192490
13	6	0	2.972986	0.239819	0.089141
14	6	0	3.060334	2.413481	0.135127
15	6	0	1.721958	0.799590	-0.021247
16	7	0	1.764973	2.145448	0.006560
17	7	0	3.824565	1.311834	0.188166
18	6	0	3.193121	-1.169081	0.083634
19	6	0	0.722881	-1.325682	-0.155663
20	7	0	1.971798	-1.856591	-0.047410
21	7	0	0.591130	0.012761	-0.140894
22	17	0	-0.994949	0.782005	-0.213547
23	8	0	4.240647	-1.777257	0.171702
24	1	0	2.049481	-2.870141	-0.068841
25	7	0	-0.312306	-2.126964	-0.270191
26	1	0	-0.148188	-3.125149	-0.273407
27	1	0	-1.294548	-1.817383	-0.383140
28	1	0	4.831602	1.274746	0.286963

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.952249	-1.921450	-0.226134
2	1	0	3.004862	-2.256026	0.676089
3	8	0	3.008296	1.775886	-0.550878
4	1	0	3.407554	1.415111	0.273299
5	1	0	3.193383	1.122850	-1.234462
6	8	0	5.073378	-0.778507	-0.473322
7	1	0	3.935037	-1.366780	-0.403559
8	1	0	5.056725	-0.149968	-1.201279
9	8	0	4.246117	0.590932	1.532255
10	1	0	4.671715	0.040294	0.797314
11	1	0	4.917602	1.207374	1.840630
12	1	0	-3.492140	-3.396928	0.177119
13	6	0	-2.969675	-0.268832	0.073831
14	6	0	-3.137714	-2.380089	0.128622

15	6	0	-1.689945	-0.761771	-0.018534
16	7	0	-1.793220	-2.106771	0.016987
17	7	0	-3.872211	-1.304642	0.164878
18	6	0	-3.183239	1.147053	0.065778
19	6	0	-0.707532	1.347097	-0.133455
20	7	0	-1.963718	1.853945	-0.042711
21	7	0	-0.559813	0.006311	-0.121768
22	17	0	1.032454	-0.785207	-0.183252
23	8	0	-4.229791	1.757579	0.137264
24	1	0	-2.056699	2.866245	-0.061338
25	7	0	0.323214	2.153210	-0.228269
26	1	0	0.154102	3.150821	-0.232277
27	1	0	1.310474	1.849785	-0.332576
28	1	0	-4.867475	-1.244915	0.241571

Standard orientation of TS-G2-n-N7 and initial structure

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

Standard orientation of transition state of TS-G2-n-N7

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -734.13 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.039167	-0.723532	0.909709
2	6	0	-1.200611	0.282706	0.424870
3	6	0	-1.653117	1.187479	-0.572037
4	6	0	-3.749252	-0.101876	-0.400046
5	6	0	-0.163846	-0.891826	1.872244
6	1	0	0.633809	-1.249522	2.509849
7	7	0	-1.376886	-1.466391	1.832541
8	1	0	0.765731	-1.036661	-0.462811
9	8	0	3.544088	-1.821294	-1.589737
10	1	0	3.643798	-1.661477	-2.536312
11	17	0	1.967508	1.088671	0.718570
12	8	0	0.992706	-1.761036	-1.063707
13	1	0	0.731684	-2.569507	-0.607659
14	1	0	2.569837	-1.774056	-1.364318
15	8	0	3.633640	1.760426	0.437064
16	1	0	4.226203	-1.050837	-0.966288
17	1	0	3.543928	2.411664	-0.271582
18	8	0	4.955457	-0.313971	-0.366695
19	1	0	4.482758	0.520850	-0.068152
20	1	0	5.306438	-0.759685	0.414395
21	7	0	0.011270	0.159446	1.065980
22	7	0	-2.977091	0.907394	-0.924251
23	7	0	-3.331266	-0.937655	0.506578
24	8	0	-1.054524	2.116967	-1.117082
25	1	0	-3.380904	1.523500	-1.621197
26	7	0	-5.039976	-0.148812	-0.852336

27	1	0	-5.503702	-1.025703	-0.661251
28	1	0	-5.204549	0.199721	-1.787140

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.039167	-0.723532	0.909709
2	6	0	-1.200611	0.282706	0.424870
3	6	0	-1.653117	1.187479	-0.572037
4	6	0	-3.749252	-0.101876	-0.400046
5	6	0	-0.163846	-0.891826	1.872244
6	1	0	0.633809	-1.249522	2.509849
7	7	0	-1.376886	-1.466391	1.832541
8	1	0	0.765731	-1.036661	-0.462811
9	8	0	3.544088	-1.821294	-1.589737
10	1	0	3.643798	-1.661477	-2.536312
11	17	0	1.967508	1.088671	0.718570
12	8	0	0.992706	-1.761036	-1.063707
13	1	0	0.731684	-2.569507	-0.607659
14	1	0	2.569837	-1.774056	-1.364318
15	8	0	3.633640	1.760426	0.437064
16	1	0	4.226203	-1.050837	-0.966288
17	1	0	3.543928	2.411664	-0.271582
18	8	0	4.955457	-0.313971	-0.366695
19	1	0	4.482758	0.520850	-0.068152
20	1	0	5.306438	-0.759685	0.414395
21	7	0	0.011270	0.159446	1.065980
22	7	0	-2.977091	0.907394	-0.924251
23	7	0	-3.331266	-0.937655	0.506578
24	8	0	-1.054524	2.116967	-1.117082
25	1	0	-3.380904	1.523500	-1.621197
26	7	0	-5.039976	-0.148812	-0.852336
27	1	0	-5.503702	-1.025703	-0.661251
28	1	0	-5.204549	0.199721	-1.787140

Standard orientation of TS-G2-n-C8 and initial structure

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

Standard orientation of transition state of TS-G2-n-C8

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -408.44 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.083975	0.422427	0.300106
2	6	0	-1.568896	-0.903164	0.591762
3	6	0	0.513931	-0.798628	1.158570

4	1	0	1.144300	-0.799571	2.040284
5	7	0	0.149300	0.493376	0.693965
6	8	0	2.353873	1.903642	0.189395
7	1	0	2.432231	2.860976	0.126546
8	17	0	1.855469	-1.352889	-0.216860
9	8	0	2.924142	0.786941	2.654609
10	1	0	2.120310	1.024815	3.127605
11	1	0	2.838179	1.206071	1.779532
12	8	0	3.347016	-1.781254	-1.675034
13	1	0	2.833781	1.503363	-0.582993
14	1	0	4.057381	-2.090700	-1.100705
15	8	0	3.633507	0.812814	-1.875535
16	1	0	3.564089	-0.186774	-1.819501
17	1	0	3.131347	1.073424	-2.654312
18	1	0	0.862990	1.244343	0.512233
19	7	0	-0.609341	-1.613372	1.138350
20	1	0	-3.848533	1.515644	-1.032583
21	8	0	-1.590375	2.535909	-0.683572
22	6	0	-1.927867	1.417168	-0.367918
23	6	0	-3.594201	-0.393297	-0.247138
24	7	0	-3.180651	0.896258	-0.582067
25	7	0	-2.834989	-1.301468	0.315700
26	7	0	-4.862216	-0.663124	-0.548038
27	1	0	-5.224871	-1.581593	-0.342806
28	1	0	-5.468162	0.015970	-0.983242

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.082157	0.421828	0.304376
2	6	0	-1.566951	-0.904934	0.590973
3	6	0	0.515686	-0.802231	1.158557
4	1	0	1.146331	-0.806050	2.040076
5	7	0	0.151024	0.491500	0.698733
6	8	0	2.357189	1.899771	0.198407
7	1	0	2.430553	2.857635	0.137561
8	17	0	1.856581	-1.350405	-0.219978
9	8	0	2.926795	0.769523	2.659167
10	1	0	2.137758	1.037943	3.140695
11	1	0	2.845115	1.188516	1.783754
12	8	0	3.346188	-1.773049	-1.684597
13	1	0	2.829010	1.504134	-0.581245
14	1	0	4.060991	-2.075058	-1.111816
15	8	0	3.610462	0.823488	-1.891428
16	1	0	3.549646	-0.176525	-1.833153
17	1	0	3.085287	1.079055	-2.656654
18	1	0	0.865694	1.242055	0.518466
19	7	0	-0.607452	-1.616987	1.135292
20	1	0	-3.846369	1.519053	-1.025747
21	8	0	-1.588957	2.538543	-0.672138
22	6	0	-1.926105	1.418522	-0.360685
23	6	0	-3.591683	-0.393155	-0.248138
24	7	0	-3.178600	0.897922	-0.577533

25	7	0	-2.832564	-1.302825	0.312373
26	7	0	-4.859116	-0.662948	-0.551542
27	1	0	-5.220670	-1.583019	-0.351663
28	1	0	-5.464413	0.016123	-0.987695

Standard orientation of TS-G2-n-N9 and initial structure

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

Standard orientation of transition state of TS-G2-n-N9

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1013.93 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.453855	2.296602	-0.364013
2	1	0	3.623064	2.439682	-1.301126
3	8	0	2.222788	-1.324158	1.944625
4	1	0	2.646101	-1.576658	1.100829
5	1	0	2.445257	-0.395822	2.068274
6	8	0	4.718383	0.344769	0.294804
7	1	0	4.100851	1.361208	-0.038079
8	1	0	4.587075	0.240923	1.242969
9	8	0	3.412663	-1.726994	-0.499398
10	1	0	3.953999	-0.900833	-0.264187
11	1	0	4.009525	-2.479085	-0.426980
12	1	0	1.308640	-1.910027	-0.733210
13	6	0	-1.116929	0.192279	-0.175053
14	6	0	0.358912	-1.422407	-0.554711
15	6	0	-1.773090	-1.017983	-0.229502
16	7	0	-0.827637	-1.996154	-0.466537
17	7	0	0.214316	-0.100743	-0.388655
18	17	0	1.562058	1.014414	-0.387373
19	7	0	-1.637863	1.404804	0.038603
20	6	0	-2.948999	1.373282	0.208901
21	7	0	-3.686642	0.214664	0.164938
22	6	0	-3.188658	-1.071955	-0.050413
23	8	0	-3.916908	-2.049483	-0.069798
24	1	0	-4.690913	0.275203	0.306601
25	7	0	-3.622584	2.502445	0.428695
26	1	0	-3.110656	3.367941	0.502403
27	1	0	-4.615289	2.502769	0.607824
28	1	0	-1.003423	-2.990647	-0.564375

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.408888	2.306396	-0.278733

2	1	0	3.565231	2.553394	-1.196433
3	8	0	2.313808	-1.321949	1.933721
4	1	0	2.704065	-1.583839	1.076891
5	1	0	2.561698	-0.398737	2.047175
6	8	0	4.732601	0.332334	0.188170
7	1	0	4.073293	1.389605	-0.054504
8	1	0	4.705128	0.203319	1.141934
9	8	0	3.378937	-1.711102	-0.557958
10	1	0	3.943790	-0.890968	-0.332933
11	1	0	3.967073	-2.472913	-0.534213
12	1	0	1.330117	-1.911562	-0.688079
13	6	0	-1.123338	0.180183	-0.169944
14	6	0	0.374968	-1.424049	-0.517718
15	6	0	-1.785443	-1.028365	-0.214296
16	7	0	-0.819363	-1.999842	-0.431019
17	7	0	0.211888	-0.107794	-0.368351
18	17	0	1.560665	1.023245	-0.349670
19	7	0	-1.643597	1.392125	0.024080
20	6	0	-2.957766	1.369134	0.186134
21	7	0	-3.697636	0.212150	0.156282
22	6	0	-3.204610	-1.079714	-0.038159
23	8	0	-3.934851	-2.053151	-0.045334
24	1	0	-4.703478	0.272874	0.287505
25	7	0	-3.620989	2.504714	0.386150
26	1	0	-3.104171	3.369966	0.422343
27	1	0	-4.619396	2.522837	0.530537
28	1	0	-0.984712	-2.981977	-0.520855

Standard orientation of TS-G2-n-N^2 and initial structure

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

Standard orientation of transition state of TS-G2-n-N^2

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -232.68 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.239071	-0.763811	1.694406
2	8	0	3.471307	-0.830986	-2.071628
3	1	0	4.290658	-1.144582	-1.672114
4	17	0	1.915204	-1.251675	-0.468194
5	8	0	2.097033	0.161633	2.457226
6	1	0	2.835162	0.519120	1.878880
7	1	0	-5.731382	-0.357514	-0.735120
8	1	0	1.588452	0.914236	2.779312
9	8	0	3.237763	1.524776	-1.433228
10	1	0	3.400898	0.237888	-1.848124
11	1	0	2.284796	1.643620	-1.359860
12	8	0	4.035842	0.991853	0.919596
13	1	0	3.703105	1.236446	-0.022766

14	1	0	4.590151	0.211295	0.814852
15	7	0	-3.917538	-1.336640	-0.187881
16	7	0	-4.019776	0.873378	-0.478700
17	6	0	-4.681869	-0.304064	-0.493036
18	6	0	-2.692398	-0.787920	0.036156
19	6	0	-2.728812	0.585139	-0.137429
20	6	0	-1.579699	1.415796	0.038581
21	6	0	-0.537741	-0.731897	0.542896
22	7	0	-0.482389	0.620144	0.400452
23	7	0	-1.561486	-1.484131	0.379551
24	8	0	-1.479662	2.624305	-0.081037
25	7	0	0.712311	-1.335736	0.903488
26	1	0	0.562451	-2.313388	1.163425
27	1	0	0.391787	1.113308	0.573118
28	1	0	-4.406635	1.787784	-0.675521

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.206789	-0.840679	1.690531
2	8	0	3.492501	-0.811336	-2.044651
3	1	0	4.315756	-1.085038	-1.624604
4	17	0	1.940027	-1.267329	-0.458709
5	8	0	2.070048	0.189919	2.476295
6	1	0	2.785782	0.564487	1.892712
7	1	0	-5.685669	-0.316631	-0.748678
8	1	0	1.536327	0.928543	2.788796
9	8	0	3.175858	1.536209	-1.472971
10	1	0	3.374371	0.282050	-1.839423
11	1	0	2.221013	1.631166	-1.389741
12	8	0	4.002861	1.059915	0.903168
13	1	0	3.663051	1.282320	-0.032977
14	1	0	4.556853	0.277982	0.807181
15	7	0	-3.907390	-1.341834	-0.214315
16	7	0	-4.012431	0.941491	-0.482841
17	6	0	-4.633873	-0.239824	-0.505376
18	6	0	-2.694131	-0.814661	0.019993
19	6	0	-2.744609	0.578346	-0.139898
20	6	0	-1.582811	1.379536	0.055636
21	6	0	-0.538670	-0.773596	0.539373
22	7	0	-0.480836	0.580364	0.413884
23	7	0	-1.560448	-1.522277	0.359233
24	8	0	-1.444256	2.596835	-0.042750
25	7	0	0.712511	-1.384477	0.898528
26	1	0	0.562369	-2.367110	1.136913
27	1	0	0.391823	1.070887	0.593454
28	1	0	-4.380316	1.852611	-0.668638

Standard orientation of TS-G1-a-N1 and initial structure

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

Standard orientation of transition state of TS-G1-a-N1

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -75.34 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.075750	0.352878	0.026087
2	6	0	2.384413	-0.826030	-0.266156
3	6	0	0.968698	-0.853805	-0.135635
4	6	0	1.175445	1.423524	0.535761
5	6	0	4.445017	-1.146340	-0.558648
6	1	0	5.386300	-1.626664	-0.795832
7	7	0	4.403583	0.150853	-0.161112
8	1	0	-0.880083	-0.081952	1.532983
9	8	0	-3.685975	-1.583366	1.274657
10	1	0	-4.319839	-1.603865	2.002114
11	17	0	-1.596853	0.800297	-0.866640
12	8	0	-1.546750	-0.317364	2.216967
13	1	0	-1.098610	-0.891971	2.848242
14	1	0	-2.879484	-1.099072	1.594281
15	8	0	-3.111013	1.095649	-1.744987
16	1	0	-4.247792	-1.066903	0.178085
17	1	0	-3.364200	2.013859	-1.571424
18	8	0	-4.727733	-0.658332	-0.723653
19	1	0	-4.157047	0.052019	-1.150285
20	1	0	-4.876204	-1.364620	-1.369172
21	8	0	0.239510	-1.861051	-0.348687
22	7	0	0.470776	2.563463	0.900450
23	1	0	-0.426213	2.377356	1.329360
24	1	0	1.024417	3.225631	1.427171
25	7	0	0.401789	0.335518	0.272533
26	7	0	2.484994	1.514023	0.447606
27	7	0	3.288146	-1.798786	-0.644546

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.075750	0.352878	0.026087
2	6	0	2.384413	-0.826030	-0.266156
3	6	0	0.968698	-0.853805	-0.135635
4	6	0	1.175445	1.423524	0.535761
5	6	0	4.445017	-1.146340	-0.558648
6	1	0	5.386300	-1.626664	-0.795832
7	7	0	4.403583	0.150853	-0.161112
8	1	0	-0.880083	-0.081952	1.532983
9	8	0	-3.685975	-1.583366	1.274657
10	1	0	-4.319839	-1.603865	2.002114
11	17	0	-1.596853	0.800297	-0.866640

12	8	0	-1.546750	-0.317364	2.216967
13	1	0	-1.098610	-0.891971	2.848242
14	1	0	-2.879484	-1.099072	1.594281
15	8	0	-3.111013	1.095649	-1.744987
16	1	0	-4.247792	-1.066903	0.178085
17	1	0	-3.364200	2.013859	-1.571424
18	8	0	-4.727733	-0.658332	-0.723653
19	1	0	-4.157047	0.052019	-1.150285
20	1	0	-4.876204	-1.364620	-1.369172
21	8	0	0.239510	-1.861051	-0.348687
22	7	0	0.470776	2.563463	0.900450
23	1	0	-0.426213	2.377356	1.329360
24	1	0	1.024417	3.225631	1.427171
25	7	0	0.401789	0.335518	0.272533
26	7	0	2.484994	1.514023	0.447606
27	7	0	3.288146	-1.798786	-0.644546

Standard orientation of TS-G1-a-N3 and initial structure

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

Standard orientation of transition state of TS-G1-a-N3

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -860.93 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.610286	0.444941	2.133809
2	1	0	2.754653	0.361686	2.568454
3	8	0	3.305114	-1.848944	0.167598
4	1	0	3.653047	-1.194896	-0.864176
5	1	0	3.579486	-1.326217	0.932192
6	8	0	3.214335	1.552200	-0.364668
7	1	0	3.448527	0.895389	1.280811
8	1	0	3.719741	2.343160	-0.581528
9	8	0	3.893317	-0.539727	-1.784683
10	1	0	3.511730	0.822100	-0.980946
11	1	0	4.843100	-0.575475	-1.936678
12	1	0	-3.473420	-3.348692	0.111464
13	6	0	-2.908179	-0.257763	-0.006951
14	6	0	-3.061389	-2.350008	0.071724
15	6	0	-1.641278	-0.833689	0.005470
16	7	0	-1.710684	-2.157749	0.054847
17	7	0	-3.830838	-1.272586	0.037390
18	6	0	-3.074201	1.147970	-0.057685
19	6	0	-0.590998	1.283668	-0.079933
20	7	0	-1.833073	1.827311	-0.097694
21	7	0	-0.486588	-0.054379	-0.032873
22	17	0	1.068133	-0.812997	0.041107
23	8	0	-4.106628	1.811067	-0.073600
24	7	0	0.469948	2.071282	-0.098998

25	1	0	0.323016	3.070378	-0.160745
26	1	0	1.439501	1.738088	-0.182707
27	1	0	-1.894127	2.840895	-0.147069

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.657113	0.285804	2.072585
2	1	0	2.786151	0.180643	2.468802
3	8	0	3.201492	-1.800351	0.091967
4	1	0	3.591665	-1.137510	-0.896632
5	1	0	3.504522	-1.298422	0.861124
6	8	0	3.208656	1.545446	-0.285710
7	1	0	3.518177	0.815927	1.259990
8	1	0	3.700868	2.349453	-0.479579
9	8	0	3.897232	-0.429413	-1.773368
10	1	0	3.500207	0.828789	-0.940375
11	1	0	4.858960	-0.423781	-1.804488
12	1	0	-3.506525	-3.322981	0.064778
13	6	0	-2.911820	-0.241224	-0.008704
14	6	0	-3.084080	-2.327575	0.041003
15	6	0	-1.649341	-0.829322	0.002671
16	7	0	-1.731426	-2.152960	0.034454
17	7	0	-3.846205	-1.245295	0.016842
18	6	0	-3.066166	1.168233	-0.043591
19	6	0	-0.578035	1.271787	-0.054086
20	7	0	-1.813939	1.832602	-0.067046
21	7	0	-0.486207	-0.063530	-0.017791
22	17	0	1.090320	-0.845144	0.031575
23	8	0	-4.087797	1.842663	-0.057773
24	7	0	0.490192	2.051770	-0.068362
25	1	0	0.348520	3.051169	-0.117543
26	1	0	1.461710	1.715216	-0.141052
27	1	0	-1.863505	2.846235	-0.103849

Standard orientation of TS-G1-a-N7 and initial structure

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

Standard orientation of transition state of TS-G1-a-N7

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -91.30 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.055310	0.601367	-1.063860
2	1	0	4.080930	0.279751	-1.973112
3	17	0	2.168486	0.933716	-0.682972

4	8	0	0.371304	-0.385433	2.640393
5	1	0	0.778470	-0.977628	1.974151
6	1	0	-0.402345	0.002593	2.215922
7	8	0	4.215235	-1.407308	0.668379
8	1	0	4.236097	-0.655719	0.022443
9	1	0	4.516650	-1.057251	1.513514
10	8	0	1.559422	-2.104321	0.846643
11	1	0	2.498903	-1.837712	0.768579
12	1	0	1.140074	-1.923415	-0.010186
13	6	0	-0.816469	0.472164	-0.335005
14	6	0	-1.889787	1.175093	0.220683
15	6	0	-3.341883	-0.485115	-0.188214
16	6	0	-1.000410	-0.831147	-0.854984
17	6	0	-0.158296	2.391873	0.371404
18	1	0	0.503007	3.217015	0.595501
19	7	0	-1.466763	2.386734	0.664745
20	7	0	0.284874	1.288423	-0.231263
21	7	0	-2.327228	-1.232326	-0.739093
22	7	0	-3.170652	0.709997	0.305440
23	8	0	-0.163928	-1.596729	-1.358042
24	1	0	-2.539797	-2.157728	-1.099943
25	7	0	-4.582717	-1.049300	-0.235436
26	1	0	-4.635085	-2.058337	-0.281568
27	1	0	-5.261434	-0.627256	0.383047

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.055183	0.600237	-1.064952
2	1	0	4.080353	0.278545	-1.974165
3	17	0	2.168485	0.933190	-0.683401
4	8	0	0.369914	-0.386656	2.640224
5	1	0	0.777547	-0.978307	1.973779
6	1	0	-0.403632	0.001491	2.215653
7	8	0	4.215107	-1.405951	0.670005
8	1	0	4.236018	-0.655508	0.022687
9	1	0	4.514867	-1.053798	1.514868
10	8	0	1.559405	-2.104210	0.846071
11	1	0	2.498808	-1.837111	0.768719
12	1	0	1.140453	-1.923001	-0.010891
13	6	0	-0.816274	0.472342	-0.335064
14	6	0	-1.889439	1.175279	0.220883
15	6	0	-3.341722	-0.484777	-0.187989
16	6	0	-1.000398	-0.830864	-0.855244
17	6	0	-0.157755	2.391784	0.371779
18	1	0	0.503638	3.216800	0.596048
19	7	0	-1.466202	2.386767	0.665185
20	7	0	0.285204	1.288387	-0.231168
21	7	0	-2.327225	-1.231937	-0.739238
22	7	0	-3.170346	0.710286	0.305739
23	8	0	-0.164043	-1.596437	-1.358508
24	1	0	-2.539844	-2.157355	-1.100028
25	7	0	-4.582540	-1.049057	-0.234900

