

Supporting Information for

**A DFT-metadynamics study disclosing key properties of ring-opening  
polymerization catalysts to produce polyethercarbonate polyols from cyclic  
ethylene carbonate as part of an emerging CCU technology**

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Gürtler\*, Martin R. Machat\*

### Metadynamics parameters for proton transfer

UNITS LENGTH= Å TIME=ps ENERGY=kcal/mol  
PACE=25 for the first run; PACE=100 for the second run

d1: DISTANCE ATOMS=atom1,atom2 (H $\cdots$ O distance (in ROH starter molecule))  
d2: DISTANCE ATOMS=atom1,atom2 (RO $\cdots$ C=O distance (alkoxide – C=O))

METAD ARG=d1,d2 SIGMA=0.4,0.4 HEIGHT=0.35 LABEL=restraint

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LABEL=uwall1

UPPER\_WALLS ARG=d2 AT=2.5 KAPPA=250.0 EXP=2 EPS=1 OFFSET=0  
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### Metadynamics parameters for ring opening of cEC

UNITS LENGTH= Å TIME=ps ENERGY=kcal/mol  
PACE=25 for the first run; PACE=100 for the second run

d1: DISTANCE ATOMS=atom1,atom2 (RO $\cdots$ C=O (alkoxide – C=O and cEC ring))  
d2: DISTANCE ATOMS=atom1,atom2 (O $\cdots$ C=O distance (first cEC ring))

METAD ARG=d1,d2 SIGMA=0.4,0.4 HEIGHT=0.35 LABEL=restraint

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UPPER\_WALLS ARG=d2 AT=2.5 KAPPA=250.0 EXP=2 EPS=1 OFFSET=0  
LABEL=uwall2

### Metadynamics parameters for CO<sub>2</sub> release

UNITS LENGTH= Å TIME=ps ENERGY=kcal/mol  
PACE=25 for the first run; PACE=100 for the second run

d1: DISTANCE ATOMS=atom1,atom2 (O $\cdots$ CH<sub>2</sub>-O (negative oxygen of the CAT and CH<sub>2</sub> of cEC))  
d2: DISTANCE ATOMS=atom1,atom2 (O(ethereal) $\cdots$ CH<sub>2</sub> in cEC)

METAD ARG=d1,d2 SIGMA=0.4,0.4 HEIGHT=0.35 LABEL=restraint

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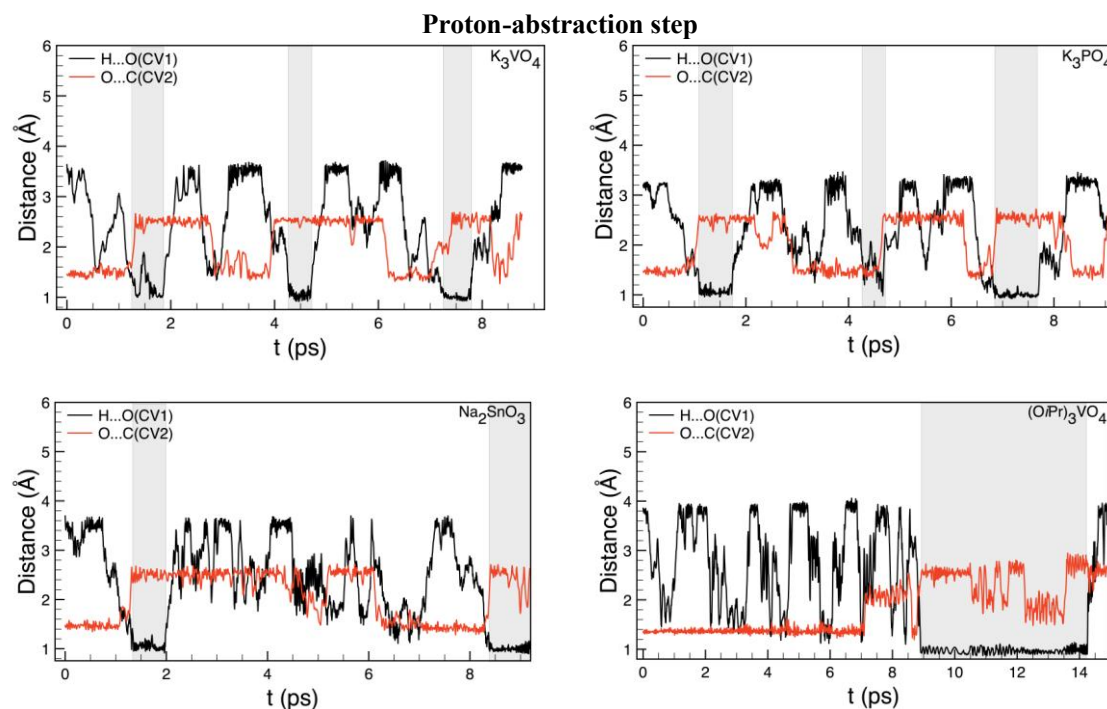
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The constraints of the MTD (harmonic walls) are defined such that the walls are at least 1.2 – 2.5 Å longer than the normal bond length in each case.

