Supporting Information

A significant role of alkaline cations on the Reimer-Tiemann reaction.

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They are only ca. 6 kcal/mol smaller than that of the PhO^-… Na^+ coordination.

(b) Charge-transfer (CT) interactions to make the hexagonal pyramid coordination stable.

Geometries in the R-T reaction with K^+, which correspond to those in Figure 1 (with Na^+). The step of Int4(K^+) to Int6(K^+) via TS4(K^+) was obtained. That is, Int5(K^+) of the $C_6H_4(CHCl_2)$-O^- form dose not intervene in the K^+ containing reaction.

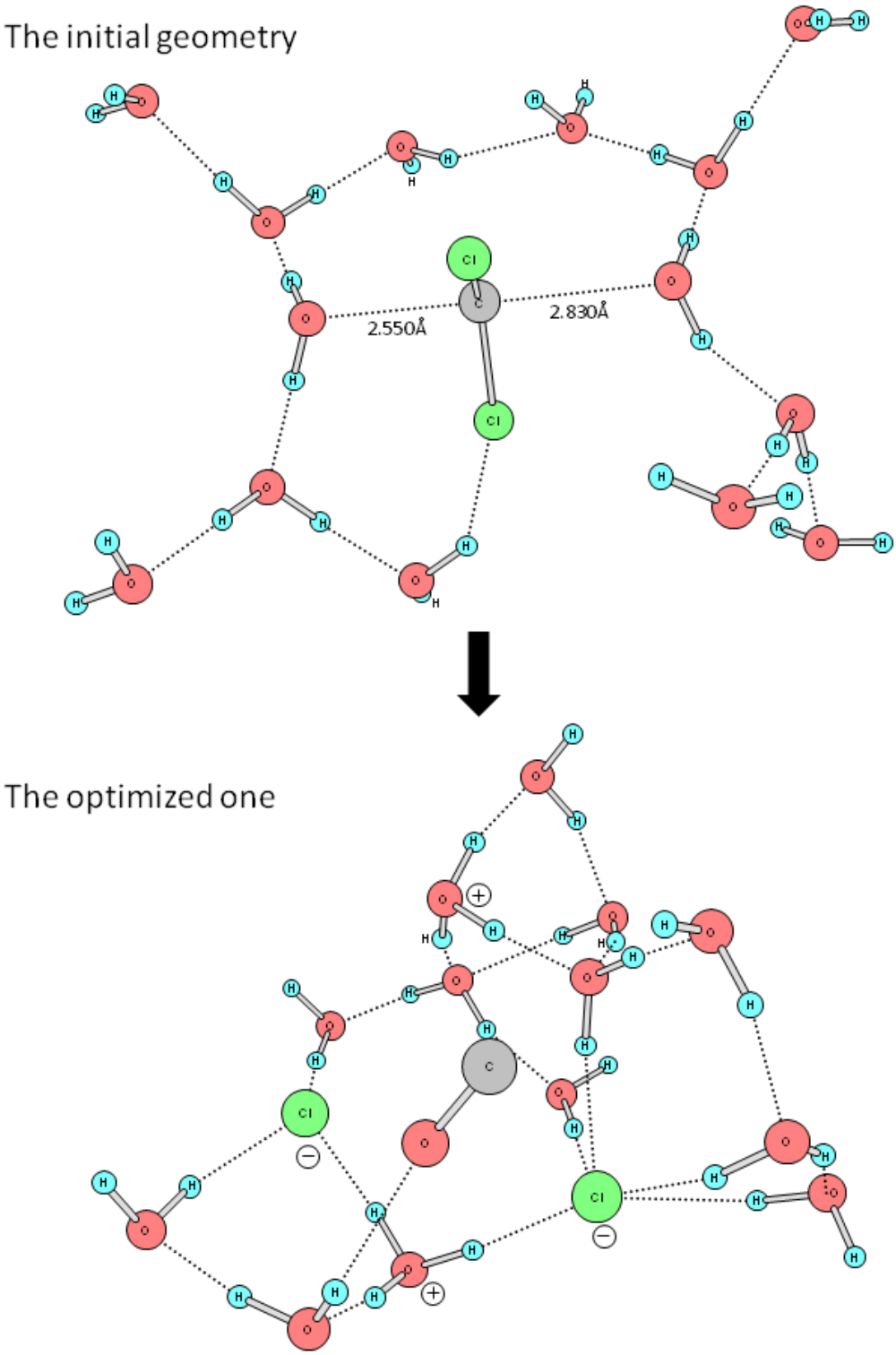
Three TS geometries obtained by two computational methods.

Energy changes along the paths in Figure 1 and Figure S4. Relative Gibbs free energies of RB3LYP/6-311+G(d,p) SCRF=PCM // RB3LYP/6-31(+)G(d) are shown in Table S1 (without square brackets).

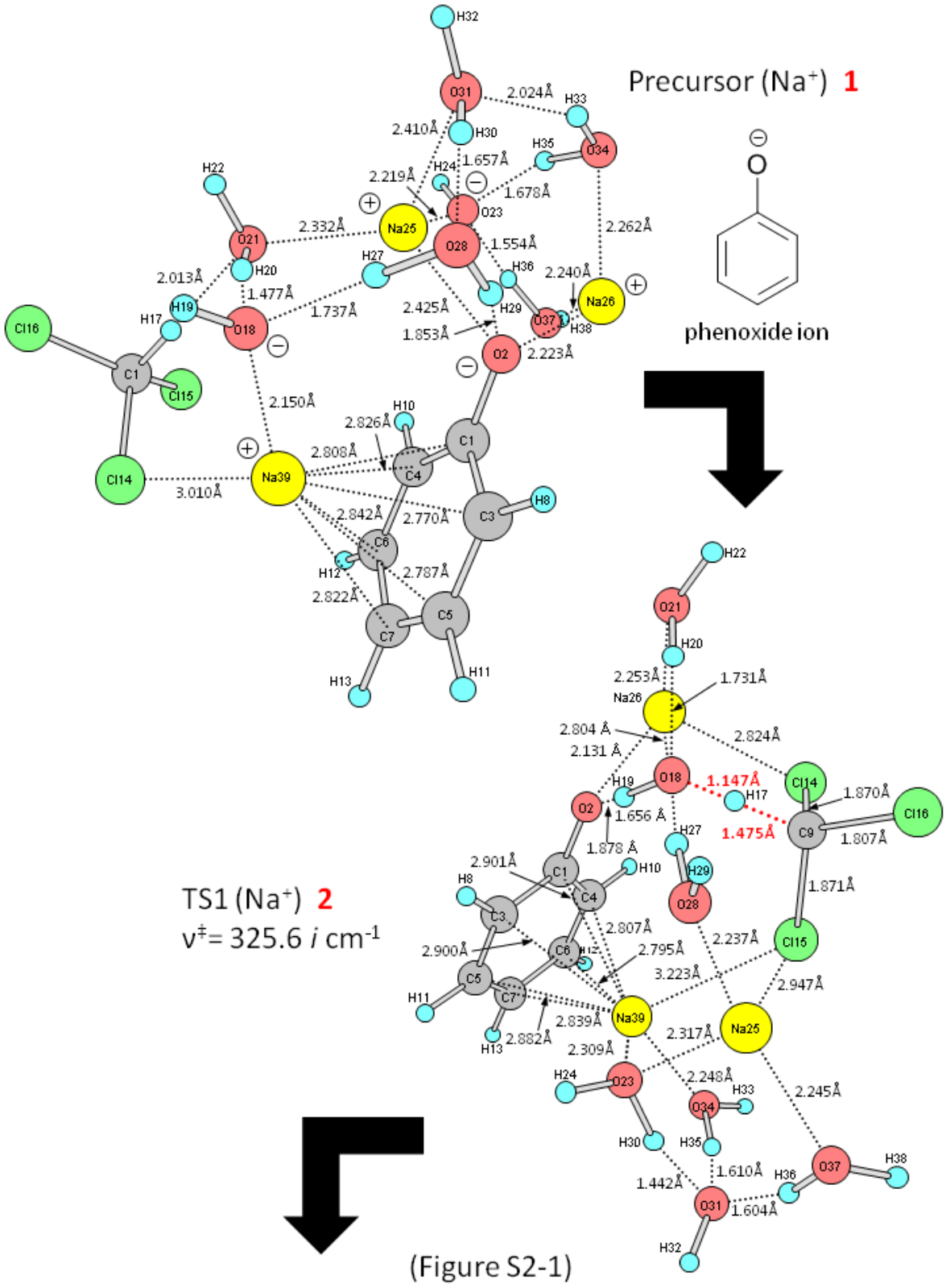
Changes of Gibbs free energies in kcal/mol (T=298.15K P=1atm). Values without square brackets are of RB3LYP/6-311+G(d,p) SCRF=PCM // RB3LYP/6-31(+)G(d). Those with

square brackets are of RB3LYP/6-311+G(d,p) SCRF=PCM // RB3LYP/6-31+G(d), which are shown in Figure 2.

Cartesian coordinates of the B3LYP /6-31(+)G(d) and B3LYP /6-31+G(d) optimized geometries which are shown in Figure 1 and Figure S2.

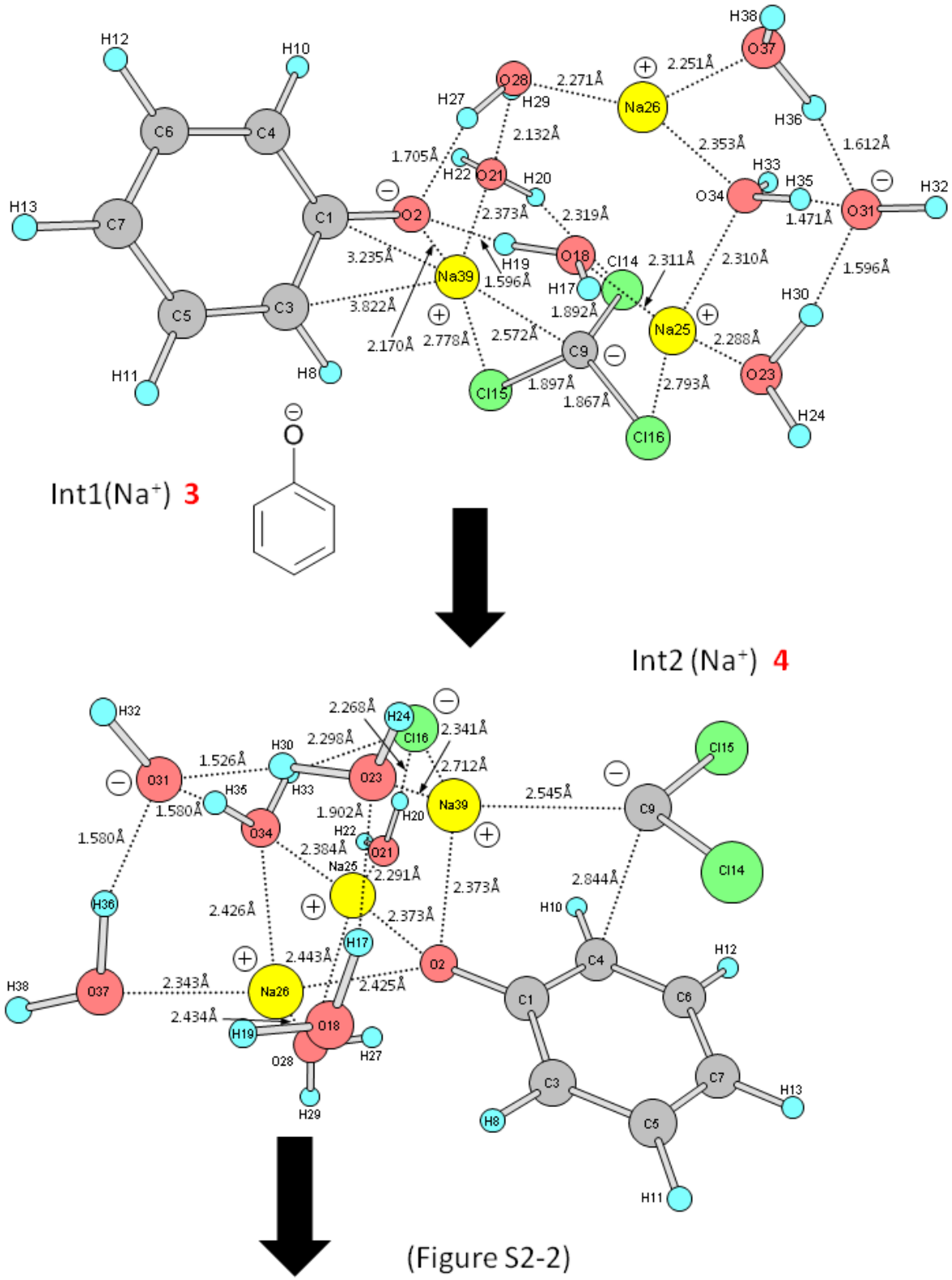


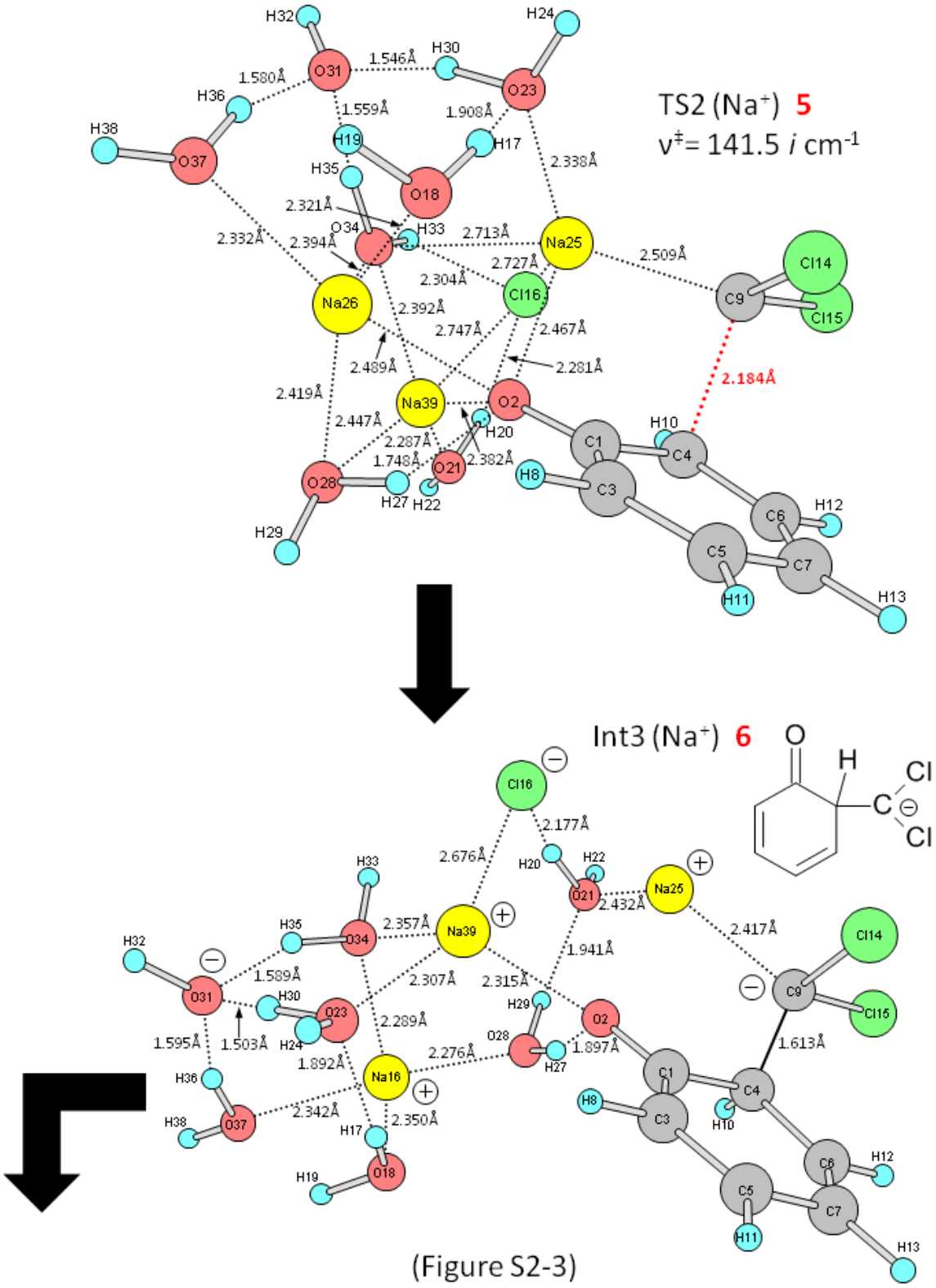
(Figure S1)


Precursor (Na⁺) 1
phenoxide ion
TS1 (Na⁺) 2
v‡= 325.6 i cm-1
H32
O31
2.024Å
H33
2.410Å
H30
H35
O34
H22
H24
1.657Å
2.219Å
1.678Å
O23
O21
2.332Å
Na25
O28
1.554Å
2.262Å
H27
H36
2.240Å
2.013Å
H20
1.477Å
Na26
H19
H17
1.737Å
2.425Å
H29
O37
H38
Cl16
O18
1.853Å
O2
2.223Å
C1
Cl15
2.150Å
H10
2.826Å
C1
2.808Å
C4
Cl14
Na39
3.010Å
2.842Å
2.770Å
C3
H8
C6
H12
2.787Å
2.822Å
C7
C5
H13
H11
H22
O21
H20
2.253Å
1.731Å
Na26
2.804 Å
2.131 Å
2.824Å
H19
O18
1.147Å
H17
Cl14
1.870Å
Cl16
O2
1.656 Å
1.475Å
C9
1.807Å
H27
1.878 Å
2.901Å
C1
H10
H29
H8
C4
O28
1.871Å
C3
2.807Å
2.900Å
C6
H12
2.795Å
2.237Å
Cl15
3.223Å
C5
2.947Å
H11
C7
Na39
2.839Å
2.317Å
Na25
H13
2.882Å
2.309Å
H24
O23
2.248Å
2.245Å
H33
O34
H30
H35
1.610Å
H36
O37
H38
1.442Å
O31
1.604Å
H32

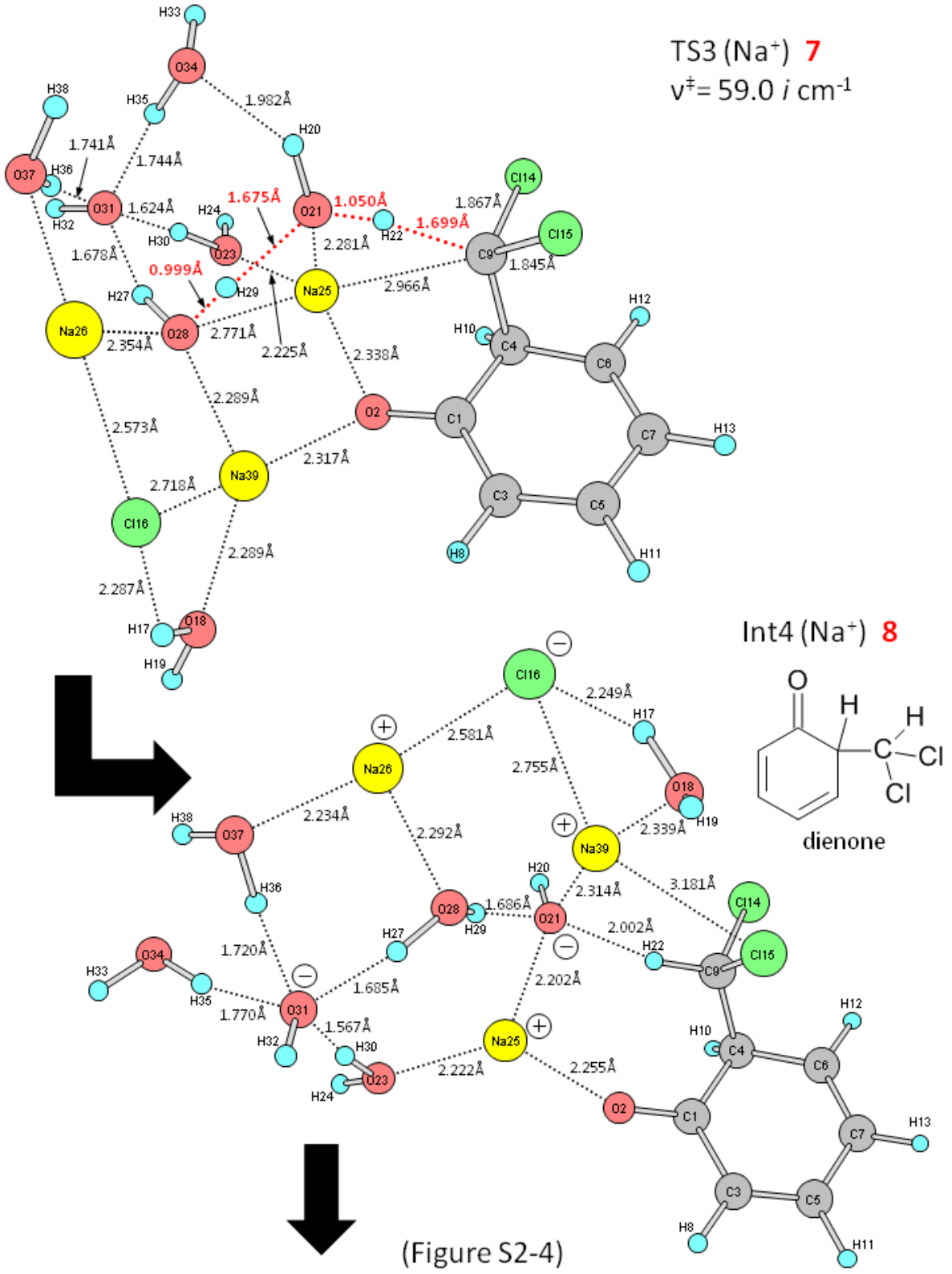
(Figure S2-1)