26	1	0	-4.634704	-2.058106	-0.281276
27	1	0	-5.260990	-0.627455	0.384178

Standard orientation of TS-G1-a-C8 and initial structure

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

Standard orientation of transition state of TS-G1-a-C8

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -448.95 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.696552	-1.425315	1.340486
2	1	0	-1.123782	-0.582641	2.081845
3	8	0	-2.915704	-1.880335	-1.663616
4	1	0	-2.370474	-1.855109	-2.460546
5	17	0	-1.667807	-1.235339	-0.252025
6	8	0	-4.082744	0.626471	1.658356
7	1	0	-3.434495	1.244534	1.270316
8	1	0	-3.598127	-0.184433	1.850993
9	8	0	-4.345647	0.403686	-1.243547
10	1	0	-3.888555	-0.433176	-1.480026
11	1	0	-4.560654	0.331671	-0.300156
12	8	0	-2.427792	2.117856	-0.031223
13	1	0	-2.877132	1.567424	-0.696404
14	1	0	-1.563142	1.707440	0.155163
15	7	0	-0.037314	0.704354	0.781943
16	6	0	-0.368677	-0.535103	1.307562
17	6	0	1.203262	0.534814	0.377904
18	6	0	1.664968	-0.777254	0.725385
19	6	0	3.691371	-0.407501	-0.177071
20	6	0	2.078168	1.448940	-0.329073
21	7	0	3.318644	0.877561	-0.547601
22	7	0	2.918209	-1.252038	0.445806
23	8	0	1.820548	2.585523	-0.701443
24	1	0	3.995611	1.451020	-1.042517
25	7	0	4.939206	-0.762093	-0.553152
26	1	0	5.313869	-1.605197	-0.142527
27	1	0	5.608695	-0.047045	-0.800560

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.705267	-1.420706	1.353127
2	1	0	-1.121299	-0.585139	2.086405
3	8	0	-2.904113	-1.911809	-1.649839
4	1	0	-2.374732	-1.839354	-2.454646

5	17	0	-1.659808	-1.252197	-0.243311
6	8	0	-4.104316	0.709300	1.657540
7	1	0	-3.488625	1.332514	1.227285
8	1	0	-3.573782	-0.057417	1.901957
9	8	0	-4.355316	0.357601	-1.225184
10	1	0	-3.892649	-0.479812	-1.452206
11	1	0	-4.559445	0.301984	-0.278433
12	8	0	-2.423186	2.105496	-0.087629
13	1	0	-2.894127	1.551785	-0.735571
14	1	0	-1.583370	1.659658	0.126615
15	7	0	-0.040825	0.698336	0.776018
16	6	0	-0.365681	-0.537744	1.312822
17	6	0	1.201205	0.535008	0.374746
18	6	0	1.670526	-0.771399	0.733646
19	6	0	3.695035	-0.397154	-0.170187
20	6	0	2.071126	1.448598	-0.339194
21	7	0	3.315787	0.882321	-0.550541
22	7	0	2.928016	-1.240661	0.460659
23	8	0	1.807944	2.579446	-0.722366
24	1	0	3.987678	1.453197	-1.055541
25	7	0	4.945709	-0.750988	-0.554811
26	1	0	5.315759	-1.588097	-0.127161
27	1	0	5.622276	-0.024200	-0.744772

Standard orientation of TS-G1-a-N9 and initial structure

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

Standard orientation of transition state of TS-G1-a-N9

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -88.36 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.155014	-0.532521	-0.840344
2	1	0	4.614252	-1.273510	-0.424386
3	17	0	2.349995	-0.934098	-0.749228
4	8	0	0.154836	-0.325501	2.602447
5	1	0	0.537940	0.414665	2.089203
6	1	0	-0.608261	-0.635176	2.098838
7	8	0	3.943260	1.558943	0.871844
8	1	0	4.131048	0.836291	0.234338
9	1	0	4.317249	2.363851	0.497752
10	8	0	1.214054	1.804095	1.169556
11	1	0	2.179474	1.698726	1.046282
12	1	0	0.795175	1.625648	0.311239
13	6	0	-0.282898	-2.472937	-0.106986
14	6	0	-0.716264	-0.418030	-0.547688
15	7	0	0.276267	-1.332190	-0.592588
16	6	0	-1.722147	1.575155	-0.722900
17	6	0	-3.050446	-0.322503	0.119851

18	6	0	-1.851710	-1.062898	-0.052118
19	7	0	-1.559747	-2.382700	0.223618
20	7	0	-0.615405	0.898802	-0.896848
21	7	0	-2.882926	1.016869	-0.252603
22	1	0	0.295859	-3.381312	-0.011022
23	8	0	-4.147111	-0.707663	0.539782
24	1	0	-3.703040	1.608191	-0.158328
25	7	0	-1.782635	2.891671	-1.060983
26	1	0	-0.884814	3.345555	-1.161122
27	1	0	-2.493321	3.458006	-0.617328

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.123465	-0.497509	-0.906670
2	1	0	4.558472	-1.211778	-0.426839
3	17	0	2.200837	-0.924503	-0.751776
4	8	0	0.217579	-0.482507	2.525023
5	1	0	0.617425	0.293779	2.084913
6	1	0	-0.638583	-0.607376	2.101287
7	8	0	3.956278	1.503593	0.796180
8	1	0	4.071323	0.760395	0.143932
9	1	0	4.145070	2.316784	0.317444
10	8	0	1.286633	1.731367	1.260736
11	1	0	2.248339	1.612273	1.104243
12	1	0	0.844130	1.597710	0.407734
13	6	0	-0.261997	-2.455925	-0.107412
14	6	0	-0.691850	-0.373034	-0.510917
15	7	0	0.296777	-1.294146	-0.551542
16	6	0	-1.690665	1.618207	-0.654148
17	6	0	-3.044504	-0.313860	0.079995
18	6	0	-1.831256	-1.043485	-0.073433
19	7	0	-1.542915	-2.369726	0.179007
20	7	0	-0.575346	0.948316	-0.816605
21	7	0	-2.864951	1.039017	-0.250199
22	1	0	0.325704	-3.358314	-0.019836
23	8	0	-4.146442	-0.712216	0.448924
24	1	0	-3.689824	1.623503	-0.162583
25	7	0	-1.736767	2.942398	-0.937503
26	1	0	-0.838963	3.399782	-1.007282
27	1	0	-2.473376	3.495544	-0.522990

Standard orientation of TS-G1-a-N^2 and initial structure

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

Standard orientation of transition state of TS-G1-a-N^2

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -616.91 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.097964	0.610087	1.563979
2	8	0	3.212897	-2.146730	-1.192888
3	1	0	3.528196	-2.941140	-0.747347
4	17	0	1.757558	-1.180118	0.205617
5	8	0	1.962912	1.909736	1.626351
6	1	0	2.771269	1.837827	1.058286
7	1	0	-5.848711	-0.981943	-0.342594
8	1	0	1.450420	2.658190	1.298750
9	8	0	4.927250	-0.438718	-1.070271
10	1	0	4.038737	-1.368471	-1.156187
11	1	0	5.241446	-0.224368	-1.954441
12	8	0	4.142293	1.715288	0.118905
13	1	0	4.444520	0.869106	-0.346395
14	1	0	4.917295	2.100859	0.540224
15	7	0	-3.987713	-1.330513	0.618955
16	7	0	-4.306350	0.337523	-0.927539
17	6	0	-4.815126	-0.682527	-0.231979
18	6	0	-2.832359	-0.660865	0.453562
19	6	0	-3.014753	0.361774	-0.488844
20	6	0	-1.940629	1.224668	-0.839896
21	6	0	-0.700796	-0.128892	0.762679
22	7	0	-0.774336	0.892667	-0.132571
23	7	0	-1.645686	-0.927960	1.095923
24	8	0	-1.924514	2.166812	-1.636857
25	7	0	0.597634	-0.317534	1.346574
26	1	0	0.508916	-0.888773	2.190171
27	1	0	0.041897	1.475305	-0.304393

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.121371	0.564445	1.610013
2	8	0	3.246112	-2.165569	-1.183351
3	1	0	3.680349	-2.882562	-0.707224
4	17	0	1.767334	-1.223586	0.233025
5	8	0	1.945772	1.816714	1.718941
6	1	0	2.753903	1.775158	1.139674
7	1	0	-5.885195	-0.905256	-0.381627
8	1	0	1.431513	2.583511	1.439166
9	8	0	4.773063	-0.251848	-1.293085
10	1	0	3.948710	-1.338527	-1.257104
11	1	0	4.878280	0.041209	-2.203769
12	8	0	4.092538	1.710481	0.195183
13	1	0	4.357935	0.922721	-0.398833
14	1	0	4.887703	2.010472	0.647280
15	7	0	-3.986190	-1.293233	0.537465
16	7	0	-4.284662	0.380352	-0.921210
17	6	0	-4.848921	-0.616055	-0.288756
18	6	0	-2.783646	-0.655292	0.426970

19	6	0	-2.983303	0.366473	-0.482786
20	6	0	-1.892164	1.231399	-0.816108
21	6	0	-0.673310	-0.167502	0.769366
22	7	0	-0.733794	0.864487	-0.105606
23	7	0	-1.633144	-0.966340	1.079268
24	8	0	-1.873791	2.180739	-1.584134
25	7	0	0.609827	-0.376177	1.370708
26	1	0	0.507208	-0.960127	2.205014
27	1	0	0.087799	1.448023	-0.258944

Standard orientation of TS-A1-n-N1 and initial structure

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

Standard orientation of transition state of TS-A1-n-N1

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -998.37 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.668143	-1.536686	-0.646292
2	1	0	-3.800442	-1.374197	-1.586494
3	8	0	-1.456707	1.258484	1.980115
4	1	0	-1.857036	1.582756	1.153599
5	1	0	-1.928466	0.446376	2.190115
6	8	0	-4.453727	0.438999	0.494399
7	1	0	-4.087129	-0.592784	-0.073986
8	1	0	-4.166233	0.378112	1.411242
9	8	0	-2.630545	1.911829	-0.471926
10	1	0	-3.419241	1.356410	-0.129177
11	1	0	-2.881971	2.840296	-0.444707
12	1	0	5.157381	1.549323	-0.147803
13	6	0	2.185271	0.475020	-0.256935
14	6	0	4.218343	1.019801	-0.119235
15	1	0	4.920554	-0.854408	0.613225
16	6	0	2.843908	-0.647078	0.217450
17	7	0	4.148588	-0.278950	0.300414
18	7	0	3.056827	1.515719	-0.464253
19	6	0	0.787793	0.403456	-0.441339
20	6	0	1.008992	-1.863764	0.336997
21	1	0	0.445036	-2.763868	0.545149
22	7	0	0.053995	1.392615	-0.902632
23	1	0	-0.973953	1.425087	-0.854079
24	1	0	0.529219	2.268255	-1.078509
25	7	0	0.259648	-0.814187	-0.125173
26	7	0	2.290148	-1.840827	0.529362
27	17	0	-1.482060	-1.116916	-0.366740

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.669865	-1.519493	-0.675036
2	1	0	-3.789151	-1.324343	-1.610925
3	8	0	-1.446750	1.243920	1.989769
4	1	0	-1.850073	1.571045	1.166149
5	1	0	-1.913989	0.428367	2.196038
6	8	0	-4.447848	0.435160	0.505577
7	1	0	-4.084006	-0.587127	-0.081249
8	1	0	-4.147004	0.363536	1.417296
9	8	0	-2.627860	1.913755	-0.460023
10	1	0	-3.415430	1.357610	-0.117480
11	1	0	-2.877299	2.842469	-0.422329
12	1	0	5.150696	1.553774	-0.160134
13	6	0	2.181034	0.474287	-0.256327
14	6	0	4.212609	1.022250	-0.127295
15	1	0	4.924255	-0.847199	0.602955
16	6	0	2.842676	-0.646248	0.216975
17	7	0	4.147375	-0.275686	0.294738
18	7	0	3.049286	1.516567	-0.468107
19	6	0	0.784265	0.400751	-0.440471
20	6	0	1.008063	-1.862802	0.346933
21	1	0	0.446273	-2.762428	0.563804
22	7	0	0.051247	1.387587	-0.908201
23	1	0	-0.976439	1.423398	-0.852190
24	1	0	0.529113	2.260664	-1.089352
25	7	0	0.257280	-0.815975	-0.119011
26	7	0	2.290175	-1.839033	0.535291
27	17	0	-1.482222	-1.118244	-0.369220

Standard orientation of TS-A1-n-C2 and initial structure

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

Standard orientation of transition state of TS-A1-n-C2

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1372.75 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.058986	-0.973721	0.236593
2	6	0	2.825186	0.150256	-0.057891
3	6	0	2.120356	1.355733	-0.251454
4	6	0	0.166851	0.172452	0.147460
5	1	0	-0.865593	0.390468	1.001686
6	8	0	-4.060039	0.657876	1.619115
7	1	0	-4.294558	1.501514	1.217988
8	17	0	-1.670819	-0.021816	-0.938871
9	8	0	-1.530294	0.700989	2.025179
10	1	0	-1.306607	0.074475	2.725332

11	1	0	-2.530572	0.655273	1.862442
12	8	0	-3.179169	-0.273024	-2.120052
13	1	0	-4.325307	-0.043781	0.977975
14	1	0	-3.466368	0.629132	-2.310155
15	8	0	-4.737310	-1.217173	-0.171558
16	1	0	-4.221135	-0.905763	-0.953734
17	1	0	-4.322085	-2.037061	0.115719
18	7	0	2.746845	2.516865	-0.508146
19	1	0	3.728628	2.516025	-0.736085
20	1	0	2.196635	3.318345	-0.776283
21	6	0	4.200669	-1.442865	0.163363
22	1	0	2.768501	-2.956317	0.589216
23	1	0	5.094777	-2.044575	0.215778
24	7	0	0.784771	1.332119	-0.147195
25	7	0	0.727935	-1.021779	0.348429
26	7	0	2.968525	-1.988122	0.377010
27	7	0	4.167614	-0.160132	-0.101381

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.992649	-1.013200	0.054069
2	6	0	2.818509	0.102653	-0.045010
3	6	0	2.179489	1.358307	-0.014488
4	6	0	0.164680	0.228960	0.183009
5	1	0	-0.860916	0.328736	1.065520
6	8	0	-4.024267	-0.033410	1.776962
7	1	0	-4.472517	0.817728	1.734711
8	17	0	-1.679949	0.329894	-0.900608
9	8	0	-1.532124	0.438781	2.126715
10	1	0	-1.172470	-0.189642	2.766163
11	1	0	-2.512238	0.222846	1.977910
12	8	0	-3.203757	0.373508	-2.089840
13	1	0	-4.240189	-0.507390	0.938690
14	1	0	-3.559655	1.262521	-1.964075
15	8	0	-4.631992	-1.249215	-0.531841
16	1	0	-4.162451	-0.668487	-1.178537
17	1	0	-4.174429	-2.096004	-0.548514
18	7	0	2.866091	2.513102	-0.063870
19	1	0	3.844563	2.502070	-0.305331
20	1	0	2.356240	3.374298	-0.187746
21	6	0	4.106017	-1.575599	-0.108293
22	1	0	2.592096	-3.061436	0.056156
23	1	0	4.967195	-2.223973	-0.161616
24	7	0	0.844425	1.387537	0.097238
25	7	0	0.660955	-1.009669	0.164762
26	7	0	2.845977	-2.083498	0.013733
27	7	0	4.142972	-0.266543	-0.148248

Standard orientation of TS-A1-n-N3 and initial structure

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

Standard orientation of transition state of TS-A1-n-N3

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -751.31 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.394019	1.961295	-0.400216
2	1	0	3.605890	2.049723	-1.335649
3	8	0	1.596152	-1.491023	1.838378
4	1	0	2.021419	-1.750230	0.996132
5	1	0	1.935296	-0.611110	2.031445
6	8	0	4.395064	-0.100707	0.377576
7	1	0	3.905567	0.997150	-0.026940
8	1	0	4.165307	-0.174678	1.309699
9	8	0	2.868096	-1.947489	-0.545735
10	1	0	3.507622	-1.213859	-0.249509
11	1	0	3.346304	-2.779339	-0.466008
12	1	0	-3.455435	3.085898	0.715818
13	6	0	-2.566734	0.118111	0.029964
14	6	0	-2.981709	2.149796	0.466312
15	1	0	-0.977434	2.865184	0.248664
16	6	0	-1.364533	0.795898	-0.054323
17	7	0	-1.628575	2.089290	0.223986
18	7	0	-3.577280	0.994892	0.360345
19	6	0	-2.554029	-1.272606	-0.217805
20	6	0	-0.277057	-1.162689	-0.583057
21	1	0	0.666850	-1.640000	-0.825004
22	7	0	-3.642061	-2.018736	-0.160468
23	1	0	-3.584534	-3.009568	-0.348257
24	1	0	-4.539172	-1.611996	0.060039
25	7	0	-1.373213	-1.873270	-0.527406
26	7	0	-0.209728	0.165476	-0.365876
27	17	0	1.344473	1.008329	-0.401828

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.364495	1.996955	-0.328022
2	1	0	3.560615	2.163342	-1.256227
3	8	0	1.707567	-1.523564	1.835469
4	1	0	2.093295	-1.764717	0.969638
5	1	0	2.039131	-0.639295	2.021704
6	8	0	4.420516	-0.094931	0.281947
7	1	0	3.900135	1.020300	-0.037312
8	1	0	4.245440	-0.213405	1.221318
9	8	0	2.856237	-1.919196	-0.622877
10	1	0	3.508754	-1.192582	-0.337281
11	1	0	3.336223	-2.753030	-0.586848

12	1	0	-3.499126	3.079658	0.645989
13	6	0	-2.578234	0.106469	0.029326
14	6	0	-3.015501	2.142262	0.420376
15	1	0	-1.015254	2.870432	0.216395
16	6	0	-1.380873	0.792265	-0.053740
17	7	0	-1.659285	2.088768	0.195206
18	7	0	-3.600047	0.980402	0.330909
19	6	0	-2.552909	-1.287165	-0.198766
20	6	0	-0.272310	-1.166627	-0.535986
21	1	0	0.677692	-1.640905	-0.762941
22	7	0	-3.638083	-2.037994	-0.145561
23	1	0	-3.575329	-3.030262	-0.323294
24	1	0	-4.539738	-1.630602	0.054035
25	7	0	-1.364662	-1.884179	-0.485241
26	7	0	-0.217091	0.164924	-0.337300
27	17	0	1.331222	1.020605	-0.354745

Standard orientation of TS-A1-n-N7 and initial structure

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

Standard orientation of transition state of TS-A1-n-N7

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -510.15 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.013683	2.235983	-0.211843
2	1	0	3.157316	2.525207	-1.119370
3	8	0	1.987613	-1.451324	1.860629
4	1	0	2.357557	-1.679063	0.984936
5	1	0	2.232461	-0.531053	2.001672
6	8	0	4.369474	0.257970	0.162521
7	1	0	3.683912	1.337837	-0.036036
8	1	0	4.347747	0.088848	1.110127
9	8	0	3.027596	-1.756191	-0.658289
10	1	0	3.590215	-0.940943	-0.402210
11	1	0	3.619006	-2.515855	-0.658607
12	1	0	0.932213	-1.939425	-0.749505
13	6	0	-1.526076	0.087526	-0.124296
14	6	0	-0.023475	-1.469243	-0.549461
15	1	0	-1.362099	-3.073333	-0.577359
16	6	0	-2.177795	-1.132699	-0.190642
17	7	0	-1.209268	-2.077300	-0.460464
18	7	0	-0.182977	-0.170580	-0.357436
19	6	0	-2.309993	1.234272	0.130450
20	6	0	-4.121394	-0.199107	0.228781
21	1	0	-5.190340	-0.279934	0.386428
22	7	0	-1.825108	2.474629	0.200693
23	1	0	-2.465059	3.236466	0.370871
24	1	0	-0.855398	2.690841	0.033441

25	7	0	-3.624842	1.037606	0.311321
26	7	0	-3.482647	-1.336402	-0.022560
27	17	0	1.175991	0.951103	-0.308141

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.999720	2.243515	-0.186351
2	1	0	3.125844	2.553670	-1.089528
3	8	0	2.054747	-1.458154	1.846737
4	1	0	2.406513	-1.689625	0.964728
5	1	0	2.294976	-0.534735	1.974167
6	8	0	4.379147	0.269368	0.115366
7	1	0	3.679084	1.349518	-0.043986
8	1	0	4.386817	0.080655	1.059395
9	8	0	3.029374	-1.740424	-0.698993
10	1	0	3.592004	-0.923235	-0.447631
11	1	0	3.629687	-2.491979	-0.737405
12	1	0	0.934737	-1.942902	-0.703178
13	6	0	-1.533043	0.083052	-0.112144
14	6	0	-0.023218	-1.472840	-0.512452
15	1	0	-1.357070	-3.080697	-0.541449
16	6	0	-2.181526	-1.138859	-0.176308
17	7	0	-1.208445	-2.083345	-0.429944
18	7	0	-0.187348	-0.173319	-0.331548
19	6	0	-2.322257	1.230323	0.120822
20	6	0	-4.132298	-0.205155	0.207641
21	1	0	-5.203347	-0.286117	0.351821
22	7	0	-1.839979	2.471812	0.187301
23	1	0	-2.482668	3.234128	0.343404
24	1	0	-0.867683	2.687102	0.035298
25	7	0	-3.639303	1.033275	0.284068
26	7	0	-3.487992	-1.343805	-0.022695
27	17	0	1.167808	0.954019	-0.279725

Standard orientation of TS-A1-n-C8 and initial structure

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

Standard orientation of transition state of TS-A1-n-C8

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -399.30 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.264767	-0.913501	-0.138372
2	6	0	1.853501	0.279479	0.421894
3	6	0	3.221411	0.558079	0.030575

4	6	0	3.121406	-1.352066	-1.248789
5	6	0	-0.171784	0.211182	1.125493
6	1	0	3.669802	-1.992765	-1.930316
7	1	0	-0.720776	0.078074	2.050631
8	7	0	0.043308	-0.965111	0.360721
9	8	0	-2.459338	-1.865370	-0.196563
10	1	0	-2.807703	-2.744426	-0.376251
11	17	0	-1.461633	1.299705	0.090056
12	8	0	-2.678913	-1.256393	2.483665
13	1	0	-1.942992	-1.757228	2.849623
14	1	0	-2.679709	-1.459600	1.529257
15	8	0	-2.974426	2.261462	-1.083543
16	1	0	-2.936176	-1.225038	-0.784247
17	1	0	-3.574478	2.541258	-0.382209
18	8	0	-3.743241	-0.135428	-1.775409
19	1	0	-3.479998	0.801787	-1.526168
20	1	0	-3.398288	-0.286214	-2.661195
21	1	0	-0.748991	-1.565949	0.073174
22	7	0	3.857702	1.612433	0.488034
23	1	0	3.412073	2.260041	1.123234
24	1	0	4.814878	1.782954	0.207843
25	7	0	3.818045	-0.292989	-0.807940
26	7	0	1.875719	-1.741496	-0.988125
27	7	0	1.026891	0.921294	1.193832

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.264567	-0.904354	-0.170723
2	6	0	1.856386	0.271021	0.420464
3	6	0	3.226230	0.554519	0.041294
4	6	0	3.122802	-1.321753	-1.285392
5	6	0	-0.168745	0.191299	1.121223
6	1	0	3.672089	-1.947853	-1.980098
7	1	0	-0.714728	0.037583	2.045071
8	7	0	0.042885	-0.965888	0.327380
9	8	0	-2.461226	-1.858728	-0.238851
10	1	0	-2.790112	-2.732811	-0.471012
11	17	0	-1.460390	1.304187	0.109566
12	8	0	-2.638588	-1.360039	2.465368
13	1	0	-1.870402	-1.838924	2.792464
14	1	0	-2.659830	-1.532923	1.505289
15	8	0	-2.965273	2.291718	-1.044812
16	1	0	-2.954801	-1.195837	-0.786955
17	1	0	-3.552293	2.587520	-0.339101
18	8	0	-3.807272	-0.085810	-1.710630
19	1	0	-3.514146	0.844927	-1.471143
20	1	0	-3.525639	-0.232478	-2.619063
21	1	0	-0.751201	-1.559733	0.029642
22	7	0	3.860612	1.596168	0.529813
23	1	0	3.409804	2.224957	1.179995
24	1	0	4.819518	1.776094	0.262077
25	7	0	3.823625	-0.277746	-0.815546

26	7	0	1.874407	-1.711933	-1.040973
27	7	0	1.031300	0.896081	1.207958

Standard orientation of TS-A1-n-N9 and initial structure

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

Standard orientation of transition state of TS-A1-n-N9

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -120.69 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.607695	-0.009584	1.602142
2	8	0	-3.677596	-1.282159	-1.011108
3	1	0	-3.709146	-1.250032	-1.975057
4	17	0	-1.847770	-1.178363	-0.567770
5	8	0	-0.949194	0.702975	2.163066
6	1	0	-1.894947	1.581709	1.330970
7	1	0	0.372468	-2.873510	1.049716
8	1	0	-1.439865	0.282720	2.878461
9	8	0	-4.463616	0.969803	-0.027976
10	1	0	-4.217309	0.082450	-0.433760
11	1	0	-5.074755	0.802201	0.698232
12	8	0	-2.518367	2.175449	0.788347
13	1	0	-3.392231	1.617108	0.419428
14	1	0	-2.026559	2.548591	0.044352
15	7	0	0.140538	-1.051256	-0.024598
16	7	0	2.143373	-1.736271	0.788128
17	6	0	0.854548	-1.989646	0.654386
18	6	0	1.055323	-0.100771	-0.372697
19	6	0	2.283830	-0.530255	0.135031
20	6	0	3.392397	0.303245	-0.096158
21	6	0	1.973060	1.733141	-1.209993
22	1	0	1.887128	2.666487	-1.756942
23	7	0	3.212450	1.440826	-0.782269
24	7	0	0.854289	1.043156	-1.059262
25	7	0	4.623468	0.012477	0.382967
26	1	0	4.806408	-0.930825	0.689061
27	1	0	5.405013	0.529513	0.008691

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.608695	-0.006119	1.604378
2	8	0	-3.675475	-1.285368	-1.012190
3	1	0	-3.705792	-1.255847	-1.976249
4	17	0	-1.845026	-1.176677	-0.566199

5	8	0	-0.954795	0.705297	2.163904
6	1	0	-1.903391	1.580444	1.328966
7	1	0	0.372049	-2.872778	1.046337
8	1	0	-1.445358	0.283275	2.878310
9	8	0	-4.468476	0.963888	-0.034150
10	1	0	-4.219062	0.076303	-0.438951
11	1	0	-5.081028	0.795574	0.690709
12	8	0	-2.527125	2.171859	0.784803
13	1	0	-3.401020	1.611247	0.414600
14	1	0	-2.034759	2.544739	0.041083
15	7	0	0.140831	-1.046611	-0.021452
16	7	0	2.144249	-1.737787	0.784335
17	6	0	0.854822	-1.988485	0.652803
18	6	0	1.056549	-0.096697	-0.368982
19	6	0	2.285335	-0.530074	0.134578
20	6	0	3.395064	0.301762	-0.096968
21	6	0	1.975962	1.737672	-1.203185
22	1	0	1.890672	2.672731	-1.747329
23	7	0	3.215798	1.441595	-0.779483
24	7	0	0.856105	1.049588	-1.051616
25	7	0	4.626670	0.007077	0.378199
26	1	0	4.808482	-0.937349	0.681461
27	1	0	5.408359	0.523782	0.003779

Standard orientation of TS-A1-n-N^6 and initial structure

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

Standard orientation of transition state of TS-A1-n-N^6

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -177.74 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.031133	-0.693350	1.576649
2	8	0	-3.102112	1.910916	-1.364248
3	1	0	-3.589863	2.439011	-0.722509
4	17	0	-1.541800	1.135239	-0.167095
5	8	0	-1.710943	-1.421395	1.945888
6	1	0	-2.708739	-1.205091	1.624590
7	1	0	4.807618	1.844696	1.118642
8	1	0	-1.451935	-2.290670	1.611160
9	8	0	-4.182789	-0.404126	-1.325533
10	1	0	-3.790489	0.535086	-1.386365
11	1	0	-3.542303	-0.988938	-1.744184
12	8	0	-4.012690	-0.916425	1.236275
13	1	0	-4.083057	-0.727893	0.255731
14	1	0	-4.314214	-0.127400	1.700456
15	7	0	4.310050	0.224064	-0.176652
16	7	0	2.764413	1.278274	1.058304
17	6	0	4.028182	1.206643	0.731272

18	6	0	3.126565	-0.394066	-0.463659
19	6	0	2.175423	0.274967	0.313562
20	6	0	0.860306	-0.177123	0.193008
21	6	0	1.599601	-1.733828	-1.323510
22	1	0	1.328874	-2.550408	-1.982406
23	7	0	0.589664	-1.188637	-0.632969
24	7	0	2.886843	-1.403631	-1.299097
25	7	0	-0.187230	0.366089	0.932813
26	1	0	0.149143	1.113934	1.534151
27	1	0	5.218331	0.007526	-0.565196

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.031307	-0.727029	1.557647
2	8	0	-3.099320	1.931158	-1.339717
3	1	0	-3.577529	2.461924	-0.693040
4	17	0	-1.540025	1.132081	-0.154912
5	8	0	-1.710295	-1.461359	1.914084
6	1	0	-2.710247	-1.235228	1.604221
7	1	0	4.804565	1.827759	1.160713
8	1	0	-1.455441	-2.323205	1.557629
9	8	0	-4.210465	-0.368135	-1.314892
10	1	0	-3.804350	0.566085	-1.368297
11	1	0	-3.589452	-0.956013	-1.757730
12	8	0	-4.014546	-0.935174	1.232150
13	1	0	-4.092783	-0.725023	0.256325
14	1	0	-4.313613	-0.157315	1.716270
15	7	0	4.313246	0.231192	-0.166432
16	7	0	2.762462	1.259268	1.084032
17	6	0	4.027240	1.195901	0.759193
18	6	0	3.131594	-0.383379	-0.468316
19	6	0	2.177246	0.269249	0.318822
20	6	0	0.863222	-0.182564	0.186172
21	6	0	1.609103	-1.709093	-1.357449
22	1	0	1.341490	-2.513459	-2.032435
23	7	0	0.596421	-1.178748	-0.659398
24	7	0	2.895733	-1.377297	-1.323411
25	7	0	-0.187018	0.345207	0.933265
26	1	0	0.146780	1.082685	1.548669
27	1	0	5.222989	0.023479	-0.556377

Standard orientation of TS-A2-n-N1 and initial structure

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

Standard orientation of transition state of TS-A2-n-N1

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -999.67cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.662891	-1.529123	-0.659062
2	1	0	-3.791270	-1.362934	-1.599170
3	8	0	-1.466899	1.258431	1.987669
4	1	0	-1.867087	1.581860	1.160872
5	1	0	-1.935808	0.444310	2.196321
6	8	0	-4.455795	0.440921	0.486057
7	1	0	-4.085986	-0.588159	-0.084460
8	1	0	-4.169997	0.377753	1.403297
9	8	0	-2.626209	1.909125	-0.472231
10	1	0	-3.418603	1.356456	-0.132806
11	1	0	-2.875433	2.838322	-0.450731
12	1	0	5.235124	1.416372	-0.095946
13	6	0	2.189532	0.437009	-0.241964
14	6	0	4.315631	0.854373	-0.051418
15	6	0	2.879256	-0.673242	0.230441
16	7	0	4.207938	-0.398421	0.345357
17	7	0	3.138763	1.409758	-0.414823
18	6	0	0.795206	0.398460	-0.432141
19	6	0	1.007570	-1.872985	0.340782
20	1	0	0.432754	-2.767352	0.545236
21	7	0	0.056098	1.388956	-0.890493
22	1	0	-0.972299	1.410733	-0.834688
23	1	0	0.508173	2.276585	-1.066087
24	7	0	0.262587	-0.816074	-0.120778
25	7	0	2.284449	-1.859127	0.533546
26	17	0	-1.478697	-1.112488	-0.369267
27	1	0	3.000637	2.356183	-0.747630

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.661712	-1.530929	-0.654594
2	1	0	-3.792543	-1.368739	-1.595051
3	8	0	-1.467965	1.261425	1.986326
4	1	0	-1.867629	1.587859	1.160441
5	1	0	-1.933571	0.443857	2.188728
6	8	0	-4.455296	0.441839	0.485532
7	1	0	-4.084716	-0.589213	-0.082907
8	1	0	-4.170232	0.380641	1.403126
9	8	0	-2.626707	1.910300	-0.473825
10	1	0	-3.418837	1.357243	-0.134083
11	1	0	-2.878457	2.838909	-0.458845
12	1	0	5.234157	1.418453	-0.094124
13	6	0	2.189216	0.437153	-0.241811
14	6	0	4.315004	0.855796	-0.050379
15	6	0	2.879532	-0.672892	0.230323
16	7	0	4.208007	-0.397242	0.345749
17	7	0	3.137917	1.410604	-0.413929
18	6	0	0.794991	0.397795	-0.432413

19	6	0	1.008577	-1.873814	0.339729
20	1	0	0.434333	-2.768676	0.543708
21	7	0	0.055481	1.387893	-0.890895
22	1	0	-0.972924	1.409070	-0.835701
23	1	0	0.506888	2.276117	-1.065214
24	7	0	0.263039	-0.817194	-0.121609
25	7	0	2.285422	-1.859310	0.532754
26	17	0	-1.478543	-1.114186	-0.368731
27	1	0	2.999221	2.357075	-0.746357

Standard orientation of TS-A2-n-C2 and initial structure

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

Standard orientation of transition state of TS-A2-n-C2

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1363.39cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.243352	-0.859422	0.427869
2	6	0	2.698077	0.301397	-0.197458
3	6	0	1.765430	1.274168	-0.599119
4	6	0	0.136463	-0.135236	0.255704
5	1	0	-0.850583	0.107015	1.144795
6	8	0	-3.393023	1.812821	0.869947
7	1	0	-2.928157	2.232453	0.137514
8	17	0	-1.681360	-0.903651	-0.558277
9	8	0	-1.524547	0.567410	2.116476
10	1	0	-1.883114	-0.174323	2.621445
11	1	0	-2.297217	1.068319	1.694342
12	8	0	-3.224423	-1.643509	-1.476375
13	1	0	-3.983133	1.128588	0.470877
14	1	0	-3.129137	-1.311680	-2.377858
15	8	0	-4.961356	-0.087983	-0.179369
16	1	0	-4.368319	-0.686245	-0.695850
17	1	0	-5.284178	-0.605229	0.565699
18	7	0	2.123996	2.447331	-1.165820
19	1	0	3.044676	2.538726	-1.568989
20	1	0	1.390763	2.997456	-1.588779
21	6	0	4.357310	-1.017049	0.321126
22	1	0	5.378440	-1.356283	0.402634
23	7	0	0.478449	1.019497	-0.358804
24	7	0	0.943595	-1.106703	0.665834
25	7	0	3.304486	-1.675875	0.747185
26	7	0	4.062222	0.175431	-0.255211
27	1	0	4.726832	0.832437	-0.641580

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.962602	-1.061075	0.062261
2	6	0	2.800553	0.045537	-0.038913
3	6	0	2.175033	1.308073	-0.013001
4	6	0	0.147919	0.201041	0.184923
5	1	0	-0.877783	0.314446	1.065664
6	8	0	-4.045842	-0.011566	1.773625
7	1	0	-4.484852	0.844213	1.728228
8	17	0	-1.693995	0.318597	-0.901633
9	8	0	-1.549258	0.434837	2.125566
10	1	0	-1.197281	-0.195524	2.767375
11	1	0	-2.531428	0.229012	1.975989
12	8	0	-3.215574	0.375075	-2.093175
13	1	0	-4.265672	-0.485673	0.936441
14	1	0	-3.562067	1.268231	-1.970536
15	8	0	-4.663365	-1.227587	-0.532463
16	1	0	-4.186698	-0.653854	-1.180189
17	1	0	-4.214913	-2.079292	-0.545989
18	7	0	2.874083	2.455269	-0.064793
19	1	0	3.852718	2.433005	-0.304815
20	1	0	2.373699	3.321527	-0.191933
21	6	0	4.070025	-1.646639	-0.095412
22	1	0	4.924254	-2.304389	-0.145591
23	7	0	0.840205	1.351985	0.096722
24	7	0	0.630869	-1.042900	0.171031
25	7	0	2.804425	-2.140599	0.026298
26	7	0	4.121113	-0.338180	-0.139163
27	1	0	4.928589	0.245424	-0.225117

Standard orientation of TS-A2-n-N3 and initial structure

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

Standard orientation of transition state of TS-A2-n-N3

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1025.12cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.443318	-1.967971	-0.429135
2	1	0	-3.633011	-2.007135	-1.372437
3	8	0	-1.590372	1.483433	1.852479
4	1	0	-2.017585	1.748227	1.013459
5	1	0	-1.910389	0.592938	2.028866
6	8	0	-4.390390	0.095485	0.396777
7	1	0	-3.936693	-0.967746	-0.019702
8	1	0	-4.140696	0.157274	1.324582
9	8	0	-2.869988	1.959835	-0.529213
10	1	0	-3.503772	1.224701	-0.238582

11	1	0	-3.351036	2.789354	-0.442600
12	1	0	3.381029	-3.122871	0.725508
13	6	0	2.536279	-0.107167	0.019014
14	6	0	2.853651	-2.218215	0.467145
15	6	0	1.360944	-0.838707	-0.044346
16	7	0	1.551932	-2.144811	0.232255
17	7	0	3.490952	-1.038156	0.354524
18	6	0	2.527494	1.278984	-0.234425
19	6	0	0.251602	1.126861	-0.587915
20	1	0	-0.696422	1.596063	-0.829106
21	7	0	3.605308	2.044737	-0.187471
22	1	0	3.522742	3.032040	-0.384797
23	1	0	4.516317	1.665653	0.026365
24	7	0	1.339800	1.856133	-0.542259
25	7	0	0.202565	-0.194571	-0.360509
26	17	0	-1.345485	-1.030031	-0.402633
27	1	0	4.481588	-0.878090	0.493328

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.391162	-2.017827	-0.319933
2	1	0	-3.589178	-2.185518	-1.247500
3	8	0	-1.733360	1.507080	1.835729
4	1	0	-2.121305	1.746788	0.970487
5	1	0	-2.063505	0.622656	2.023738
6	8	0	-4.448175	0.073576	0.289972
7	1	0	-3.927252	-1.041439	-0.029157
8	1	0	-4.271123	0.193344	1.228809
9	8	0	-2.887996	1.898548	-0.620488
10	1	0	-3.539048	1.171532	-0.332581
11	1	0	-3.368842	2.731881	-0.584351
12	1	0	3.475849	-3.091650	0.639910
13	6	0	2.550213	-0.120223	0.021857
14	6	0	2.990659	-2.155064	0.414293
15	6	0	1.353445	-0.807466	-0.057719
16	7	0	1.633881	-2.103363	0.192110
17	7	0	3.573689	-0.992651	0.322160
18	6	0	2.522800	1.273114	-0.207799
19	6	0	0.241587	1.149610	-0.539753
20	1	0	-0.709458	1.622551	-0.765124
21	7	0	3.607242	2.025228	-0.157908
22	1	0	3.542967	3.017217	-0.336654
23	1	0	4.509803	1.619087	0.040136
24	7	0	1.333239	1.868453	-0.492298
25	7	0	0.188320	-0.181770	-0.339393
26	17	0	-1.359059	-1.039216	-0.352362
27	1	0	4.543827	-0.781896	0.442218

Standard orientation of TS-A2-n-N7 and initial structure

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

Standard orientation of transition state of TS-A2-n-N7

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -83.68cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.488137	0.071107	1.570511
2	8	0	-3.208420	-1.438277	-1.267317
3	1	0	-3.131858	-1.302562	-2.222322
4	17	0	-1.577553	-1.270701	-0.598482
5	8	0	-0.893960	0.786252	2.094325
6	1	0	-2.099626	1.522994	1.307113
7	1	0	0.758822	-2.954198	1.168464
8	1	0	-1.234385	0.381540	2.899388
9	8	0	-4.502768	0.495644	-0.094115
10	1	0	-4.075947	-0.267970	-0.580423
11	1	0	-5.065782	0.141379	0.607495
12	8	0	-2.858117	1.989633	0.855580
13	1	0	-3.728899	1.183393	0.342129
14	1	0	-2.493400	2.593243	0.197764
15	7	0	0.544093	-1.015617	0.350507
16	7	0	2.586603	-1.958810	0.752329
17	6	0	1.255324	-2.067077	0.795973
18	6	0	1.522724	-0.131091	-0.038680
19	6	0	2.769248	-0.714818	0.217534
20	1	0	4.705474	1.655696	-0.769600
21	7	0	2.657679	1.775146	-0.828691
22	7	0	3.947976	-0.098163	-0.035899
23	6	0	1.494762	1.162307	-0.578694
24	6	0	3.794080	1.110081	-0.545768
25	7	0	0.332873	1.796064	-0.902967
26	1	0	-0.516131	1.469503	-0.463639
27	1	0	0.392990	2.795047	-1.039631

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.488137	0.071107	1.570511
2	8	0	-3.208420	-1.438277	-1.267317
3	1	0	-3.131858	-1.302562	-2.222322
4	17	0	-1.577553	-1.270701	-0.598482
5	8	0	-0.893960	0.786252	2.094325
6	1	0	-2.099626	1.522994	1.307113
7	1	0	0.758822	-2.954198	1.168464
8	1	0	-1.234385	0.381540	2.899388
9	8	0	-4.502768	0.495644	-0.094115
10	1	0	-4.075947	-0.267970	-0.580423
11	1	0	-5.065782	0.141379	0.607495

12	8	0	-2.858117	1.989633	0.855580
13	1	0	-3.728899	1.183393	0.342129
14	1	0	-2.493400	2.593243	0.197764
15	7	0	0.544093	-1.015617	0.350507
16	7	0	2.586603	-1.958810	0.752329
17	6	0	1.255324	-2.067077	0.795973
18	6	0	1.522724	-0.131091	-0.038680
19	6	0	2.769248	-0.714818	0.217534
20	1	0	4.705474	1.655696	-0.769600
21	7	0	2.657679	1.775146	-0.828691
22	7	0	3.947976	-0.098163	-0.035899
23	6	0	1.494762	1.162307	-0.578694
24	6	0	3.794080	1.110081	-0.545768
25	7	0	0.332873	1.796064	-0.902967
26	1	0	-0.516131	1.469503	-0.463639
27	1	0	0.392990	2.795047	-1.039631

Standard orientation of TS-A2-n-C8 and initial structure

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

Standard orientation of transition state of TS-A2-n-C8

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -359.89cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.472339	0.200085	0.298671
2	6	0	-1.851281	-1.194918	0.226269
3	6	0	0.190916	-1.091409	0.922283
4	1	0	0.724626	-1.264207	1.851822
5	7	0	-0.265495	0.256320	0.767332
6	8	0	1.763887	1.942947	0.660675
7	1	0	1.729974	2.892400	0.815531
8	17	0	1.612975	-1.219909	-0.391196
9	8	0	2.658605	0.139307	2.570474
10	1	0	3.163195	-0.503865	2.062811
11	1	0	2.449849	0.858376	1.948919
12	8	0	3.295127	-1.127319	-1.804655
13	1	0	2.268298	1.777757	-0.184588
14	1	0	4.003720	-1.400567	-1.210709
15	8	0	3.092560	1.435332	-1.560535
16	1	0	3.202793	0.432122	-1.668288
17	1	0	2.528222	1.722909	-2.285385
18	1	0	0.407277	1.074833	0.803976
19	7	0	-0.864368	-1.952815	0.625163
20	7	0	-2.104372	2.483052	-0.171124
21	1	0	-1.203707	2.814271	0.145994
22	1	0	-2.774716	3.159504	-0.511451
23	1	0	-4.824850	-0.841062	-0.945029
24	6	0	-2.417680	1.198471	-0.176515

25	6	0	-3.834189	-0.584501	-0.586946
26	7	0	-3.583639	0.759419	-0.601939
27	7	0	-3.077734	-1.584908	-0.219932

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.530974	0.300352	0.169742
2	6	0	-1.854374	-1.074361	0.464420
3	6	0	0.169039	-0.773807	1.107880
4	1	0	0.745092	-0.743395	2.025735
5	7	0	-0.307176	0.476362	0.634218
6	8	0	1.944544	1.947361	0.241444
7	1	0	2.091360	2.898306	0.226139
8	17	0	1.562405	-1.338959	-0.184192
9	8	0	2.409448	0.858390	2.729607
10	1	0	1.593578	1.086351	3.186579
11	1	0	2.327728	1.257384	1.842918
12	8	0	3.131565	-1.709248	-1.588864
13	1	0	2.508094	1.544142	-0.467981
14	1	0	3.813183	-2.046095	-0.995526
15	8	0	3.476801	0.875386	-1.662307
16	1	0	3.375867	-0.124268	-1.655026
17	1	0	3.106657	1.178284	-2.497367
18	1	0	0.341773	1.266745	0.472876
19	7	0	-0.873539	-1.697832	1.048252
20	7	0	-1.997466	2.482487	-0.756463
21	1	0	-1.132880	2.713228	-0.310089
22	1	0	-1.898898	2.583664	-1.746437
23	1	0	-4.896722	-0.896348	-0.829413
24	6	0	-2.339963	1.159057	-0.454427
25	6	0	-3.974666	-0.637409	-0.541727
26	7	0	-3.511556	0.604375	-0.754711
27	7	0	-3.174399	-1.518790	0.063632

Standard orientation of TS-A2-n-N9 and initial structure

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

Standard orientation of transition state of TS-A2-n-N9

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -994.07cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.531611	2.061434	-0.209710
2	1	0	3.715824	2.266720	-1.132292
3	8	0	1.836668	-1.556895	1.824168

4	1	0	2.221875	-1.789835	0.956643
5	1	0	2.184114	-0.682108	2.025947
6	8	0	4.523856	-0.091781	0.263756
7	1	0	4.047335	1.026644	0.023580
8	1	0	4.390770	-0.250962	1.203981
9	8	0	2.938395	-1.891651	-0.666053
10	1	0	3.593026	-1.170460	-0.375856
11	1	0	3.426952	-2.721105	-0.680926
12	1	0	0.833222	-1.773077	-0.840798
13	6	0	-1.282447	0.582060	-0.091347
14	6	0	-0.040004	-1.176203	-0.607773
15	1	0	-1.581482	-2.562591	-0.673153
16	6	0	-2.102209	-0.526468	-0.198776
17	7	0	-1.292157	-1.601576	-0.523770
18	7	0	-0.001865	0.133198	-0.360776
19	17	0	1.485609	1.054575	-0.304778
20	7	0	-1.665290	1.819799	0.209832
21	6	0	-2.978552	1.883757	0.403899
22	1	0	-3.373365	2.861038	0.655205
23	7	0	-3.883940	0.904286	0.331516
24	6	0	-3.483142	-0.339520	0.026992
25	7	0	-4.381320	-1.320723	-0.050118
26	1	0	-4.115462	-2.271725	-0.256403
27	1	0	-5.352268	-1.115796	0.133259