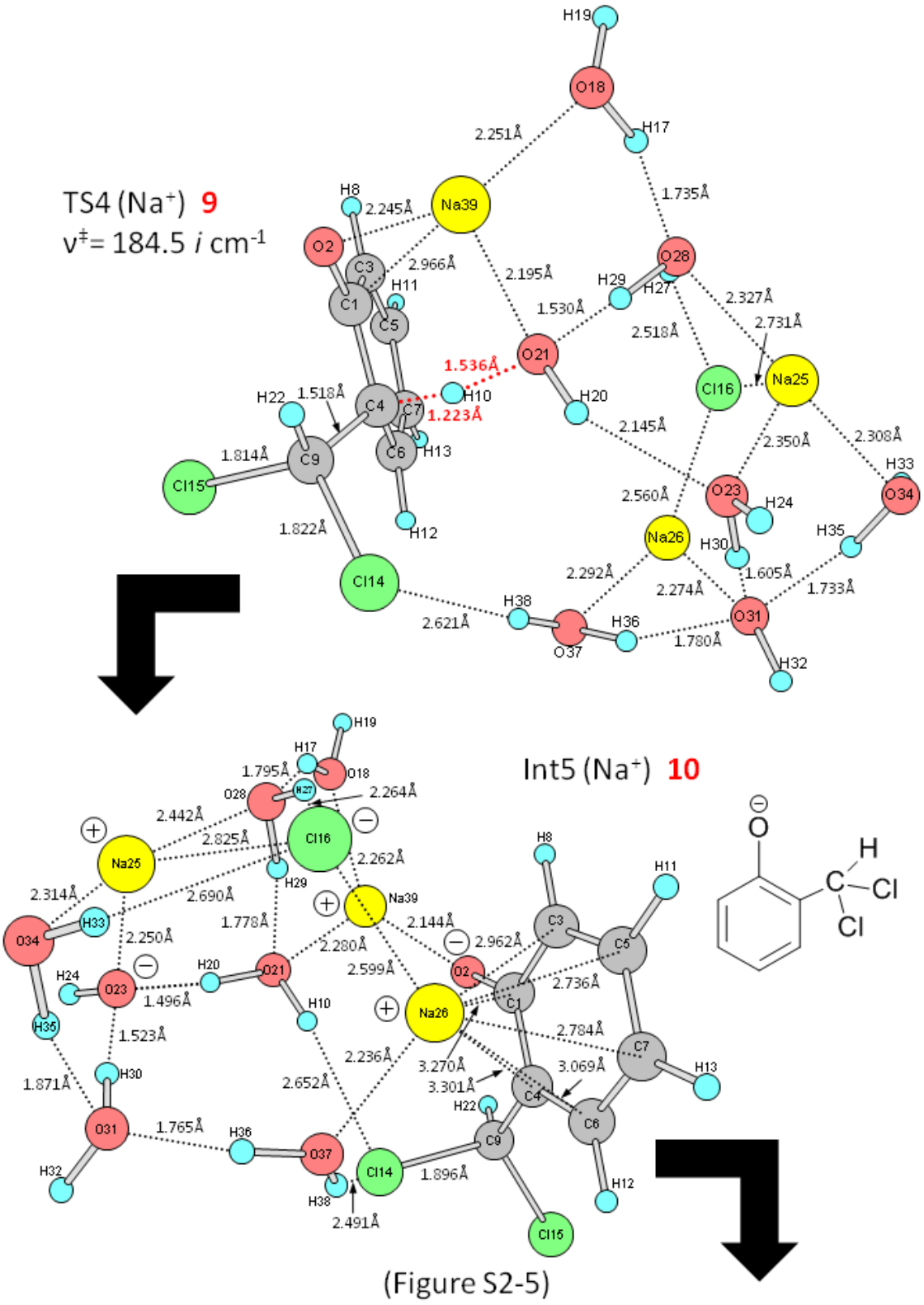
4


H12
H10
C6
C4
H13
C7
C1
O2
C5
C3
H11
H8
O
H38
O37
2.251Å
O28
2.271Å
H27
H29
Na26
H36
2.132Å
2.353Å
1.612Å
1.705Å
H22
O21
H20
H33
H35
O34
O31
H32
1.471Å
2.373Å
2.319Å
3.235Å
O18
H19
Cl14
2.311Å
2.310Å
1.596Å
Na39
1.596Å
H17
H30
3.822Å
1.892Å
Na25
2.170Å
2.778Å
2.572Å
C9
2.288Å
O23
Cl15
1.897Å
2.793Å
1.867Å
H24
Cl16
Int1(Na⁺) 3
Int2 (Na⁺) 4
H32
2.268Å
H24
Cl16
2.341Å
O31
1.526Å
H30
2.298Å
O23
2.712Å
Cl15
H35
H33
Na39
2.545Å
C9
1.580Å
1.902Å
H20
O34
H22
1.580Å
2.384Å
O21
Cl14
Na25
2.291Å
H36
2.373Å
2.844Å
2.426Å
2.373Å
H10
H17
2.443Å
C4
H12
O2
H38
O37
2.343Å
Na26
2.425Å
C1
C6
2.434Å
H19
O18
C3
C7
H13
H8
C5
O28
H27
H29
H11
(Figure S2-2)

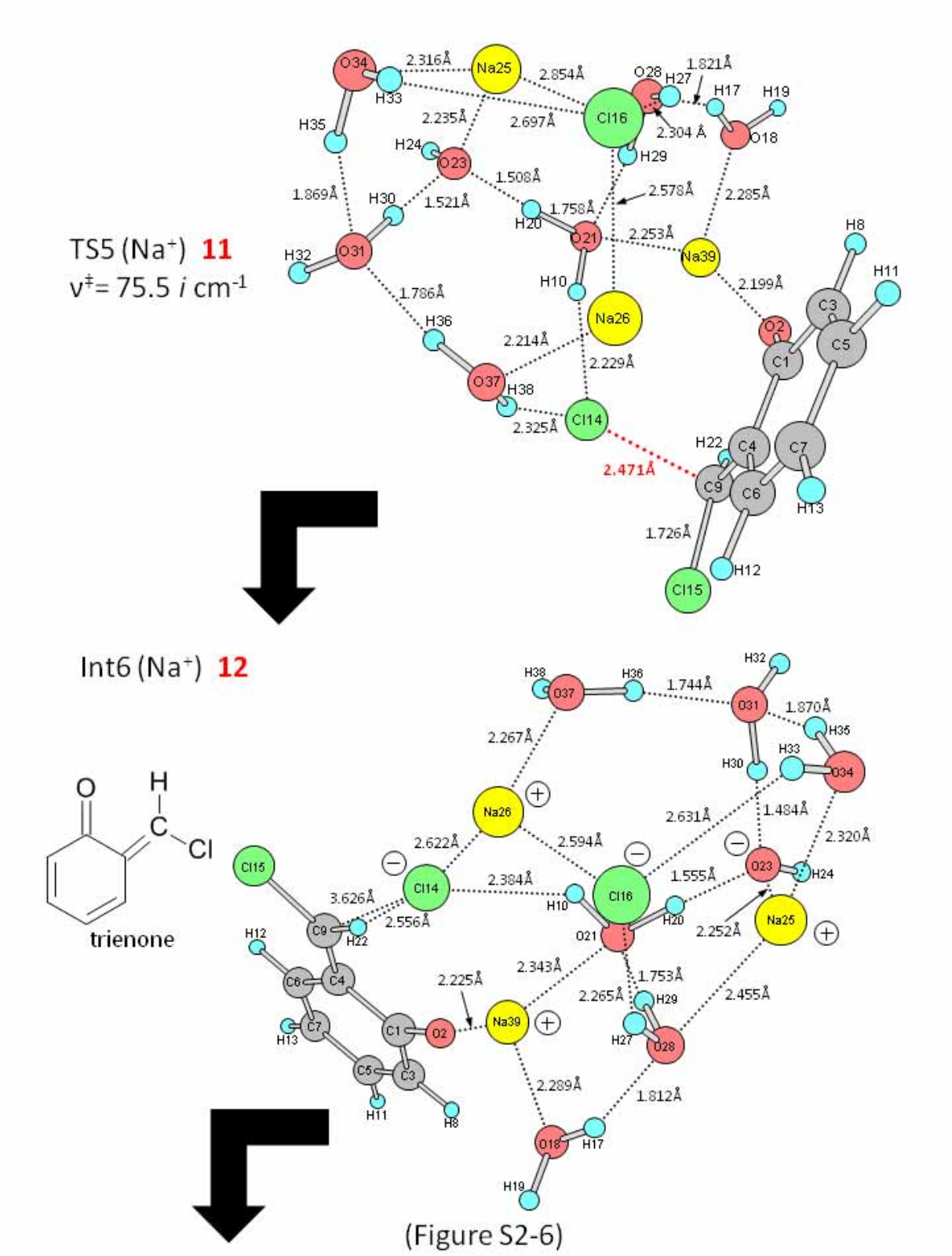

TS2 (Na+) 5
v‡= 141.5 i cm-1
Int3 (Na+) 6
H32
H24
O31
1.546Å
H30
O23
1.580Å
H36
1.559Å
1.908Å
H38
O37
H19
H17
H35
O18
2.338Å
2.321Å
O34
H33
2.713Å
Na25
2.332Å
2.394Å
2.727Å
2.509Å
Cl14
2.304Å
Cl16
C9
Na26
2.392Å
Cl15
2.747Å
2.467Å
2.489Å
2.281Å
2.184Å
2.419Å
Na39
O2
2.447Å
H10
H20
C1
2.287Å
1.748Å
O21
2.382Å
C4
O28
H8
C3
H27
H22
C6
H12
H29
C5
C7
H11
H13
2.177Å
2.676Å
H20
H22
O21
Na25
2.432Å
2.417Å
H33
H35
O34
2.357Å
Na39
H32
1.589Å
2.307Å
2.315Å
1.941Å
O31
H30
O23
H29
O2
2.289Å
1.595Å
1.503Å
H24
O28
1.897Å
1.613Å
1.892Å
2.276Å
H27
H36
Na16
C1
C4
H38
O37
2.342Å
2.350Å
H8
C3
H10
H17
C6
H12
H19
O18
C5
C7
H11
H13

(Figure S2-3)

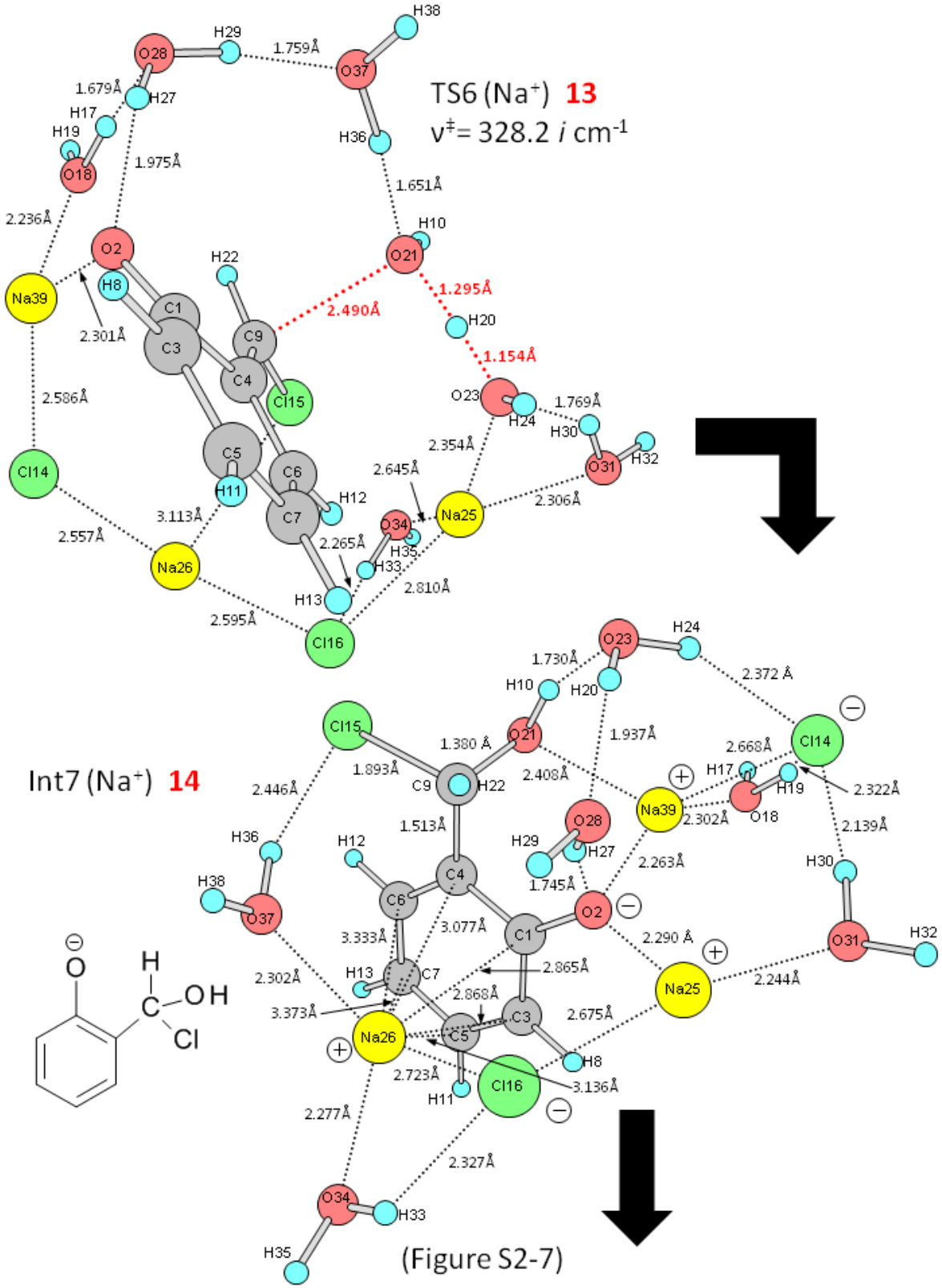

TS3 (Na+) 7
v‡= 59.0 i cm-1
Int4 (Na+) 8
dienone
(Figure S2-4)

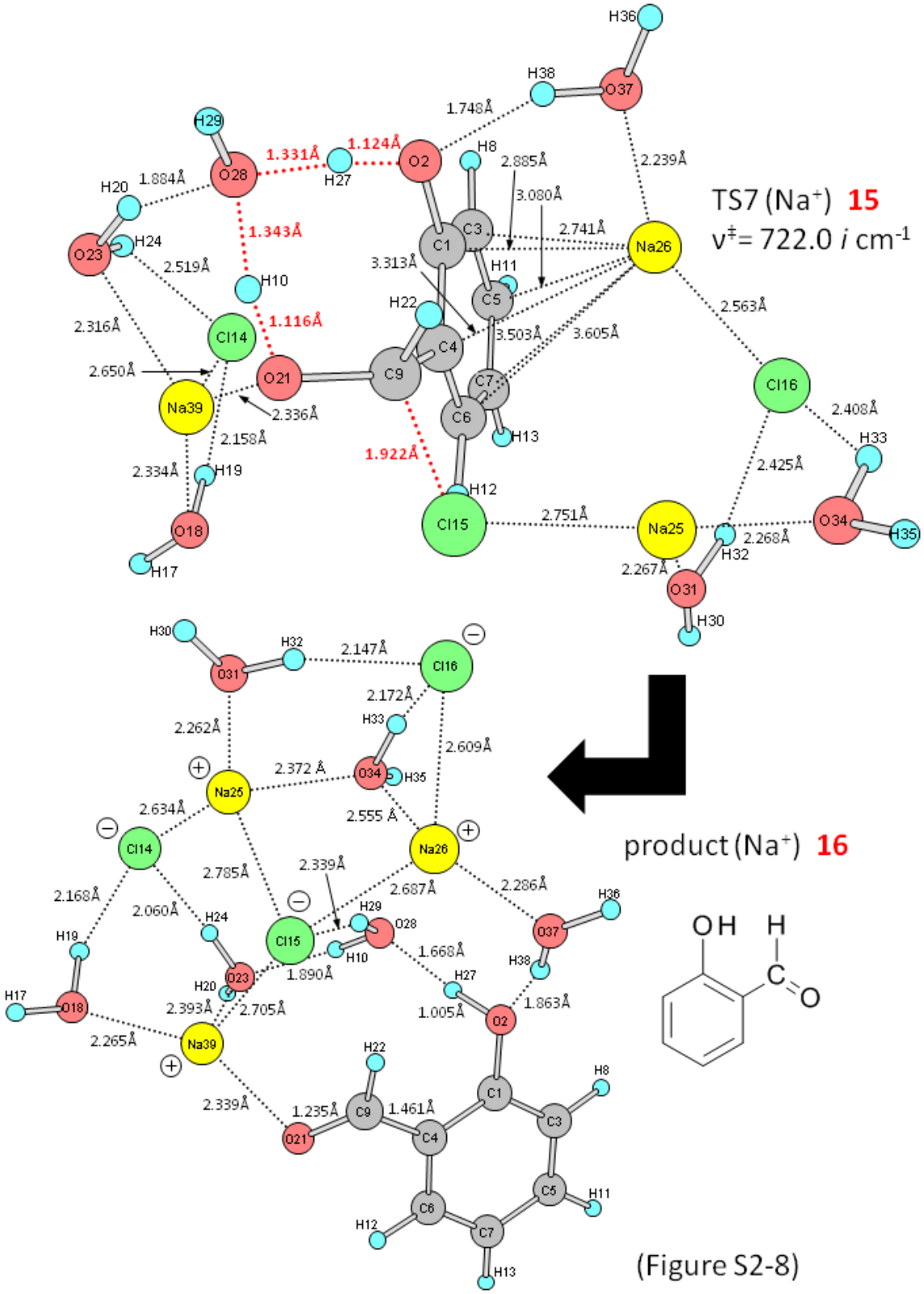

TS4 (Na⁺) 9
v‡= 184.5 i cm-1
Int5 (Na⁺) 10
H19
O18
H17
2.251Å
1.735Å
H8
2.245Å
Na39
O2
C3
2.966Å
2.195Å
H11
C1
C5
O28
H29
H27
1.530Å
2.327Å
2.731Å
2.518Å
O21
1.536Å
Cl16
Na25
H22
1.518Å
C4
C7
H10
1.223Å
H20
2.145Å
1.814Å
C9
C6
H13
2.350Å
2.308Å
H33
Cl15
2.560Å
O23
H24
O34
1.822Å
H12
Na26
H30
H35
Cl14
2.292Å
2.274Å
1.605Å
1.733Å
H38
2.621Å
O31
H36
O37
1.780Å
H32
H19
H17
1.795Å
O18
O28
H27
2.264Å
2.442Å
2.825Å
Cl16
2.262Å
Na25
H29
2.314Å
2.690Å
Na39
H33
O34
1.778Å
2.144Å
2.962Å
2.250Å
2.280Å
H8
H11
C3
C5
H24
O23
H20
O21
2.599Å
O2
1.496Å
2.736Å
H10
C1
Na26
H35
2.784Å
1.523Å
C7
2.236Å
3.270Å
3.069Å
H13
1.871Å
H30
2.652Å
3.301Å
C4
H22
O31
1.765Å
H36
C6
C9
O37
Cl14
1.896Å
H12
H32
H38
2.491Å
Cl15
O
H
C
Cl
Cl

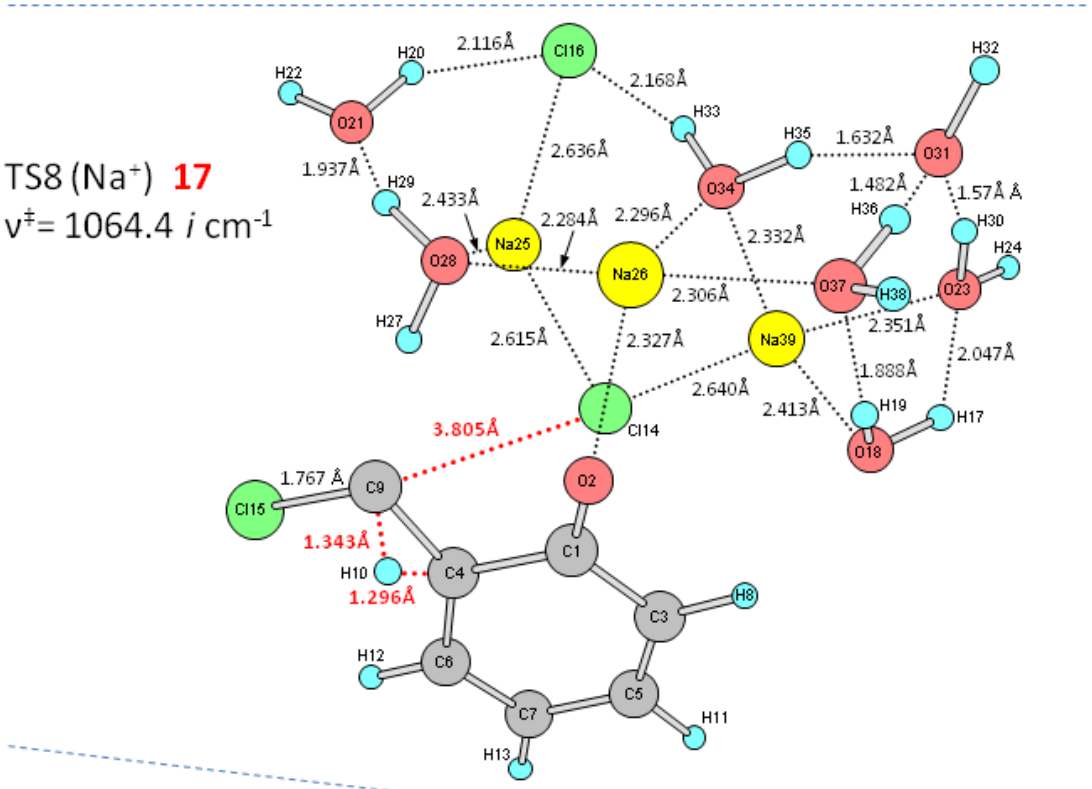
(Figure S2-5)

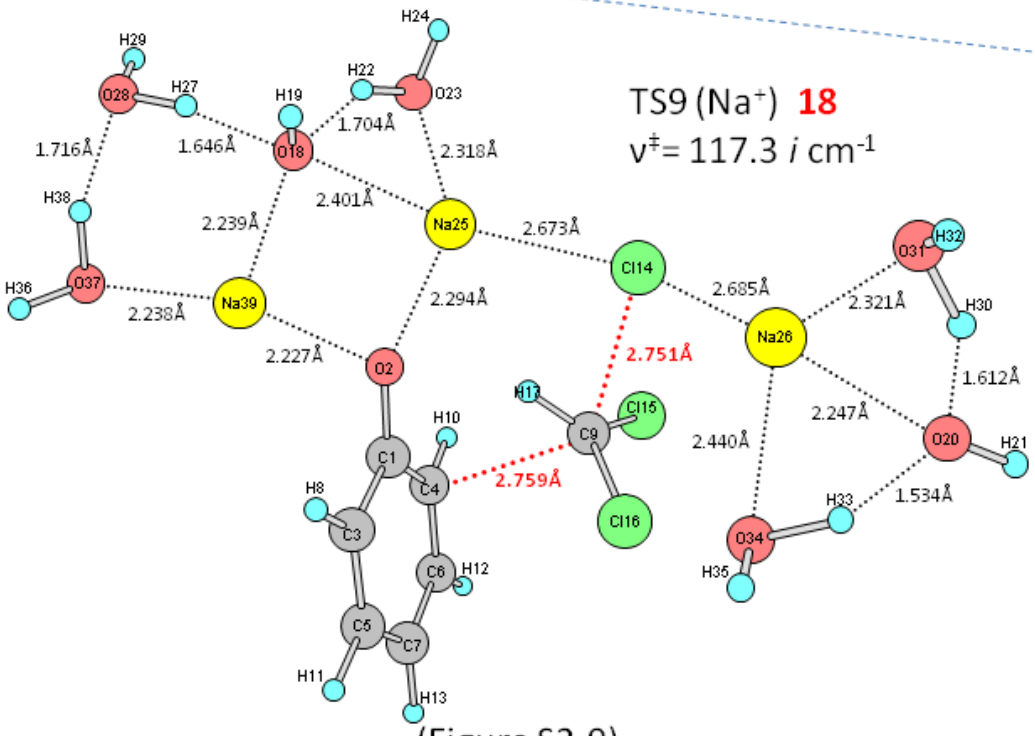


(Figure S2-6)


TS6 (Na⁺) 13
ν‡= 328.2 i cm-1
Int7 (Na⁺) 14
(Figure S2-7)

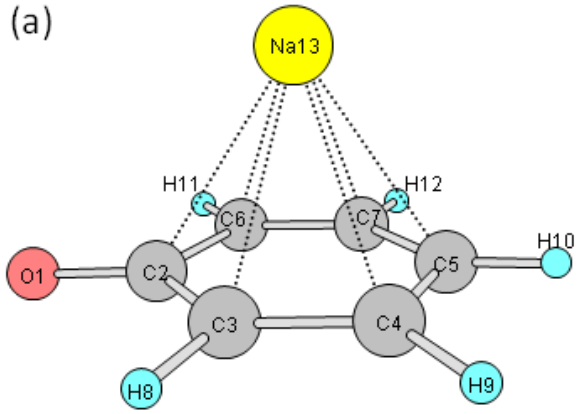

TS7 (Na⁺) 15
v‡= 722.0 i cm-1
product (Na⁺) 16
OH H
C=O
(Figure S2-8)


TS8 (Na+) 17
v‡= 1064.4 i cm-1
2.116Å
2.168Å
1.937Å
2.636Å
2.433Å
2.284Å
2.296Å
1.632Å
1.482Å
1.57Å Å
2.332Å
2.306Å
2.615Å
2.327Å
2.640Å
2.351Å
1.888Å
2.047Å
2.413Å
3.805Å
1.767 Å
1.343Å
1.296Å
Cl16
O21
H20
H22
H29
O28
H27
Na25
Na26
H33
H35
O34
O31
H32
H36
H30
H24
O37
H38
O23
Na39
O18
H19
H17
Cl14
Cl15
C9
O2
C1
C4
H10
C3
H8
H12
C6
C5
C7
H11
H13