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.520740	2.052715	-0.141285
2	1	0	3.706920	2.321418	-1.047157
3	8	0	1.875403	-1.575133	1.787931
4	1	0	2.245229	-1.795904	0.910504
5	1	0	2.272378	-0.729487	2.020314
6	8	0	4.546023	-0.112159	0.206488
7	1	0	4.048563	1.035707	0.029216
8	1	0	4.462096	-0.309317	1.145163
9	8	0	2.925298	-1.866718	-0.725463
10	1	0	3.596722	-1.158813	-0.428950
11	1	0	3.399743	-2.703549	-0.763231
12	1	0	0.825714	-1.775100	-0.793560
13	6	0	-1.278514	0.594289	-0.092391
14	6	0	-0.046106	-1.171198	-0.568942
15	1	0	-1.595423	-2.554715	-0.649853
16	6	0	-2.113660	-0.516262	-0.200685
17	7	0	-1.302008	-1.595089	-0.499250
18	7	0	0.003363	0.139033	-0.335372
19	17	0	1.501284	1.055612	-0.264917
20	7	0	-1.675381	1.822027	0.185851
21	6	0	-2.991348	1.906169	0.357872
22	1	0	-3.382075	2.888668	0.589385
23	7	0	-3.894892	0.916027	0.278391
24	6	0	-3.470043	-0.311005	-0.001800
25	7	0	-4.456211	-1.397629	-0.089105

26	1	0	-4.078281	-2.224948	0.326481
27	1	0	-5.289203	-1.131559	0.396003

Standard orientation of TS-A2-n-N^6 and initial structure

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

Standard orientation of transition state of TS-A2-n-N^6

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -190.15cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.990234	0.329092	1.725911
2	8	0	3.184850	-1.762628	-1.497366
3	1	0	3.730407	-2.266631	-0.883323
4	17	0	1.572625	-1.201725	-0.263283
5	8	0	1.644228	0.989560	2.229929
6	1	0	2.617550	1.007033	1.778813
7	1	0	-5.003170	-1.731218	0.745662
8	1	0	1.262879	1.877851	2.215857
9	8	0	4.010626	0.657304	-1.334552
10	1	0	3.723823	-0.312535	-1.446401
11	1	0	3.296433	1.191232	-1.698681
12	8	0	3.897917	1.022399	1.255053
13	1	0	3.933011	0.888752	0.263726
14	1	0	4.417375	0.317622	1.657709
15	7	0	-4.377979	-0.001026	-0.319507
16	7	0	-2.926811	-1.297494	0.789525
17	6	0	-4.212430	-1.069342	0.427411
18	6	0	-3.110703	0.510461	-0.458112
19	6	0	-2.184762	-0.287412	0.227548
20	6	0	-0.839236	0.078791	0.201507
21	6	0	-1.463866	1.860199	-1.107973
22	1	0	-1.127342	2.737166	-1.648959
23	7	0	-0.499073	1.171621	-0.477496
24	7	0	-2.762418	1.606332	-1.146985
25	7	0	0.163204	-0.610150	0.881692
26	1	0	-0.195412	-1.437334	1.351450
27	1	0	-2.593854	-2.065935	1.356659

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.990234	0.329092	1.725911
2	8	0	3.184850	-1.762628	-1.497366
3	1	0	3.730407	-2.266631	-0.883323
4	17	0	1.572625	-1.201725	-0.263283

5	8	0	1.644228	0.989560	2.229929
6	1	0	2.617550	1.007033	1.778813
7	1	0	-5.003170	-1.731218	0.745662
8	1	0	1.262879	1.877851	2.215857
9	8	0	4.010626	0.657304	-1.334552
10	1	0	3.723823	-0.312535	-1.446401
11	1	0	3.296433	1.191232	-1.698681
12	8	0	3.897917	1.022399	1.255053
13	1	0	3.933011	0.888752	0.263726
14	1	0	4.417375	0.317622	1.657709
15	7	0	-4.377979	-0.001026	-0.319507
16	7	0	-2.926811	-1.297494	0.789525
17	6	0	-4.212430	-1.069342	0.427411
18	6	0	-3.110703	0.510461	-0.458112
19	6	0	-2.184762	-0.287412	0.227548
20	6	0	-0.839236	0.078791	0.201507
21	6	0	-1.463866	1.860199	-1.107973
22	1	0	-1.127342	2.737166	-1.648959
23	7	0	-0.499073	1.171621	-0.477496
24	7	0	-2.762418	1.606332	-1.146985
25	7	0	0.163204	-0.610150	0.881692
26	1	0	-0.195412	-1.437334	1.351450
27	1	0	-2.593854	-2.065935	1.356659

Standard orientation of TS-A1-a-N1 and initial structure

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

Standard orientation of transition state of TS-A1-a-N1

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1022.52cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.876873	-1.454977	-0.769209
2	1	0	-3.983742	-1.157770	-1.678987
3	8	0	-0.997906	1.304913	1.959620
4	1	0	-1.511543	1.642131	1.201915
5	1	0	-1.474346	0.531473	2.281648
6	8	0	-4.350463	0.407500	0.701051
7	1	0	-4.142324	-0.503173	-0.008150
8	1	0	-4.001952	0.185551	1.571404
9	8	0	-2.538193	2.000975	-0.273998
10	1	0	-3.294636	1.438433	0.071883
11	1	0	-2.835925	2.916592	-0.293357
12	1	0	5.167786	1.390893	-0.177011
13	6	0	2.195285	0.418985	-0.322576
14	6	0	4.226087	0.861014	-0.126375
15	6	0	2.849197	-0.673044	0.270380
16	7	0	4.155655	-0.386209	0.396155
17	7	0	3.097049	1.411358	-0.574561

18	6	0	0.814738	0.365839	-0.543270
19	6	0	0.950722	-1.844628	0.427067
20	1	0	0.350531	-2.707001	0.687560
21	7	0	0.099887	1.328960	-1.119279
22	1	0	-0.909318	1.414563	-0.977431
23	1	0	0.592009	2.195661	-1.293380
24	7	0	0.240866	-0.813056	-0.153474
25	7	0	2.219686	-1.825018	0.655045
26	17	0	-1.456308	-1.070346	-0.410846

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.637266	-1.506729	-0.677546
2	1	0	-3.751976	-1.314475	-1.614606
3	8	0	-1.406985	1.253383	1.984691
4	1	0	-1.805325	1.579771	1.158358
5	1	0	-1.879932	0.441492	2.192391
6	8	0	-4.407575	0.457170	0.492709
7	1	0	-4.047856	-0.569572	-0.088857
8	1	0	-4.110471	0.387241	1.405785
9	8	0	-2.575125	1.920920	-0.471938
10	1	0	-3.367305	1.370906	-0.130128
11	1	0	-2.819029	2.851273	-0.438721
12	1	0	5.199956	1.514773	-0.142371
13	6	0	2.224133	0.453013	-0.245218
14	6	0	4.258532	0.989098	-0.110903
15	6	0	2.877213	-0.669689	0.234790
16	7	0	4.183858	-0.306776	0.315875
17	7	0	3.099485	1.489164	-0.457842
18	6	0	0.827616	0.387267	-0.434159
19	6	0	1.034756	-1.874546	0.362747
20	1	0	0.466709	-2.769891	0.581028
21	7	0	0.102326	1.376731	-0.908341
22	1	0	-0.925318	1.419011	-0.856207
23	1	0	0.586160	2.246177	-1.091106
24	7	0	0.292061	-0.824978	-0.109945
25	7	0	2.316300	-1.857851	0.555675
26	17	0	-1.448336	-1.117621	-0.365317

Standard orientation of TS-A1-a-C2 and initial structure

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

Standard orientation of transition state of TS-A1-a-C2

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -534.44cm^{-1}

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.248771	-0.741810	0.602855
2	6	0	2.416529	0.454974	-0.182089
3	6	0	1.329299	1.396037	-0.196120
4	6	0	0.142599	-0.134557	1.118494
5	1	0	-0.536155	-0.117575	1.964563
6	8	0	-2.385099	2.025103	-0.172327
7	1	0	-1.457705	1.757280	-0.022945
8	17	0	-1.090284	-1.224227	-0.137254
9	8	0	-3.605921	0.492953	1.835915
10	1	0	-2.960635	-0.177493	2.088188
11	1	0	-3.114216	1.166841	1.330090
12	8	0	-2.431449	-2.143467	-1.496356
13	1	0	-2.808479	1.335390	-0.715155
14	1	0	-1.951276	-2.034700	-2.326349
15	8	0	-4.069295	-0.086697	-0.987285
16	1	0	-3.502717	-0.862985	-1.225297
17	1	0	-4.161118	-0.105319	-0.021797
18	6	0	4.147146	-0.735740	-0.294767
19	1	0	5.146908	-1.016286	-0.596120
20	7	0	0.255593	1.101345	0.491113
21	7	0	1.181664	-1.034089	1.281885
22	7	0	3.415674	-1.480383	0.493809
23	7	0	3.599217	0.463002	-0.749093
24	7	0	1.448531	2.570021	-0.852112
25	1	0	0.612942	3.118783	-1.002043
26	1	0	2.190575	2.672102	-1.528843

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.254661	-0.735060	0.600694
2	6	0	2.402929	0.464498	-0.184010
3	6	0	1.307794	1.396405	-0.182780
4	6	0	0.148276	-0.148485	1.139535
5	1	0	-0.524247	-0.141434	1.990773
6	8	0	-2.370777	2.028628	-0.232709
7	1	0	-1.454204	1.746290	-0.047503
8	17	0	-1.080484	-1.247998	-0.111638
9	8	0	-3.615056	0.548753	1.810180
10	1	0	-2.972304	-0.110990	2.094880
11	1	0	-3.116812	1.209048	1.294108
12	8	0	-2.412482	-2.174722	-1.471022
13	1	0	-2.798857	1.322110	-0.749886
14	1	0	-1.931061	-2.064405	-2.300101
15	8	0	-4.049596	-0.110575	-0.992015
16	1	0	-3.482436	-0.890222	-1.218266
17	1	0	-4.142160	-0.115389	-0.026263
18	6	0	4.141684	-0.711769	-0.320481
19	1	0	5.139673	-0.983805	-0.635211
20	7	0	0.243744	1.089929	0.514448
21	7	0	1.197788	-1.038059	1.291025

22	7	0	3.426318	-1.463620	0.476000
23	7	0	3.578364	0.483326	-0.765599
24	7	0	1.409496	2.573231	-0.836411
25	1	0	0.567989	3.116144	-0.974209
26	1	0	2.143898	2.684762	-1.519940

Standard orientation of TS-A1-a-N3 and initial structure

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

Standard orientation of transition state of TS-A1-a-N3

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -120.17cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.730047	-1.520546	-0.575281
2	1	0	-4.039829	-1.523451	-1.488221
3	8	0	0.263320	1.507480	2.049005
4	1	0	-0.536990	1.659616	1.507596
5	1	0	0.481253	0.572222	1.969575
6	8	0	-4.298036	0.748321	0.615984
7	1	0	-4.149580	-0.135719	0.174611
8	1	0	-4.591816	0.569035	1.515404
9	8	0	-1.982633	2.209801	0.616496
10	1	0	-2.788752	1.649301	0.618879
11	1	0	-2.249861	3.071826	0.954064
12	1	0	2.614526	-3.001264	1.692726
13	6	0	2.300176	-0.370703	0.002649
14	6	0	2.285201	-2.167586	1.087033
15	6	0	1.022605	-0.946766	-0.041181
16	7	0	1.002263	-2.096418	0.648441
17	7	0	3.115025	-1.183785	0.746406
18	6	0	2.507208	0.860496	-0.639365
19	6	0	0.299786	0.845717	-1.291122
20	1	0	-0.519206	1.330145	-1.809622
21	7	0	1.477788	1.447410	-1.295935
22	7	0	0.015966	-0.318805	-0.714590
23	17	0	-1.770957	-0.935986	-0.679164
24	7	0	3.689968	1.487507	-0.631301
25	1	0	4.476603	1.096801	-0.136537
26	1	0	3.792152	2.384493	-1.081556

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.729089	-1.521645	-0.575735
2	1	0	-4.038384	-1.525398	-1.488832

3	8	0	0.259182	1.502907	2.050190
4	1	0	-0.540264	1.656388	1.507876
5	1	0	0.474570	0.566928	1.972361
6	8	0	-4.299216	0.747030	0.614395
7	1	0	-4.149865	-0.136986	0.173136
8	1	0	-4.592601	0.567620	1.513918
9	8	0	-1.984356	2.209311	0.616048
10	1	0	-2.790474	1.648792	0.617871
11	1	0	-2.251112	3.070397	0.956386
12	1	0	2.616523	-3.002717	1.688750
13	6	0	2.300829	-0.369805	0.002595
14	6	0	2.286761	-2.168267	1.084360
15	6	0	1.023456	-0.946259	-0.041712
16	7	0	1.003677	-2.096913	0.646199
17	7	0	3.116153	-1.183695	0.744950
18	6	0	2.507342	0.862201	-0.637993
19	6	0	0.299749	0.847660	-1.289224
20	1	0	-0.519538	1.332473	-1.806882
21	7	0	1.477561	1.449651	-1.293555
22	7	0	0.016467	-0.317721	-0.714099
23	17	0	-1.769709	-0.935463	-0.679112
24	7	0	3.690003	1.489420	-0.629766
25	1	0	4.476634	1.098790	-0.134924
26	1	0	3.791534	2.387391	-1.078208

Standard orientation of TS-A1-a-N7 and initial structure

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

Standard orientation of transition state of TS-A1-a-N7

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -111.33cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.356699	1.675973	-0.736860
2	1	0	-3.203129	2.495593	-0.252162
3	17	0	-1.563446	0.787001	-0.858805
4	8	0	-0.301414	-1.125236	2.163759
5	1	0	-0.978101	-1.489559	1.557867
6	8	0	-4.267236	-0.219457	0.862692
7	1	0	-3.971729	0.540189	0.290714
8	1	0	-4.261698	0.098960	1.771722
9	8	0	-2.383366	-2.192294	0.712994
10	1	0	-3.061788	-1.481553	0.717957
11	1	0	-2.173106	-2.366040	-0.210866
12	6	0	1.312224	0.190255	-0.361702
13	6	0	0.276954	-1.379463	-1.426150
14	7	0	0.114941	-0.131045	-0.957276
15	1	0	0.452237	-0.869917	1.619301
16	7	0	1.482290	-1.901626	-1.219406

17	1	0	-0.524569	-1.891935	-1.940358
18	6	0	2.148016	-0.917743	-0.542065
19	6	0	1.814824	1.305951	0.330160
20	6	0	3.788834	0.132341	0.539686
21	7	0	3.422356	-0.966161	-0.093893
22	7	0	3.073636	1.246184	0.779553
23	1	0	4.802280	0.150336	0.925730
24	7	0	1.101387	2.440258	0.526677
25	1	0	0.099007	2.419798	0.410127
26	1	0	1.461510	3.101906	1.199812

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.354626	1.668558	-0.752354
2	1	0	-3.202105	2.490815	-0.271746
3	17	0	-1.563227	0.779780	-0.865430
4	8	0	-0.315141	-1.104894	2.167288
5	1	0	-0.989084	-1.478644	1.564189
6	8	0	-4.268718	-0.209257	0.869312
7	1	0	-3.973550	0.541555	0.286053
8	1	0	-4.249399	0.119469	1.774529
9	8	0	-2.391287	-2.189446	0.717982
10	1	0	-3.068272	-1.477402	0.725193
11	1	0	-2.176712	-2.355733	-0.206291
12	6	0	1.314713	0.186707	-0.361006
13	6	0	0.283292	-1.388298	-1.420497
14	7	0	0.118169	-0.139047	-0.955455
15	1	0	0.447459	-0.874893	1.624024
16	7	0	1.489850	-1.907335	-1.211730
17	1	0	-0.516731	-1.904282	-1.933546
18	6	0	2.153110	-0.919825	-0.537408
19	6	0	1.814053	1.305612	0.328204
20	6	0	3.791361	0.138011	0.541351
21	7	0	3.427996	-0.963539	-0.088585
22	7	0	3.073100	1.250663	0.777891
23	1	0	4.804786	0.160096	0.927286
24	7	0	1.097162	2.437111	0.522674
25	1	0	0.095479	2.417422	0.400723
26	1	0	1.458047	3.107431	1.186635

Standard orientation of TS-A1-a-C8 and initial structure

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

Standard orientation of transition state of TS-A1-a-C8

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -452.74cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.073842	-1.778607	1.079164
2	1	0	-0.615578	-1.019206	2.137403
3	8	0	-2.822901	-1.751443	-1.585800
4	1	0	-2.297858	-1.823556	-2.392765
5	17	0	-1.401942	-1.333116	-0.180318
6	8	0	-3.539223	0.924289	1.731560
7	1	0	-2.885559	1.516153	1.316124
8	1	0	-3.106946	0.064147	1.793718
9	8	0	-3.837321	0.708846	-1.194861
10	1	0	-3.505207	-0.197314	-1.403091
11	1	0	-4.102270	0.685953	-0.262995
12	8	0	-1.746680	2.194886	-0.031242
13	1	0	-2.289612	1.684703	-0.660019
14	1	0	-0.996716	1.630461	0.231490
15	7	0	0.350990	0.429487	0.909925
16	6	0	0.030606	-0.879716	1.279855
17	6	0	1.537597	0.299208	0.367012
18	6	0	1.994005	-1.056199	0.475142
19	6	0	3.890807	-0.493797	-0.561287
20	6	0	2.394609	1.244130	-0.302791
21	1	0	4.868599	-0.760016	-0.949382
22	7	0	2.012916	2.508056	-0.465522
23	1	0	2.618158	3.167017	-0.934797
24	1	0	1.111219	2.823083	-0.137260
25	7	0	3.569749	0.818356	-0.745700
26	7	0	3.209367	-1.463410	-0.003276

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.081008	-1.813556	1.043315
2	1	0	-0.599250	-1.081517	2.130729
3	8	0	-2.856244	-1.717299	-1.615618
4	1	0	-2.317627	-1.661710	-2.414133
5	17	0	-1.407250	-1.350201	-0.182557
6	8	0	-3.470269	0.918312	1.719540
7	1	0	-2.827865	1.534325	1.322554
8	1	0	-3.008764	0.074242	1.776858
9	8	0	-3.783897	0.732508	-1.140163
10	1	0	-3.467058	-0.176562	-1.376058
11	1	0	-3.995567	0.694725	-0.194935
12	8	0	-1.706470	2.207583	-0.009582
13	1	0	-2.278213	1.724798	-0.635939
14	1	0	-0.998484	1.595086	0.258406
15	7	0	0.334146	0.394236	0.912662
16	6	0	0.023382	-0.929816	1.257586
17	6	0	1.518408	0.285481	0.370796
18	6	0	1.991617	-1.068798	0.458003
19	6	0	3.881279	-0.461054	-0.561021
20	6	0	2.360074	1.250939	-0.293809

21	1	0	4.866099	-0.705369	-0.946704
22	7	0	1.951503	2.506399	-0.449445
23	1	0	2.537367	3.172410	-0.931706
24	1	0	1.029334	2.790351	-0.152632
25	7	0	3.541679	0.849589	-0.736155
26	7	0	3.215915	-1.450482	-0.021195

Standard orientation of TS-A1-a-N9 and initial structure

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

Standard orientation of transition state of TS-A1-a-N9

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -70.82cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.911279	-1.032193	-0.820767
2	1	0	4.296028	-1.672137	-0.208741
3	17	0	2.049566	-1.098674	-0.533271
4	8	0	0.670618	0.228054	2.556516
5	1	0	0.991080	0.901312	1.921306
6	1	0	0.413104	-0.534029	2.024077
7	8	0	4.147619	1.464991	0.150814
8	1	0	4.164040	0.560799	-0.238868
9	1	0	4.531822	2.058636	-0.503029
10	8	0	1.533570	2.113066	0.729098
11	1	0	2.446715	1.865799	0.478445
12	1	0	0.944946	1.845101	0.000818
13	6	0	-0.724208	-2.158397	0.260055
14	6	0	-0.878023	-0.121921	-0.419807
15	7	0	0.012572	-1.131495	-0.232868
16	6	0	-1.744569	1.863374	-0.925588
17	6	0	-3.216888	0.273033	-0.139738
18	1	0	-1.622627	2.883335	-1.274967
19	6	0	-2.128396	-0.609365	-0.030557
20	7	0	-2.017816	-1.912382	0.403458
21	7	0	-0.644399	1.127134	-0.880203
22	7	0	-2.997559	1.517931	-0.594962
23	1	0	-0.263684	-3.104756	0.509582
24	7	0	-4.478910	-0.096832	0.166881
25	1	0	-4.628739	-0.949515	0.684706
26	1	0	-5.184703	0.620739	0.244667

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.003197	-0.906504	-0.760970

2	1	0	4.319638	-1.513485	-0.082946
3	17	0	1.918224	-1.054271	-0.554795
4	8	0	0.281070	0.247669	2.453759
5	1	0	0.713750	0.911868	1.878690
6	1	0	0.649403	-0.601971	2.193576
7	8	0	4.037580	1.413904	0.347059
8	1	0	4.057414	0.502829	-0.096054
9	1	0	4.298934	2.050663	-0.325278
10	8	0	1.456602	2.072734	0.783131
11	1	0	2.389252	1.796875	0.633233
12	1	0	0.957806	1.841611	-0.015982
13	6	0	-0.601348	-2.161752	0.255280
14	6	0	-0.801366	-0.131118	-0.511781
15	7	0	0.090697	-1.144910	-0.333327
16	6	0	-1.697530	1.824154	-1.029442
17	6	0	-3.117412	0.253697	-0.119538
18	1	0	-1.598515	2.833840	-1.413878
19	6	0	-2.016276	-0.620089	-0.040337
20	7	0	-1.876430	-1.904851	0.441864
21	7	0	-0.589225	1.094108	-1.025495
22	7	0	-2.927086	1.485747	-0.623801
23	1	0	-0.110819	-3.087984	0.518070
24	7	0	-4.347164	-0.105988	0.278274
25	1	0	-4.487350	-0.978967	0.761329
26	1	0	-5.078862	0.586818	0.309217

Standard orientation of TS-A1-a-N^6 and initial structure

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

Standard orientation of transition state of TS-A1-a-N^6

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -966.74cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.829694	-1.082091	-1.204590
2	8	0	3.386078	2.383936	0.729392
3	1	0	3.718894	2.684755	-0.122873
4	17	0	1.438009	1.056865	-0.235878
5	8	0	1.521791	-2.020386	-1.419364
6	1	0	2.493821	-1.819241	-1.178558
7	1	0	-4.778317	1.354904	-1.723955
8	1	0	1.226029	-2.780995	-0.901005
9	8	0	4.231074	0.088850	1.257643
10	1	0	3.883131	1.056238	1.026462
11	1	0	3.639241	-0.267169	1.929257
12	8	0	3.945029	-1.482757	-0.848287
13	1	0	4.047696	-0.867436	-0.070631
14	1	0	4.379011	-1.067175	-1.601786
15	7	0	-4.402838	0.316795	0.083914

16	7	0	-2.752147	0.849176	-1.440759
17	6	0	-4.040848	0.883375	-1.087005
18	6	0	-3.221129	-0.143893	0.554723
19	6	0	-1.707390	-1.112214	1.894229
20	6	0	-0.923718	-0.216288	-0.044979
21	7	0	-0.666049	-0.863469	1.081999
22	7	0	0.178179	0.014595	-0.935546
23	1	0	-0.152373	0.476812	-1.784093
24	1	0	-1.467775	-1.638090	2.811029
25	7	0	-2.980712	-0.794645	1.705141
26	6	0	-2.202252	0.183767	-0.381577

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.851047	-1.056782	-1.250313
2	8	0	3.352787	2.381549	0.871576
3	1	0	3.665541	2.725803	0.028275
4	17	0	1.418968	1.052564	-0.183708
5	8	0	1.553968	-1.974475	-1.489018
6	1	0	2.523704	-1.760628	-1.248503
7	1	0	-4.739576	1.582320	-1.580037
8	1	0	1.275628	-2.753014	-0.987975
9	8	0	4.239702	0.086742	1.269084
10	1	0	3.872214	1.061732	1.095729
11	1	0	3.643611	-0.325056	1.904369
12	8	0	3.963779	-1.404515	-0.897383
13	1	0	4.058985	-0.814316	-0.099642
14	1	0	4.412846	-0.973446	-1.632990
15	7	0	-4.390350	0.365029	0.117771
16	7	0	-2.728102	0.994336	-1.356834
17	6	0	-4.014630	1.030846	-0.995027
18	6	0	-3.221345	-0.172066	0.536345
19	6	0	-1.733407	-1.309440	1.767757
20	6	0	-0.928593	-0.254390	-0.081057
21	7	0	-0.687651	-1.014721	0.977316
22	7	0	0.180932	0.028226	-0.947026
23	1	0	-0.144927	0.524252	-1.777909
24	1	0	-1.507602	-1.928383	2.628169
25	7	0	-2.997326	-0.937509	1.616951
26	6	0	-2.195081	0.215380	-0.369260

Standard orientation of TS-Gua-n-N1 and initial structure

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

Standard orientation of transition state of TS-Gua-n-N1

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -89.74cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.609941	-0.735997	0.038133
2	6	0	-0.153434	-0.327547	-1.037710
3	6	0	-1.563684	-0.163129	-0.842087
4	6	0	-1.113263	-0.829464	1.419837
5	6	0	1.839874	-0.449465	-1.763100
6	1	0	2.716595	-0.436104	-2.391550
7	7	0	1.897200	-0.831907	-0.435253
8	1	0	-3.402010	-1.674752	0.000612
9	8	0	-5.549096	-0.527987	-1.907790
10	1	0	-6.273220	-1.058941	-2.259352
11	17	0	-3.820854	0.706647	1.059630
12	8	0	-4.128334	-2.191993	-0.390636
13	1	0	-3.712704	-2.815233	-0.996774
14	1	0	-5.003713	-1.122456	-1.330942
15	8	0	-5.303904	1.660193	1.466099
16	1	0	-6.057624	0.546042	-1.275441
17	1	0	-5.750458	1.183678	2.179432
18	8	0	-6.480623	1.428823	-0.787626
19	1	0	-6.098433	1.547887	0.146900
20	1	0	-6.265994	2.216698	-1.306636
21	8	0	-2.374840	0.174173	-1.718106
22	7	0	-1.654002	-1.026456	2.660005
23	1	0	-2.642298	-1.229113	2.691125
24	1	0	-1.087504	-1.572580	3.292330
25	7	0	-1.976598	-0.430072	0.453455
26	7	0	0.196228	-1.011470	1.288599
27	7	0	0.635752	-0.156678	-2.164099
28	6	0	3.050693	-1.054603	0.426512
29	1	0	2.848547	-1.927932	1.043284
30	6	0	4.788506	0.287303	-0.518178
31	6	0	4.123587	0.994952	0.672737
32	1	0	4.428516	0.694561	-1.465071
33	1	0	4.888603	1.275257	1.400617
34	6	0	4.355883	-1.186629	-0.345972
35	1	0	4.249559	-1.722349	-1.291821
36	8	0	3.250756	0.042062	1.294391
37	6	0	3.325636	2.219141	0.266604
38	1	0	2.832870	2.641957	1.147648
39	1	0	2.556098	1.936457	-0.462995
40	8	0	4.250935	3.135644	-0.296673
41	1	0	3.762408	3.890506	-0.641032
42	8	0	6.194346	0.431000	-0.434212
43	1	0	6.578418	0.250654	-1.300498
44	8	0	5.265715	-1.849109	0.507984
45	1	0	6.114729	-1.390977	0.419393

Standard orientation of initial structure

Standard orientation:

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

1	6	0	0.604347	-0.731223	0.028662
2	6	0	-0.156949	-0.314055	-1.045066
3	6	0	-1.567822	-0.152353	-0.851648
4	6	0	-1.121051	-0.838202	1.407048
5	6	0	1.837931	-0.427257	-1.766841
6	1	0	2.716317	-0.406198	-2.392729
7	7	0	1.892630	-0.821715	-0.442508
8	1	0	-3.405007	-1.683955	-0.011838
9	8	0	-5.572084	-0.515895	-1.895418
10	1	0	-6.300725	-1.046858	-2.237208
11	17	0	-3.807863	0.696384	1.055851
12	8	0	-4.136033	-2.193246	-0.403600
13	1	0	-3.727275	-2.817212	-1.013564
14	1	0	-5.017993	-1.111598	-1.329378
15	8	0	-5.292175	1.655648	1.478802
16	1	0	-6.075584	0.564694	-1.247261
17	1	0	-5.736091	1.175188	2.190964
18	8	0	-6.484691	1.443580	-0.755010
19	1	0	-6.089108	1.556991	0.178779
20	1	0	-6.269879	2.230820	-1.274933
21	8	0	-2.377616	0.189281	-1.726373
22	7	0	-1.664424	-1.048923	2.643224
23	1	0	-2.652600	-1.252425	2.671190
24	1	0	-1.098189	-1.599578	3.271856
25	7	0	-1.982527	-0.427806	0.442468
26	7	0	0.188004	-1.019410	1.275448
27	7	0	0.634484	-0.132083	-2.168004
28	6	0	3.044416	-1.053360	0.418851
29	1	0	2.836819	-1.929227	1.030234
30	6	0	4.797364	0.281711	-0.511062
31	6	0	4.130468	0.988136	0.679570
32	1	0	4.447977	0.697831	-1.457991
33	1	0	4.893430	1.259448	1.412993
34	6	0	4.350965	-1.189553	-0.351281
35	1	0	4.241963	-1.717345	-1.301131
36	8	0	3.248031	0.038542	1.292257
37	6	0	3.344283	2.220429	0.274364
38	1	0	2.846336	2.640559	1.153821
39	1	0	2.579729	1.947958	-0.464251
40	8	0	4.281199	3.134525	-0.273541
41	1	0	3.799888	3.884206	-0.638604
42	8	0	6.203661	0.412968	-0.415385
43	1	0	6.593522	0.232241	-1.279027
44	8	0	5.253267	-1.867589	0.498868
45	1	0	6.100786	-1.402657	0.433830

Standard orientation of TS-Gua-n-N3 and initial structure

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

Standard orientation of transition state of TS-Gua-n-N3

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1085.83cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.184761	-3.388298	-0.840502
2	1	0	-2.211597	-3.490405	-1.796467
3	8	0	-0.581204	-3.328675	1.348055
4	1	0	-1.222525	-2.746605	1.795110
5	1	0	-0.986305	-3.477529	0.471840
6	8	0	-4.086814	-2.204783	0.056560
7	1	0	-3.222464	-2.859558	-0.429117
8	1	0	-4.899663	-2.707094	0.159346
9	8	0	-2.717111	-1.803013	2.329622
10	1	0	-3.283426	-1.979725	1.538960
11	1	0	-3.080899	-2.332624	3.046215
12	1	0	2.612469	2.284909	0.145329
13	6	0	-0.502491	2.803140	-0.108177
14	6	0	1.540249	2.274427	0.028606
15	6	0	-0.457890	1.428671	-0.146763
16	7	0	0.850772	1.077926	-0.050677
17	7	0	0.765743	3.319368	0.001384
18	6	0	-1.760428	3.490614	-0.079827
19	6	0	-2.806480	1.240435	-0.151949
20	7	0	-2.848617	2.590834	-0.066058
21	7	0	-1.588442	0.644949	-0.228857
22	17	0	-1.571686	-1.039153	-0.604651
23	8	0	-1.963917	4.685153	-0.037820
24	1	0	-3.766673	3.022926	0.001132
25	7	0	-3.912314	0.533943	-0.174958
26	1	0	-4.791410	1.035141	-0.137768
27	1	0	-3.960990	-0.511699	-0.131699
28	6	0	1.515061	-0.234395	0.057380
29	1	0	0.778555	-0.967238	0.382468
30	6	0	3.370244	-1.494753	-0.687435
31	6	0	3.772455	-0.658349	0.522814
32	1	0	4.183474	-1.603606	-1.410340
33	1	0	4.178861	-1.281385	1.322406
34	6	0	2.204116	-0.672416	-1.237110
35	1	0	2.596049	0.210290	-1.751490
36	8	0	2.531359	-0.106643	1.020648
37	8	0	2.844953	-2.751558	-0.303438
38	1	0	3.542587	-3.255191	0.131801
39	8	0	1.295838	-1.370815	-2.048820
40	1	0	1.707035	-1.516770	-2.908940
41	6	0	4.756852	0.441717	0.183375
42	1	0	5.710591	-0.024671	-0.085608
43	1	0	4.409188	1.031017	-0.672536
44	8	0	4.894535	1.265031	1.330701
45	1	0	5.502671	1.980539	1.117067

Standard orientation of initial structure

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	-2.091533	-3.335011	-0.817346
2	1	0	-1.877792	-3.482607	-1.743379
3	8	0	-1.398905	-3.527387	1.764507
4	1	0	-2.106559	-2.914273	2.028559
5	1	0	-1.502676	-3.596358	0.795514
6	8	0	-4.119827	-2.082947	-0.455478
7	1	0	-3.184853	-2.760681	-0.700567
8	1	0	-4.946018	-2.520783	-0.677300
9	8	0	-3.655716	-1.928799	2.166739
10	1	0	-3.892973	-2.000869	1.208881
11	1	0	-4.198378	-2.578439	2.624748
12	1	0	2.745729	2.171327	0.126833
13	6	0	-0.357533	2.826756	0.000403
14	6	0	1.670300	2.212457	0.063967
15	6	0	-0.356570	1.461100	-0.143132
16	7	0	0.929995	1.063795	-0.105898
17	7	0	0.933905	3.285245	0.131561
18	6	0	-1.601718	3.538857	0.007696
19	6	0	-2.694897	1.314215	-0.264350
20	7	0	-2.706760	2.663465	-0.135760
21	7	0	-1.487256	0.697938	-0.280151
22	17	0	-1.439206	-1.012673	-0.490035
23	8	0	-1.791338	4.730660	0.121203
24	1	0	-3.616084	3.118786	-0.118849
25	7	0	-3.811480	0.635495	-0.373941
26	1	0	-4.680077	1.154906	-0.347014
27	1	0	-3.885108	-0.408680	-0.450393
28	6	0	1.458372	-0.303652	-0.214550
29	1	0	0.621387	-1.011704	-0.445034
30	6	0	3.653136	-0.716710	-0.949656
31	6	0	3.661033	-0.987307	0.551084
32	1	0	4.342300	0.120093	-1.232176
33	1	0	3.962512	-2.042823	0.760712
34	6	0	2.336642	-0.319528	-1.343421
35	1	0	2.635615	0.562825	-1.869699
36	8	0	2.239756	-0.719820	1.027120
37	8	0	3.978307	-1.883157	-1.710291
38	1	0	4.911778	-1.869900	-1.934021
39	8	0	1.493065	-1.112403	-2.182842
40	1	0	1.902515	-1.212897	-3.045310
41	6	0	4.666305	-0.064941	1.265415
42	1	0	5.590424	-0.585614	1.406144
43	1	0	4.835634	0.807496	0.669528
44	8	0	4.138436	0.321427	2.537018
45	1	0	4.851930	0.376081	3.176970

Standard orientation of TS-Gua-n-N7 and initial structure

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

Standard orientation of transition state of TS-Gua-n-N7

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -694.13cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.441331	4.572908	-0.728533
2	1	0	-2.418269	4.699469	-1.682903
3	8	0	1.675848	1.868297	2.527719
4	1	0	1.520377	2.384573	1.710438
5	1	0	1.813283	0.958675	2.235066
6	8	0	-0.278329	5.212866	0.154153
7	1	0	-1.422816	4.912016	-0.316432
8	1	0	-0.407832	5.428538	1.082713
9	8	0	1.268013	3.174738	0.160805
10	1	0	0.628847	3.972487	0.152019
11	1	0	2.148401	3.521562	-0.017856
12	17	0	-1.926894	2.385000	-0.444340
13	6	0	1.165846	-1.637425	0.734037
14	6	0	2.713226	-1.271184	-1.010363
15	6	0	3.230804	-0.641221	0.282261
16	1	0	0.889715	-2.334422	1.523795
17	1	0	4.053046	-1.247019	0.676250
18	6	0	-1.315091	-1.448072	0.239612
19	6	0	-2.905235	-2.992576	0.249346
20	6	0	-3.557463	-0.668651	-0.292464
21	7	0	-3.366015	-4.233199	0.399295
22	1	0	-4.344040	-4.455909	0.292992
23	1	0	-2.722408	-4.963141	0.663195
24	7	0	-3.821274	-2.025964	-0.086246
25	8	0	-4.441483	0.113165	-0.594097
26	6	0	-0.142599	0.424890	0.116703
27	1	0	0.662943	1.148162	0.146032
28	7	0	-1.394249	0.732029	-0.161376
29	7	0	-0.057011	-0.894563	0.369167
30	7	0	-1.617635	-2.738815	0.420493
31	6	0	-2.164335	-0.413563	-0.094150
32	1	0	2.143267	-0.529597	-1.583921
33	1	0	-4.793027	-2.298460	-0.204182
34	6	0	1.776412	-2.348301	-0.471864
35	1	0	1.020593	-2.673503	-1.190306
36	8	0	2.118995	-0.715534	1.195937
37	6	0	3.676339	0.794752	0.099200
38	1	0	2.855282	1.392204	-0.299956
39	1	0	4.007996	1.233829	1.043385
40	8	0	4.712508	0.814227	-0.877458
41	1	0	5.513720	0.453728	-0.478960
42	8	0	3.723133	-1.861070	-1.796671
43	1	0	4.398012	-1.185580	-1.950610
44	8	0	2.520421	-3.436875	0.034042
45	1	0	3.273774	-3.572697	-0.557403

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.501320	4.531156	-0.762624
2	1	0	-2.437705	4.663336	-1.714405
3	8	0	1.648465	1.895418	2.522286
4	1	0	1.472989	2.408049	1.706895
5	1	0	1.802477	0.988907	2.228233
6	8	0	-0.393843	5.200771	0.226483
7	1	0	-1.507033	4.884774	-0.302029
8	1	0	-0.567261	5.326097	1.164632
9	8	0	1.200188	3.195087	0.158158
10	1	0	0.544289	3.977751	0.175629
11	1	0	2.070657	3.566564	-0.019780
12	17	0	-1.956320	2.355136	-0.466415
13	6	0	1.192332	-1.617462	0.733200
14	6	0	2.736624	-1.232572	-1.010214
15	6	0	3.243308	-0.592350	0.281779
16	1	0	0.926695	-2.316838	1.524437
17	1	0	4.072914	-1.185987	0.678768
18	6	0	-1.291859	-1.465513	0.240647
19	6	0	-2.861469	-3.031025	0.259066
20	6	0	-3.544487	-0.718452	-0.294129
21	7	0	-3.306462	-4.277093	0.413581
22	1	0	-4.282706	-4.510584	0.313927
23	1	0	-2.654584	-4.996878	0.685024
24	7	0	-3.790250	-2.077774	-0.079621
25	8	0	-4.439064	0.049823	-0.599439
26	6	0	-0.144644	0.422655	0.106192
27	1	0	0.650451	1.157709	0.133077
28	7	0	-1.400413	0.711121	-0.173170
29	7	0	-0.041268	-0.894251	0.366006
30	7	0	-1.577165	-2.759478	0.427750
31	6	0	-2.154844	-0.444148	-0.098412
32	1	0	2.156374	-0.500369	-1.585636
33	1	0	-4.758772	-2.362645	-0.194662
34	6	0	1.814700	-2.321963	-0.470410
35	1	0	1.064667	-2.659668	-1.189171
36	8	0	2.130583	-0.679459	1.193161
37	6	0	3.670271	0.848934	0.095803
38	1	0	2.842615	1.435044	-0.306664
39	1	0	3.994574	1.294721	1.039358
40	8	0	4.707918	0.878657	-0.879005
41	1	0	5.513615	0.532316	-0.477038
42	8	0	3.755500	-1.809369	-1.794560
43	1	0	4.421190	-1.124910	-1.948840
44	8	0	2.573585	-3.398437	0.039241
45	1	0	3.325221	-3.530181	-0.555261

Standard orientation of TS-Gua-n-C8 and initial structure

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

Standard orientation of transition state of TS-Gua-n-C8

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -432.43cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.014752	-0.336268	-0.808762
2	1	0	0.151103	1.104395	-1.901821
3	8	0	2.072151	2.076337	1.861945
4	1	0	1.563700	2.288801	2.654025
5	17	0	0.695420	1.596176	0.472274
6	8	0	4.243811	0.748297	0.777287
7	1	0	4.031764	0.925349	-0.154616
8	1	0	3.499385	1.117703	1.284780
9	8	0	3.175082	3.736449	0.068520
10	1	0	2.769414	3.244701	0.816898
11	1	0	4.119229	3.767572	0.257087
12	8	0	3.404543	1.693109	-1.742359
13	1	0	3.184513	2.480362	-1.201846
14	1	0	2.572505	1.301030	-2.027556
15	7	0	-1.602184	1.854301	-0.984094
16	6	0	-0.548347	0.976953	-1.085428
17	6	0	-2.602659	1.158535	-0.509569
18	6	0	-2.276516	-0.228538	-0.374040
19	6	0	-4.274785	-0.782776	0.425554
20	6	0	-3.938326	1.597329	-0.123762
21	7	0	-4.699881	0.521721	0.325377
22	7	0	-3.054064	-1.198017	0.087511
23	8	0	-4.381663	2.722513	-0.169560
24	7	0	-5.147319	-1.659170	0.890287
25	1	0	-6.087226	-1.396215	1.151371
26	1	0	-4.869643	-2.626450	0.972514
27	6	0	-0.265839	-1.590744	-0.778756
28	6	0	2.112615	-1.364162	-0.672459
29	6	0	1.582633	-2.084621	0.568249
30	1	0	-0.967133	-2.364431	-1.093285
31	1	0	1.767924	-3.162153	0.466886
32	1	0	2.217568	-0.301006	-0.464920
33	1	0	-5.650135	0.742330	0.610947
34	6	0	0.981421	-1.605941	-1.674420
35	1	0	0.945410	-0.877606	-2.486279
36	8	0	0.166580	-1.846205	0.544191
37	8	0	3.365932	-1.824622	-1.114232
38	1	0	3.224581	-2.687479	-1.527947
39	8	0	1.188162	-2.912690	-2.175149
40	1	0	0.583655	-3.074741	-2.908315
41	6	0	2.156808	-1.590669	1.873206
42	1	0	3.248151	-1.659046	1.819582
43	1	0	1.882148	-0.544870	2.027520
44	8	0	1.650694	-2.315858	2.985560
45	1	0	1.973965	-3.222045	2.923011

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.022717	-0.331893	-0.808661
2	1	0	0.148871	1.113365	-1.888112
3	8	0	2.116430	2.052341	1.860282
4	1	0	1.646938	2.105038	2.701444
5	17	0	0.704281	1.578660	0.482696
6	8	0	4.235111	0.709410	0.767511
7	1	0	4.077010	0.926466	-0.166533
8	1	0	3.495460	1.119264	1.255530
9	8	0	3.073192	3.810722	0.069245
10	1	0	2.757003	3.293493	0.840066
11	1	0	3.951224	4.130259	0.300343
12	8	0	3.535825	1.802764	-1.713706
13	1	0	3.306439	2.567070	-1.140899
14	1	0	2.709358	1.432632	-2.040542
15	7	0	-1.600547	1.863308	-0.962104
16	6	0	-0.550311	0.982043	-1.072171
17	6	0	-2.605099	1.166597	-0.498049
18	6	0	-2.285173	-0.223575	-0.376116
19	6	0	-4.288813	-0.778220	0.409718
20	6	0	-3.939946	1.606740	-0.110022
21	7	0	-4.708497	0.528856	0.321717
22	7	0	-3.067710	-1.194198	0.073460
23	8	0	-4.377446	2.734574	-0.141932
24	7	0	-5.166993	-1.657205	0.858417
25	1	0	-6.105514	-1.393374	1.123720
26	1	0	-4.891837	-2.625840	0.933313
27	6	0	-0.268894	-1.580926	-0.767130
28	6	0	2.116362	-1.405944	-0.681749
29	6	0	1.573261	-2.114237	0.559786
30	1	0	-0.969712	-2.363610	-1.061221
31	1	0	1.702783	-3.198390	0.442666
32	1	0	2.246134	-0.346009	-0.472064
33	1	0	-5.659602	0.749810	0.604212
34	6	0	0.970950	-1.610403	-1.676626
35	1	0	0.943278	-0.866676	-2.475050
36	8	0	0.174558	-1.801295	0.558466
37	8	0	3.354654	-1.900446	-1.130656
38	1	0	3.180025	-2.725224	-1.605314
39	8	0	1.147774	-2.908981	-2.208085
40	1	0	0.513275	-3.054312	-2.919069
41	6	0	2.189235	-1.661857	1.859821
42	1	0	3.273249	-1.801979	1.800034
43	1	0	1.991909	-0.599598	2.016923
44	8	0	1.641874	-2.348577	2.976670
45	1	0	1.990965	-3.247094	2.977775

Standard orientation of TS-Gua-n-N^2 and initial structure

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

Standard orientation of transition state of TS-Gua-n-N^2

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -172.39cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.362207	-1.100127	-1.418493
2	8	0	-5.176513	-1.020318	2.594279
3	1	0	-5.826213	-1.710785	2.420396
4	17	0	-3.674059	-1.256160	0.877077
5	8	0	-4.530903	-0.756541	-2.221085
6	1	0	-5.324438	-0.576021	-1.628066
7	1	0	3.148299	2.113367	0.305367
8	1	0	-4.366884	0.036543	-2.744106
9	8	0	-5.930234	0.993898	1.387034
10	1	0	-5.546064	-0.121074	2.128503
11	1	0	-5.100262	1.416429	1.140879
12	8	0	-6.553312	-0.391830	-0.632561
13	1	0	-6.303264	0.199068	0.180568
14	1	0	-6.728322	-1.271765	-0.282519
15	7	0	1.724508	0.523488	0.170262
16	7	0	1.166481	2.652706	-0.240418
17	6	0	2.130235	1.829494	0.092086
18	6	0	0.400345	0.520661	-0.151055
19	6	0	0.072170	1.842079	-0.396538
20	6	0	-1.275926	2.175544	-0.754657
21	6	0	-1.621454	-0.236756	-0.531167
22	7	0	-2.074291	1.013063	-0.793858
23	7	0	-0.421726	-0.562646	-0.204216
24	8	0	-1.756107	3.264350	-1.009779
25	7	0	-2.614768	-1.266858	-0.604836
26	1	0	-2.161049	-2.181000	-0.676186
27	1	0	-3.048333	1.154652	-1.055794
28	6	0	2.547878	-0.656765	0.461664
29	6	0	4.447857	-0.564641	-0.944438
30	6	0	4.875861	-0.453724	0.518974
31	1	0	1.922964	-1.361348	1.010007
32	1	0	5.321353	-1.401290	0.837627
33	1	0	4.298310	0.432679	-1.374251
34	6	0	3.109715	-1.285477	-0.811468
35	1	0	2.450827	-1.145652	-1.671778
36	6	0	5.830362	0.675038	0.789675
37	1	0	6.691133	0.558125	0.119013
38	1	0	5.345801	1.632371	0.569473
39	8	0	6.228727	0.608279	2.149976
40	1	0	6.816949	1.349446	2.328593
41	8	0	3.645939	-0.253675	1.243915
42	8	0	5.315578	-1.340304	-1.739875
43	1	0	6.158018	-0.879570	-1.829411
44	8	0	3.317469	-2.655281	-0.532365
45	1	0	4.023563	-2.968939	-1.113400