TS9 (Na+) 18
v‡= 117.3 i cm-1
1.716Å
1.646Å
1.704Å
2.318Å
2.401Å
2.239Å
2.673Å
2.238Å
2.294Å
2.227Å
2.751Å
2.685Å
2.321Å
1.612Å
2.247Å
2.440Å
2.759Å
1.534Å
H29
O28
H27
H19
O18
H22
H24
O23
H38
H36
O37
Na39
Na25
Cl14
O31
H32
H30
Na26
O20
H21
H33
O34
H35
H17
Cl15
C9
Cl16
H10
C1
C4
H8
C3
C6
H12
C5
C7
H11
H13
O2

(Figure S2-9)

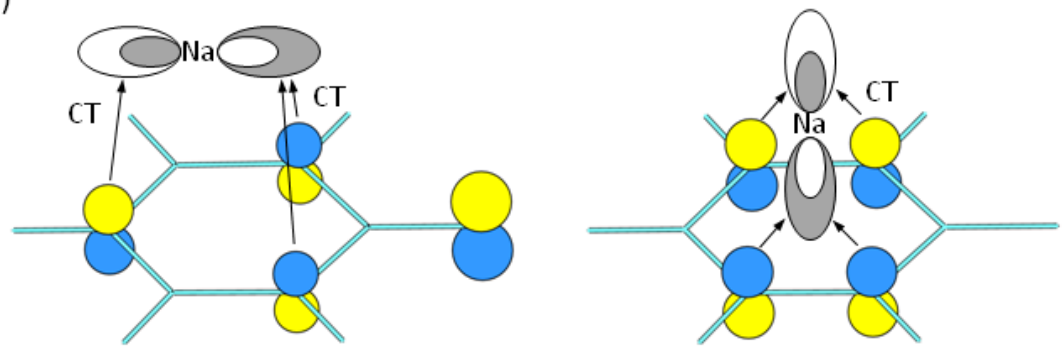
(a)



ΔE = a) +125.76 kcal/mol
b) +118.52 kcal/mol
c) +118.93 kcal/mol

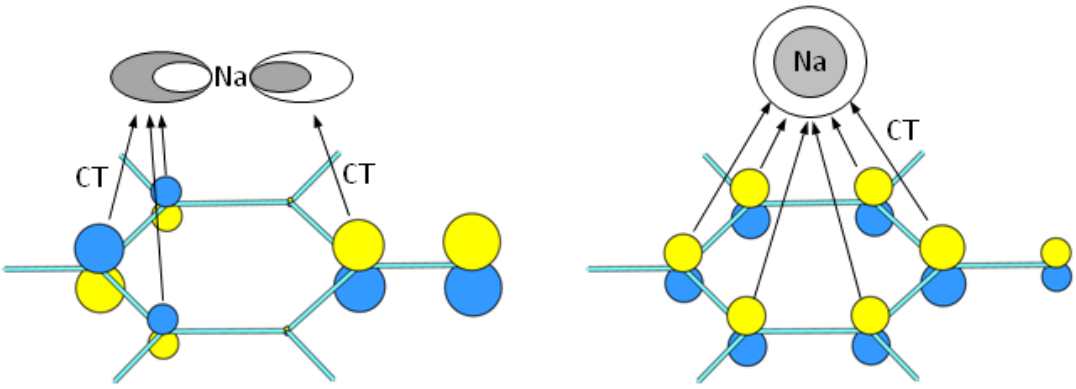
a) B3LYP/6-31(+)G(d) // B3LYP/6-31(+)G(d)
b) B3LYP/6-311+G(d,p) // B3LYP/6-31(+)G(d)
c) B3PW91/6-311++G(2df,2p) // B3LYP/6-31(+)G(d)

(b)



occupied MO no. 25 (HOMO)
eigenvalue: 2.121 eV; symmetry: A

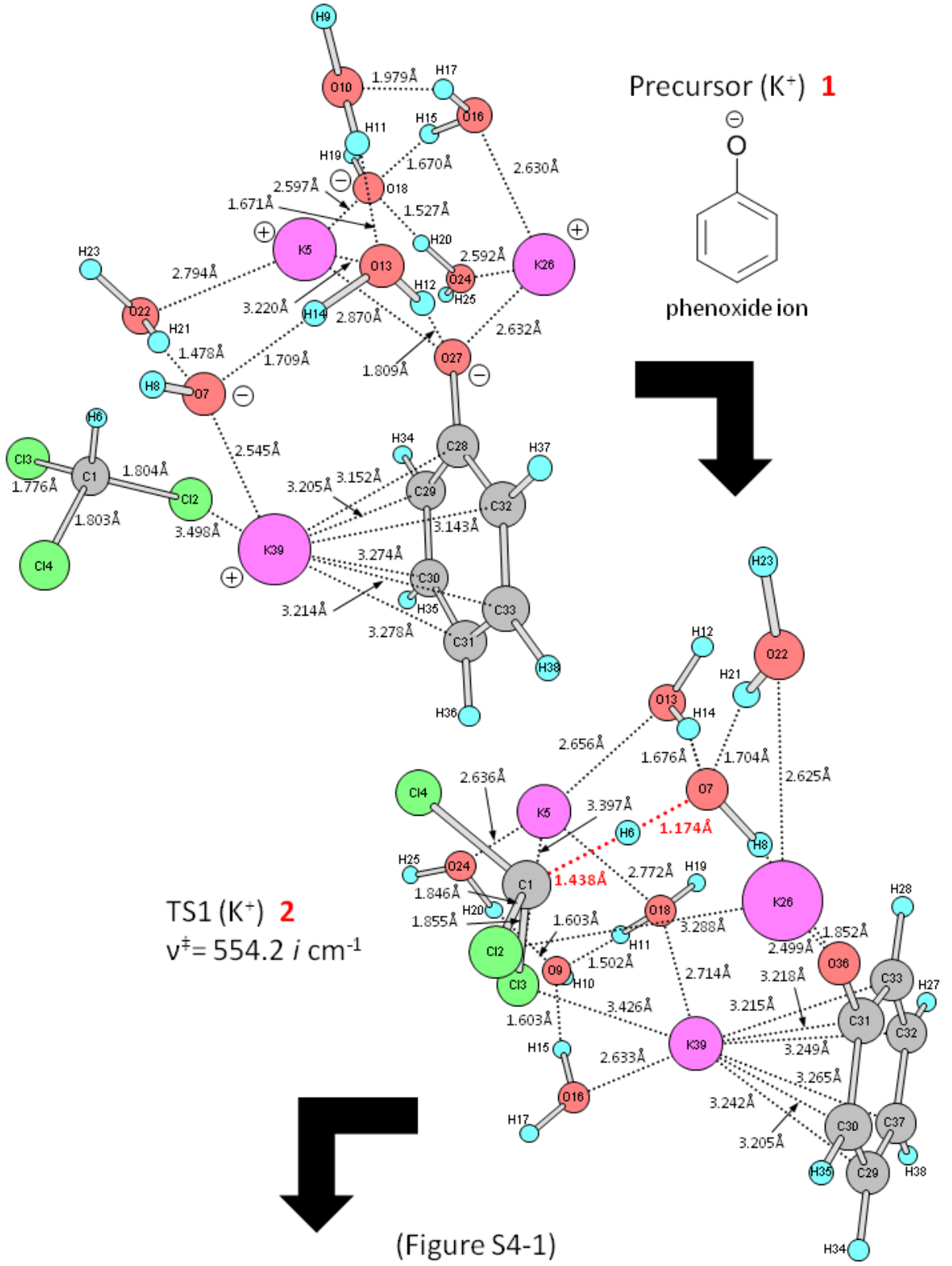
occupied MO no. 23 (HOMO-2)
eigenvalue: -1.995 eV; symmetry: A



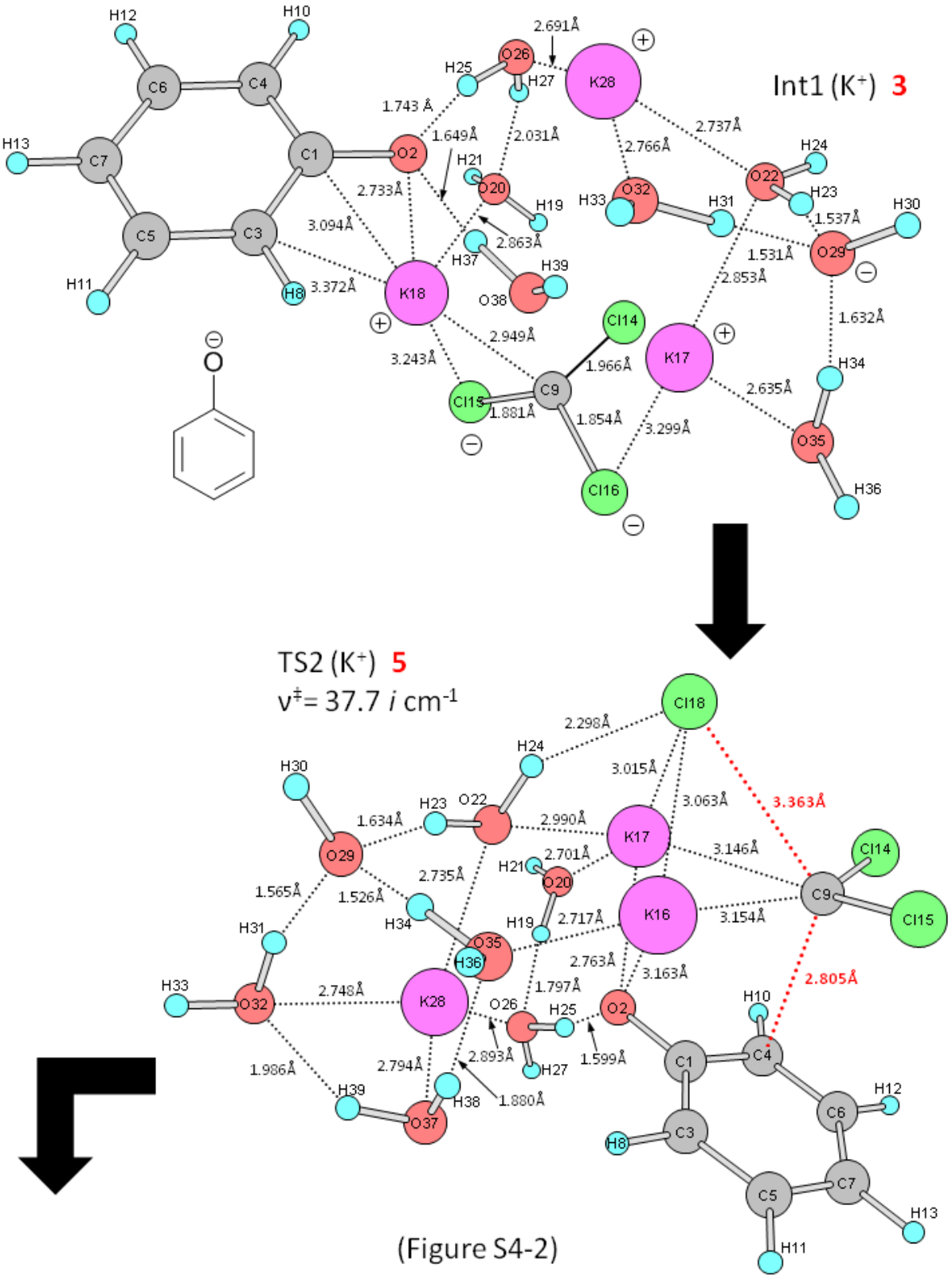
occupied MO no. 22 (HOMO-3)
eigenvalue: -3.630 eV; symmetry: A

occupied MO no. 19 (HOMO-6)
eigenvalue: -6.667 eV; symmetry: A

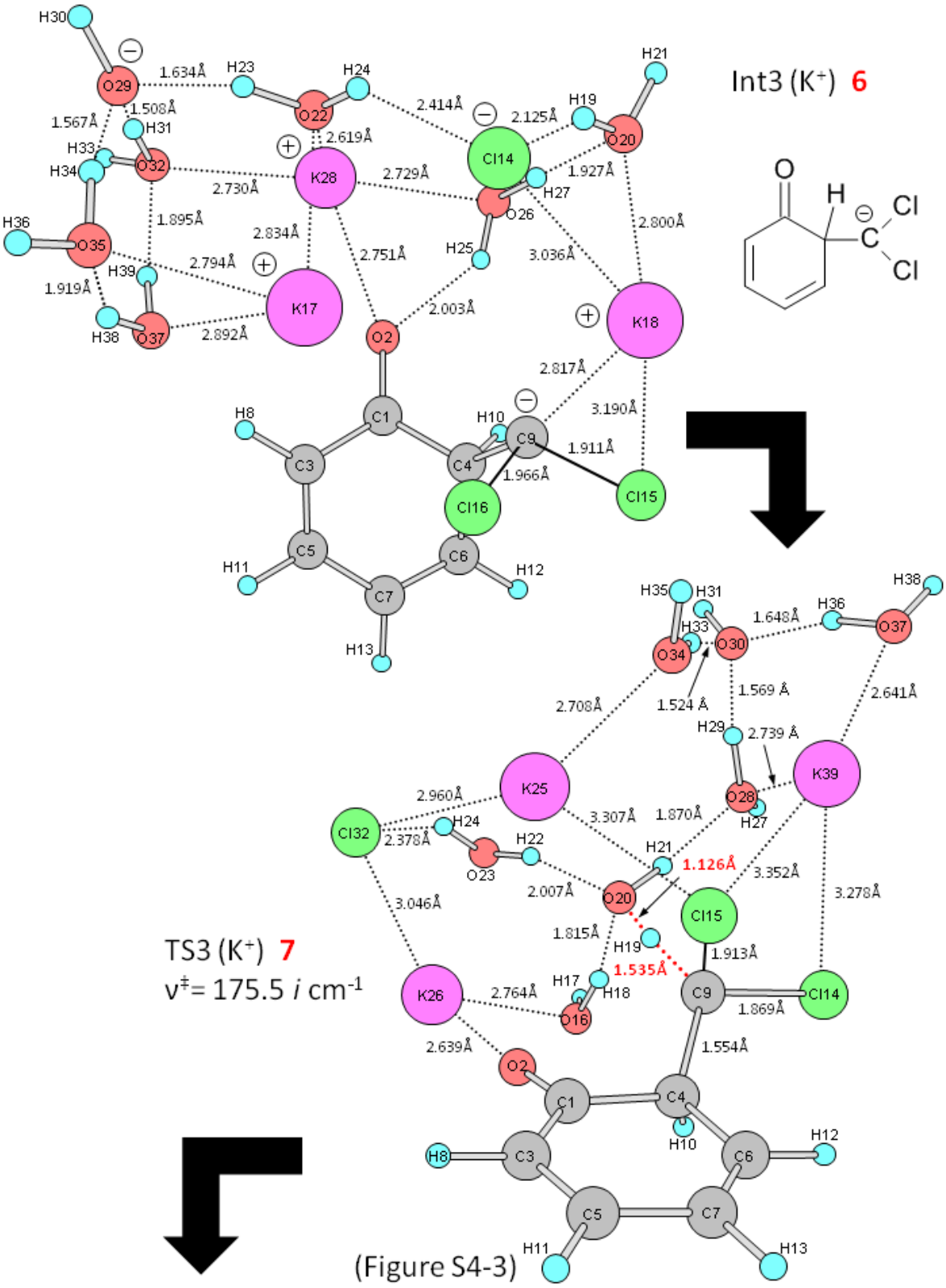
(Figure S3)

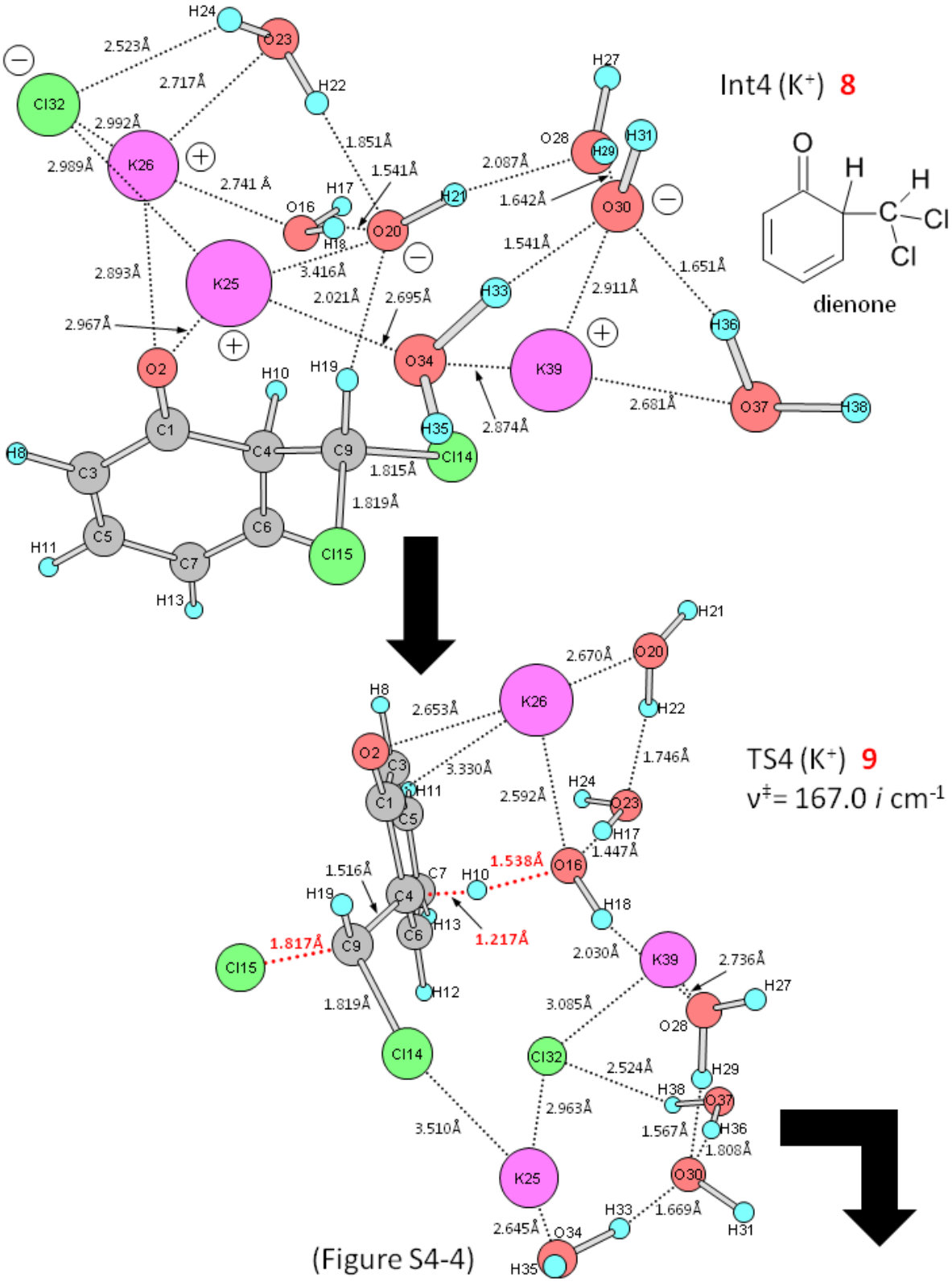


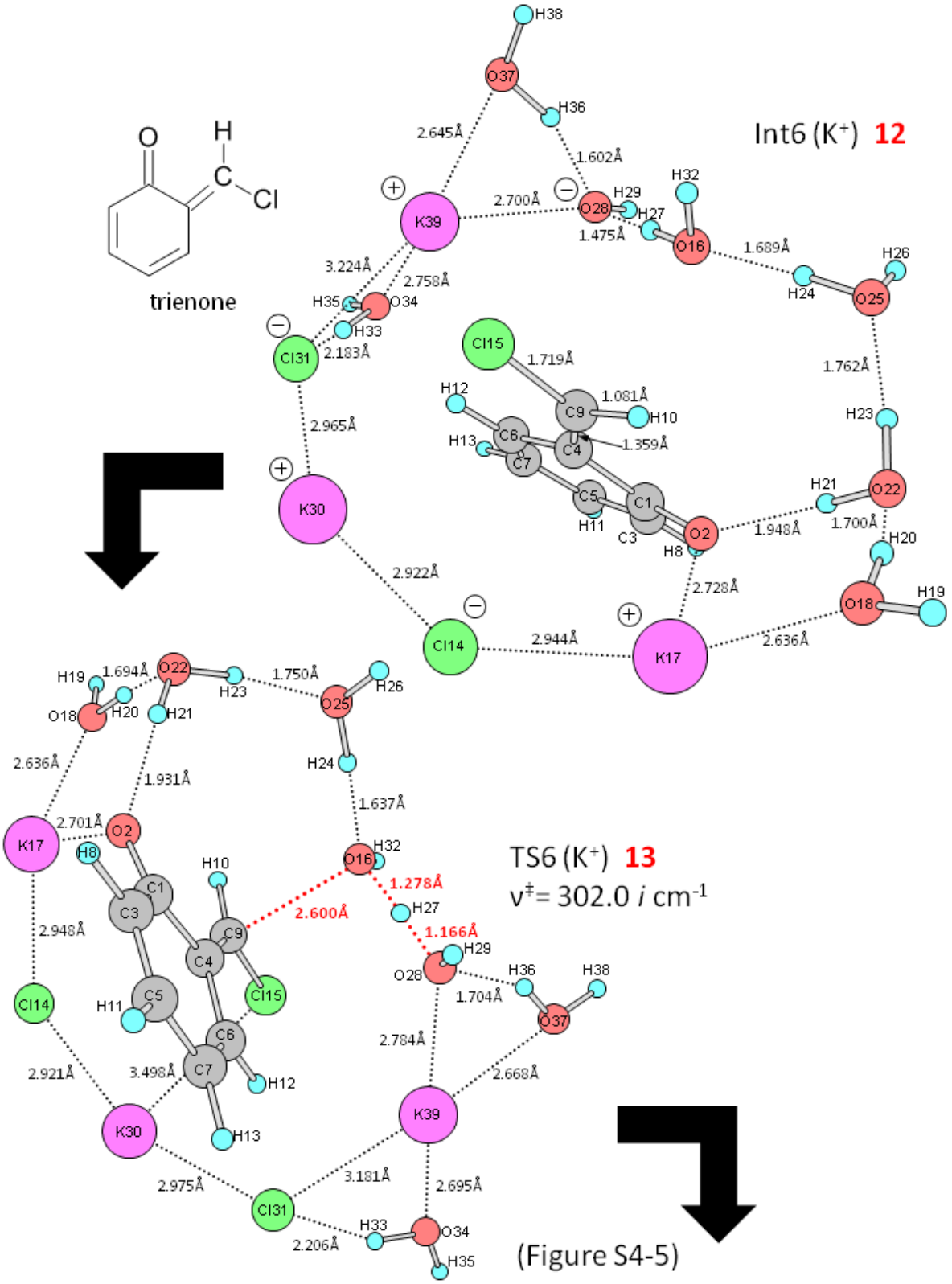
(Figure S4-1)