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.384314	-0.092183	1.803169
2	8	0	-5.009370	2.747293	-1.109266
3	1	0	-5.625618	3.179505	-0.507083
4	17	0	-3.584159	1.646039	0.265331
5	8	0	-4.563518	-0.807419	2.142750
6	1	0	-5.350746	-0.468120	1.611926
7	1	0	3.026303	-1.952205	-1.463320
8	1	0	-4.457978	-1.745741	1.947844
9	8	0	-5.956431	0.549999	-1.636312
10	1	0	-5.465840	1.793471	-1.400388
11	1	0	-5.183102	-0.001974	-1.794776
12	8	0	-6.555138	0.166860	0.798662
13	1	0	-6.317159	0.290304	-0.197031
14	1	0	-6.667861	1.053077	1.158778
15	7	0	1.701621	-0.743166	-0.297875
16	7	0	0.952287	-2.400862	-1.603760
17	6	0	2.004046	-1.747489	-1.180789
18	6	0	0.346224	-0.765756	-0.150970
19	6	0	-0.099520	-1.790488	-0.966596
20	6	0	-1.503167	-2.073108	-1.036379
21	6	0	-1.655773	-0.223585	0.559511
22	7	0	-2.221209	-1.194394	-0.199169
23	7	0	-0.402699	0.056557	0.632222
24	8	0	-2.084587	-2.923787	-1.684980
25	7	0	-2.580502	0.547557	1.329690
26	1	0	-2.076234	1.115961	2.013185
27	1	0	-3.229131	-1.338691	-0.164128
28	6	0	2.655722	0.151940	0.347944
29	6	0	4.930232	-0.306664	0.523321
30	6	0	4.801893	1.100743	-0.028875
31	1	0	2.084939	0.758912	1.051591
32	1	0	4.800028	1.835983	0.784171
33	1	0	5.197278	-1.000123	-0.281102
34	6	0	3.624589	-0.612388	1.035487
35	1	0	3.824300	-1.662994	1.000243
36	6	0	5.932253	1.383957	-1.035689
37	1	0	6.878368	1.202127	-0.570174
38	1	0	5.823076	0.741674	-1.884484
39	8	0	5.863347	2.748327	-1.458355
40	1	0	6.732411	3.039681	-1.743731
41	8	0	3.414786	1.046156	-0.646905
42	8	0	5.865665	-0.426820	1.598229
43	1	0	6.545561	-1.062015	1.361865
44	8	0	3.019119	-0.284055	2.288684
45	1	0	3.459961	-0.764554	2.993226

Standard orientation of TS-Gua-a-N1 and initial structure

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

Standard orientation of transition state of TS-Gua-a-N1
State=1-A Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -120.61cm^{-1}
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.587340	0.784412	-0.164125
2	6	0	-4.854952	0.129734	-0.510622
3	6	0	-4.574965	0.300184	0.981710
4	1	0	-2.054595	1.723743	-0.020282
5	8	0	6.086835	-1.199404	1.020988
6	1	0	6.226465	-0.859120	1.912695
7	8	0	3.884555	1.479000	-1.727800
8	1	0	4.032825	1.898456	-0.862230
9	1	0	3.239595	0.776403	-1.582045
10	8	0	6.600568	0.732510	-0.746085
11	1	0	6.502871	-0.025573	-0.115656
12	1	0	5.827475	0.710377	-1.329807
13	8	0	4.970369	2.376564	0.744699
14	1	0	5.746376	1.930574	0.351982
15	1	0	5.190493	3.309953	0.836217
16	6	0	-0.287087	-0.188613	-0.215058
17	6	0	1.609998	0.467943	0.736529
18	6	0	1.650383	-1.583265	-0.569650
19	7	0	2.322793	1.312697	1.533905
20	1	0	3.316427	1.420976	1.351396
21	1	0	1.850170	2.189913	1.706091
22	7	0	2.260458	-0.621455	0.233038
23	17	0	4.142443	-0.921440	0.657462
24	8	0	2.282084	-2.547069	-1.021088
25	6	0	-1.781056	-1.327091	-1.360606
26	1	0	-2.736637	-1.581127	-1.794402
27	7	0	-0.688668	-2.023813	-1.500481
28	7	0	-1.606049	-0.187116	-0.601568
29	7	0	0.326015	0.735074	0.543579
30	6	0	0.263615	-1.318930	-0.783694
31	6	0	-3.753359	0.982426	-1.137776
32	1	0	-3.503887	0.685632	-2.158545
33	1	0	-4.719213	-0.921262	-0.791411
34	8	0	-3.151502	0.373532	1.078549
35	1	0	-5.022923	1.237437	1.330672
36	6	0	-5.076109	-0.861693	1.808882
37	1	0	-4.877028	-0.701534	2.872009
38	1	0	-4.577637	-1.780836	1.484068
39	8	0	-6.476417	-0.927835	1.554680
40	1	0	-6.847848	-1.696428	2.002297
41	8	0	-4.095757	2.355490	-1.083164
42	1	0	-5.009873	2.449847	-1.385124
43	8	0	-6.122074	0.598338	-0.917873
44	1	0	-6.790480	0.149688	-0.380890

Standard orientation of initial structure
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.633396	-0.510972	-0.390040
2	6	0	4.918921	0.029220	-0.427641
3	6	0	4.635746	-0.658671	0.905602
4	1	0	2.261559	-1.503220	-0.646402
5	8	0	-6.055664	0.729680	1.503918
6	1	0	-6.148435	0.110462	2.237827
7	8	0	-3.970787	-0.834254	-2.050594
8	1	0	-4.052134	-1.542627	-1.388051
9	1	0	-3.363406	-0.184258	-1.675897
10	8	0	-6.627246	-0.544529	-0.780231
11	1	0	-6.513510	-0.024649	0.053869
12	1	0	-5.881542	-0.316013	-1.356053
13	8	0	-4.919002	-2.556795	0.010964
14	1	0	-5.710010	-2.015647	-0.181763
15	1	0	-5.138759	-3.470759	-0.199702
16	6	0	0.262267	0.287333	-0.246731
17	6	0	-1.588285	-0.673901	0.521944
18	6	0	-1.713955	1.667835	-0.124470
19	7	0	-2.261776	-1.735744	1.051082
20	1	0	-3.257070	-1.811288	0.860323
21	1	0	-1.767866	-2.611419	0.941378
22	7	0	-2.276259	0.496320	0.378261
23	17	0	-4.138859	0.617317	0.973859
24	8	0	-2.380474	2.704271	-0.248948
25	6	0	1.698537	1.756082	-1.023045
26	1	0	2.641600	2.141952	-1.378566
27	7	0	0.583247	2.430896	-0.943892
28	7	0	1.563469	0.439873	-0.645112
29	7	0	-0.306611	-0.836169	0.227741
30	6	0	-0.332786	1.517710	-0.451440
31	6	0	3.734186	-0.195024	-1.215127
32	1	0	3.669416	0.711536	-1.779799
33	1	0	5.075437	1.077396	-0.280232
34	8	0	3.125225	-0.478240	1.073177
35	1	0	4.889327	-1.697034	0.856636
36	6	0	5.397026	0.037009	2.049316
37	1	0	5.090665	-0.378805	2.986408
38	1	0	5.180629	1.084817	2.036259
39	8	0	6.802567	-0.161632	1.876410
40	1	0	7.251185	-0.023093	2.713757
41	8	0	3.735047	-1.312970	-2.106809
42	1	0	4.349584	-1.148887	-2.825851
43	8	0	6.056905	-0.561452	-1.060885
44	1	0	6.666577	0.128553	-1.332534

Standard orientation of TS-Gua-a-N3 and initial structure

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

Standard orientation of transition state of TS-Gua-a-N3

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1130.65cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.525357	3.334041	-2.204514
2	1	0	0.155999	4.001405	-2.338822
3	8	0	0.645962	1.069352	2.267726
4	1	0	0.972202	1.899496	1.873957
5	1	0	-0.017740	0.717814	1.655397
6	8	0	-1.145646	3.334588	0.136105
7	1	0	-0.866523	3.360605	-1.018539
8	1	0	-1.242688	2.401240	0.363411
9	8	0	1.334572	3.515450	1.035803
10	1	0	0.395361	3.555216	0.696974
11	1	0	1.426511	4.194702	1.712826
12	1	0	-0.606011	-3.594520	-0.363439
13	6	0	2.162094	-2.082848	0.002111
14	6	0	0.226290	-2.915564	-0.273763
15	6	0	1.342846	-1.046533	-0.363338
16	7	0	0.086795	-1.561293	-0.531035
17	7	0	1.442027	-3.258323	0.038117
18	6	0	3.538453	-1.812610	0.345889
19	6	0	3.077595	0.474770	0.022344
20	7	0	3.894933	-0.485092	0.394998
21	7	0	1.804173	0.238970	-0.452750
22	17	0	0.921237	1.460316	-1.291135
23	6	0	-1.159651	-0.823767	-0.716656
24	1	0	-1.105992	-0.276152	-1.657929
25	6	0	-3.468687	-0.692059	-0.265795
26	6	0	-2.716022	0.121267	0.774301
27	8	0	4.354865	-2.701866	0.624079
28	7	0	3.475629	1.761794	0.048764
29	1	0	4.371156	1.907208	0.494283
30	1	0	2.776221	2.483795	0.227309
31	6	0	-2.405040	-1.703181	-0.705295
32	1	0	-2.331069	-2.480316	0.058560
33	8	0	-1.326695	0.077344	0.363728
34	1	0	-4.351629	-1.182555	0.150411
35	8	0	-3.814210	0.162435	-1.340813
36	1	0	-4.011172	-0.386491	-2.112657
37	8	0	-2.610922	-2.249402	-1.986038
38	1	0	-3.179342	-3.026200	-1.915119
39	1	0	-3.046017	1.162299	0.755597
40	6	0	-2.810217	-0.422347	2.187285
41	1	0	-2.576938	-1.492574	2.203902
42	1	0	-2.081270	0.102974	2.811540
43	8	0	-4.134268	-0.182600	2.638761
44	1	0	-4.219365	-0.503205	3.543775

Standard orientation of initial structure

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	-0.501599	3.358047	-2.177495
2	1	0	0.184427	4.022518	-2.302042
3	8	0	0.662806	1.048808	2.268798
4	1	0	0.990236	1.881453	1.881324
5	1	0	-0.009014	0.708688	1.658592
6	8	0	-1.124795	3.331044	0.162299
7	1	0	-0.843925	3.370892	-0.992317
8	1	0	-1.198931	2.394702	0.384812
9	8	0	1.360736	3.503742	1.059097
10	1	0	0.422082	3.554412	0.722278
11	1	0	1.461138	4.181449	1.736446
12	1	0	-0.636791	-3.582092	-0.384836
13	6	0	2.142789	-2.094052	-0.010237
14	6	0	0.200408	-2.909877	-0.291792
15	6	0	1.332699	-1.050052	-0.373808
16	7	0	0.072623	-1.553668	-0.545581
17	7	0	1.412831	-3.263633	0.020994
18	6	0	3.520929	-1.836234	0.336184
19	6	0	3.079139	0.456017	0.020074
20	7	0	3.888288	-0.511845	0.390085
21	7	0	1.805328	0.231590	-0.459384
22	17	0	0.930838	1.465576	-1.287334
23	6	0	-1.167528	-0.803466	-0.726107
24	1	0	-1.107354	-0.246525	-1.661283
25	6	0	-3.476083	-0.662244	-0.265259
26	6	0	-2.713670	0.125282	0.787651
27	8	0	4.329595	-2.733146	0.612572
28	7	0	3.486516	1.740066	0.053310
29	1	0	4.381718	1.878263	0.501709
30	1	0	2.791358	2.466578	0.229561
31	6	0	-2.421279	-1.672064	-0.728172
32	1	0	-2.353663	-2.465336	0.019245
33	8	0	-1.328325	0.088956	0.362631
34	1	0	-4.360949	-1.154861	0.144252
35	8	0	-3.818864	0.215852	-1.321920
36	1	0	-4.014080	-0.315529	-2.106451
37	8	0	-2.633167	-2.189773	-2.019681
38	1	0	-3.221225	-2.953275	-1.965996
39	1	0	-3.041026	1.167229	0.795458
40	6	0	-2.793124	-0.451253	2.188711
41	1	0	-2.547401	-1.518905	2.178915
42	1	0	-2.064909	0.067970	2.818791
43	8	0	-4.115704	-0.237544	2.657148
44	1	0	-4.186186	-0.570225	3.559197

Standard orientation of TS-Gua-a-N7 and initial structure

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

Standard orientation of transition state of TS-Gua-a-N7

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1153.27cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.700208	3.898274	-0.542763
2	1	0	-3.741522	4.236632	-1.443243
3	8	0	-0.023161	0.237362	2.174745
4	1	0	0.004221	1.130322	1.777866
5	1	0	0.723423	-0.246338	1.793296
6	8	0	-1.625879	4.618252	0.466642
7	1	0	-2.674598	4.294533	-0.032680
8	1	0	-1.798725	5.217601	1.199450
9	8	0	0.159064	2.773673	1.083011
10	1	0	-0.537870	3.443254	0.829808
11	1	0	0.882763	2.862990	0.453383
12	17	0	-2.554134	1.750177	-0.704563
13	6	0	1.690369	-1.166331	-0.756456
14	6	0	3.187053	0.704836	-0.836649
15	6	0	3.319230	-0.022971	0.495849
16	1	0	1.748187	-2.232367	-0.968184
17	1	0	4.233509	-0.625873	0.496886
18	6	0	-0.739409	-1.679912	-0.356885
19	6	0	-1.773284	-3.499131	0.343867
20	6	0	-3.127389	-1.595623	0.071627
21	7	0	-1.725611	-4.801519	0.756457
22	1	0	-2.604056	-5.298435	0.765930
23	1	0	-0.925768	-5.338709	0.454864
24	7	0	-2.974327	-2.905246	0.403478
25	8	0	-4.237413	-1.022620	0.108002
26	6	0	-0.266208	0.398994	-0.955733
27	1	0	0.256542	1.291274	-1.265175
28	7	0	-1.561546	0.343168	-0.710246
29	7	0	0.269489	-0.824704	-0.788954
30	7	0	-0.599597	-2.961446	-0.035097
31	6	0	-1.905845	-0.946412	-0.323944
32	8	0	2.183338	-0.904002	0.547023
33	6	0	2.550857	-0.368456	-1.736622
34	1	0	1.970175	0.050232	-2.561592
35	1	0	2.513389	1.562452	-0.737161
36	8	0	4.458491	1.111510	-1.291180
37	1	0	4.360099	1.840812	-1.915375
38	8	0	3.545425	-1.250578	-2.216351
39	1	0	4.326874	-0.721163	-2.434892
40	6	0	3.298404	0.902799	1.681759
41	1	0	4.125077	1.614090	1.579562
42	1	0	2.355729	1.459922	1.695067
43	8	0	3.439228	0.123816	2.861101
44	1	0	3.350221	0.701734	3.627581

Standard orientation of initial structure

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	-3.696738	3.903497	-0.533093
2	1	0	-3.746233	4.240322	-1.433730
3	8	0	-0.022497	0.240946	2.174742
4	1	0	0.007132	1.133156	1.776311
5	1	0	0.723782	-0.244506	1.794959
6	8	0	-1.613669	4.625854	0.457034
7	1	0	-2.666441	4.300295	-0.033069
8	1	0	-1.782548	5.221829	1.193558
9	8	0	0.162679	2.773443	1.076230
10	1	0	-0.531397	3.445630	0.822019
11	1	0	0.889992	2.863673	0.450948
12	17	0	-2.553618	1.752570	-0.699949
13	6	0	1.687781	-1.167445	-0.756296
14	6	0	3.187408	0.701345	-0.836023
15	6	0	3.319646	-0.028292	0.495416
16	1	0	1.745166	-2.233533	-0.967921
17	1	0	4.231809	-0.634400	0.494267
18	6	0	-0.742298	-1.679495	-0.356875
19	6	0	-1.777653	-3.498370	0.342544
20	6	0	-3.130117	-1.593445	0.071992
21	7	0	-1.731104	-4.801184	0.753976
22	1	0	-2.610019	-5.297282	0.762971
23	1	0	-0.931846	-5.338828	0.451635
24	7	0	-2.978149	-2.903457	0.402839
25	8	0	-4.239681	-1.019557	0.108888
26	6	0	-0.267391	0.399318	-0.954744
27	1	0	0.256109	1.291385	-1.263516
28	7	0	-1.562743	0.344504	-0.708986
29	7	0	0.267204	-0.824947	-0.788807
30	7	0	-0.603553	-2.961410	-0.036144
31	6	0	-1.908048	-0.944981	-0.323129
32	8	0	2.180452	-0.904983	0.547266
33	6	0	2.549044	-0.370160	-1.736681
34	1	0	1.968339	0.049971	-2.560888
35	1	0	2.514598	1.559396	-0.734670
36	8	0	4.458887	1.107322	-1.290932
37	1	0	4.360633	1.835429	-1.916554
38	8	0	3.542108	-1.253113	-2.218025
39	1	0	4.324789	-0.724763	-2.434826
40	6	0	3.303506	0.896395	1.682175
41	1	0	4.132458	1.604926	1.579663
42	1	0	2.362609	1.456699	1.696733
43	8	0	3.442791	0.116139	2.860811
44	1	0	3.375065	0.696768	3.627457

Standard orientation of TS-Gua-a-C8 and initial structure

Cartesian coordinates of the transition state optimized at the M06-2X/6-311+G(d) level:
Standard orientation of transition state of TS-Gua-a-C8
State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -458.19cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.566042	-0.808197	-0.618946
2	1	0	0.440383	0.779321	-1.681728
3	8	0	1.546388	2.364512	2.243958
4	1	0	0.978750	2.174042	3.002775
5	17	0	0.624308	1.496170	0.747610
6	8	0	2.156067	2.529330	-2.150217
7	1	0	1.333827	3.003182	-1.909056
8	1	0	2.523020	2.192182	-1.325291
9	8	0	0.884012	4.726451	1.040178
10	1	0	1.181134	3.939592	1.547220
11	1	0	1.664489	5.270307	0.888727
12	8	0	-0.149258	3.868523	-1.389893
13	1	0	0.154010	4.170640	-0.509310
14	1	0	-0.789550	3.156464	-1.236639
15	7	0	-1.505381	1.224313	-0.953503
16	6	0	-0.322799	0.540371	-0.951904
17	6	0	-2.414574	0.394717	-0.480898
18	6	0	-1.862858	-0.899768	-0.246793
19	6	0	-3.814855	-1.659847	0.477215
20	6	0	-3.830237	0.591920	-0.169615
21	7	0	-4.475676	-0.499085	0.304511
22	7	0	-2.505923	-1.943941	0.236733
23	8	0	-4.395523	1.687310	-0.336209
24	7	0	-4.538568	-2.682788	0.955768
25	1	0	-5.518305	-2.558844	1.156058
26	1	0	-4.109984	-3.583182	1.101637
27	6	0	0.395019	-1.891985	-0.527192
28	6	0	2.668081	-1.199489	-0.782780
29	6	0	2.458453	-1.815608	0.595602
30	1	0	-0.174109	-2.814322	-0.640913
31	1	0	2.867128	-2.832808	0.601488
32	6	0	1.506359	-1.815248	-1.575878
33	1	0	1.222365	-1.232062	-2.454133
34	1	0	2.563440	-0.110339	-0.740632
35	8	0	1.032174	-1.882786	0.744081
36	8	0	3.931972	-1.565871	-1.292847
37	1	0	4.188258	-0.945675	-1.986476
38	8	0	1.823781	-3.145192	-1.940170
39	1	0	2.754132	-3.161800	-2.209153
40	6	0	3.053114	-1.021133	1.733364
41	1	0	4.130750	-0.944074	1.577875
42	1	0	2.627283	-0.014391	1.753699
43	8	0	2.864104	-1.666217	2.986478
44	1	0	1.926925	-1.627310	3.212949

Standard orientation of initial structure

Standard orientation:

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

1	7	0	-0.636764	-0.753421	-0.624364
2	1	0	0.453633	0.812076	-1.634176
3	8	0	1.756992	2.245010	2.252431
4	1	0	1.143773	2.217792	2.999108
5	17	0	0.723662	1.451173	0.792968
6	8	0	2.256755	2.388074	-2.087686
7	1	0	1.464982	2.931418	-1.893967
8	1	0	2.609702	2.109161	-1.235152
9	8	0	1.497066	4.616216	0.904236
10	1	0	1.671768	3.816916	1.445413
11	1	0	2.329178	4.876917	0.497011
12	8	0	0.027155	3.881684	-1.341022
13	1	0	0.433930	4.145027	-0.491052
14	1	0	-0.634846	3.201625	-1.140449
15	7	0	-1.454978	1.341648	-0.866168
16	6	0	-0.317055	0.589273	-0.906775
17	6	0	-2.413026	0.547143	-0.429430
18	6	0	-1.937008	-0.785034	-0.251757
19	6	0	-3.929848	-1.464424	0.439010
20	6	0	-3.811661	0.813801	-0.096641
21	7	0	-4.520096	-0.259221	0.326276
22	7	0	-2.638765	-1.811551	0.186171
23	8	0	-4.311052	1.948298	-0.201798
24	7	0	-4.713794	-2.465614	0.866485
25	1	0	-5.689632	-2.298462	1.054121
26	1	0	-4.342929	-3.398785	0.951451
27	6	0	0.264515	-1.888525	-0.560982
28	6	0	2.574275	-1.312172	-0.785397
29	6	0	2.322174	-1.958890	0.571988
30	1	0	-0.351282	-2.775688	-0.706558
31	1	0	2.672754	-2.997254	0.546534
32	6	0	1.383629	-1.834251	-1.602592
33	1	0	1.134483	-1.203520	-2.458515
34	1	0	2.533773	-0.220745	-0.709349
35	8	0	0.892525	-1.951947	0.712735
36	8	0	3.817156	-1.735703	-1.302421
37	1	0	4.111830	-1.111719	-1.977151
38	8	0	1.630408	-3.164228	-2.017049
39	1	0	2.563350	-3.224316	-2.270447
40	6	0	2.953844	-1.235027	1.735756
41	1	0	4.034044	-1.204698	1.582191
42	1	0	2.577281	-0.210045	1.791061
43	8	0	2.732665	-1.913074	2.965921
44	1	0	1.796329	-1.844544	3.188806

Standard orientation of TS-Gua-a-N^2 and initial structure

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

Standard orientation of transition state of TS-Gua-a-N^2

State=1-A Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1145.61cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.327727	-0.521959	-1.519979
2	8	0	-5.107148	-1.377552	2.493827
3	1	0	-5.502797	-2.240472	2.328802
4	17	0	-3.640793	-1.105682	0.674083
5	8	0	-4.732882	-0.190823	-2.336863
6	1	0	-5.509057	-0.409771	-1.768129
7	1	0	3.300286	2.027712	0.611507
8	1	0	-4.799434	0.744552	-2.558966
9	8	0	-6.587876	0.301513	1.579768
10	1	0	-5.853848	-0.543044	2.071030
11	1	0	-6.059205	1.093848	1.437237
12	8	0	-6.789582	-0.914266	-0.741809
13	1	0	-6.722491	-0.424372	0.129866
14	1	0	-6.615139	-1.841036	-0.542307
15	7	0	1.790377	0.546972	0.281305
16	7	0	1.361502	2.738772	0.109906
17	6	0	2.271154	1.830075	0.354383
18	6	0	0.467388	0.658456	-0.056904
19	6	0	0.214241	2.016495	-0.154475
20	6	0	-1.111019	2.441613	-0.498327
21	6	0	-1.589114	0.175382	-0.566947
22	7	0	-2.009812	1.414487	-0.700908
23	7	0	-0.418548	-0.338328	-0.257079
24	8	0	-1.459144	3.635082	-0.620159
25	7	0	-2.626611	-0.827041	-0.790086
26	1	0	-2.204759	-1.722171	-1.047140
27	6	0	2.534687	-0.705574	0.401025
28	6	0	4.431947	-0.582720	-1.010039
29	6	0	4.877666	-0.682749	0.450336
30	1	0	1.873145	-1.435707	0.867721
31	1	0	5.255804	-1.690864	0.649139
32	1	0	4.348038	0.468915	-1.308064
33	6	0	3.041101	-1.207961	-0.951023
34	1	0	2.394532	-0.900488	-1.775936
35	6	0	5.910391	0.340089	0.836525
36	1	0	6.760388	0.245001	0.150158
37	1	0	5.493419	1.347407	0.737739
38	8	0	6.314290	0.091562	2.176706
39	1	0	6.948971	0.766970	2.442583
40	8	0	3.669584	-0.484010	1.209120
41	8	0	5.245947	-1.299094	-1.911608
42	1	0	6.077649	-0.825922	-2.038381
43	8	0	3.121679	-2.617357	-0.857806
44	1	0	3.667752	-2.945111	-1.584997

Standard orientation of initial structure

Standard orientation:

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

1	1	0	-3.338074	-0.634329	-1.538103
2	8	0	-5.120032	-1.455307	2.416655
3	1	0	-5.649582	-2.198633	2.108247
4	17	0	-3.645683	-1.231385	0.653442
5	8	0	-4.710441	-0.163041	-2.290088
6	1	0	-5.476561	-0.339679	-1.688806
7	1	0	3.224470	2.045090	0.627912
8	1	0	-4.653096	0.793152	-2.389472
9	8	0	-6.217662	0.535354	1.592978
10	1	0	-5.673809	-0.481122	2.066156
11	1	0	-5.495038	1.121698	1.345133
12	8	0	-6.732176	-0.704164	-0.618868
13	1	0	-6.559153	-0.189544	0.233845
14	1	0	-6.593344	-1.631593	-0.399839
15	7	0	1.752808	0.529276	0.284056
16	7	0	1.277312	2.710947	0.104386
17	6	0	2.203503	1.823825	0.359998
18	6	0	0.431134	0.609973	-0.065898
19	6	0	0.149134	1.961510	-0.169308
20	6	0	-1.184726	2.361426	-0.524776
21	6	0	-1.608320	0.079565	-0.588543
22	7	0	-2.056538	1.306230	-0.731536
23	7	0	-0.429381	-0.410126	-0.268011
24	8	0	-1.557697	3.539641	-0.650566
25	7	0	-2.623419	-0.943713	-0.816241
26	1	0	-2.186912	-1.830779	-1.072062
27	6	0	2.522771	-0.704718	0.427477
28	6	0	4.388297	-0.537715	-1.014732
29	6	0	4.859941	-0.605902	0.438559
30	1	0	1.881327	-1.439423	0.914939
31	1	0	5.274615	-1.600038	0.634401
32	1	0	4.263167	0.505975	-1.325946
33	6	0	3.029241	-1.222300	-0.917030
34	1	0	2.355025	-0.974214	-1.740217
35	6	0	5.871100	0.444198	0.805093
36	1	0	6.709438	0.367675	0.100885
37	1	0	5.426431	1.440499	0.708650
38	8	0	6.299596	0.204265	2.136901
39	1	0	6.937082	0.884915	2.376848
40	8	0	3.660347	-0.441696	1.218813
41	8	0	5.206633	-1.246754	-1.918084
42	1	0	6.056554	-0.797152	-1.992347
43	8	0	3.194484	-2.620653	-0.784764
44	1	0	3.871729	-2.897589	-1.416164

Standard orientation of TS-Ado-n-N1 and initial structure

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

Standard orientation of transition state of TS-Ado-n-N1

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -970.01cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	5.990191	-1.029576	-1.267047
2	1	0	6.331891	-1.667328	-0.630924
3	8	0	3.362093	2.312904	-0.077546
4	1	0	3.948401	1.905817	0.584720
5	1	0	3.709714	2.033770	-0.930372
6	8	0	6.561257	1.153808	-0.412974
7	1	0	6.299639	0.037786	-0.882486
8	1	0	6.057063	1.801139	-0.916804
9	8	0	5.073323	0.894700	1.624029
10	1	0	5.739998	0.991699	0.853104
11	1	0	5.349712	1.479830	2.336247
12	1	0	-2.592711	-0.305423	2.377884
13	6	0	0.273730	-0.510250	1.067516
14	6	0	-1.718726	-0.421052	1.756285
15	6	0	-0.513009	-0.872006	-0.009344
16	7	0	-1.800251	-0.825734	0.444176
17	7	0	-0.493594	-0.229894	2.170818
18	6	0	1.674725	-0.476024	0.893735
19	6	0	1.200813	-1.162362	-1.364963
20	1	0	1.669347	-1.409745	-2.308727
21	7	0	2.528167	-0.173429	1.846339
22	1	0	3.522187	0.046312	1.689383
23	1	0	2.137193	0.096464	2.739735
24	7	0	2.072628	-0.823303	-0.364662
25	7	0	-0.089471	-1.201871	-1.249639
26	17	0	3.812713	-0.914235	-0.750083
27	6	0	-2.970018	-1.008133	-0.425053
28	1	0	-2.762290	-1.869744	-1.056133
29	6	0	-4.739508	0.285197	0.524730
30	6	0	-4.132987	1.002789	-0.685941
31	1	0	-4.358376	0.703627	1.459549
32	1	0	-4.903199	1.159352	-1.445304
33	6	0	-4.273030	-1.172866	0.345291
34	1	0	-4.155432	-1.712785	1.287584
35	8	0	-3.150389	0.114472	-1.251861
36	8	0	-6.147817	0.399706	0.481915
37	1	0	-6.502769	0.209167	1.358392
38	8	0	-5.160768	-1.846662	-0.521713
39	1	0	-6.031809	-1.440092	-0.401598
40	6	0	-3.499324	2.318549	-0.309325
41	1	0	-4.252393	2.932957	0.198539
42	1	0	-2.670113	2.135278	0.386183
43	8	0	-3.041192	2.942579	-1.497045
44	1	0	-2.584083	3.755008	-1.256435

Standard orientation of initial structure

Standard orientation:

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

1	8	0	5.988741	-1.030517	-1.265492
2	1	0	6.333005	-1.667417	-0.629901
3	8	0	3.362894	2.313112	-0.085303
4	1	0	3.950334	1.908391	0.577240
5	1	0	3.704697	2.025744	-0.937730
6	8	0	6.558231	1.154624	-0.414441
7	1	0	6.297476	0.037805	-0.882300
8	1	0	6.052576	1.800536	-0.918632
9	8	0	5.073969	0.898877	1.625158
10	1	0	5.739904	0.995233	0.853364
11	1	0	5.344709	1.492512	2.332487
12	1	0	-2.593939	-0.294656	2.377607
13	6	0	0.272584	-0.508364	1.068957
14	6	0	-1.719885	-0.414383	1.756941
15	6	0	-0.514263	-0.874989	-0.006225
16	7	0	-1.801550	-0.825541	0.446858
17	7	0	-0.494713	-0.221936	2.170725
18	6	0	1.673459	-0.474418	0.894627
19	6	0	1.199611	-1.173002	-1.360212
20	1	0	1.668013	-1.425601	-2.302655
21	7	0	2.527538	-0.165354	1.844669
22	1	0	3.520483	0.055923	1.683271
23	1	0	2.137427	0.112661	2.735956
24	7	0	2.071431	-0.828718	-0.361790
25	7	0	-0.090723	-1.211405	-1.244738
26	17	0	3.811931	-0.918688	-0.747774
27	6	0	-2.971469	-1.010134	-0.421808
28	1	0	-2.764802	-1.874499	-1.049417
29	6	0	-4.738061	0.289988	0.523711
30	6	0	-4.129797	1.001906	-0.689593
31	1	0	-4.356148	0.710714	1.457182
32	1	0	-4.899930	1.158648	-1.449005
33	6	0	-4.274730	-1.169802	0.349448
34	1	0	-4.158137	-1.706552	1.293703
35	8	0	-3.150429	0.109007	-1.253180
36	8	0	-6.146121	0.407075	0.480473
37	1	0	-6.501342	0.224073	1.358425
38	8	0	-5.164144	-1.845033	-0.514781
39	1	0	-6.034261	-1.436057	-0.396107
40	6	0	-3.492248	2.316979	-0.317157
41	1	0	-4.243476	2.934893	0.189180
42	1	0	-2.663294	2.133803	0.378625
43	8	0	-3.032735	2.936660	-1.506587
44	1	0	-2.574454	3.749089	-1.268104

Standard orientation of TS-Ado-n-C2 and initial structure

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

Standard orientation of transition state of TS-Ado-n-C2

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1393.92cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.244018	0.827005	-0.077696
2	6	0	0.061066	2.139610	-0.499817
3	6	0	-1.272752	2.588594	-0.587535
4	6	0	-1.932569	0.483549	0.134417
5	1	0	-2.754799	0.108314	1.160446
6	8	0	-5.787056	0.397876	1.497443
7	1	0	-5.707707	1.061470	0.802823
8	17	0	-3.346765	-0.945572	-0.633586
9	8	0	-3.361744	0.068771	2.252379
10	1	0	-3.234521	-0.805359	2.644326
11	1	0	-4.345515	0.181682	2.027659
12	8	0	-4.523560	-2.184528	-1.518882
13	1	0	-6.058739	-0.442107	1.054214
14	1	0	-4.792814	-1.712150	-2.316884
15	8	0	-6.442399	-1.925439	0.334869
16	1	0	-5.783437	-2.067952	-0.384719
17	1	0	-6.258667	-2.592786	1.004058
18	7	0	-1.586302	3.827075	-0.996375
19	1	0	-0.864377	4.515972	-1.135682
20	1	0	-2.545735	4.133739	-0.953612
21	6	0	2.156293	1.829195	-0.483070
22	1	0	3.226644	1.955925	-0.558238
23	7	0	-2.250734	1.730387	-0.262406
24	7	0	-0.712493	-0.046646	0.247369
25	7	0	1.606516	0.643016	-0.071166
26	7	0	1.270297	2.754638	-0.748197
27	6	0	2.321852	-0.568962	0.278280
28	1	0	1.591691	-1.242803	0.730932
29	6	0	4.213972	-1.903183	-0.248441
30	6	0	4.596874	-0.853619	0.778397
31	1	0	5.020053	-2.109154	-0.958936
32	1	0	5.045656	-1.301630	1.666139
33	6	0	2.994704	-1.255617	-0.912918
34	1	0	3.307681	-0.516217	-1.654393
35	8	0	3.346956	-0.255861	1.196302
36	8	0	3.808366	-3.077795	0.430088
37	1	0	3.167916	-3.526836	-0.139346
38	8	0	2.093047	-2.186644	-1.467979
39	1	0	2.382612	-2.405930	-2.361041
40	6	0	5.497411	0.235092	0.218713
41	1	0	6.509228	-0.153305	0.096518
42	1	0	5.135920	0.567345	-0.761925
43	8	0	5.568627	1.331317	1.115108
44	1	0	4.659825	1.595663	1.307445

Standard orientation of initial structure

Standard orientation:

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

1	6	0	0.253946	0.841760	-0.067477
2	6	0	0.075928	2.152942	-0.494450
3	6	0	-1.256475	2.609015	-0.577399
4	6	0	-1.924164	0.508357	0.152102
5	1	0	-2.755285	0.142498	1.174182
6	8	0	-5.863859	0.338054	1.466902
7	1	0	-5.839192	1.014566	0.780715
8	17	0	-3.330489	-0.923425	-0.629258
9	8	0	-3.424309	0.149664	2.233524
10	1	0	-3.283754	-0.691046	2.689242
11	1	0	-4.404246	0.207853	1.973037
12	8	0	-4.494947	-2.158361	-1.536319
13	1	0	-6.104541	-0.506984	1.016324
14	1	0	-4.789616	-1.664365	-2.311990
15	8	0	-6.413762	-2.025933	0.325638
16	1	0	-5.741160	-2.123675	-0.389364
17	1	0	-6.176212	-2.660680	1.009556
18	7	0	-1.563537	3.849091	-0.978203
19	1	0	-0.839982	4.519391	-1.181488
20	1	0	-2.525250	4.150032	-0.981928
21	6	0	2.169346	1.830509	-0.490875
22	1	0	3.239382	1.950060	-0.579324
23	7	0	-2.237469	1.756057	-0.246815
24	7	0	-0.705566	-0.026220	0.264365
25	7	0	1.615762	0.649663	-0.068435
26	7	0	1.286859	2.759717	-0.753927
27	6	0	2.320101	-0.569374	0.279153
28	1	0	1.580564	-1.235228	0.728505
29	6	0	4.201442	-1.917889	-0.249772
30	6	0	4.592663	-0.873491	0.779132
31	1	0	5.005719	-2.130059	-0.960489
32	1	0	5.041011	-1.328496	1.663425
33	6	0	2.987038	-1.260402	-0.913791
34	1	0	3.303828	-0.523825	-1.656476
35	8	0	3.345326	-0.271791	1.202252
36	8	0	3.787309	-3.089707	0.428628
37	1	0	3.135814	-3.528532	-0.136142
38	8	0	2.077858	-2.184321	-1.468579
39	1	0	2.369575	-2.411999	-2.358997
40	6	0	5.502223	0.209981	0.222592
41	1	0	6.511176	-0.186700	0.102502
42	1	0	5.146209	0.546747	-0.758474
43	8	0	5.581732	1.301950	1.123074
44	1	0	4.676873	1.575619	1.319428

Standard orientation of TS-Ado-n-N3 and initial structure

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

Standard orientation of transition state of TS-Ado-n-N3

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -533.04cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.831473	-3.462176	0.031847
2	1	0	-1.813258	-3.782236	-0.876454
3	8	0	-3.931435	0.033840	1.831036
4	1	0	-4.355763	-0.278276	1.005895
5	1	0	-3.352042	-0.686409	2.100003
6	8	0	-4.150069	-3.217339	0.700861
7	1	0	-2.920551	-3.391045	0.347750
8	1	0	-4.126906	-2.899308	1.609572
9	8	0	-4.925331	-1.069568	-0.463156
10	1	0	-4.631136	-1.959347	-0.061228
11	1	0	-5.886133	-1.044380	-0.406600
12	1	0	2.578752	2.057516	0.848174
13	6	0	-0.397733	2.629097	-0.069285
14	6	0	1.550145	2.061604	0.528711
15	6	0	-0.393695	1.245711	-0.009085
16	7	0	0.855673	0.877952	0.378683
17	7	0	0.837460	3.123090	0.274249
18	6	0	-1.593006	3.280278	-0.447733
19	6	0	-2.608861	1.225630	-0.660028
20	1	0	-3.480284	0.620889	-0.888367
21	7	0	-2.684774	2.527996	-0.742708
22	7	0	-1.507757	0.530249	-0.312835
23	17	0	-1.614806	-1.236369	-0.177857
24	7	0	-1.688692	4.594529	-0.527240
25	1	0	-0.898174	5.184531	-0.312751
26	1	0	-2.561108	5.023172	-0.801966
27	6	0	1.425822	-0.481844	0.548498
28	1	0	0.760905	-1.050199	1.195149
29	6	0	3.075520	-0.731150	-1.127445
30	6	0	3.728440	-0.758524	0.253418
31	1	0	3.071334	0.291679	-1.522703
32	1	0	4.016562	-1.784851	0.500056
33	6	0	1.649154	-1.164638	-0.800481
34	1	0	0.929854	-0.856618	-1.562986
35	8	0	2.681295	-0.349320	1.158693
36	8	0	3.636320	-1.638619	-2.047924
37	1	0	4.530481	-1.351463	-2.267154
38	8	0	1.592933	-2.554430	-0.561382
39	1	0	2.109057	-2.992635	-1.251401
40	6	0	4.915146	0.154315	0.383669
41	1	0	5.643639	-0.128440	-0.386451
42	1	0	4.607778	1.190645	0.205902
43	8	0	5.457432	-0.002968	1.684939
44	1	0	6.202350	0.600104	1.777338

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.202153	-3.569292	-0.214370

2	1	0	-1.285180	-3.833242	-1.136777
3	8	0	-3.501526	-0.520235	2.145191
4	1	0	-4.006687	-0.846044	1.373770
5	1	0	-2.793537	-1.160356	2.270293
6	8	0	-3.410620	-3.680077	0.764603
7	1	0	-2.268872	-3.655770	0.263617
8	1	0	-3.311559	-3.413807	1.684563
9	8	0	-4.675447	-1.606948	-0.084543
10	1	0	-4.196588	-2.461743	0.182015
11	1	0	-5.610358	-1.741092	0.102029
12	1	0	2.470830	2.341699	-0.014328
13	6	0	-0.742836	2.672751	-0.250259
14	6	0	1.407554	2.175088	-0.097136
15	6	0	-0.502045	1.308798	-0.259355
16	7	0	0.811237	1.003797	-0.164215
17	7	0	0.530525	3.207162	-0.142804
18	6	0	-2.064497	3.165727	-0.332746
19	6	0	-2.786314	0.970543	-0.444711
20	1	0	-3.594438	0.251167	-0.531397
21	7	0	-3.059188	2.251872	-0.438146
22	7	0	-1.552503	0.451894	-0.361058
23	17	0	-1.331793	-1.298934	-0.320479
24	7	0	-2.405122	4.443131	-0.316284
25	1	0	-1.739475	5.195534	-0.231118
26	1	0	-3.385288	4.683180	-0.379894
27	6	0	1.430750	-0.329081	-0.141011
28	1	0	0.645994	-1.110205	-0.311326
29	6	0	3.658318	-0.659226	-0.816979
30	6	0	3.662857	-0.789077	0.702436
31	1	0	4.294330	0.192512	-1.170583
32	1	0	4.030761	-1.798009	1.011711
33	6	0	2.324078	-0.389758	-1.256468
34	1	0	2.570620	0.458766	-1.859896
35	8	0	2.220336	-0.575283	1.140176
36	8	0	4.071005	-1.866270	-1.463226
37	1	0	5.002143	-1.806622	-1.689114
38	8	0	1.547848	-1.312214	-2.025520
39	1	0	1.960142	-1.441186	-2.882829
40	6	0	4.594408	0.260941	1.335899
41	1	0	5.555136	-0.175391	1.513423
42	1	0	4.697926	1.093128	0.671333
43	8	0	4.037108	0.706917	2.575020
44	1	0	4.743885	0.871363	3.203528

Standard orientation of TS-Ado-n-N7 and initial structure

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

Standard orientation of transition state of TS-Ado-n-N7

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -475.90cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.149796	2.734329	-0.747428
2	1	0	-4.349706	2.741280	-1.689362
3	8	0	-0.466386	1.204650	2.910218
4	1	0	-0.398820	1.932991	2.260222
5	1	0	-1.347093	0.834939	2.790291
6	8	0	-2.183290	4.128107	-0.408461
7	1	0	-3.255636	3.413703	-0.593490
8	1	0	-2.432452	4.889069	0.124645
9	8	0	-0.263937	3.035558	0.914570
10	1	0	-0.994875	3.469293	0.357120
11	1	0	0.612603	3.290962	0.589844
12	1	0	-0.092278	1.187217	0.281808
13	6	0	-1.584665	-1.669096	-0.089317
14	6	0	-0.352959	0.137698	0.183186
15	6	0	-0.302722	-2.062978	0.267563
16	7	0	0.445668	-0.905523	0.415367
17	7	0	-1.564984	-0.281932	-0.133779
18	6	0	-2.542205	-2.682236	-0.308205
19	6	0	-0.868413	-4.188142	0.217325
20	1	0	-0.610256	-5.233383	0.339986
21	7	0	-3.805456	-2.453570	-0.668426
22	1	0	-4.178267	-1.525718	-0.791690
23	7	0	-2.131767	-3.949049	-0.138945
24	7	0	0.110600	-3.317020	0.439793
25	17	0	-2.817413	0.913612	-0.433718
26	6	0	1.855476	-0.771953	0.865885
27	1	0	1.923439	-1.209452	1.861091
28	6	0	3.030246	-0.252075	-1.120722
29	6	0	2.991730	0.971935	-0.208090
30	1	0	2.214996	-0.219287	-1.850048
31	1	0	3.994069	1.177488	0.176919
32	6	0	2.811316	-1.406115	-0.134054
33	1	0	2.405295	-2.304721	-0.602360
34	8	0	4.285937	-0.319430	-1.760434
35	1	0	4.217617	-0.908501	-2.521273
36	8	0	4.010113	-1.673880	0.560836
37	1	0	4.735991	-1.520647	-0.061671
38	8	0	2.161870	0.592830	0.913390
39	6	0	2.444744	2.190761	-0.905940
40	1	0	3.091985	2.396264	-1.763833
41	1	0	1.431725	1.994079	-1.276026
42	8	0	2.441235	3.290267	-0.002748
43	1	0	2.394584	4.106427	-0.513843
44	1	0	-4.426584	-3.239986	-0.788512

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.146492	2.752957	-0.733196

2	1	0	-4.352925	2.767719	-1.673611
3	8	0	-0.437427	1.187649	2.897533
4	1	0	-0.378506	1.919832	2.250890
5	1	0	-1.317150	0.813864	2.782962
6	8	0	-2.173453	4.139282	-0.396437
7	1	0	-3.250546	3.427167	-0.580447
8	1	0	-2.418665	4.898032	0.141629
9	8	0	-0.252694	3.034860	0.915201
10	1	0	-0.984180	3.472557	0.361583
11	1	0	0.623475	3.287485	0.587587
12	1	0	-0.085106	1.187557	0.263278
13	6	0	-1.594015	-1.662028	-0.091627
14	6	0	-0.352169	0.139347	0.170377
15	6	0	-0.314216	-2.060955	0.266904
16	7	0	0.440605	-0.906940	0.407961
17	7	0	-1.566516	-0.275271	-0.144452
18	6	0	-2.556222	-2.671439	-0.307750
19	6	0	-0.890421	-4.183286	0.225671
20	1	0	-0.637486	-5.229239	0.353071
21	7	0	-3.817435	-2.437887	-0.670411
22	1	0	-4.184709	-1.508852	-0.801235
23	7	0	-2.152244	-3.939530	-0.132505
24	7	0	0.092834	-3.316231	0.444586
25	17	0	-2.815811	0.924385	-0.436174
26	6	0	1.850321	-0.779217	0.860549
27	1	0	1.914810	-1.218651	1.855180
28	6	0	3.032655	-0.260387	-1.121939
29	6	0	2.998571	0.961373	-0.206178
30	1	0	2.218978	-0.221520	-1.852714
31	1	0	4.000600	1.159538	0.183497
32	6	0	2.805417	-1.415816	-0.138686
33	1	0	2.395237	-2.310884	-0.610260
34	8	0	4.289296	-0.332081	-1.759258
35	1	0	4.221096	-0.923114	-2.518617
36	8	0	4.001294	-1.692260	0.557771
37	1	0	4.729417	-1.538302	-0.061957
38	8	0	2.161406	0.584359	0.910473
39	6	0	2.461219	2.185801	-0.901805
40	1	0	3.113401	2.391763	-1.755822
41	1	0	1.449060	1.995607	-1.277504
42	8	0	2.458867	3.281138	0.006439
43	1	0	2.420207	4.099991	-0.500990
44	1	0	-4.442145	-3.221666	-0.789093