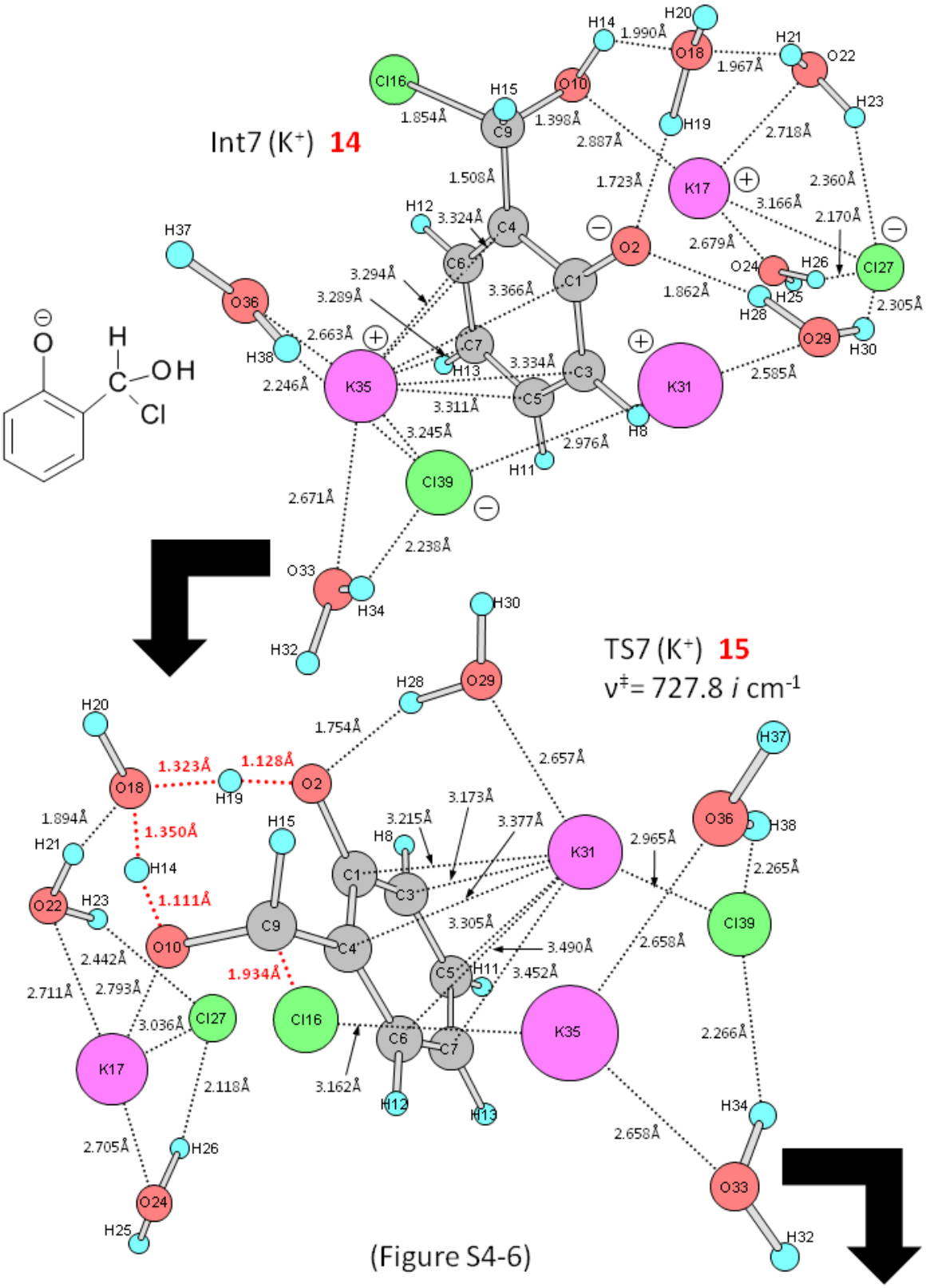

Int1 (K⁺) 3
TS2 (K⁺) 5
ν‡= 37.7 i cm-1
2.691Å
1.743 Å
1.649Å
2.031Å
2.737Å
2.766Å
2.733Å
3.094Å
2.863Å
1.537Å
1.531Å
2.853Å
1.632Å
3.372Å
2.949Å
3.243Å
1.966Å
1.881Å
1.854Å
3.299Å
2.635Å
2.298Å
3.015Å
3.063Å
3.363Å
1.634Å
2.990Å
3.146Å
2.701Å
2.735Å
1.565Å
1.526Å
2.717Å
3.154Å
2.763Å
3.163Å
2.805Å
2.748Å
1.797Å
1.599Å
2.893Å
2.794Å
1.880Å
1.986Å
H12
H10
C6
C4
H13
C7
C1
O2
H25
O26
H27
K28
H24
O22
H23
H30
O29
H21
O20
H19
H33
O32
H31
C5
C3
H11
H8
K18
O38
H37
H39
Cl14
K17
H34
Cl15
C9
O35
Cl16
H36
Cl18
K16
H38
O37
C1
C4
H10
H12
C6
C3
H8
C5
C7
H13
H11

(Figure S4-2)


Int3 (K⁺) 6
TS3 (K⁺) 7
v‡= 175.5 i cm-1
(Figure S4-3)


Int4 (K⁺) 8
dienone
TS4 (K⁺) 9
v‡= 167.0 i cm-1
(Figure S4-4)


trienone
Int6 (K⁺) 12
TS6 (K⁺) 13
ν‡= 302.0 i cm-1
(Figure S4-5)


Int7 (K⁺) 14
TS7 (K⁺) 15
v‡= 727.8 i cm-1
O
H
C
OH
Cl
H14
H20
1.990Å
O18
H21
O22
1.967Å
Cl16
H15
1.854Å
O10
1.398Å
C9
2.887Å
H19
2.718Å
H23
1.508Å
1.723Å
K17
2.360Å
3.166Å
2.170Å
H12
3.324Å
C4
O2
2.679Å
H37
C6
O24
H26
Cl27
3.294Å
3.289Å
3.366Å
C1
1.862Å
H25
2.305Å
O36
H28
2.663Å
C7
O29
H30
H38
3.334Å
C3
2.585Å
2.246Å
K35
H13
C5
K31
3.311Å
3.245Å
H8
2.976Å
H11
Cl39
2.671Å
2.238Å
O33
H34
H32
H30
H28
O29
1.754Å
2.657Å
H20
1.323Å
1.128Å
O18
H19
O2
H37
3.173Å
1.894Å
1.350Å
H15
3.215Å
3.377Å
O36
H21
H8
K31
2.965Å
H38
H14
C1
2.265Å
O22
H23
1.111Å
C3
Cl39
C9
3.305Å
3.490Å
2.658Å
O10
C4
2.442Å
C5
H11
3.452Å
1.934Å
2.711Å
2.793Å
Cl27
Cl16
K35
2.266Å
3.036Å
C6
C7
K17
2.118Å
3.162Å
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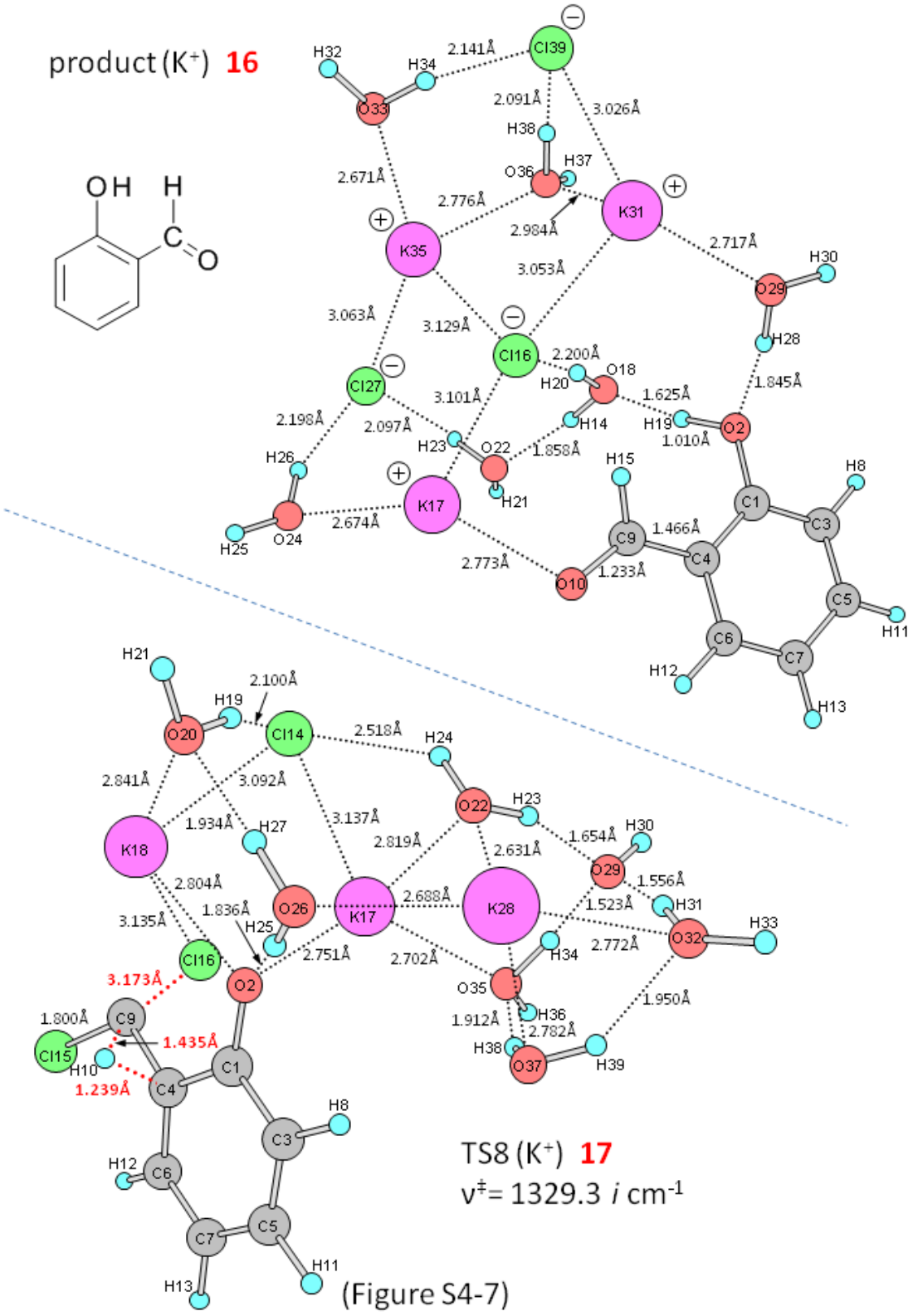
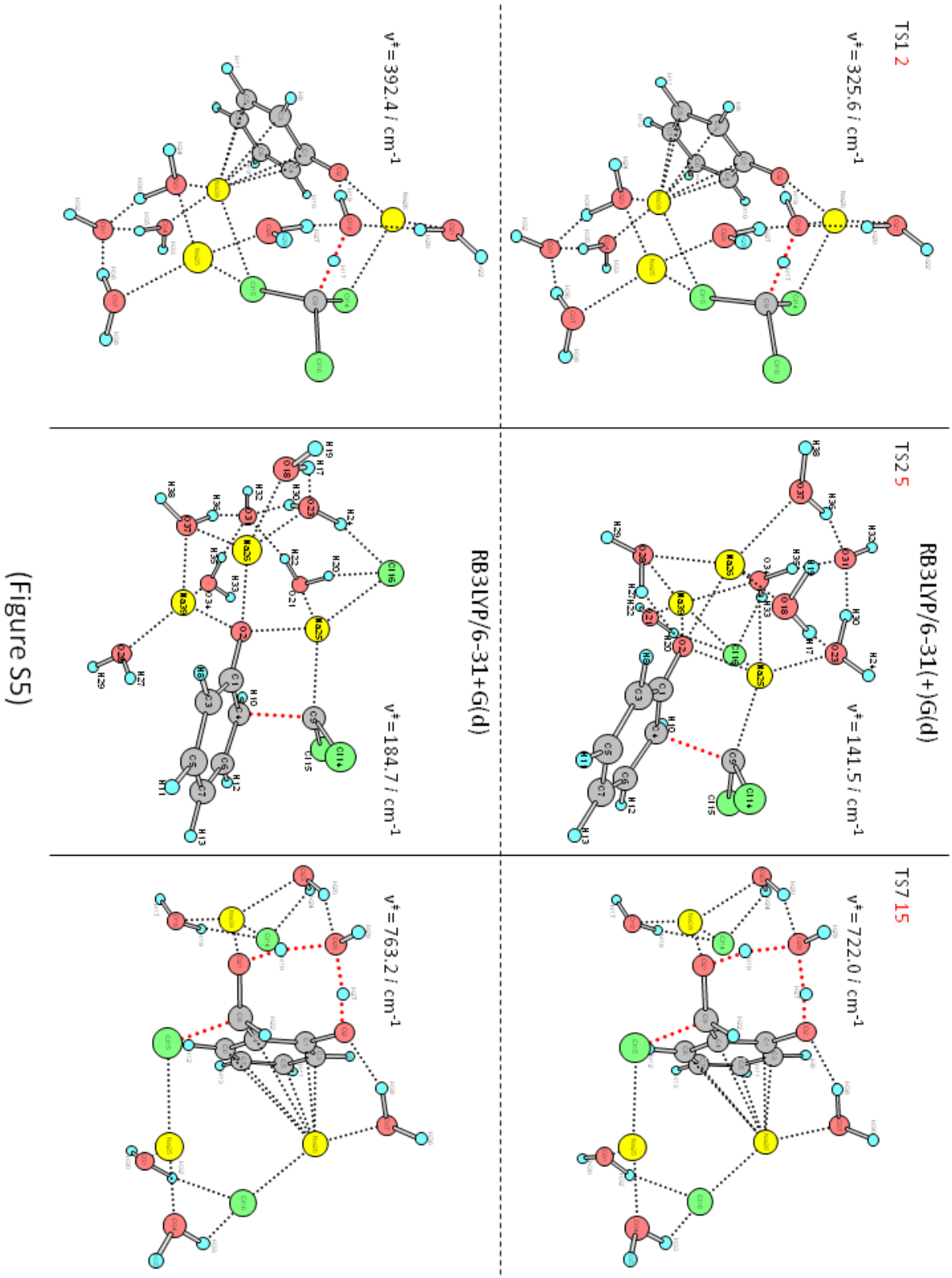
H13
H34
2.658Å
2.705Å
H26
O24
O33
H25
H32

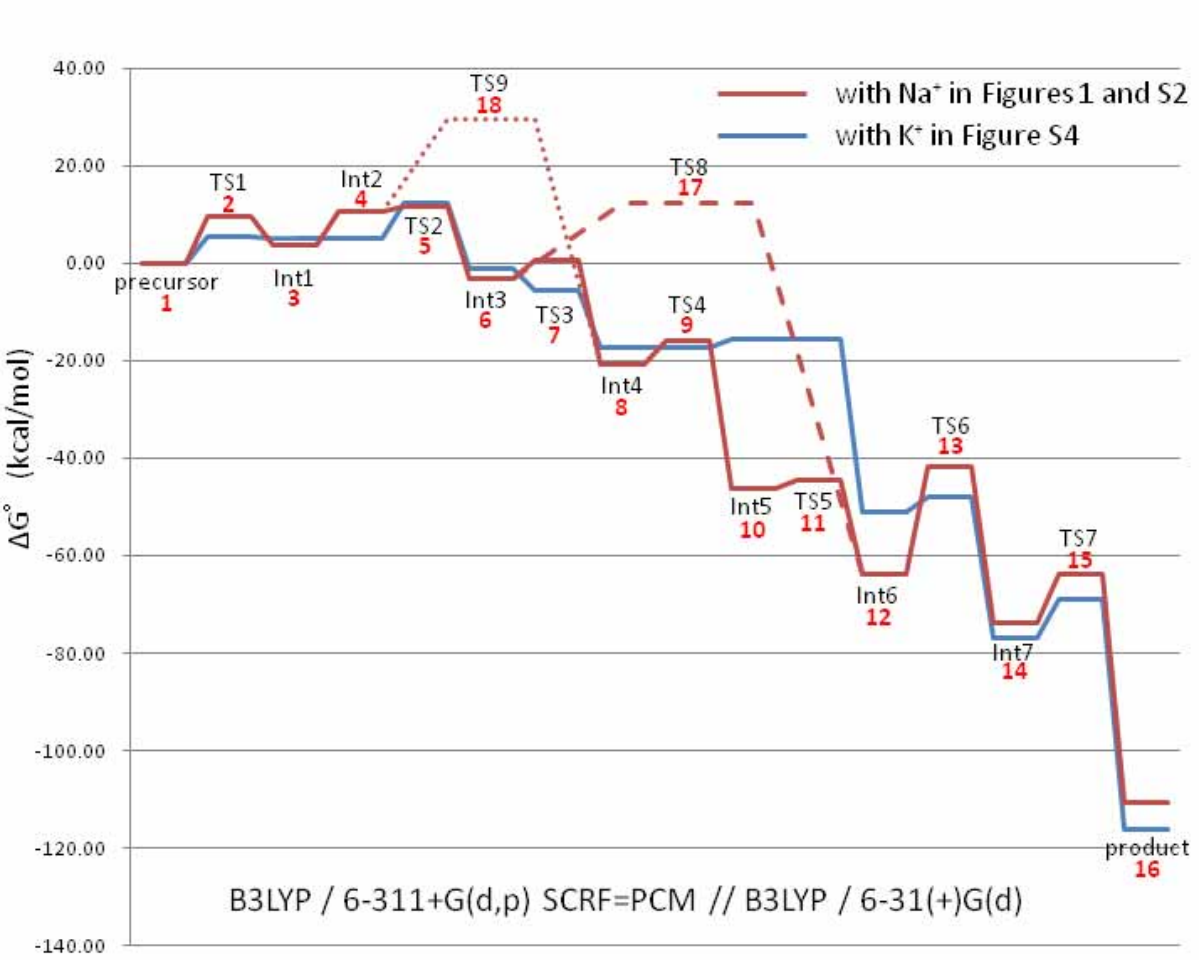
(Figure S4-6)



(Figure S4-7)


RB3LYP/6-31(+)G(d)
RB3LYP/6-31+G(d)
TS1 2
TS2 5
TS7 15
ν‡= 325.6 i cm-1
ν‡= 392.4 i cm-1
ν‡= 141.5 i cm-1
ν‡= 184.7 i cm-1
ν‡= 722.0 i cm-1
ν‡= 763.2 i cm-1

(Figure S5)



(Figure S6)

	precursor 1	TS1 2	Int1 3	Int2 4	TS2 5	Int3 6	TS3 7	Int4 8	TS4 9
Na^+	0.00	9.59 [9.43]	3.84 [4.70]	10.61 [6.45]	11.69 [9.29]	-3.28 [-3.63]	0.62 [0.21]	-20.82 [-22.08]	-16.03 [-15.84]
K^+	0.00	5.27	5.05		12.30 [11.38]	-0.94	-5.57	-17.48	-15.60
	Int5 10	**TS5 11**	**Int6 12**	**TS6 13**	**Int7 14**	**TS7 15**	**product 16**	**TS8 17**	**TS9 18**
Na^+	-46.15 [-46.64]	-44.60 [-45.72]	-63.90 [-6230]	-41.91 [-42.22]	-73.76 [-74.01]	-63.75 [-63.48]	-110.80 [-113.83]	12.34 [12.36]	29.58 [29.54]
K^+			-51.02	-48.09	-76.97	-69.00	-116.24		

(Table S1)

=Figure 1=

RB3LYP/6-31(+)G(d)
precursor in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.step0revna.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.359715	-0.967891	-0.254296
2	17	0	3.690867	0.799156	0.024753
3	17	0	3.191018	-1.298343	-1.996059
4	17	0	4.648053	-1.955355	0.482568
5	11	0	-1.463993	-1.511812	0.349476
6	1	0	2.414977	-1.204163	0.244185
7	8	0	0.659181	0.511653	2.642383
8	1	0	1.102250	0.458610	3.500740
9	1	0	-2.813233	-2.652743	3.024731
10	8	0	-2.774559	-1.998422	2.312626
11	1	0	-2.547369	-1.109271	2.730919
12	1	0	-2.277441	0.752815	1.966952
13	8	0	-2.055881	0.466098	2.884579
14	1	0	-1.056321	0.514701	2.915856
15	1	0	-3.902191	-2.334502	-0.479237
16	8	0	-4.606635	-1.851501	0.060748
17	1	0	-4.299438	-1.945249	0.982679
18	8	0	-2.484437	-2.481513	-1.365499
19	1	0	-2.303138	-3.369652	-1.702897
20	1	0	-2.900460	-1.529609	-2.521481
21	1	0	0.717805	-0.769125	1.909380
22	8	0	0.696431	-1.573679	1.224271
23	1	0	0.870437	-2.375491	1.740216
24	8	0	-3.288947	-0.716236	-3.034389
25	1	0	-3.667780	-1.044765	-3.860749
26	11	0	-3.998262	0.026432	-1.044169
27	8	0	-2.252786	0.769477	0.114318
28	6	0	-1.425035	1.724320	-0.251589
29	6	0	-0.482460	1.539187	-1.306103
30	6	0	0.425864	2.541642	-1.654673
31	6	0	0.450620	3.767219	-0.970946
32	6	0	-1.395827	2.984864	0.415990
33	6	0	-0.482472	3.978933	0.056601
34	1	0	-0.505256	0.601362	-1.856325
35	1	0	1.122082	2.364123	-2.471049
36	1	0	1.147292	4.549040	-1.258519
37	1	0	-2.108126	3.157248	1.218657
38	1	0	-0.499901	4.931143	0.583034
39	11	0	1.067301	1.877752	1.032809

SCF Done: E(RB+HF-LYP) = -2747.15905882 A.U. after 1 cycles
Zero-point correction= 0.267324 (Hartree/Particle)
Thermal correction to Energy= 0.300651

Thermal correction to Enthalpy= 0.301595
Thermal correction to Gibbs Free Energy= 0.197462
Sum of electronic and zero-point Energies= -2746.891734
Sum of electronic and thermal Energies= -2746.858408
Sum of electronic and thermal Enthalpies= -2746.857464
Sum of electronic and thermal Free Energies= -2746.961597

TS1 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts1na.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.004053	-0.966187	-0.717165
2	17	0	2.750667	0.177091	-1.994987
3	17	0	0.243935	-1.271636	-1.271936
4	17	0	2.878827	-2.543382	-0.829214
5	11	0	-0.826878	-2.430382	1.217422
6	1	0	2.005045	-0.372185	0.633125
7	8	0	2.004618	0.096046	1.680233
8	1	0	1.429362	0.896024	1.589243
9	8	0	-3.957062	-2.385759	-0.127360
10	1	0	-4.885929	-2.551207	0.088669
11	1	0	-3.269293	-1.482847	0.762832
12	1	0	1.122944	-2.316313	3.514955
13	8	0	0.629625	-1.862321	2.818067
14	1	0	1.201512	-1.092522	2.508564
15	1	0	-3.691336	-1.353300	-1.333998
16	8	0	-3.347087	-0.569735	-1.884162
17	1	0	-3.262238	-0.872171	-2.798474
18	8	0	-2.527783	-0.856847	1.213359
19	1	0	-2.858999	-0.559146	2.073080
20	1	0	-2.932268	-3.585701	0.162655
21	1	0	3.598092	0.745034	1.867631
22	8	0	4.345076	1.361984	1.615658
23	1	0	5.176692	0.882539	1.732667
24	8	0	-2.109125	-4.109208	0.456785
25	1	0	-1.965130	-4.807358	-0.196577
26	11	0	2.959553	2.144240	0.020690
27	1	0	-3.356206	3.088434	1.919063
28	1	0	-0.993112	2.524799	2.417357
29	6	0	-2.064005	3.389276	-1.210122
30	6	0	-0.733105	3.064409	-0.937239
31	6	0	-0.292621	2.749359	0.385854
32	6	0	-2.625398	3.078012	1.112438
33	6	0	-1.298832	2.755132	1.399709
34	1	0	-2.352075	3.637554	-2.229772
35	1	0	0.006217	3.065203	-1.735129
36	8	0	0.947438	2.450511	0.651589
37	6	0	-3.030968	3.393464	-0.193807
38	1	0	-4.062990	3.652425	-0.409582
39	11	0	-2.168941	0.701354	-0.452962

SCF Done: E(RB+HF-LYP) = -2747.13199000 A.U. after 1 cycles
Zero-point correction= 0.260518 (Hartree/Particle)
Thermal correction to Energy= 0.294471
Thermal correction to Enthalpy= 0.295415
Thermal correction to Gibbs Free Energy= 0.190242
Sum of electronic and zero-point Energies= -2746.871472
Sum of electronic and thermal Energies= -2746.837519
Sum of electronic and thermal Enthalpies= -2746.836575
Sum of electronic and thermal Free Energies= -2746.941748