Standard orientation of TS-Ado-n-C8 and initial structure

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

Standard orientation of transition state of TS-Ado-n-C8

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -422.86cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.296836	-0.279534	0.930168
2	1	0	1.061120	1.446460	2.172333
3	8	0	-1.420135	3.043805	-1.062216
4	1	0	-1.080950	3.935563	-1.200764
5	17	0	0.074620	2.097827	0.022257
6	8	0	-2.355763	1.103475	-2.645767
7	1	0	-3.121063	0.809797	-2.123240
8	1	0	-1.971032	1.855437	-2.148614
9	8	0	-3.400909	2.516960	0.594469
10	1	0	-2.644034	2.785363	0.011725
11	1	0	-3.030698	1.990918	1.311577
12	8	0	-4.577421	0.590142	-0.958151
13	1	0	-4.240360	1.331003	-0.410066
14	1	0	-4.460392	-0.187599	-0.395790
15	7	0	2.648561	1.556807	0.801236
16	6	0	1.394934	1.117878	1.194986
17	6	0	3.220732	0.535688	0.228316
18	6	0	2.409405	-0.647009	0.292340
19	6	0	3.961341	-1.819315	-0.747291
20	6	0	4.503348	0.392676	-0.426904
21	7	0	4.832867	-0.815425	-0.898271
22	7	0	2.748702	-1.838500	-0.189019
23	6	0	0.154214	-1.163864	1.138268
24	6	0	-2.155808	-0.653963	0.722456
25	6	0	-1.669371	-1.876151	-0.046464
26	1	0	0.498333	-1.997701	1.755335
27	1	0	-1.856250	-2.784485	0.543319
28	1	0	-2.148723	0.214430	0.059099
29	1	0	4.297524	-2.769867	-1.145935
30	7	0	5.324091	1.409323	-0.553815
31	1	0	5.086349	2.326086	-0.200210
32	6	0	-1.073715	-0.516398	1.811306
33	1	0	-0.930259	0.519150	2.117660
34	8	0	-3.458016	-0.766478	1.244013
35	1	0	-3.475175	-1.510871	1.861416
36	8	0	-1.393543	-1.319101	2.932024
37	1	0	-1.989970	-0.822786	3.504691
38	8	0	-0.260398	-1.636071	-0.129277
39	6	0	-2.243017	-2.031558	-1.423882
40	1	0	-3.336163	-2.035027	-1.340139
41	1	0	-1.939777	-1.180020	-2.038817
42	8	0	-1.768828	-3.256834	-1.965643
43	1	0	-2.094640	-3.332088	-2.868612
44	1	0	6.217952	1.279388	-1.009830

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.318363	-0.277089	0.929104
2	1	0	1.059681	1.438318	2.181717

3	8	0	-1.439290	3.006083	-1.030082
4	1	0	-1.116315	3.906241	-1.154666
5	17	0	0.048480	2.081473	0.030466
6	8	0	-2.493927	1.155938	-2.659530
7	1	0	-3.226417	0.830961	-2.109329
8	1	0	-2.071025	1.871218	-2.141699
9	8	0	-3.442470	2.496853	0.626663
10	1	0	-2.679772	2.751714	0.048711
11	1	0	-3.081002	1.991714	1.363022
12	8	0	-4.625665	0.551052	-0.893147
13	1	0	-4.285539	1.295994	-0.352519
14	1	0	-4.478931	-0.226569	-0.337189
15	7	0	2.653849	1.565940	0.814581
16	6	0	1.403861	1.119644	1.205371
17	6	0	3.233242	0.556441	0.234735
18	6	0	2.426946	-0.624103	0.292573
19	6	0	3.927975	-1.861209	-0.766172
20	6	0	4.539514	0.508762	-0.418911
21	7	0	4.782754	-0.811909	-0.893029
22	7	0	2.753727	-1.834439	-0.201893
23	6	0	0.178365	-1.175686	1.126691
24	6	0	-2.138644	-0.675092	0.736967
25	6	0	-1.643358	-1.868134	-0.071738
26	1	0	0.535482	-2.017443	1.724885
27	1	0	-1.821486	-2.796815	0.487955
28	1	0	-2.152536	0.213058	0.100214
29	1	0	4.286704	-2.794227	-1.184373
30	7	0	5.394453	1.426131	-0.587581
31	1	0	5.210650	2.349183	-0.249657
32	6	0	-1.049164	-0.550597	1.821080
33	1	0	-0.908646	0.479790	2.145758
34	8	0	-3.434629	-0.821569	1.265328
35	1	0	-3.448416	-1.604748	1.832532
36	8	0	-1.351378	-1.377151	2.928282
37	1	0	-1.956698	-0.900792	3.508467
38	8	0	-0.235217	-1.617434	-0.149564
39	6	0	-2.215778	-1.980370	-1.453884
40	1	0	-3.308682	-2.002980	-1.370641
41	1	0	-1.927006	-1.101765	-2.036866
42	8	0	-1.723517	-3.176244	-2.042082
43	1	0	-2.039188	-3.214606	-2.950937
44	1	0	6.253947	1.228112	-1.058812

Standard orientation of TS-Ado-n-N^6 and initial structure

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

Standard orientation of transition state of TS-Ado-n-N^6

State=1-A Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -170.42cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.679745	1.212540	1.268962
2	8	0	-5.484253	-0.267090	-2.494344
3	1	0	-5.623445	0.504576	-3.054285
4	17	0	-4.009128	0.429184	-1.163579
5	8	0	-4.439335	1.223388	2.002791
6	1	0	-5.118817	0.406560	1.830967
7	1	0	2.363819	2.050039	-0.382107
8	1	0	-4.035998	1.135672	2.876979
9	8	0	-7.254695	-0.158182	-0.659726
10	1	0	-6.579561	-0.213157	-1.422097
11	1	0	-7.885968	-0.872486	-0.790707
12	8	0	-5.979419	-0.631795	1.548848
13	1	0	-6.479925	-0.450394	0.695783
14	1	0	-5.463490	-1.433787	1.409097
15	7	0	1.798309	0.112224	0.321270
16	7	0	0.280855	1.674820	-0.228305
17	6	0	1.550882	1.379103	-0.145294
18	6	0	0.573698	-0.457560	0.549690
19	6	0	-0.355726	0.527193	0.202651
20	6	0	-1.700323	0.182571	0.360363
21	6	0	-1.016658	-1.880384	1.105226
22	1	0	-1.322013	-2.853757	1.470880
23	7	0	-2.011598	-1.031635	0.818025
24	7	0	0.292917	-1.678729	1.001440
25	7	0	-2.731104	1.077291	0.100782
26	1	0	-2.365749	1.948172	-0.276301
27	6	0	3.100593	-0.522284	0.452832
28	1	0	2.970939	-1.370993	1.128004
29	6	0	5.187998	-0.831063	-0.628635
30	6	0	5.218988	0.444501	0.194657
31	1	0	6.054606	0.446505	0.896785
32	6	0	3.686603	-0.996138	-0.880104
33	1	0	3.358707	-0.342640	-1.692407
34	1	0	5.763356	-0.750085	-1.555249
35	8	0	5.647860	-1.902850	0.174075
36	1	0	5.223106	-2.706450	-0.157529
37	8	0	3.294062	-2.331033	-1.106178
38	1	0	3.405861	-2.533615	-2.042233
39	8	0	4.009213	0.412458	0.984809
40	6	0	5.264818	1.689921	-0.664899
41	1	0	4.466854	1.672081	-1.416308
42	1	0	6.228382	1.716274	-1.184569
43	8	0	5.115323	2.809864	0.193596
44	1	0	5.133324	3.607778	-0.345210

Standard orientation of initial structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.346819	1.512535	-0.752877
2	8	0	-5.684963	-2.246829	-0.344562

3	1	0	-5.922544	-2.492699	-1.245168
4	17	0	-4.023721	-0.976026	-0.671771
5	8	0	-4.002760	2.321965	-0.542971
6	1	0	-4.708748	2.025461	0.219395
7	1	0	2.316878	-0.989443	-2.185041
8	1	0	-3.485102	3.074307	-0.225903
9	8	0	-7.150527	-0.264191	0.282035
10	1	0	-6.593983	-1.085692	0.034781
11	1	0	-7.738262	-0.526702	0.997280
12	8	0	-5.593891	1.603353	1.179270
13	1	0	-6.193403	0.874052	0.830917
14	1	0	-5.093636	1.233760	1.915421
15	7	0	1.891391	-0.675872	-0.097423
16	7	0	0.324083	-0.512962	-1.708427
17	6	0	1.580580	-0.739942	-1.437562
18	6	0	0.717862	-0.340864	0.533897
19	6	0	-0.240818	-0.253211	-0.475565
20	6	0	-1.536573	0.065549	-0.066411
21	6	0	-0.766209	0.138459	2.094535
22	1	0	-1.014872	0.303458	3.136263
23	7	0	-1.781370	0.260080	1.229962
24	7	0	0.504887	-0.152583	1.834377
25	7	0	-2.582538	0.228665	-0.969863
26	1	0	-2.263178	0.057616	-1.919998
27	6	0	3.181068	-0.651038	0.604761
28	1	0	3.056972	-1.242412	1.510199
29	6	0	5.360643	0.031248	-0.210339
30	6	0	4.434858	1.205867	0.055819
31	1	0	4.944493	2.016608	0.575106
32	6	0	4.370885	-1.168919	-0.222054
33	1	0	4.091788	-1.404101	-1.249313
34	1	0	5.890203	0.118041	-1.162621
35	8	0	6.262904	-0.061834	0.873007
36	1	0	6.909579	-0.747606	0.672689
37	8	0	4.872284	-2.324904	0.414722
38	1	0	5.546061	-2.721075	-0.150597
39	8	0	3.480129	0.671461	0.984333
40	6	0	3.776380	1.713199	-1.223138
41	1	0	3.595295	0.896089	-1.930985
42	1	0	4.466363	2.412893	-1.703473
43	8	0	2.556408	2.348462	-0.877591
44	1	0	2.262286	2.864093	-1.635957

Transition state of chlorination of C8 in the anion form of isomer G1 by HOCl

Ts-G1-anion-C8:

1\1\GINC-GSNEW2315\FTS\RM062X\6-311+G(d)\C5H11Cl1N5O5(1-)\ROOT\28-Feb-2023\0\\# opt=(calcfc,ts,maxcyc=100,noeigentest) freq=noraman 6-311+g(d) scrf=smd em=gd3 m062x\\Title Card Required\\-1,1\N,0.696552,-1.425315,1.340486\H,-1.123782,-0.582641,2.081845\O,-2.915704,-1.880335,-1.663616\H,-2.370474,-1.855109,-2.460546\Cl,-1.667807,-1.235339,-0.252025\O,-4.082744,0.626471,1.658356\H,-3.434495,1.244534,1.270316\H,-3.598127,-0.184433,1.850993\O,-4.345647,0.403686,-1.243547\H,-3.888555,-0.433176,-1.480026\H,-4.560654,0.331671,-0.300156\O,-2.427792,2.117856,-0.0

31223\H,-2.877132,1.567424,-0.696404\H,-1.563142,1.70744,0.155163\N,-0
.037314,0.704354,0.781943\C,-0.368677,-0.535103,1.307562\C,1.203262,0.
534814,0.377904\C,1.664968,-0.777254,0.725385\C,3.691371,-0.407501,-0.
177071\C,2.078168,1.44894,-0.329073\N,3.318644,0.877561,-0.547601\N,2.
918209,-1.252038,0.445806\O,1.820548,2.585523,-0.701443\H,3.995611,1.4
5102,-1.042517\N,4.939206,-0.762093,-0.553152\H,5.313869,-1.605197,-0.
142527\H,5.608695,-0.047045,-0.80056\\Version=ES64L-G16RevC.01\State=1
-A\HF=-1307.30595\RMSD=7.066e-09\RMSF=4.894e-06\Dipole=7.4799457,-0.64
2529,-0.2743483\Polar=0.,0.,0.,0.,0.,0.\Quadrupole=6.3843901,-16.64236
6,10.2579758,8.2380713,-12.6508027,1.9334779\PG=C01 [X(C5H11Cl1N5O5)]\
\@

Reactant complex of chlorination of C8 in the anion form of isomer G1 by HOCl
R-G1-anion-C8:

1\1\GINC-GSNEW2431\FOpt\RM062X\6-311+G(d)\C5H11Cl1N5O5(1-)\ROOT\29-Feb
-2023\0\\# opt freq 6-311+g(d) scrf=smd em=gd3 m062x\\Title Card Requi
red\\-1,1\N,-0.4535028876,1.9599030384,-1.3771803885\H,1.255753686,2.9
529098767,-0.5846807991\O,1.613758368,-2.7010882194,-0.6781082895\H,1.
313306164,-3.4588606073,-0.1515753611\Cl,0.6125710954,-1.3813469105,-0
.2535595707\O,3.5097318085,1.1123946558,-1.2634696606\H,3.29067075,1.3
356479208,-0.3395465242\H,2.665745284,1.0359048714,-1.7245366348\O,3.9
756489274,-1.3255439872,0.0850149372\H,3.3249494488,-1.991706518,-0.18
20431889\H,3.9304844718,-0.6214931365,-0.5860273246\O,2.9063396169,0.9
435023577,1.4799269678\H,3.0758523629,0.0098818265,1.2726366821\H,1.94
5739416,1.1061247104,1.3827463143\N,0.2537285883,1.7054263339,0.790417
6356\C,0.436344617,2.2691008045,-0.4018211309\C,-0.8636502691,0.930286
7184,0.5734419134\C,-1.2877238531,1.1011199119,-0.7542903064\C,-3.0308
066854,-0.2914000381,-0.5105960712\C,-1.6016135348,0.1004329665,1.4550
005497\N,-2.6908150878,-0.4867769887,0.8073217948\N,-2.3767825281,0.49
17512018,-1.3207594417\O,-1.3892640116,-0.1471075712,2.6509244127\H,-3
.25409704,-1.1189322514,1.367728438\N,-4.0944594303,-1.0283655633,-0.9
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07.3304818\RMSD=2.503e-09\RMSF=1.346e-05\Dipole=-4.450208,-3.994358,-1
.1692506\Quadrupole=2.0633805,12.0698273,-14.1332077,4.7748673,-4.5733
852,-0.4515491\PG=C01 [X(C5H11Cl1N5O5)]\\@

Product complex of chlorination of C8 in the anion form of isomer G1 by HOCl
P-G1-anion-C8:

1\1\GINC-GSNEW2314\FOpt\RM062X\6-311+G(d)\C5H11Cl1N5O5(1-)\ROOT\29-Feb
-2023\0\\# opt freq 6-311+g(d) scrf=smd em=gd3 iop(1/8=3) m062x\\Title
Card Required\\-1,1\N,0.69674,-1.825942,-0.692221\H,-0.895331,-1.9691
31,0.660149\O,-2.317008,2.420631,-1.919797\H,-1.654366,1.727892,-2.008
759\Cl,-1.78404,-1.009302,-1.285371\O,-3.674429,-2.010391,1.907137\H,-

3.362654,-1.090977,1.771178\H,-2.985477,-2.591602,1.568669\O,-4.214853
,1.496784,-0.59926\H,-3.405904,1.871666,-1.178281\H,-4.550519,0.717524
,-1.054489\O,-2.929509,0.610699,1.590796\H,-3.407768,0.932799,0.788273
\H,-1.988029,0.607934,1.365284\N,-0.182057,-0.011798,0.588163\C,-0.483
054,-1.284868,-0.081514\C,1.072628,0.10944,0.426016\C,1.640226,-1.0056
41,-0.367253\C,3.712664,-0.12944,-0.202178\C,1.96631,1.181292,0.932219
\N,3.268036,0.950202,0.561435\N,2.95401,-1.09688,-0.669206\O,1.618928,
2.135164,1.588736\H,3.951732,1.636703,0.871778\N,5.016236,-0.134787,-0
.447174\H,5.406172,-0.88995,-0.992643\H,5.632385,0.591915,-0.111464\\V
ersion=ES64L-G16RevC.01\State=1-A\HF=-1307.342941\RMSD=5.100e-09\RMSF=
9.612e-06\Dipole=11.9093824,-3.6387087,1.0640423\Quadrupole=17.0818604
,-13.8149596,-3.2669007,29.1096363,4.6542652,8.9569586\PG=C01 [X(C5H11
Cl1N5O5)]\\@

Transition state of chlorination of C8 in the neutral form of isomer G1 by HOCl

Ts-G1-neutral-C8:

1\1\GINC-GSNEW2441\FTS\RM062X\6-311G(d)\C5H12Cl1N5O5\ROOT\28-Feb-2023\
0\\# opt=(calcfc,ts,maxcyc=100,noeigentest) freq=noraman 6-311g(d) scr
f=smd em=gd3 m062x\\Title Card Required\\0,1\C,-1.0890099323,0.5077260
517,0.4268953542\C,-1.487500352,-0.8742856099,0.447812707\C,-2.8346725
472,-1.2166036755,0.0059397371\C,-3.0421359298,1.2105030063,-0.3748166
11\C,0.5598539058,-0.8331803927,1.0621520805\H,1.2334121515,-1.0439269
184,1.88136871\N,0.1566470295,0.5104518492,0.883279355\O,2.4657732634,
1.9510147603,0.5573422565\H,2.6926256164,2.8686445361,0.7385108769\Cl,
1.8477512412,-1.1985092668,-0.5019629764\O,3.0928946257,0.3256505924,2
.6923360181\H,2.3246246907,0.4614371803,3.2557846764\H,2.945199923,0.8
968054114,1.9152470848\O,3.1908344401,-1.3342588136,-2.0466934031\H,2.
9009446371,1.6968136123,-0.293305666\H,3.9263203852,-1.7885991093,-1.6
176934335\O,3.6311636321,1.2655265828,-1.7625265588\H,3.5107795715,0.2
885819235,-1.9022084757\H,3.1052460736,1.6999931437,-2.4416407211\H,0.
8437868436,1.278601334,0.8301448384\N,-3.533788369,-0.0766770146,-0.37
47537731\N,-1.8172872864,1.5443879262,0.017852065\N,-0.5285539766,-1.6
573652537,0.8643334336\O,-3.3315162397,-2.3201837314,-0.0404554909\H,-
4.4856104536,-0.2292722617,-0.6958091565\N,-3.8679700321,2.1539340714,
-0.798372625\H,-4.8069177043,1.9474164665,-1.1080376938\H,-3.547811207
7,3.1110765995,-0.8119336084\\Version=ES64L-G16RevC.01\State=1-A\HF=-1
307.727443\RMSD=7.637e-09\RMSF=4.871e-06\Dipole=-5.6205052,5.2387069,0
.068427\Quadrupole=9.4420491,-2.7212461,-6.720803,-14.2123501,10.30875
66,-5.1975369\PG=C01 [X(C5H12Cl1N5O5)]\\@

Reactant complex of chlorination of C8 in the neutral form of isomer G1 by HOCl

R-G1-neutral-C8:

1\1\GINC-GSNEW2314\FOpt\RM062X\6-311G(d)\C5H12Cl1N5O5\ROOT\29-Feb-2023
\0\\# opt freq 6-311g(d) scrf=smd m062x em=gd3 scf=tight\\Title Card R

equired\\0,1\C,-0.858382967,-0.0096916613,0.7736897426\C,-1.3668431634
,-1.1673230397,0.2018989369\C,-2.6384137126,-1.1122487958,-0.439316063
2\C,-2.5828537795,1.2698779991,0.2131722412\C,0.5234036692,-1.69208800
45,1.0002849781\H,1.4226963892,-2.213666782,1.2880165005\N,0.340036481
6,-0.3688451316,1.3074337553\O,2.4596584584,1.4168822636,1.6027936536\
H,2.5524410211,2.0995716638,2.274314332\Cl,1.7332331822,-0.8095448249,
-1.5935804816\O,3.5806379666,-1.0486569759,2.0537471244\H,2.9983533539
,-1.3484140102,2.759130813\H,3.2869370498,-0.1423313837,1.8514094564\O
,2.5038395069,0.347878804,-2.5787480673\H,2.3861880038,1.8608517152,0.
7284385169\H,3.4338129692,0.0770899547,-2.6416276732\O,2.1401435899,2.
5565072486,-0.8242112727\H,2.3505873413,1.916946839,-1.5218405427\H,1.
1994093738,2.7444639457,-0.9084077954\H,1.0671398299,0.2795710653,1.63
5631548\N,-3.1756801298,0.1809362303,-0.3727461619\N,-1.4155043489,1.2
230554532,0.8117370519\N,-0.4837391796,-2.2187307535,0.3506387283\O,-3
.2589524467,-2.0097047439,-1.0008792611\H,-4.0789489616,0.3006431333,-
0.8194389424\N,-3.2477942722,2.4420006473,0.1062703891\H,-4.2385327217
,2.4230451405,-0.0892311127\H,-2.9308875039,3.1857330034,0.7104316059\
\Version=ES64L-G16RevC.01\State=1-A\HF=-1307.7559041\RMSD=8.978e-09\RM
SF=6.345e-05\Dipole=-0.3649826,4.8024226,0.7328533\Quadrupole=6.820377
2,-9.6697295,2.8493523,-18.7918064,-8.6269769,-0.238472\PG=C01 [X(C5H1
2Cl1N5O5)]\\@

Product complex of chlorination of C8 in the neutral form of isomer G1 by HOCl

P-G1-neutral-C8:

1\1\GINC-GSNEW2417\FOpt\RM062X\6-311G(d)\C5H12Cl1N5O5\ROOT\29-Feb-2023
\0\\# opt freq 6-311g(d) scrf=smd m062x em=gd3\\Title Card Required\\0
,1\C,-1.2040251915,0.5485212448,0.1061537274\C,-1.5718540407,-0.879992
6753,0.2343333071\C,-2.9758477265,-1.295883638,0.0014826802\C,-3.32004
61625,1.1033905209,-0.4271921202\C,0.5090519491,-0.6460222987,0.692635
9538\H,0.8955019608,-0.689984038,1.7105677351\N,0.0564718165,0.6792376
527,0.363970751\O,2.5671774199,1.9135961834,0.7543730292\H,2.627683468
5,2.8396776432,1.0129751141\Cl,1.8820042108,-1.1262252872,-0.357883566
3\O,2.6212060635,0.2552798352,2.9807094023\H,1.8242335622,0.5338207217
,3.443009532\H,2.6859337746,0.8423674741,2.2055289113\O,4.6591392379,-
1.2403978394,-1.6717042052\H,3.4182091587,1.5651788187,-0.7551618319\H
,4.774610746,-1.5139672512,-0.7569438632\O,3.8391812976,1.3894747235,-
1.6198549462\H,4.3829766063,-0.303878743,-1.6333887442\H,3.1218220396,
1.3832559891,-2.2621984833\H,1.6287870165,1.7295513144,0.5549190541\N,
-3.7611939695,-0.2118762189,-0.3191898138\N,-2.0841697434,1.5138633241
,-0.225290862\N,-0.5796978598,-1.6132067798,0.549192577\O,-3.400300941
9,-2.4230380398,0.0791498101\H,-4.743815893,-0.4063247582,-0.489918887
6\N,-4.2565250881,1.9780817884,-0.7630231485\H,-5.2159883579,1.7076230
472,-0.9243409751\H,-4.0014153537,2.9504122862,-0.8527401372\\Version=
ES64L-G16RevC.01\State=1-A\HF=-1307.7929041\RMSD=8.323e-09\RMSF=1.423e

-05\Dipole=-7.2088736,4.4751472,0.4240875\Quadrupole=7.6169277,-3.0424438,-4.5744839,-9.4578983,16.4571358,-1.0131961\PG=C01 [X(C5H12Cl1N5O5)]\\@