Int1 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.k1na.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.384770	-0.249064	-0.123189
2	8	0	2.098899	-0.185044	0.279307
3	6	0	3.712405	-0.656446	-1.432651
4	6	0	4.439300	0.091292	0.747616
5	6	0	5.041408	-0.720022	-1.850732
6	6	0	5.765073	0.023332	0.320861
7	6	0	6.078902	-0.381539	-0.979097
8	1	0	2.905768	-0.916275	-2.116580
9	6	0	-1.931077	-1.918871	-0.233669
10	1	0	4.198923	0.409571	1.759461
11	1	0	5.266012	-1.036367	-2.866986
12	1	0	6.560675	0.291633	1.012451
13	1	0	7.113386	-0.432263	-1.306745
14	17	0	-3.042038	-2.036635	1.293169
15	17	0	-1.208514	-3.661111	-0.440529
16	17	0	-3.115011	-1.716230	-1.662636
17	11	0	-1.852824	0.694719	-1.033025
18	11	0	0.541760	-1.688902	0.434504
19	1	0	-1.123013	-1.880727	2.584896
20	8	0	-0.154668	-1.774933	2.701005
21	1	0	0.107687	-2.432296	3.364088
22	8	0	-2.424690	1.991374	0.791070
23	1	0	-2.630612	2.898822	0.282904
24	1	0	-3.158763	1.807974	1.394539
25	1	0	1.587688	0.552761	1.729288
26	8	0	1.000882	0.968231	2.427576
27	1	0	0.594869	0.212082	2.884942
28	11	0	-0.189358	2.531751	1.289422
29	8	0	-2.504035	4.073101	-0.594388
30	1	0	-3.289577	4.636433	-0.641024
31	1	0	-1.258905	4.666932	0.239926
32	8	0	-0.450123	4.724481	0.854381
33	1	0	0.094962	5.463200	0.551792
34	1	0	-2.139372	3.209071	-1.885838
35	8	0	-1.832217	2.450472	-2.499448

36	1	0	-2.174318	2.639862	-3.384106
37	1	0	1.138572	0.834051	-0.486567
38	8	0	0.325769	1.399178	-0.722292
39	1	0	0.502022	1.892906	-1.538949

SCF Done: E(RB+HF-LYP) = -2747.14138951 A.U. after 1 cycles
Zero-point correction= 0.264199 (Hartree/Particle)
Thermal correction to Energy= 0.298761
Thermal correction to Enthalpy= 0.299705
Thermal correction to Gibbs Free Energy= 0.192263
Sum of electronic and zero-point Energies= -2746.877190
Sum of electronic and thermal Energies= -2746.842628
Sum of electronic and thermal Enthalpies= -2746.841684
Sum of electronic and thermal Free Energies= -2746.949127

Int2 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts2na10.g09.reva.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.959063	-0.309018	1.462385
2	8	0	0.289508	0.041117	1.145092
3	6	0	-1.269431	-1.618427	1.899090
4	6	0	-2.025218	0.625305	1.361990
5	6	0	-2.569758	-1.955022	2.257149
6	6	0	-3.323247	0.278588	1.759735
7	6	0	-3.607827	-1.009481	2.199922
8	1	0	-0.474889	-2.359800	1.926929
9	6	0	-2.403603	-0.026032	-1.380297
10	1	0	-1.794344	1.638722	1.042975
11	1	0	-2.783561	-2.969197	2.586744
12	1	0	-4.112602	1.023917	1.701301
13	1	0	-4.616229	-1.283310	2.495654
14	17	0	-3.182145	-1.577864	-1.280511
15	17	0	-3.573472	1.212610	-1.780802
16	17	0	0.764363	2.957321	-1.331545
17	11	0	0.110294	0.328913	-1.203426
18	11	0	1.686896	1.958662	1.100760
19	8	0	1.396541	4.208098	1.425708
20	1	0	1.110354	4.270307	0.484532
21	1	0	1.827477	5.045266	1.648915
22	8	0	2.820714	0.725548	-0.595976
23	1	0	3.255953	0.075151	-1.256788
24	1	0	2.519682	1.486780	-1.137963
25	1	0	1.278066	0.110465	2.512328
26	8	0	2.220022	0.289230	2.802796
27	1	0	2.266882	0.245474	3.768675
28	11	0	2.373976	-1.164765	0.857436
29	8	0	3.547653	-1.225706	-2.105553
30	1	0	4.128396	-1.123658	-2.872719
31	1	0	4.102828	-2.044026	-0.873285

32	8	0	4.165548	-2.449805	0.066034
33	1	0	5.104077	-2.557291	0.274601
34	1	0	2.061674	-1.428580	-2.386817
35	8	0	1.026043	-1.517767	-2.312406
36	1	0	0.704231	-1.868677	-3.155660
37	8	0	1.403782	-3.109055	-0.011043
38	1	0	1.106085	-2.772935	-0.885724
39	1	0	2.274798	-3.513421	-0.174634

SCF Done: E(RB3LYP) = -2747.13360683 A.U. after 1 cycles
Zero-point correction= 0.263791 (Hartree/Particle)
Thermal correction to Energy= 0.299107
Thermal correction to Enthalpy= 0.300051
Thermal correction to Gibbs Free Energy= 0.192964
Sum of electronic and zero-point Energies= -2746.869816
Sum of electronic and thermal Energies= -2746.834500
Sum of electronic and thermal Enthalpies= -2746.833556
Sum of electronic and thermal Free Energies= -2746.940643

TS2 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts2na10.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.102314	-0.224604	1.359298
2	8	0	0.146566	0.092629	1.103087
3	6	0	-1.444654	-1.407319	2.058093
4	6	0	-2.179898	0.608623	0.886671
5	6	0	-2.766720	-1.683475	2.368515
6	6	0	-3.509305	0.351559	1.321464
7	6	0	-3.811522	-0.798241	2.018592
8	1	0	-0.651856	-2.098912	2.331107
9	6	0	-2.228736	-0.067452	-1.189171
10	1	0	-1.916602	1.601130	0.532927
11	1	0	-3.003568	-2.601663	2.901046
12	1	0	-4.293745	1.043756	1.030188
13	1	0	-4.835005	-1.027024	2.298482
14	17	0	-2.869559	-1.731080	-1.189194
15	17	0	-3.466574	1.019249	-1.918058
16	17	0	0.924571	2.991252	-1.370402
17	11	0	0.240077	0.351937	-1.348184
18	11	0	1.600470	1.979531	1.092553
19	8	0	1.244343	4.209216	1.456226
20	1	0	1.050598	4.298915	0.494329
21	1	0	1.579253	5.063819	1.762576
22	8	0	2.799992	0.667435	-0.507501
23	1	0	3.296819	0.004002	-1.119251
24	1	0	2.615693	1.456853	-1.060904
25	1	0	1.095531	0.152245	2.570189
26	8	0	2.032795	0.331853	2.849580
27	1	0	2.080023	0.322986	3.816670

28	11	0	2.295676	-1.155697	0.960041
29	8	0	3.675295	-1.294000	-1.896259
30	1	0	4.326695	-1.197144	-2.605218
31	1	0	4.118437	-2.102036	-0.612837
32	8	0	4.103338	-2.490164	0.336285
33	1	0	5.020939	-2.633471	0.606941
34	1	0	2.201409	-1.501477	-2.315607
35	8	0	1.167343	-1.564355	-2.313802
36	1	0	0.891319	-1.949434	-3.158416
37	8	0	1.320769	-3.066853	0.074439
38	1	0	1.080259	-2.758548	-0.827666
39	1	0	2.177274	-3.518287	-0.030154

SCF Done: E(RB3LYP) = -2747.13221810 A.U. after 1 cycles
Zero-point correction= 0.263927 (Hartree/Particle)
Thermal correction to Energy= 0.298384
Thermal correction to Enthalpy= 0.299328
Thermal correction to Gibbs Free Energy= 0.194806
Sum of electronic and zero-point Energies= -2746.868291
Sum of electronic and thermal Energies= -2746.833835
Sum of electronic and thermal Enthalpies= -2746.832890
Sum of electronic and thermal Free Energies= -2746.937412

Int3 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts2naa.g09.fora.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.200951	-1.145931	-0.055633
2	8	0	-0.283067	-0.266710	-0.072833
3	6	0	-1.119317	-2.343792	-0.826215
4	6	0	-2.439740	-0.884844	0.767575
5	6	0	-2.122484	-3.277898	-0.766959
6	6	0	-3.411124	-2.005046	0.825731
7	6	0	-3.282286	-3.116033	0.059702
8	1	0	-0.240012	-2.496696	-1.445683
9	6	0	-3.075672	0.490360	0.215026
10	1	0	-2.134044	-0.588526	1.779624
11	1	0	-2.035614	-4.180801	-1.367747
12	1	0	-4.284424	-1.857210	1.453409
13	1	0	-4.041977	-3.891765	0.062206
14	17	0	-3.833609	0.148905	-1.467948
15	17	0	-4.452075	0.950394	1.359873
16	17	0	0.935183	2.813070	-1.666439
17	11	0	1.569363	0.230843	-1.368545
18	11	0	-1.267909	2.004051	-0.314475
19	8	0	0.112107	3.275285	1.232293
20	1	0	-0.027811	4.142832	1.641620
21	1	0	0.636171	3.419968	0.403197
22	8	0	3.381567	1.115288	-0.147907
23	1	0	4.187886	0.650882	-0.570977

24	1	0	3.292160	2.015939	-0.500437
25	1	0	0.455425	0.313400	1.575470
26	8	0	1.021139	0.754727	2.245060
27	1	0	0.802563	1.702469	2.135954
28	11	0	3.096893	-0.062328	1.794255
29	8	0	5.077218	-0.608025	-0.957907
30	1	0	5.845545	-0.479279	-1.531742
31	1	0	5.330377	-0.944411	0.580589
32	8	0	5.186842	-1.098859	1.583476
33	1	0	6.059405	-1.138910	1.999686
34	1	0	3.875765	-1.267275	-1.575717
35	8	0	2.904271	-1.602424	-1.793908
36	1	0	2.973827	-2.255363	-2.505375
37	8	0	2.670455	-2.215700	0.955733
38	1	0	2.636923	-2.221423	-0.026322
39	1	0	3.589709	-2.461883	1.167980

SCF Done: E(RB3LYP) = -2747.15306464 A.U. after 1 cycles
Zero-point correction= 0.266558 (Hartree/Particle)
Thermal correction to Energy= 0.300554
Thermal correction to Enthalpy= 0.301498
Thermal correction to Gibbs Free Energy= 0.198465
Sum of electronic and zero-point Energies= -2746.886507
Sum of electronic and thermal Energies= -2746.852511
Sum of electronic and thermal Enthalpies= -2746.851567
Sum of electronic and thermal Free Energies= -2746.954600

TS3 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts3naa3.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.907748	1.194062	0.696539
2	8	0	0.744251	0.984062	1.135033
3	6	0	2.342795	2.487460	0.255150
4	6	0	2.879767	0.031841	0.627000
5	6	0	3.652655	2.693792	-0.080380
6	6	0	4.294868	0.402627	0.342957
7	6	0	4.648181	1.654650	-0.023482
8	1	0	1.617545	3.296066	0.229460
9	6	0	2.288330	-1.052507	-0.390583
10	1	0	2.832304	-0.488144	1.593812
11	1	0	3.962568	3.687631	-0.396084
12	1	0	5.019648	-0.405664	0.362273
13	1	0	5.672577	1.893605	-0.292197
14	17	0	3.195082	-2.640564	-0.012333
15	17	0	2.723900	-0.552062	-2.112094
16	8	0	-2.243191	-0.014718	0.480013
17	1	0	-2.802386	-0.760883	0.861164
18	1	0	-1.599643	-0.514242	-0.097669
19	1	0	0.650892	-1.400533	-0.682073

20	8	0	-0.393322	-1.509758	-0.695771
21	1	0	-0.695314	-2.386279	-1.009595
22	1	0	-2.256497	4.733811	2.205072
23	8	0	-1.917702	4.102794	1.554568
24	1	0	-2.425481	4.230961	0.721024
25	11	0	-3.602483	0.652720	-1.322406
26	11	0	-1.286303	2.042123	0.783064
27	1	0	-1.357594	-3.268568	3.217742
28	8	0	-1.390090	-2.446840	2.709269
29	1	0	-2.225765	-2.484801	2.125928
30	8	0	-3.420568	-2.311009	1.040297
31	1	0	-4.226667	-2.522095	1.535626
32	17	0	-2.784158	3.089976	-1.227976
33	1	0	-4.095418	-1.829220	-0.490628
34	8	0	-4.321480	-1.488936	-1.405294
35	1	0	-3.937280	-2.164490	-1.988379
36	1	0	-2.677281	-3.354954	-0.143242
37	8	0	-2.216134	-3.656930	-0.975854
38	1	0	-2.113410	-4.617425	-0.913311
39	11	0	0.029242	-1.207626	1.525763

SCF Done: E(RB3LYP) = -2747.14331184 A.U. after 1 cycles
Zero-point correction= 0.265886 (Hartree/Particle)
Thermal correction to Energy= 0.299536
Thermal correction to Enthalpy= 0.300480
Thermal correction to Gibbs Free Energy= 0.196745
Sum of electronic and zero-point Energies= -2746.877426
Sum of electronic and thermal Energies= -2746.843776
Sum of electronic and thermal Enthalpies= -2746.842832
Sum of electronic and thermal Free Energies= -2746.946567

Int4 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts3naa3a.rev.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.068434	-1.751443	-0.292317
2	8	0	-1.943354	-2.202904	-0.044398
3	6	0	-3.891057	-2.285956	-1.360573
4	6	0	-3.652575	-0.624911	0.580932
5	6	0	-5.122433	-1.773466	-1.614926
6	6	0	-5.005339	-0.121130	0.163156
7	6	0	-5.690584	-0.678433	-0.850558
8	1	0	-3.468274	-3.095258	-1.947320
9	6	0	-2.612550	0.491191	0.802356
10	1	0	-3.772268	-1.091542	1.574360
11	1	0	-5.711750	-2.187584	-2.429862
12	1	0	-5.414983	0.708307	0.731558
13	1	0	-6.675353	-0.310935	-1.122224
14	17	0	-3.124132	1.578761	2.148842
15	17	0	-2.356991	1.445601	-0.719630

16	8	0	2.409680	-0.016209	-0.445355
17	1	0	2.856849	-0.891066	-0.656076
18	1	0	1.806158	-0.159874	0.344201
19	1	0	-1.613873	0.118012	1.067849
20	8	0	0.379243	0.016341	1.225479
21	1	0	0.565631	0.275760	2.139969
22	1	0	0.858165	3.267211	-2.967379
23	8	0	0.662066	3.284917	-2.019746
24	1	0	1.434555	3.714184	-1.581508
25	11	0	4.195000	1.367137	-0.056344
26	11	0	0.778735	1.736918	-0.269797
27	1	0	2.301705	-4.152563	1.055835
28	8	0	1.907717	-3.504672	0.454854
29	1	0	2.694684	-3.079017	-0.054262
30	8	0	3.803060	-2.275546	-0.816608
31	1	0	3.820489	-2.601017	-1.729824
32	17	0	2.816094	3.535215	0.183801
33	1	0	4.988952	-1.039815	-0.655389
34	8	0	5.626746	-0.315499	-0.386989
35	1	0	6.253184	-0.802616	0.176309
36	1	0	5.138696	-2.902572	0.160449
37	8	0	5.927876	-2.997998	0.759174
38	1	0	6.454420	-3.726856	0.400733
39	11	0	0.195541	-2.103884	0.661745

SCF Done: E(RB3LYP) = -2747.18234110 A.U. after 1 cycles
Zero-point correction= 0.267919 (Hartree/Particle)
Thermal correction to Energy= 0.302503
Thermal correction to Enthalpy= 0.303447
Thermal correction to Gibbs Free Energy= 0.194607
Sum of electronic and zero-point Energies= -2746.914422
Sum of electronic and thermal Energies= -2746.879838
Sum of electronic and thermal Enthalpies= -2746.878894
Sum of electronic and thermal Free Energies= -2746.987734

TS4 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts4na.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.732906	1.152788	0.576917
2	8	0	3.086576	1.899684	-0.370297
3	6	0	2.719819	1.607587	1.947434
4	6	0	2.168582	-0.215122	0.301328
5	6	0	2.295476	0.793064	2.957860
6	6	0	1.847095	-1.053390	1.466392
7	6	0	1.853152	-0.554806	2.727131
8	1	0	3.084554	2.612567	2.137935
9	6	0	2.860102	-0.906382	-0.859390
10	1	0	1.123701	0.165594	-0.206728
11	1	0	2.307862	1.165664	3.979834

12	1	0	1.565107	-2.087057	1.286165
13	1	0	1.559681	-1.169639	3.572256
14	17	0	1.841597	-2.232904	-1.582946
15	17	0	4.477467	-1.587514	-0.399464
16	8	0	0.100478	0.924936	-1.064857
17	1	0	-0.968865	1.805787	-0.415290
18	1	0	-0.456794	0.283485	-1.540496
19	1	0	3.049354	-0.205966	-1.666487
20	8	0	-0.069595	4.350879	-1.136940
21	1	0	-0.126885	5.282731	-0.885501
22	1	0	-0.801930	3.863912	-0.666413
23	8	0	-1.697512	2.485363	-0.111856
24	1	0	-1.836395	2.309247	0.840159
25	11	0	-2.599275	-1.802993	1.356001
26	11	0	1.348281	2.657773	-1.571634
27	1	0	-2.543889	-0.478948	-3.051432
28	8	0	-2.404014	-0.424306	-2.094909
29	1	0	-2.802750	-1.274280	-1.692765
30	8	0	-3.455135	-2.336436	-0.682142
31	1	0	-3.920300	-3.082943	-1.087312
32	17	0	-3.202154	0.582323	2.061777
33	1	0	-1.843909	-3.023643	-0.367681
34	8	0	-1.090717	-3.146099	0.273597
35	1	0	-0.272558	-2.945398	-0.207910
36	1	0	-4.737534	-1.172882	-0.625187
37	8	0	-5.299172	-0.342328	-0.634380
38	1	0	-5.707459	-0.297154	0.244195
39	11	0	-3.466146	1.059816	-0.614216

SCF Done: E(RB+HF-LYP) = -2747.17505619 A.U. after 1 cycles
Zero-point correction= 0.266153 (Hartree/Particle)
Thermal correction to Energy= 0.298979
Thermal correction to Enthalpy= 0.299923
Thermal correction to Gibbs Free Energy= 0.198045
Sum of electronic and zero-point Energies= -2746.908903
Sum of electronic and thermal Energies= -2746.876077
Sum of electronic and thermal Enthalpies= -2746.875133
Sum of electronic and thermal Free Energies= -2746.977011

Int5 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts4ana.g09.reva.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.885556	1.235873	0.762871
2	8	0	1.679996	2.098130	-0.172836
3	6	0	1.343190	1.384810	2.081201
4	6	0	2.672662	0.045742	0.536291
5	6	0	1.564356	0.442311	3.078467
6	6	0	2.857904	-0.903617	1.548950
7	6	0	2.308805	-0.726607	2.820818

8	1	0	0.769764	2.284726	2.288756
9	6	0	3.272425	-0.069735	-0.814554
10	1	0	-0.126573	0.549656	-1.641931
11	1	0	1.150957	0.610410	4.071157
12	1	0	3.463600	-1.781812	1.342824
13	1	0	2.498155	-1.450110	3.608237
14	17	0	2.080313	-0.859828	-2.060057
15	17	0	4.816669	-0.977966	-0.895974
16	8	0	-0.910683	1.121423	-1.726573
17	1	0	-1.963126	1.566316	-0.364884
18	1	0	-1.678254	0.500694	-2.086141
19	1	0	3.432213	0.907399	-1.259702
20	8	0	-1.630772	4.339572	-0.465309
21	1	0	-1.891283	5.190503	-0.086767
22	1	0	-2.221498	3.643961	-0.080012
23	8	0	-2.691051	1.933896	0.199637
24	1	0	-2.560657	1.521357	1.084314
25	11	0	-0.201251	-1.110041	1.678059
26	11	0	0.102826	3.100543	-1.223073
27	1	0	-3.245141	-0.271933	-3.151581
28	8	0	-2.858901	-0.398480	-2.273173
29	1	0	-2.565973	-1.867761	-2.001036
30	8	0	-2.399981	-2.813741	-1.592726
31	1	0	-2.405812	-3.457441	-2.316590
32	17	0	-2.656986	-0.442489	2.206415
33	1	0	-0.927289	-2.685298	-0.627965
34	8	0	-0.124317	-2.488573	-0.080933
35	1	0	0.599314	-2.342402	-0.713376
36	1	0	-3.850560	-2.743909	-0.413602
37	8	0	-4.528334	-2.303751	0.148475
38	1	0	-4.175582	-2.340659	1.055188
39	11	0	-3.910595	-0.120442	-0.304092

SCF Done: E(RB3LYP) = -2747.23020867 A.U. after 1 cycles
Zero-point correction= 0.269691 (Hartree/Particle)
Thermal correction to Energy= 0.303230
Thermal correction to Enthalpy= 0.304174
Thermal correction to Gibbs Free Energy= 0.202094
Sum of electronic and zero-point Energies= -2746.960518
Sum of electronic and thermal Energies= -2746.926979
Sum of electronic and thermal Enthalpies= -2746.926035
Sum of electronic and thermal Free Energies= -2747.028114

TS5 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts4ana.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.101702	1.184084	0.953911
2	8	0	2.008966	2.146285	0.135726
3	6	0	1.468936	1.225329	2.252483

4	6	0	2.828352	-0.049682	0.630502
5	6	0	1.525726	0.159390	3.117477
6	6	0	2.841650	-1.138869	1.552112
7	6	0	2.208585	-1.047560	2.770813
8	1	0	0.938563	2.135713	2.515350
9	6	0	3.458033	-0.082925	-0.620885
10	1	0	-0.289297	0.472404	-1.833998
11	1	0	1.029482	0.226974	4.082581
12	1	0	3.377482	-2.043269	1.280366
13	1	0	2.254699	-1.867797	3.481153
14	17	0	1.685855	-0.447452	-2.303426
15	17	0	4.581899	-1.320991	-1.050170
16	8	0	-0.997737	1.129250	-1.652974
17	1	0	-1.842177	1.622007	-0.191661
18	1	0	-1.884016	0.682265	-1.982599
19	1	0	3.597544	0.837191	-1.167736
20	8	0	-1.067118	4.269803	-0.349751
21	1	0	-1.069341	5.107899	0.133190
22	1	0	-1.722273	3.674951	0.091956
23	8	0	-2.456009	2.049733	0.459740
24	1	0	-2.278784	1.590331	1.309922
25	11	0	-0.216782	-1.344446	1.279699
26	11	0	0.443951	2.814668	-1.256254
27	1	0	-3.644175	0.205557	-2.941782
28	8	0	-3.199939	-0.041452	-2.118479
29	1	0	-2.947400	-1.538416	-2.032251
30	8	0	-2.771802	-2.526060	-1.741047
31	1	0	-2.929937	-3.092928	-2.510591
32	17	0	-2.420523	-0.483777	2.303888
33	1	0	-1.111670	-2.568913	-1.084505
34	8	0	-0.237698	-2.460570	-0.631842
35	1	0	0.371720	-2.081372	-1.298602
36	1	0	-4.050742	-2.461329	-0.379910
37	8	0	-4.618217	-2.039326	0.306065
38	1	0	-4.161765	-2.191005	1.152024
39	11	0	-3.947379	0.153194	-0.021250

SCF Done: E(RB+HF-LYP) = -2747.22445158 A.U. after 1 cycles
Zero-point correction= 0.269197 (Hartree/Particle)
Thermal correction to Energy= 0.302317
Thermal correction to Enthalpy= 0.303261
Thermal correction to Gibbs Free Energy= 0.201153
Sum of electronic and zero-point Energies= -2746.955255
Sum of electronic and thermal Energies= -2746.922135
Sum of electronic and thermal Enthalpies= -2746.921190
Sum of electronic and thermal Free Energies= -2747.023298

Int6 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts4ana.g09.fora.chk
Standard orientation:

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

1	6	0	4.099240	-1.074948	0.285165
2	8	0	2.892348	-1.336994	0.120417
3	6	0	5.052403	-2.110877	0.646950
4	6	0	4.652253	0.309392	0.123877
5	6	0	6.371278	-1.828030	0.818424
6	6	0	6.071010	0.529638	0.322039
7	6	0	6.895980	-0.493559	0.654678
8	1	0	4.656730	-3.114140	0.769606
9	6	0	3.770640	1.293715	-0.201721
10	1	0	-1.023974	-0.068618	0.826521
11	1	0	7.059960	-2.625590	1.087101
12	1	0	6.455380	1.536485	0.198162
13	1	0	7.957407	-0.321206	0.802227
14	17	0	0.185188	1.258914	-0.741461
15	17	0	4.204305	2.942844	-0.430243
16	8	0	-1.202310	-1.014565	1.001768
17	1	0	-2.122715	-1.769147	-0.285346
18	1	0	-2.027006	-1.044337	1.624344
19	1	0	2.706294	1.117261	-0.343357
20	8	0	-0.132612	-3.081827	-1.588432
21	1	0	0.094777	-3.577733	-2.387002
22	1	0	-1.118854	-3.009036	-1.554083
23	8	0	-2.660776	-2.266524	-0.958261
24	1	0	-2.950890	-1.580051	-1.601840
25	11	0	-2.340675	1.853192	-1.121259
26	11	0	0.708638	-1.385513	-0.301416
27	1	0	-3.494385	-1.619186	3.008063
28	8	0	-3.466356	-1.069863	2.211732
29	1	0	-4.043044	0.274656	2.460919
30	8	0	-4.498091	1.227076	2.421058
31	1	0	-4.743280	1.481717	3.322794
32	17	0	-4.216350	0.265551	-1.952491
33	1	0	-3.460121	2.282260	1.499058
34	8	0	-2.833368	2.762816	0.895606
35	1	0	-2.061845	2.989485	1.435884
36	1	0	-5.872370	0.662254	1.286340
37	8	0	-6.318147	0.101896	0.610368
38	1	0	-6.185914	0.567853	-0.235139
39	11	0	-4.594500	-1.418159	0.294179

SCF Done: E(RB3LYP) = -2747.24980984 A.U. after 1 cycles
Zero-point correction= 0.268592 (Hartree/Particle)
Thermal correction to Energy= 0.303391
Thermal correction to Enthalpy= 0.304335
Thermal correction to Gibbs Free Energy= 0.195735
Sum of electronic and zero-point Energies= -2746.981218
Sum of electronic and thermal Energies= -2746.946419
Sum of electronic and thermal Enthalpies= -2746.945475
Sum of electronic and thermal Free Energies= -2747.054075

TS6 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk= reimer.ts5na.chk

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.080221	0.058382	1.486199
2	8	0	-3.107409	-0.014335	0.755846
3	6	0	-2.174557	0.075395	2.925788
4	6	0	-0.715017	0.040194	0.905954
5	6	0	-1.065754	-0.122377	3.698398
6	6	0	0.407489	-0.219162	1.773176
7	6	0	0.237740	-0.301956	3.123255
8	1	0	-3.166564	0.169487	3.356077
9	6	0	-0.614505	0.318408	-0.433550
10	1	0	-1.471758	0.624992	-1.016968
11	1	0	-1.168103	-0.164603	4.780192
12	1	0	1.398122	-0.315396	1.342936
13	1	0	1.089429	-0.480939	3.771989
14	17	0	-1.329071	-3.442952	-0.640262
15	17	0	0.762068	-0.053746	-1.413851
16	8	0	-0.067145	2.744092	-0.560028
17	11	0	-3.158717	-1.630824	-0.881415
18	8	0	-3.850691	-0.134194	-2.391239
19	1	0	-4.161886	-0.082166	-3.305478
20	1	0	-4.105939	0.727125	-1.940464
21	1	0	-4.208496	1.427830	-0.025291
22	8	0	-4.431098	1.939966	-0.826122
23	1	0	-3.789762	2.695348	-0.807331
24	1	0	-1.547159	3.472048	-0.481129
25	8	0	-2.478419	3.845991	-0.579531
26	1	0	-2.545266	4.604773	0.016824
27	1	0	1.045887	2.614547	0.088929
28	8	0	2.045720	2.428068	0.633219
29	1	0	1.869803	2.587317	1.572453
30	11	0	1.094833	-2.848232	-0.083479
31	17	0	3.459675	-1.916071	0.436507
32	1	0	0.183945	2.957731	-1.473810
33	1	0	4.090880	-1.185584	-1.612636
34	8	0	4.078034	-0.351221	-2.133275
35	1	0	4.817437	-0.387835	-2.757125
36	1	0	3.585865	3.154735	0.156024
37	8	0	4.509335	2.921921	-0.127036
38	1	0	4.904940	3.691034	-0.558809
39	11	0	3.558932	0.821878	-0.185749

SCF Done: E(RB+HF-LYP) = -2747.19829643 A.U. after 1 cycles
Zero-point correction= 0.262710 (Hartree/Particle)
Thermal correction to Energy= 0.298428
Thermal correction to Enthalpy= 0.299372
Thermal correction to Gibbs Free Energy= 0.190222
Sum of electronic and zero-point Energies= -2746.935587
Sum of electronic and thermal Energies= -2746.899868
Sum of electronic and thermal Enthalpies= -2746.898924

Sum of electronic and thermal Free Energies= -2747.008075

Int7 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.step5revna.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.487433	-0.205574	1.090021
2	8	0	0.486788	0.480961	0.519709
3	6	0	-1.176283	0.292444	2.226826
4	6	0	-0.892149	-1.484306	0.581874
5	6	0	-2.176781	-0.449639	2.854732
6	6	0	-1.886230	-2.216260	1.239727
7	6	0	-2.534268	-1.712959	2.370397
8	1	0	-0.883551	1.266726	2.609927
9	6	0	-0.189825	-1.927098	-0.682774
10	8	0	1.122334	-2.293036	-0.465076
11	1	0	-2.673405	-0.041315	3.731718
12	1	0	-2.163359	-3.190870	0.852201
13	1	0	-3.300313	-2.300833	2.866171
14	1	0	1.658167	-2.038980	-1.274266
15	1	0	-0.249992	-1.157975	-1.452895
16	17	0	-1.127073	-3.331167	-1.540205
17	11	0	2.354108	-0.739190	0.901062
18	8	0	0.716525	1.112808	-2.096799
19	1	0	0.517223	0.715708	-1.209385
20	1	0	-0.115718	1.529323	-2.385244
21	8	0	2.536227	-1.042567	-2.382522
22	1	0	1.978752	-0.266589	-2.604552
23	1	0	3.322339	-0.652148	-1.942175
24	8	0	4.049940	-1.142578	2.404752
25	1	0	4.562700	-1.869235	2.786682
26	1	0	4.648193	-0.653910	1.795929
27	17	0	4.437891	0.510753	-0.201665
28	1	0	3.470597	2.389922	0.127834
29	8	0	2.896874	3.186303	0.285073
30	1	0	3.485198	3.950714	0.207524
31	11	0	0.745667	2.671746	-0.092887
32	1	0	-5.373163	2.771756	0.585585
33	8	0	-4.515698	2.350392	0.432965
34	1	0	-3.919039	3.017741	0.029502
35	11	0	-3.002780	0.691456	0.052377
36	8	0	-3.436609	-0.862650	-1.589221
37	1	0	-2.952545	-1.708270	-1.662841
38	1	0	-3.735215	-0.646487	-2.485637
39	17	0	-1.789467	2.933583	-0.905073

SCF Done: E(RB+HF-LYP) = -2747.27151805 A.U. after 1 cycles
Zero-point correction= 0.270136 (Hartree/Particle)
Thermal correction to Energy= 0.305820
Thermal correction to Enthalpy= 0.306764

Thermal correction to Gibbs Free Energy= 0.199037
Sum of electronic and zero-point Energies= -2747.001382
Sum of electronic and thermal Energies= -2746.965698
Sum of electronic and thermal Enthalpies= -2746.964754
Sum of electronic and thermal Free Energies= -2747.072481

TS7 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts6na.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.461459	1.515002	0.155295
2	8	0	0.694347	2.413807	-0.835807
3	6	0	0.411981	1.983546	1.482072
4	6	0	0.207409	0.139340	-0.097673
5	6	0	0.142587	1.113327	2.541063
6	6	0	-0.030210	-0.718973	0.983155
7	6	0	-0.076886	-0.243854	2.294029
8	1	0	0.646521	3.029582	1.659584
9	6	0	0.359046	-0.315782	-1.536009
10	8	0	1.638876	-0.593754	-1.895788
11	1	0	0.149420	1.490203	3.560225
12	1	0	-0.175148	-1.778545	0.794573
13	1	0	-0.252732	-0.932788	3.113469
14	1	0	2.045114	0.360985	-2.305505
15	1	0	-0.112312	0.398241	-2.217821
16	17	0	-0.703826	-1.880142	-1.875841
17	11	0	3.391564	-1.163885	-0.460776
18	8	0	2.420456	1.646845	-2.396341
19	1	0	1.487900	2.130058	-1.579168
20	1	0	2.408401	2.032832	-3.284523
21	1	0	4.078935	1.194735	-1.625828
22	8	0	4.723446	0.570190	-1.225091
23	1	0	4.822162	0.833947	-0.287525
24	8	0	3.672042	-2.990676	0.965348
25	1	0	4.388615	-3.630586	1.084828
26	1	0	3.862416	-2.238383	1.589792
27	17	0	3.986638	-0.105858	1.894608
28	1	0	-0.716377	3.445606	-0.837772
29	8	0	-1.633016	3.700743	-0.548793
30	1	0	-1.906910	4.466604	-1.071713
31	11	0	-2.262402	2.110434	0.896096
32	1	0	-3.577589	-3.246082	2.198024
33	8	0	-3.421799	-2.527056	1.569103
34	1	0	-3.836091	-1.717248	1.930735
35	11	0	-3.074766	-1.663256	-0.498146
36	8	0	-4.892430	-1.106009	-1.734450
37	1	0	-5.451373	-1.093440	-2.524359
38	1	0	-5.189235	-0.384660	-1.143004
39	17	0	-4.208564	0.443315	0.894176

SCF Done: E(RB+HF-LYP) = -2747.22458483 A.U. after 1 cycles
Zero-point correction= 0.262445 (Hartree/Particle)
Thermal correction to Energy= 0.297746
Thermal correction to Enthalpy= 0.298690
Thermal correction to Gibbs Free Energy= 0.186071
Sum of electronic and zero-point Energies= -2746.962140
Sum of electronic and thermal Energies= -2746.926839
Sum of electronic and thermal Enthalpies= -2746.925895
Sum of electronic and thermal Free Energies= -2747.038514

product in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.step5forna.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.628348	-1.135131	0.416670
2	8	0	2.437032	-1.723282	0.751439
3	6	0	4.805232	-1.797553	0.776873
4	6	0	3.700756	0.101737	-0.267388
5	6	0	6.040380	-1.224754	0.487586
6	6	0	4.961704	0.678724	-0.517056
7	6	0	6.125805	0.022448	-0.148779
8	1	0	4.729460	-2.743599	1.303179
9	6	0	2.485308	0.728942	-0.781228
10	8	0	2.394914	1.902709	-1.155659
11	1	0	6.948547	-1.747422	0.775321
12	1	0	4.992360	1.633822	-1.032777
13	1	0	7.095165	0.463586	-0.358773
14	1	0	0.530897	0.801574	1.755513
15	1	0	1.598393	0.082278	-0.854230
16	17	0	-1.039758	0.220926	-1.317799
17	11	0	0.173637	2.616422	-0.993821
18	8	0	0.442215	-0.161681	1.577760
19	1	0	1.757598	-1.066008	1.092316
20	1	0	-0.183038	-0.183743	0.820256
21	1	0	0.677714	3.324415	1.914114
22	8	0	0.233673	2.633551	1.398164
23	1	0	-0.748261	2.777621	1.537913
24	8	0	-1.293517	4.336882	-1.123132
25	1	0	-1.802014	4.800392	-1.803673
26	1	0	-1.938893	4.086813	-0.413308
27	17	0	-2.777566	2.995237	1.260987
28	1	0	1.308067	-2.914203	-0.129614
29	8	0	0.529803	-3.383084	-0.503640
30	1	0	0.633495	-4.315834	-0.264023
31	11	0	-1.500857	-2.376142	-0.803688
32	1	0	-5.807066	-0.533519	-0.937424
33	8	0	-4.984518	-0.647247	-0.441041
34	1	0	-4.778162	-1.617881	-0.457073
35	11	0	-3.247985	0.571512	0.343191
36	8	0	-2.383938	-1.380469	1.377413

37	1	0	-1.958939	-1.466254	2.244982
38	1	0	-2.979146	-2.163285	1.246216
39	17	0	-3.784996	-3.511103	-0.254477

SCF Done: E(RB3LYP) = -2747.32261446 A.U. after 1 cycles
Zero-point correction= 0.269105 (Hartree/Particle)
Thermal correction to Energy= 0.304969
Thermal correction to Enthalpy= 0.305913
Thermal correction to Gibbs Free Energy= 0.197873
Sum of electronic and zero-point Energies= -2747.053510
Sum of electronic and thermal Energies= -2747.017646
Sum of electronic and thermal Enthalpies= -2747.016702
Sum of electronic and thermal Free Energies= -2747.124742

TS8 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.h12na.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.701102	-1.473469	0.627172
2	8	0	-0.857119	-1.116843	1.443925
3	6	0	-1.596667	-2.734554	-0.105301
4	6	0	-2.998719	-0.643048	0.408146
5	6	0	-2.654285	-3.222908	-0.789463
6	6	0	-4.090080	-1.278476	-0.344231
7	6	0	-3.907759	-2.490443	-0.906841
8	1	0	-0.649711	-3.257305	-0.011408
9	6	0	-2.893559	0.716793	0.801166
10	1	0	-3.211210	-0.285642	1.635833
11	1	0	-2.579368	-4.188128	-1.282675
12	1	0	-5.014496	-0.727172	-0.469766
13	1	0	-4.707242	-2.935028	-1.493155
14	17	0	2.532813	3.445116	-0.890060
15	17	0	-4.324729	1.692670	0.450561
16	17	0	-0.486925	-0.119120	-2.024820
17	11	0	1.853856	-1.164817	-1.396648
18	11	0	0.234705	2.155563	-0.955343
19	1	0	0.857317	4.381973	0.000381
20	8	0	-0.102014	4.375140	0.271099
21	1	0	-0.423758	5.285927	0.199509
22	8	0	2.564170	0.482163	0.094468
23	1	0	3.426693	0.040817	0.393142
24	1	0	2.769551	1.408888	-0.184348
25	1	0	-1.270896	1.529067	1.325738
26	8	0	-0.327277	1.860593	1.393251
27	1	0	-0.362983	2.838577	1.420851
28	11	0	1.083776	0.114201	1.809817
29	8	0	4.406374	-1.156135	0.913748
30	1	0	5.284888	-0.892613	1.221788
31	1	0	3.389024	-1.452856	1.949664
32	8	0	2.477706	-1.604283	2.460696

33	1	0	2.672017	-2.079970	3.281062
34	1	0	4.281636	-1.901601	-0.464280
35	8	0	3.895878	-2.327374	-1.317916
36	1	0	4.638540	-2.539426	-1.900736
37	8	0	1.627632	-3.007089	0.145912
38	1	0	2.488265	-3.309754	-0.202687
39	1	0	1.826550	-2.680253	1.053068

SCF Done: E(RB3LYP) = -2747.12062827 A.U. after 1 cycles
Zero-point correction= 0.262337 (Hartree/Particle)
Thermal correction to Energy= 0.296148
Thermal correction to Enthalpy= 0.297092
Thermal correction to Gibbs Free Energy= 0.195364
Sum of electronic and zero-point Energies= -2746.858291
Sum of electronic and thermal Energies= -2746.824480
Sum of electronic and thermal Enthalpies= -2746.823536
Sum of electronic and thermal Free Energies= -2746.925264

TS9 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.ts9na.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.393735	1.782281	-0.205371
2	8	0	-1.729679	0.547561	0.085065
3	6	0	-1.105684	2.731559	0.825966
4	6	0	-1.220056	2.219164	-1.549896
5	6	0	-0.684875	4.033138	0.518934
6	6	0	-0.784797	3.503792	-1.832537
7	6	0	-0.505358	4.423549	-0.801631
8	1	0	-1.310659	2.442258	1.853300
9	6	0	1.140265	1.157313	1.126243
10	1	0	-1.396855	1.505706	-2.352568
11	1	0	-0.492692	4.734572	1.327155
12	1	0	-0.646804	3.803911	-2.868622
13	1	0	-0.165791	5.426272	-1.042154
14	17	0	1.394201	-1.581147	1.059279
15	17	0	1.553473	1.473217	2.736176
16	17	0	2.172819	1.594750	-0.107610
17	1	0	0.197882	0.678840	0.908422
18	11	0	-1.266423	-1.580328	0.805982
19	11	0	3.555815	-1.805417	-0.517731
20	8	0	-3.155806	-2.457562	-0.387673
21	1	0	-2.854010	-3.113733	-1.033677
22	8	0	5.720798	-1.261570	-0.776912
23	1	0	6.538446	-0.983429	-0.345747
24	1	0	-3.019005	-2.993028	1.223758
25	8	0	-2.651514	-2.866383	2.147912
26	1	0	-2.540995	-3.736340	2.556248
27	1	0	-4.783163	-2.693457	-0.457613
28	8	0	-5.791467	-2.663474	-0.576558

29	1	0	-6.182833	-2.924742	0.270018
30	1	0	5.455107	-2.788857	-1.219455
31	8	0	4.809054	-3.564978	-1.366149
32	1	0	5.044586	-3.994338	-2.199313
33	1	0	4.865824	-0.258309	-1.561788
34	8	0	3.980627	0.129682	-1.941883
35	1	0	4.080416	0.152485	-2.904284
36	1	0	-6.398549	0.240224	-1.973554
37	8	0	-5.716199	-0.137041	-1.402092
38	1	0	-5.999923	-1.058955	-1.147426
39	11	0	-3.547614	-0.307861	-0.876431

SCF Done: E(RB3LYP) = -2747.09188890 A.U. after 1 cycles
Zero-point correction= 0.262014 (Hartree/Particle)
Thermal correction to Energy= 0.297586
Thermal correction to Enthalpy= 0.298531
Thermal correction to Gibbs Free Energy= 0.186064
Sum of electronic and zero-point Energies= -2746.829874
Sum of electronic and thermal Energies= -2746.794303
Sum of electronic and thermal Enthalpies= -2746.793358
Sum of electronic and thermal Free Energies= -2746.905825

RB3LYP/6-31+G(d)
precursor in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.pre.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.368817	-0.952123	-0.284252
2	17	0	3.682720	0.812347	0.015833
3	17	0	3.299657	-1.279348	-2.033880
4	17	0	4.612047	-1.944155	0.523404
5	11	0	-1.481920	-1.552537	0.305407
6	1	0	2.397897	-1.191225	0.160279
7	8	0	0.664460	0.411632	2.641909
8	1	0	1.118141	0.324048	3.491964
9	1	0	-2.822039	-2.724353	2.962314
10	8	0	-2.786765	-2.052797	2.266265
11	1	0	-2.551681	-1.175898	2.704657
12	1	0	-2.261671	0.699628	1.986112
13	8	0	-2.046043	0.392877	2.897996
14	1	0	-1.045544	0.423780	2.928228
15	1	0	-3.941083	-2.307983	-0.524808
16	8	0	-4.631367	-1.824107	0.032261
17	1	0	-4.321305	-1.948531	0.949459
18	8	0	-2.531067	-2.465707	-1.423569
19	1	0	-2.375241	-3.348896	-1.785886
20	1	0	-2.938250	-1.474237	-2.550189
21	1	0	0.717189	-0.846479	1.857020
22	8	0	0.690368	-1.622868	1.143702

23	1	0	0.896588	-2.439839	1.622563
24	8	0	-3.312695	-0.638281	-3.036109
25	1	0	-3.693868	-0.932569	-3.874152
26	11	0	-4.002043	0.072046	-1.030241
27	8	0	-2.225743	0.758486	0.127600
28	6	0	-1.410290	1.727460	-0.221213
29	6	0	-0.456893	1.568840	-1.271546
30	6	0	0.438494	2.588992	-1.603777
31	6	0	0.438038	3.809712	-0.909134
32	6	0	-1.406819	2.984207	0.457069
33	6	0	-0.506041	3.996620	0.114313
34	1	0	-0.458665	0.636188	-1.831163
35	1	0	1.144899	2.429704	-2.415580
36	1	0	1.127341	4.603813	-1.181631
37	1	0	-2.128683	3.138829	1.255370
38	1	0	-0.542929	4.943631	0.649626
39	11	0	1.048751	1.859029	1.098975

SCF Done: E(RB3LYP) = -2747.16921784 A.U. after 1 cycles
Zero-point correction= 0.267146 (Hartree/Particle)
Thermal correction to Energy= 0.300565
Thermal correction to Enthalpy= 0.301509
Thermal correction to Gibbs Free Energy= 0.196959
Sum of electronic and zero-point Energies= -2746.902072
Sum of electronic and thermal Energies= -2746.868653
Sum of electronic and thermal Enthalpies= -2746.867709
Sum of electronic and thermal Free Energies= -2746.972258

TS1 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.ts1.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.057111	-0.897706	-0.721338
2	17	0	2.754852	0.283705	-1.986629
3	17	0	0.316003	-1.279035	-1.274675
4	17	0	3.003677	-2.433626	-0.834162
5	11	0	-0.713252	-2.482095	1.224020
6	1	0	2.027641	-0.308147	0.618775
7	8	0	1.999610	0.166346	1.670626
8	1	0	1.378460	0.929816	1.579643
9	8	0	-3.841256	-2.549316	-0.124556
10	1	0	-4.759608	-2.753750	0.103128
11	1	0	-3.186703	-1.626124	0.761820
12	1	0	1.238959	-2.280070	3.513577
13	8	0	0.724400	-1.851900	2.815680
14	1	0	1.258775	-1.056553	2.503466
15	1	0	-3.640133	-1.497645	-1.328205
16	8	0	-3.341539	-0.691689	-1.872119
17	1	0	-3.288641	-0.966889	-2.797292
18	8	0	-2.468715	-0.970117	1.213313

19	1	0	-2.810834	-0.687478	2.073981
20	1	0	-2.768099	-3.711650	0.154231
21	1	0	3.549156	0.902339	1.870734
22	8	0	4.264501	1.560611	1.631309
23	1	0	5.118873	1.120754	1.739450
24	8	0	-1.925858	-4.203899	0.446537
25	1	0	-1.752995	-4.891692	-0.210881
26	11	0	2.853355	2.280356	0.032654
27	1	0	-3.496808	3.001759	1.924855
28	1	0	-1.117364	2.498643	2.412045
29	6	0	-2.228250	3.335228	-1.212356
30	6	0	-0.887308	3.043198	-0.946384
31	6	0	-0.431492	2.737214	0.375123
32	6	0	-2.769794	3.010522	1.114445
33	6	0	-1.433157	2.721657	1.395422
34	1	0	-2.528005	3.575668	-2.230751
35	1	0	-0.152918	3.060957	-1.749024
36	8	0	0.813969	2.462994	0.632451
37	6	0	-3.190152	3.315363	-0.190551
38	1	0	-4.230578	3.544124	-0.401629
39	11	0	-2.195455	0.607294	-0.448227

SCF Done: E(RB3LYP) = -2747.14204245 A.U. after 1 cycles
Zero-point correction= 0.260020 (Hartree/Particle)
Thermal correction to Energy= 0.294108
Thermal correction to Enthalpy= 0.295052
Thermal correction to Gibbs Free Energy= 0.189205
Sum of electronic and zero-point Energies= -2746.882023
Sum of electronic and thermal Energies= -2746.847934
Sum of electronic and thermal Enthalpies= -2746.846990
Sum of electronic and thermal Free Energies= -2746.952837

Int1 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.int1.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.405884	-0.293922	-0.139427
2	8	0	2.118497	-0.200382	0.233794
3	6	0	3.756919	-0.728745	-1.436381
4	6	0	4.451674	0.039315	0.748692
5	6	0	5.094876	-0.829372	-1.823479
6	6	0	5.786591	-0.064344	0.353623
7	6	0	6.122296	-0.498999	-0.933545
8	1	0	2.961964	-0.985002	-2.135146
9	6	0	-2.007157	-1.895623	-0.226595
10	1	0	4.197877	0.380504	1.750051
11	1	0	5.335029	-1.168189	-2.829325
12	1	0	6.572069	0.198881	1.059301
13	1	0	7.162847	-0.577890	-1.236774
14	17	0	-3.081616	-1.991588	1.325398

15	17	0	-1.295649	-3.633344	-0.438126
16	17	0	-3.221750	-1.692399	-1.629536
17	11	0	-1.931614	0.698237	-0.963324
18	11	0	0.493682	-1.647633	0.376163
19	1	0	-1.115214	-1.880286	2.583582
20	8	0	-0.143457	-1.776136	2.661044
21	1	0	0.147272	-2.452056	3.293167
22	8	0	-2.423845	2.102471	0.803155
23	1	0	-2.567226	2.999577	0.256494
24	1	0	-3.162087	2.004488	1.421407
25	1	0	1.607519	0.539863	1.689835
26	8	0	1.026202	0.955050	2.391980
27	1	0	0.627516	0.198740	2.855352
28	11	0	-0.156355	2.548325	1.286392
29	8	0	-2.360824	4.126907	-0.665721
30	1	0	-3.118674	4.721098	-0.761956
31	1	0	-1.111049	4.705308	0.185672
32	8	0	-0.319292	4.744678	0.820854
33	1	0	0.270796	5.444522	0.510046
34	1	0	-1.997795	3.207332	-1.905297
35	8	0	-1.705037	2.413886	-2.485097
36	1	0	-1.996413	2.594823	-3.389725
37	1	0	1.121723	0.834225	-0.531104
38	8	0	0.278426	1.363073	-0.708757
39	1	0	0.352405	1.834221	-1.555968

SCF Done: E(RB3LYP) = -2747.15560165 A.U. after 1 cycles
Zero-point correction= 0.264237 (Hartree/Particle)
Thermal correction to Energy= 0.298739
Thermal correction to Enthalpy= 0.299683
Thermal correction to Gibbs Free Energy= 0.193040
Sum of electronic and zero-point Energies= -2746.891365
Sum of electronic and thermal Energies= -2746.856863
Sum of electronic and thermal Enthalpies= -2746.855918
Sum of electronic and thermal Free Energies= -2746.962561

TS2 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.ts2.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.197500	-1.034176	0.453262
2	8	0	-0.057557	-0.725192	0.326949
3	6	0	1.714937	-1.680354	1.611074
4	6	0	2.144531	-0.697689	-0.593966
5	6	0	3.057834	-2.024380	1.696654
6	6	0	3.485699	-1.174117	-0.516109
7	6	0	3.956617	-1.780087	0.630815
8	1	0	1.039062	-1.886942	2.438139
9	6	0	2.281129	1.372603	-0.245160
10	1	0	1.730224	-0.481637	-1.574800

11	1	0	3.424800	-2.500409	2.603517
12	1	0	4.153464	-0.981713	-1.351221
13	1	0	4.998120	-2.073892	0.719062
14	17	0	3.148893	1.611575	1.289841
15	17	0	3.327156	1.957221	-1.596141
16	17	0	-1.756865	3.588677	0.346415
17	11	0	-1.064922	-2.244218	-1.177895
18	11	0	-0.249786	1.608349	-0.426524
19	8	0	-1.868797	1.507425	-2.138731
20	1	0	-2.101129	2.419084	-1.870113
21	1	0	-2.654194	0.963055	-1.874034
22	8	0	-2.029485	-1.397439	-3.036326
23	1	0	-2.814497	-1.003197	-2.549814
24	1	0	-1.654544	-0.644118	-3.520382
25	1	0	1.130527	-3.621992	-0.033782
26	8	0	0.447555	-3.909390	-0.666528
27	1	0	0.781158	-4.720914	-1.077717
28	11	0	-1.934199	-0.731517	1.655556
29	8	0	-3.787892	-0.308545	-1.327934
30	1	0	-4.704701	-0.264484	-1.638580
31	1	0	-3.465767	-1.450429	-0.463340
32	8	0	-2.959602	-2.165998	0.136520
33	1	0	-3.597207	-2.858419	0.361974
34	1	0	-3.660206	0.684061	0.160628
35	8	0	-3.304444	1.015286	1.027587
36	1	0	-2.942425	1.927390	0.857695
37	8	0	-3.228471	-0.121081	3.453722
38	1	0	-3.587083	0.534811	2.811310
39	1	0	-3.283712	0.272603	4.335505

SCF Done: E(RB+HF-LYP) = -2747.13915723 A.U. after 1 cycles
Zero-point correction= 0.264407 (Hartree/Particle)
Thermal correction to Energy= 0.299001
Thermal correction to Enthalpy= 0.299945
Thermal correction to Gibbs Free Energy= 0.194439
Sum of electronic and zero-point Energies= -2746.874750
Sum of electronic and thermal Energies= -2746.840157
Sum of electronic and thermal Enthalpies= -2746.839212
Sum of electronic and thermal Free Energies= -2746.944718

Int3 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.int3.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.212412	-1.155936	-0.061541
2	8	0	-0.289622	-0.285885	-0.069657
3	6	0	-1.140933	-2.348189	-0.847287
4	6	0	-2.449828	-0.898037	0.768375
5	6	0	-2.148026	-3.278747	-0.795610
6	6	0	-3.426663	-2.016183	0.817723

7	6	0	-3.305014	-3.120552	0.039345
8	1	0	-0.264942	-2.499001	-1.472140
9	6	0	-3.080370	0.484354	0.238039
10	1	0	-2.138594	-0.618218	1.783659
11	1	0	-2.068239	-4.174991	-1.407817
12	1	0	-4.299884	-1.871523	1.447038
13	1	0	-4.070719	-3.891172	0.034630
14	17	0	-3.855434	0.172240	-1.443644
15	17	0	-4.441428	0.945886	1.398316
16	17	0	0.904389	2.805595	-1.688623
17	11	0	1.573960	0.230521	-1.357664
18	11	0	-1.300199	2.019048	-0.334959
19	8	0	0.115527	3.256849	1.224299
20	1	0	-0.017460	4.123661	1.637741
21	1	0	0.631846	3.402872	0.391056
22	8	0	3.405673	1.118946	-0.168625
23	1	0	4.207134	0.639141	-0.588442
24	1	0	3.343676	2.023427	-0.515810
25	1	0	0.478960	0.287499	1.599464
26	8	0	1.054601	0.751865	2.242881
27	1	0	0.818877	1.693640	2.115829
28	11	0	3.141198	-0.041295	1.792831
29	8	0	5.088014	-0.617915	-0.967488
30	1	0	5.850660	-0.490903	-1.549323
31	1	0	5.359593	-0.939479	0.571990
32	8	0	5.226210	-1.081912	1.577750
33	1	0	6.102798	-1.120005	1.985610
34	1	0	3.876574	-1.280190	-1.574651
35	8	0	2.903223	-1.611435	-1.782453
36	1	0	2.964039	-2.265183	-2.494039
37	8	0	2.700940	-2.198472	0.977667
38	1	0	2.656405	-2.220096	-0.003580
39	1	0	3.619704	-2.450328	1.184391

SCF Done: E(RB3LYP) = -2747.16595579 A.U. after 1 cycles
Zero-point correction= 0.266233 (Hartree/Particle)
Thermal correction to Energy= 0.300367
Thermal correction to Enthalpy= 0.301312
Thermal correction to Gibbs Free Energy= 0.197896
Sum of electronic and zero-point Energies= -2746.899723
Sum of electronic and thermal Energies= -2746.865588
Sum of electronic and thermal Enthalpies= -2746.864644
Sum of electronic and thermal Free Energies= -2746.968060

TS3 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.ts3.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.952154	1.036926	0.745716
2	8	0	0.785480	0.854360	1.186329

3	6	0	2.438361	2.337902	0.379171
4	6	0	2.870140	-0.162436	0.595923
5	6	0	3.750633	2.505243	0.028126
6	6	0	4.294671	0.162231	0.296970
7	6	0	4.697720	1.418500	-0.002917
8	1	0	1.748459	3.176761	0.422001
9	6	0	2.207353	-1.174173	-0.450300
10	1	0	2.824058	-0.723432	1.540013
11	1	0	4.101125	3.502112	-0.232368
12	1	0	4.983544	-0.676290	0.248024
13	1	0	5.726339	1.624956	-0.284732
14	17	0	3.055249	-2.814148	-0.172050
15	17	0	2.621301	-0.612295	-2.162046
16	8	0	-2.264787	0.083534	0.510792
17	1	0	-2.855798	-0.638045	0.894278
18	1	0	-1.661129	-0.442384	-0.084177
19	1	0	0.520093	-1.453529	-0.728104
20	8	0	-0.518933	-1.512461	-0.704787
21	1	0	-0.873689	-2.362982	-1.035209
22	1	0	-0.799964	5.074614	1.689106
23	8	0	-0.740113	4.337456	1.064210
24	1	0	-1.421257	4.495715	0.371644
25	11	0	-3.692065	0.868137	-1.190020
26	11	0	-1.161679	2.072489	0.810484
27	1	0	-1.552760	-3.260841	3.216487
28	8	0	-1.532653	-2.437802	2.709464
29	1	0	-2.376081	-2.413375	2.137552
30	8	0	-3.566860	-2.143671	1.065853
31	1	0	-4.377618	-2.304865	1.572346
32	17	0	-2.810911	3.280604	-0.987713
33	1	0	-4.241497	-1.624796	-0.441582
34	8	0	-4.492630	-1.235257	-1.330546
35	1	0	-4.181879	-1.904525	-1.961742
36	1	0	-2.894589	-3.221449	-0.141073
37	8	0	-2.460519	-3.538290	-0.981550
38	1	0	-2.421227	-4.504405	-0.936082
39	11	0	-0.046262	-1.292633	1.516820

SCF Done: E(RB3LYP) = -2747.15552274 A.U. after 1 cycles
Zero-point correction= 0.266072 (Hartree/Particle)
Thermal correction to Energy= 0.299610
Thermal correction to Enthalpy= 0.300554
Thermal correction to Gibbs Free Energy= 0.197332
Sum of electronic and zero-point Energies= -2746.889451
Sum of electronic and thermal Energies= -2746.855912
Sum of electronic and thermal Enthalpies= -2746.854968
Sum of electronic and thermal Free Energies= -2746.958191

Int4 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.int4.chk
Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.437339	-1.651689	-0.220026
2	8	0	2.286046	-2.101345	-0.229629
3	6	0	4.572624	-2.469624	0.172996
4	6	0	3.717634	-0.211243	-0.689684
5	6	0	5.821255	-1.939649	0.257893
6	6	0	5.121430	0.275601	-0.459263
7	6	0	6.102703	-0.548202	-0.045295
8	1	0	4.364123	-3.502325	0.435824
9	6	0	2.618125	0.757789	-0.217570
10	1	0	3.585422	-0.268531	-1.786774
11	1	0	6.645556	-2.570389	0.584291
12	1	0	5.320691	1.320696	-0.677173
13	1	0	7.117064	-0.181135	0.081434
14	17	0	2.767952	2.352296	-1.055179
15	17	0	2.691633	0.975609	1.578836
16	8	0	-2.668621	-0.044151	0.479242
17	1	0	-2.993398	-0.948589	0.775905
18	1	0	-1.897449	-0.190279	-0.142522
19	1	0	1.604179	0.402815	-0.448581
20	8	0	-0.362287	0.135920	-0.810084
21	1	0	-0.429217	0.320764	-1.759631
22	1	0	-1.323468	4.339538	2.288350
23	8	0	-1.285226	3.910833	1.421894
24	1	0	-2.110821	4.149209	0.941191
25	11	0	-4.555477	0.958739	-0.321351
26	11	0	-1.306592	1.911136	0.292064
27	1	0	-1.773229	-4.295813	-0.384496
28	8	0	-1.538590	-3.488011	0.093856
29	1	0	-2.422629	-3.127115	0.478957
30	8	0	-3.722239	-2.439733	1.018521
31	1	0	-3.804617	-2.642125	1.963128
32	17	0	-3.483836	3.289956	-0.671844
33	1	0	-5.042006	-1.465322	0.508345
34	8	0	-5.732148	-0.903865	0.047636
35	1	0	-6.188118	-1.561781	-0.505148
36	1	0	-4.789751	-3.430352	0.015939
37	8	0	-5.452490	-3.758414	-0.650010
38	1	0	-5.923010	-4.490643	-0.226280
39	11	0	0.037590	-1.972606	-0.278832

SCF Done: E(RB3LYP) = -2747.19258446 A.U. after 1 cycles
Zero-point correction= 0.267303 (Hartree/Particle)
Thermal correction to Energy= 0.302188
Thermal correction to Enthalpy= 0.303132
Thermal correction to Gibbs Free Energy= 0.192236
Sum of electronic and zero-point Energies= -2746.925281
Sum of electronic and thermal Energies= -2746.890396
Sum of electronic and thermal Enthalpies= -2746.889452
Sum of electronic and thermal Free Energies= -2747.000349

TS4 in Figure 1

Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.ts4.chk

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.758871	1.141810	0.564566
2	8	0	3.088791	1.889339	-0.387353
3	6	0	2.790079	1.591146	1.938913
4	6	0	2.180400	-0.225622	0.297047
5	6	0	2.385785	0.775666	2.957517
6	6	0	1.878027	-1.063323	1.470943
7	6	0	1.921990	-0.568234	2.732516
8	1	0	3.165893	2.593605	2.123118
9	6	0	2.858811	-0.920081	-0.871950
10	1	0	1.138981	0.145550	-0.191702
11	1	0	2.427391	1.144052	3.980707
12	1	0	1.574155	-2.092046	1.296295
13	1	0	1.636232	-1.180631	3.582523
14	17	0	1.837614	-2.254531	-1.570641
15	17	0	4.489100	-1.586155	-0.435169
16	8	0	0.093217	0.929574	-1.064451
17	1	0	-0.961225	1.808034	-0.409417
18	1	0	-0.469720	0.292288	-1.538649
19	1	0	3.030377	-0.221500	-1.684677
20	8	0	-0.058162	4.356269	-1.119759
21	1	0	-0.098486	5.281538	-0.841747
22	1	0	-0.788282	3.866488	-0.647884
23	8	0	-1.686057	2.491370	-0.095807
24	1	0	-1.811931	2.318090	0.858034
25	11	0	-2.673009	-1.821029	1.365960
26	11	0	1.342753	2.655483	-1.582995
27	1	0	-2.572833	-0.447228	-3.048950
28	8	0	-2.426178	-0.405691	-2.092770
29	1	0	-2.836956	-1.252216	-1.698498
30	8	0	-3.510639	-2.313475	-0.692494
31	1	0	-3.977664	-3.054934	-1.104896
32	17	0	-3.197760	0.582620	2.087170
33	1	0	-1.903599	-3.007310	-0.375475
34	8	0	-1.156573	-3.146519	0.269835
35	1	0	-0.333958	-2.940150	-0.201156
36	1	0	-4.774721	-1.133253	-0.642834
37	8	0	-5.318095	-0.290359	-0.650398
38	1	0	-5.760306	-0.257092	0.211877
39	11	0	-3.463361	1.079328	-0.594012

SCF Done: E(RB3LYP) = -2747.18567379 A.U. after 1 cycles
Zero-point correction= 0.266149 (Hartree/Particle)
Thermal correction to Energy= 0.299033
Thermal correction to Enthalpy= 0.299977
Thermal correction to Gibbs Free Energy= 0.197931
Sum of electronic and zero-point Energies= -2746.919525
Sum of electronic and thermal Energies= -2746.886641

Sum of electronic and thermal Enthalpies= -2746.885697
Sum of electronic and thermal Free Energies= -2746.987743

Int5 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.int5.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.871939	1.215707	0.773426
2	8	0	1.635351	2.074063	-0.156658
3	6	0	1.339150	1.347557	2.098840
4	6	0	2.684563	0.044108	0.534218
5	6	0	1.584743	0.401540	3.088222
6	6	0	2.896736	-0.907533	1.539831
7	6	0	2.350216	-0.751367	2.816648
8	1	0	0.748889	2.234298	2.316840
9	6	0	3.279162	-0.048046	-0.821480
10	1	0	-0.139782	0.563286	-1.621908
11	1	0	1.176132	0.555764	4.085443
12	1	0	3.518141	-1.773138	1.325072
13	1	0	2.556660	-1.478632	3.596586
14	17	0	2.108351	-0.869490	-2.060877
15	17	0	4.854014	-0.903990	-0.914407
16	8	0	-0.923907	1.131421	-1.725212
17	1	0	-1.987692	1.567262	-0.373965
18	1	0	-1.683815	0.505537	-2.091363
19	1	0	3.406584	0.936241	-1.261636
20	8	0	-1.658235	4.341428	-0.435485
21	1	0	-1.908383	5.183033	-0.029883
22	1	0	-2.250369	3.639686	-0.063423
23	8	0	-2.720005	1.925772	0.191180
24	1	0	-2.585065	1.514004	1.075369
25	11	0	-0.227822	-1.133479	1.698489
26	11	0	0.080674	3.115677	-1.202261
27	1	0	-3.239538	-0.276264	-3.166573
28	8	0	-2.858958	-0.400071	-2.285280
29	1	0	-2.552623	-1.865047	-2.016055
30	8	0	-2.380563	-2.811265	-1.609486
31	1	0	-2.378467	-3.453194	-2.334975
32	17	0	-2.677417	-0.436786	2.213466
33	1	0	-0.918200	-2.681178	-0.636699
34	8	0	-0.124608	-2.486986	-0.074655
35	1	0	0.612273	-2.347549	-0.693061
36	1	0	-3.837087	-2.752353	-0.440742
37	8	0	-4.520838	-2.316987	0.118019
38	1	0	-4.184479	-2.371860	1.029643
39	11	0	-3.927603	-0.127306	-0.323990

SCF Done: E(RB3LYP) = -2747.24039844 A.U. after 1 cycles
Zero-point correction= 0.269310 (Hartree/Particle)
Thermal correction to Energy= 0.302992

Thermal correction to Enthalpy= 0.303936
Thermal correction to Gibbs Free Energy= 0.201138
Sum of electronic and zero-point Energies= -2746.971088
Sum of electronic and thermal Energies= -2746.937407
Sum of electronic and thermal Enthalpies= -2746.936463
Sum of electronic and thermal Free Energies= -2747.039261

TS5 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.ts5.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.100536	1.302349	0.785113
2	8	0	2.018412	2.157157	-0.143004
3	6	0	1.454112	1.502493	2.064128
4	6	0	2.830355	0.036486	0.622275
5	6	0	1.492702	0.547475	3.050272
6	6	0	2.830582	-0.932263	1.672337
7	6	0	2.178791	-0.694270	2.860927
8	1	0	0.923523	2.439233	2.209153
9	6	0	3.473324	-0.152603	-0.605003
10	1	0	-0.210377	0.328976	-1.848063
11	1	0	0.981636	0.730464	3.992580
12	1	0	3.369316	-1.863171	1.520965
13	1	0	2.213021	-1.422829	3.666155
14	17	0	1.681994	-0.777165	-2.246646
15	17	0	4.606085	-1.426233	-0.867729
16	8	0	-0.923283	0.996146	-1.724638
17	1	0	-1.782743	1.581311	-0.305724
18	1	0	-1.803251	0.521829	-2.026177
19	1	0	3.591741	0.680384	-1.281391
20	8	0	-1.119871	4.251860	-0.659745
21	1	0	-1.236974	5.151378	-0.324292
22	1	0	-1.749326	3.666063	-0.169996
23	8	0	-2.409933	2.051143	0.303453
24	1	0	-2.239924	1.661160	1.189095
25	11	0	-0.248001	-1.320337	1.401000
26	11	0	0.412238	2.797097	-1.499324
27	1	0	-3.558312	-0.026909	-2.965097
28	8	0	-3.130373	-0.206854	-2.116087
29	1	0	-2.924244	-1.699057	-1.902106
30	8	0	-2.792549	-2.666063	-1.529533
31	1	0	-2.957000	-3.286233	-2.255471
32	17	0	-2.419035	-0.312678	2.355301
33	1	0	-1.138664	-2.712781	-0.857989
34	8	0	-0.265170	-2.594368	-0.407591
35	1	0	0.354664	-2.277640	-1.097857
36	1	0	-4.077259	-2.462023	-0.200725
37	8	0	-4.644259	-1.972314	0.439899
38	1	0	-4.217799	-2.084966	1.306906
39	11	0	-3.922234	0.164733	-0.060589

SCF Done: E(RB3LYP) = -2747.23466823 A.U. after 1 cycles
Zero-point correction= 0.268875 (Hartree/Particle)
Thermal correction to Energy= 0.302159
Thermal correction to Enthalpy= 0.303103
Thermal correction to Gibbs Free Energy= 0.200442
Sum of electronic and zero-point Energies= -2746.965793
Sum of electronic and thermal Energies= -2746.932509
Sum of electronic and thermal Enthalpies= -2746.931565
Sum of electronic and thermal Free Energies= -2747.034226

Int6 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.int6.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.100898	-1.076154	0.281371
2	8	0	2.892923	-1.335551	0.131374
3	6	0	5.057501	-2.116184	0.631580
4	6	0	4.655831	0.307427	0.113297
5	6	0	6.381215	-1.837760	0.784045
6	6	0	6.079006	0.522995	0.290024
7	6	0	6.907455	-0.503650	0.611312
8	1	0	4.660954	-3.118767	0.760049
9	6	0	3.770635	1.295733	-0.195642
10	1	0	-1.057308	-0.090360	0.874349
11	1	0	7.071359	-2.637737	1.043307
12	1	0	6.466977	1.528287	0.160852
13	1	0	7.971741	-0.333066	0.742889
14	17	0	0.198984	1.272102	-0.638131
15	17	0	4.204113	2.943878	-0.429241
16	8	0	-1.236480	-1.040748	1.019427
17	1	0	-2.137240	-1.758853	-0.302048
18	1	0	-2.075118	-1.087042	1.624011
19	1	0	2.702965	1.122557	-0.318069
20	8	0	-0.130694	-3.067003	-1.580917
21	1	0	0.111294	-3.529922	-2.394942
22	1	0	-1.116735	-2.985413	-1.568141
23	8	0	-2.664982	-2.239200	-0.995021
24	1	0	-2.934107	-1.540108	-1.633762
25	11	0	-2.310251	1.872173	-1.096985
26	11	0	0.699137	-1.397702	-0.252145
27	1	0	-3.571517	-1.689477	2.959465
28	8	0	-3.522635	-1.120260	2.178238
29	1	0	-4.088778	0.228430	2.451049
30	8	0	-4.529108	1.186609	2.423757
31	1	0	-4.782228	1.427708	3.327034
32	17	0	-4.183202	0.314185	-1.993598
33	1	0	-3.450392	2.237058	1.538525
34	8	0	-2.806031	2.712580	0.950475
35	1	0	-2.024786	2.890791	1.495316

36	1	0	-5.887645	0.666543	1.253174
37	8	0	-6.325482	0.124599	0.557163
38	1	0	-6.195203	0.617680	-0.272595
39	11	0	-4.619592	-1.409358	0.233141

SCF Done: E(RB3LYP) = -2747.26147853 A.U. after 1 cycles
Zero-point correction= 0.268613 (Hartree/Particle)
Thermal correction to Energy= 0.303325
Thermal correction to Enthalpy= 0.304269
Thermal correction to Gibbs Free Energy= 0.196637
Sum of electronic and zero-point Energies= -2746.992865
Sum of electronic and thermal Energies= -2746.958153
Sum of electronic and thermal Enthalpies= -2746.957209
Sum of electronic and thermal Free Energies= -2747.064841

TS6 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.ts6.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.054669	0.034383	1.488935
2	8	0	-3.087329	-0.008264	0.766160
3	6	0	-2.137726	0.025087	2.931083
4	6	0	-0.694227	0.012582	0.898246
5	6	0	-1.023242	-0.193498	3.692284
6	6	0	0.432165	-0.274708	1.750983
7	6	0	0.274379	-0.374706	3.102156
8	1	0	-3.125587	0.120011	3.371855
9	6	0	-0.602628	0.305337	-0.438928
10	1	0	-1.462548	0.623679	-1.011962
11	1	0	-1.117349	-0.252805	4.774514
12	1	0	1.417942	-0.374934	1.310276
13	1	0	1.130472	-0.574233	3.739772
14	17	0	-1.335746	-3.406725	-0.660338
15	17	0	0.767206	-0.055966	-1.429692
16	8	0	-0.072422	2.742837	-0.556280
17	11	0	-3.207695	-1.623193	-0.869196
18	8	0	-3.955857	-0.109245	-2.336204
19	1	0	-4.294805	-0.047317	-3.239942
20	1	0	-4.184335	0.753163	-1.873527
21	1	0	-4.216789	1.453870	0.040974
22	8	0	-4.458908	1.971295	-0.750299
23	1	0	-3.802820	2.714338	-0.755372
24	1	0	-1.554715	3.481617	-0.489111
25	8	0	-2.481394	3.861540	-0.591061
26	1	0	-2.544645	4.616837	0.010206
27	1	0	1.013955	2.608749	0.092059
28	8	0	2.019684	2.404835	0.654082
29	1	0	1.826058	2.519505	1.596513
30	11	0	1.112707	-2.872212	-0.116006
31	17	0	3.480573	-1.921699	0.365798

32	1	0	0.188639	2.952580	-1.468166
33	1	0	4.121428	-1.115647	-1.669428
34	8	0	4.108171	-0.261313	-2.155289
35	1	0	4.872702	-0.257543	-2.749367
36	1	0	3.560368	3.153678	0.247554
37	8	0	4.495455	2.947272	-0.021205
38	1	0	4.878683	3.731970	-0.435732
39	11	0	3.557286	0.843459	-0.179068

SCF Done: E(RB3LYP) = -2747.20921913 A.U. after 1 cycles
Zero-point correction= 0.262241 (a.u.)
Thermal correction to Energy= 0.298085
Thermal correction to Enthalpy= 0.299029
Thermal correction to Gibbs Free Energy= 0.189230
Sum of electronic and zero-point Energies= -2746.946978
Sum of electronic and thermal Energies= -2746.911134
Sum of electronic and thermal Enthalpies= -2746.910190
Sum of electronic and thermal Free Energies= -2747.019989

Int7 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.int7.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.521382	-0.256771	1.080615
2	8	0	0.420232	0.478855	0.517482
3	6	0	-1.222317	0.191977	2.231484
4	6	0	-0.877477	-1.541752	0.550543
5	6	0	-2.178016	-0.608081	2.859838
6	6	0	-1.824258	-2.332505	1.210108
7	6	0	-2.478576	-1.880552	2.359913
8	1	0	-0.969785	1.172183	2.628948
9	6	0	-0.164013	-1.932124	-0.724854
10	8	0	1.158146	-2.260638	-0.514977
11	1	0	-2.685149	-0.237042	3.747666
12	1	0	-2.062894	-3.312414	0.809182
13	1	0	-3.211637	-2.511811	2.853173
14	1	0	1.687457	-1.972859	-1.317948
15	1	0	-0.250217	-1.148703	-1.478043
16	17	0	-1.060808	-3.346073	-1.611896
17	11	0	2.332811	-0.710328	0.908136
18	8	0	0.686208	1.176535	-2.075581
19	1	0	0.458335	0.755786	-1.206619
20	1	0	-0.135492	1.599082	-2.383238
21	8	0	2.538423	-0.949208	-2.408078
22	1	0	1.971801	-0.173141	-2.605043
23	1	0	3.322014	-0.564746	-1.959194
24	8	0	4.028908	-1.184506	2.384117
25	1	0	4.522463	-1.940239	2.733777
26	1	0	4.641607	-0.685168	1.800359
27	17	0	4.426384	0.558173	-0.173197

28	1	0	3.448159	2.433466	0.183798
29	8	0	2.854555	3.211019	0.354834
30	1	0	3.430216	3.988896	0.341327
31	11	0	0.711756	2.690839	-0.046420
32	1	0	-5.441823	2.641046	0.453151
33	8	0	-4.525187	2.339295	0.525421
34	1	0	-3.955925	3.029307	0.121746
35	11	0	-2.975107	0.724863	0.029120
36	8	0	-3.369697	-0.822551	-1.629973
37	1	0	-2.914215	-1.685033	-1.682188
38	1	0	-3.642036	-0.612879	-2.536315
39	17	0	-1.819305	3.006346	-0.858176

SCF Done: E(RB3LYP) = -2747.28337253 A.U. after 2 cycles
Zero-point correction= 0.269811 (Hartree/Particle)
Thermal correction to Energy= 0.305606
Thermal correction to Enthalpy= 0.306550
Thermal correction to Gibbs Free Energy= 0.198484
Sum of electronic and zero-point Energies= -2747.013562
Sum of electronic and thermal Energies= -2746.977767
Sum of electronic and thermal Enthalpies= -2746.976823
Sum of electronic and thermal Free Energies= -2747.084889

TS7 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.ts7.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.382860	1.476518	0.108005
2	8	0	0.554227	2.333818	-0.931595
3	6	0	0.344011	2.006987	1.412259
4	6	0	0.202731	0.078222	-0.071627
5	6	0	0.159277	1.175395	2.519564
6	6	0	0.047377	-0.737886	1.055810
7	6	0	0.013263	-0.202483	2.343802
8	1	0	0.530096	3.071068	1.535058
9	6	0	0.344650	-0.438623	-1.490324
10	8	0	1.627860	-0.668717	-1.868214
11	1	0	0.177575	1.600752	3.519588
12	1	0	-0.038820	-1.812269	0.920767
13	1	0	-0.089661	-0.858928	3.202276
14	1	0	1.980649	0.290578	-2.327838
15	1	0	-0.178866	0.216817	-2.193199
16	17	0	-0.646871	-2.068350	-1.722328
17	11	0	3.436791	-1.125071	-0.464955
18	8	0	2.294005	1.577731	-2.482792
19	1	0	1.348988	2.053127	-1.672829
20	1	0	2.243939	1.914610	-3.389498
21	1	0	3.981265	1.230399	-1.721969
22	8	0	4.657724	0.648313	-1.310252
23	1	0	4.785857	0.970008	-0.396020

24	8	0	3.766237	-2.889268	1.015841
25	1	0	4.491168	-3.516147	1.152528
26	1	0	3.943438	-2.123116	1.625137
27	17	0	4.032357	0.028198	1.876533
28	1	0	-0.760424	3.476685	-0.901054
29	8	0	-1.643813	3.808659	-0.587920
30	1	0	-1.915257	4.530997	-1.170453
31	11	0	-2.338690	2.215359	0.818601
32	1	0	-3.263315	-3.083854	2.385783
33	8	0	-3.505083	-2.526986	1.631907
34	1	0	-3.854256	-1.684927	1.986851
35	11	0	-3.050602	-1.708162	-0.433750
36	8	0	-4.796971	-1.149071	-1.773648
37	1	0	-5.487278	-1.375060	-2.413372
38	1	0	-5.145297	-0.440245	-1.196225
39	17	0	-4.201416	0.458475	0.853093

SCF Done: E(RB3LYP) = -2747.23579979 A.U. after 2 cycles
Zero-point correction= 0.262033 (Hartree/Particle)
Thermal correction to Energy= 0.297472
Thermal correction to Enthalpy= 0.298416
Thermal correction to Gibbs Free Energy= 0.187066
Sum of electronic and zero-point Energies= -2746.973767
Sum of electronic and thermal Energies= -2746.938328
Sum of electronic and thermal Enthalpies= -2746.937383
Sum of electronic and thermal Free Energies= -2747.048734

product in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.pro.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.561276	0.735681	0.521046
2	8	0	-2.464059	1.458386	0.890545
3	6	0	-4.819505	1.289657	0.790537
4	6	0	-3.475611	-0.515605	-0.137834
5	6	0	-5.975920	0.597848	0.441705
6	6	0	-4.661813	-1.207613	-0.462020
7	6	0	-5.904170	-0.662082	-0.176354
8	1	0	-4.865721	2.251533	1.291853
9	6	0	-2.177676	-1.057804	-0.532416
10	8	0	-1.996880	-2.190646	-0.989996
11	1	0	-6.945502	1.036562	0.663582
12	1	0	-4.569754	-2.169651	-0.957758
13	1	0	-6.812951	-1.196930	-0.436162
14	1	0	-0.239468	-0.756970	1.845588
15	1	0	-1.315184	-0.381088	-0.434607
16	17	0	1.234912	-0.180116	-1.652716
17	11	0	0.284454	-2.610149	-1.029741
18	8	0	-0.462168	0.182311	2.035960
19	1	0	-1.718731	0.908255	1.296346

20	1	0	0.393723	0.664055	1.967226
21	1	0	-0.048432	-3.157202	1.926704
22	8	0	0.317300	-2.458959	1.360924
23	1	0	1.309513	-2.508020	1.484623
24	8	0	1.943139	-4.155864	-1.103467
25	1	0	2.492969	-4.544374	-1.798912
26	1	0	2.569088	-3.815693	-0.415463
27	17	0	3.350112	-2.586376	1.205585
28	1	0	-1.696313	2.707111	-0.201217
29	8	0	-1.131783	3.268830	-0.778574
30	1	0	-0.927718	4.061876	-0.257813
31	11	0	0.816627	2.386931	-1.544472
32	1	0	5.509512	1.703585	-0.750860
33	8	0	4.666634	1.535138	-0.306657
34	1	0	4.164309	2.385235	-0.313619
35	11	0	3.234360	-0.151544	0.213267
36	8	0	2.120308	1.299446	1.777028
37	1	0	2.549846	1.417602	2.639258
38	1	0	2.187980	2.183090	1.320416
39	17	0	2.461380	3.751419	-0.061862

SCF Done: E(RB3LYP) = -2747.34188870 A.U. after 1 cycles
Zero-point correction= 0.270371 (Hartree/Particle)
Thermal correction to Energy= 0.305578
Thermal correction to Enthalpy= 0.306522
Thermal correction to Gibbs Free Energy= 0.199995
Sum of electronic and zero-point Energies= -2747.071518
Sum of electronic and thermal Energies= -2747.036311
Sum of electronic and thermal Enthalpies= -2747.035367
Sum of electronic and thermal Free Energies= -2747.141894

TS8 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.ts8.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.716615	-1.464193	0.628490
2	8	0	-0.871720	-1.109647	1.444392
3	6	0	-1.613488	-2.725440	-0.106866
4	6	0	-3.012434	-0.630957	0.407743
5	6	0	-2.671530	-3.213065	-0.792651
6	6	0	-4.104529	-1.264867	-0.347129
7	6	0	-3.924879	-2.478944	-0.909575
8	1	0	-0.666310	-3.249198	-0.015789
9	6	0	-2.905487	0.728974	0.798192
10	1	0	-3.223763	-0.271628	1.635902
11	1	0	-2.595204	-4.176871	-1.289371
12	1	0	-5.028951	-0.712926	-0.474160
13	1	0	-4.725638	-2.921405	-1.496643
14	17	0	2.572320	3.448906	-0.879017
15	17	0	-4.329980	1.710688	0.440527

16	17	0	-0.487888	-0.110367	-2.012287
17	11	0	1.855946	-1.175371	-1.399235
18	11	0	0.255914	2.165955	-0.958253
19	1	0	0.883908	4.385555	0.006176
20	8	0	-0.077234	4.371935	0.266284
21	1	0	-0.401963	5.281952	0.197715
22	8	0	2.571099	0.469490	0.097522
23	1	0	3.428930	0.016481	0.396916
24	1	0	2.789657	1.393370	-0.176325
25	1	0	-1.258477	1.540039	1.333396
26	8	0	-0.314477	1.863170	1.400056
27	1	0	-0.344913	2.841293	1.426686
28	11	0	1.085373	0.103637	1.813500
29	8	0	4.397020	-1.183415	0.913515
30	1	0	5.275401	-0.921744	1.223546
31	1	0	3.378051	-1.481977	1.946920
32	8	0	2.464864	-1.630691	2.455521
33	1	0	2.655155	-2.107314	3.276306
34	1	0	4.274000	-1.928062	-0.467872
35	8	0	3.888873	-2.349942	-1.323005
36	1	0	4.631850	-2.556372	-1.907461
37	8	0	1.610047	-3.016332	0.136677
38	1	0	2.465439	-3.333543	-0.211389
39	1	0	1.813601	-2.696552	1.045601

SCF Done: E(RB3LYP) = -2747.13248383 A.U. after 1 cycles
Zero-point correction= 0.262124 (Hartree/Particle)
Thermal correction to Energy= 0.296007
Thermal correction to Enthalpy= 0.296952
Thermal correction to Gibbs Free Energy= 0.195062
Sum of electronic and zero-point Energies= -2746.870360
Sum of electronic and thermal Energies= -2746.836477
Sum of electronic and thermal Enthalpies= -2746.835532
Sum of electronic and thermal Free Energies= -2746.937422

TS9 in Figure 1
Stoichiometry C7H18CL3NA3O8 %chk=reimer.na.ts9.chk
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.429858	1.773262	-0.202734
2	8	0	-1.758246	0.526877	0.027993
3	6	0	-1.147062	2.676743	0.872302
4	6	0	-1.261155	2.277026	-1.526400
5	6	0	-0.742183	3.997478	0.627602
6	6	0	-0.842307	3.580193	-1.748751
7	6	0	-0.571145	4.454631	-0.674800
8	1	0	-1.343680	2.336960	1.886092
9	6	0	1.137243	1.121680	1.087284
10	1	0	-1.436244	1.602724	-2.362519
11	1	0	-0.555413	4.661629	1.468591

12	1	0	-0.711112	3.931132	-2.770130
13	1	0	-0.243872	5.472208	-0.867246
14	17	0	1.380374	-1.651547	0.860930
15	17	0	1.532881	1.343245	2.715412
16	17	0	2.181072	1.621619	-0.107651
17	1	0	0.208980	0.633134	0.833792
18	11	0	-1.281653	-1.627208	0.698963
19	11	0	3.655470	-1.792939	-0.554376
20	8	0	-3.218579	-2.474347	-0.430669
21	1	0	-2.947704	-3.131279	-1.089478
22	8	0	5.801706	-1.117329	-0.600920
23	1	0	6.557245	-0.812078	-0.083346
24	1	0	-3.036929	-3.015366	1.176781
25	8	0	-2.640029	-2.891627	2.088713
26	1	0	-2.523900	-3.762674	2.493223
27	1	0	-4.852301	-2.698004	-0.446049
28	8	0	-5.863396	-2.658775	-0.527037
29	1	0	-6.225042	-2.927010	0.330515
30	1	0	5.663638	-2.643091	-1.106151
31	8	0	5.079161	-3.448658	-1.330121
32	1	0	5.408151	-3.834718	-2.152766
33	1	0	4.960220	-0.131865	-1.415754
34	8	0	4.088543	0.224815	-1.855737
35	1	0	4.268115	0.300960	-2.803757
36	1	0	-6.494461	0.267700	-1.866600
37	8	0	-5.797758	-0.121709	-1.321132
38	1	0	-6.080487	-1.044455	-1.069496
39	11	0	-3.611196	-0.319157	-0.884515

SCF Done: E(RB3LYP) = -2747.10382284 A.U. after 1 cycles
Zero-point correction= 0.261809 (Hartree/Particle)
Thermal correction to Energy= 0.297422
Thermal correction to Enthalpy= 0.298366
Thermal correction to Gibbs Free Energy= 0.185365
Sum of electronic and zero-point Energies= -2746.842014
Sum of electronic and thermal Energies= -2746.806401
Sum of electronic and thermal Enthalpies= -2746.805456
Sum of electronic and thermal Free Energies= -2746.918458

Results of IRC calculations starting from the B3LYP/6-31+G(d) TS geomerty.

Int2 (Na^+)
Stoichiometry C7H18Cl3Na3O8
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.135544	1.058619	-0.737511
2	8	0	-0.107196	0.788855	-0.406763
3	6	0	1.566074	1.121794	-2.093539
4	6	0	2.130717	1.308086	0.259833

5	6	0	2.878756	1.435502	-2.419693
6	6	0	3.445809	1.655021	-0.086944
7	6	0	3.835086	1.711568	-1.422597
8	1	0	0.842028	0.909791	-2.876903
9	6	0	2.531659	-1.530020	0.608639
10	1	0	1.832508	1.264483	1.305419
11	1	0	3.171702	1.469398	-3.467016
12	1	0	4.169753	1.850305	0.701702
13	1	0	4.856340	1.963197	-1.693564
14	17	0	3.543782	-1.889921	-0.742207
15	17	0	3.476307	-1.480908	2.087489
16	17	0	-1.403662	-2.433271	-1.549830
17	11	0	-1.229238	2.302152	0.910726
18	11	0	-0.035344	-1.414685	0.452904
19	8	0	-1.349677	-1.724692	2.317701
20	1	0	-1.553049	-2.632855	2.586074
21	1	0	-2.242666	-1.271687	2.179839
22	8	0	-1.772469	1.445169	2.942103
23	1	0	-2.483223	0.793333	2.651023
24	1	0	-1.185454	0.930499	3.515601
25	1	0	1.172628	3.540539	0.312910
26	8	0	0.342866	3.957542	0.612678
27	1	0	0.583880	4.822748	0.974955
28	11	0	-1.993312	0.137841	-1.577869
29	8	0	-3.507634	-0.266007	1.834959
30	1	0	-4.286062	-0.313147	2.410833
31	1	0	-3.475586	0.888429	0.722779
32	8	0	-3.182167	1.557516	0.010838
33	1	0	-3.926165	1.643800	-0.609665
34	1	0	-4.067769	-1.251402	0.459025
35	8	0	-4.331901	-1.668655	-0.405041
36	1	0	-3.560656	-2.211098	-0.678495
37	8	0	-4.268518	0.265403	-2.236693
38	1	0	-4.462324	-0.499820	-1.613727
39	1	0	-4.756641	0.090350	-3.054237

SCF Done: E(RB3LYP) = -2747.15230193 A.U. after 1 cycles
Zero-point correction= 0.265451 (Hartree/Particle)
Thermal correction to Energy= 0.300841
Thermal correction to Enthalpy= 0.301785
Thermal correction to Gibbs Free Energy= 0.194597
Sum of electronic and zero-point Energies= -2746.886851
Sum of electronic and thermal Energies= -2746.851461
Sum of electronic and thermal Enthalpies= -2746.850517
Sum of electronic and thermal Free Energies= -2746.957705

TS2 (Na^+)
Stoichiometry C7H18Cl3Na3O8
Standard orientation:

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

1	6	0	1.197500	-1.034176	0.453262
2	8	0	-0.057557	-0.725192	0.326949
3	6	0	1.714937	-1.680354	1.611074
4	6	0	2.144531	-0.697689	-0.593966
5	6	0	3.057834	-2.024380	1.696654
6	6	0	3.485699	-1.174117	-0.516109
7	6	0	3.956617	-1.780087	0.630815
8	1	0	1.039062	-1.886942	2.438139
9	6	0	2.281129	1.372603	-0.245160
10	1	0	1.730224	-0.481637	-1.574800
11	1	0	3.424800	-2.500409	2.603517
12	1	0	4.153464	-0.981713	-1.351221
13	1	0	4.998120	-2.073892	0.719062
14	17	0	3.148893	1.611575	1.289841
15	17	0	3.327156	1.957221	-1.596141
16	17	0	-1.756865	3.588677	0.346415
17	11	0	-1.064922	-2.244218	-1.177895
18	11	0	-0.249786	1.608349	-0.426524
19	8	0	-1.868797	1.507425	-2.138731
20	1	0	-2.101129	2.419084	-1.870113
21	1	0	-2.654194	0.963055	-1.874034
22	8	0	-2.029485	-1.397439	-3.036326
23	1	0	-2.814497	-1.003197	-2.549814
24	1	0	-1.654544	-0.644118	-3.520382
25	1	0	1.130527	-3.621992	-0.033782
26	8	0	0.447555	-3.909390	-0.666528
27	1	0	0.781158	-4.720914	-1.077717
28	11	0	-1.934199	-0.731517	1.655556
29	8	0	-3.787892	-0.308545	-1.327934
30	1	0	-4.704701	-0.264484	-1.638580
31	1	0	-3.465767	-1.450429	-0.463340
32	8	0	-2.959602	-2.165998	0.136520
33	1	0	-3.597207	-2.858419	0.361974
34	1	0	-3.660206	0.684061	0.160628
35	8	0	-3.304444	1.015286	1.027587
36	1	0	-2.942425	1.927390	0.857695
37	8	0	-3.228471	-0.121081	3.453722
38	1	0	-3.587083	0.534811	2.811310
39	1	0	-3.283712	0.272603	4.335505

SCF Done: E(RB+HF-LYP) = -2747.13915723 A.U. after 1 cycles
Zero-point correction= 0.264407 (Hartree/Particle)
Thermal correction to Energy= 0.299001
Thermal correction to Enthalpy= 0.299945
Thermal correction to Gibbs Free Energy= 0.194439
Sum of electronic and zero-point Energies= -2746.874750
Sum of electronic and thermal Energies= -2746.840157
Sum of electronic and thermal Enthalpies= -2746.839212
Sum of electronic and thermal Free Energies= -2746.944718

Int3 (Na^+)
Stoichiometry C7H18Cl3Na3O8
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.424217	-1.423970	-1.061787
2	8	0	0.402393	-0.928725	-1.595100
3	6	0	1.476929	-2.793523	-0.615426
4	6	0	2.644205	-0.536938	-0.848501
5	6	0	2.622737	-3.301896	-0.072511
6	6	0	3.845204	-1.221107	-0.285316
7	6	0	3.823242	-2.517871	0.096830
8	1	0	0.577467	-3.394415	-0.706085
9	6	0	2.130244	0.747829	-0.081475
10	1	0	2.905823	-0.112375	-1.830342
11	1	0	2.632394	-4.338445	0.258865
12	1	0	4.733715	-0.611122	-0.148452
13	1	0	4.696473	-2.984160	0.544845
14	17	0	1.914929	0.211253	1.785819
15	17	0	3.535394	1.964230	-0.059249
16	17	0	-1.944095	-2.370414	1.015268
17	11	0	0.080063	1.562713	-1.259405
18	11	0	-0.709678	-0.463673	2.229128
19	8	0	-2.043485	1.213864	2.872569
20	1	0	-2.570906	1.335967	3.674431
21	1	0	-2.625472	1.495693	2.086430
22	8	0	-0.773429	2.994418	0.486258
23	1	0	-1.733463	2.716352	0.581859
24	1	0	-0.403133	2.946169	1.381481
25	1	0	1.799968	3.753320	-1.388344
26	8	0	0.874395	3.741692	-1.684906
27	1	0	0.347407	3.972140	-0.893829
28	11	0	-1.856867	-1.332154	-1.404312
29	8	0	-3.205867	1.865055	0.628662
30	1	0	-3.892793	2.549185	0.615393
31	1	0	-2.653078	1.393340	-0.797418
32	8	0	-2.150424	1.015883	-1.601120
33	1	0	-2.803070	0.974560	-2.318764
34	1	0	-4.152925	0.365467	0.477927
35	8	0	-4.579365	-0.513264	0.285487
36	1	0	-4.028936	-1.167597	0.761531
37	8	0	-4.005097	-1.150274	-2.251784
38	1	0	-4.387138	-0.915588	-1.353820
39	1	0	-4.650537	-1.724734	-2.687886

SCF Done: E(RB3LYP) = -2747.17054342 A.U. after 1 cycles
Zero-point correction= 0.267479 (Hartree/Particle)
Thermal correction to Energy= 0.301860
Thermal correction to Enthalpy= 0.302805
Thermal correction to Gibbs Free Energy= 0.199615
Sum of electronic and zero-point Energies= -2746.903064
Sum of electronic and thermal Energies= -2746.868683
Sum of electronic and thermal Enthalpies= -2746.867739
Sum of electronic and thermal Free Energies= -2746.970928