The accuracy of the calculated free energies is 10E-9, which is the precision applied by “sumhills” command running in Plumed.

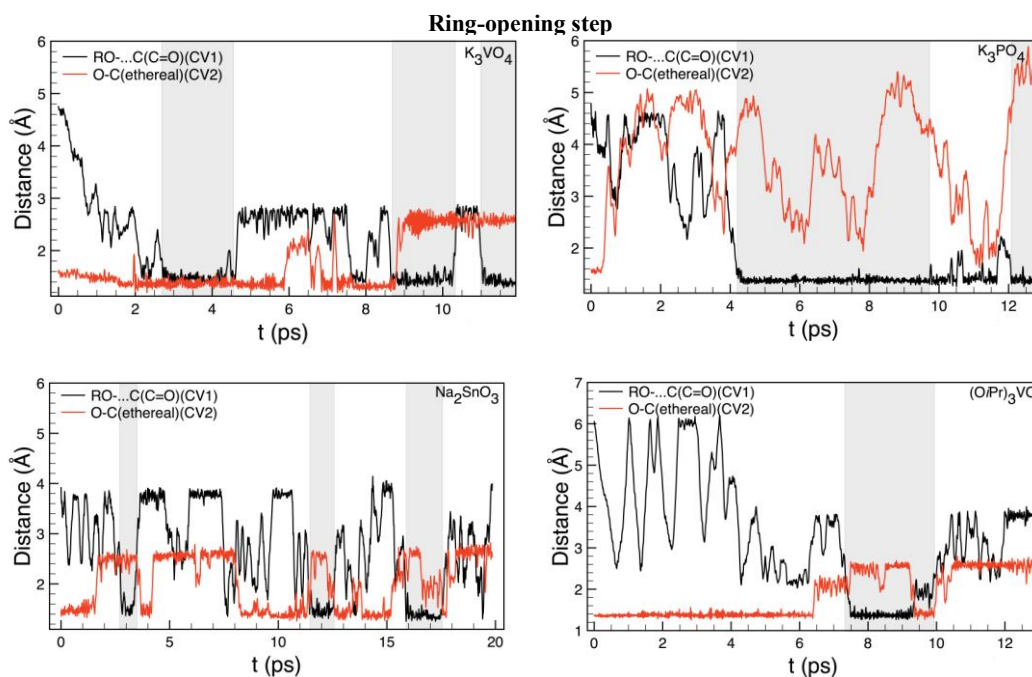
### Variation of the collective variables (CVs) for each step of the reaction

In proton-abstraction step, CV1 is the O...H distance of the ROH (that is elongated in the intermediate structure) and CV2 is the RO...C(C=O) distance with a cEC molecule in the proximity of the alkoxide ion generated from the starter ROH molecule (**Scheme 4**). Variations of the CVs alongside the time evolution of the metadynamics simulations for this step are depicted in **Figure S1**. The regions highlighted with gray in each plot indicate the RO-H bond formation (production of the reactant complex with the ROH molecule). As can be seen in **Figure S1**, multiple transitions between the reactant and intermediate states (bond cleavage and/or formation) can be detected from the CVs behavior.



**Figure S1.** Variation of the two CVs alongside the time evolution for the proton abstraction step; the gray highlighted regions show reactant-complex formation (O...H is ca. 1.0 Å).

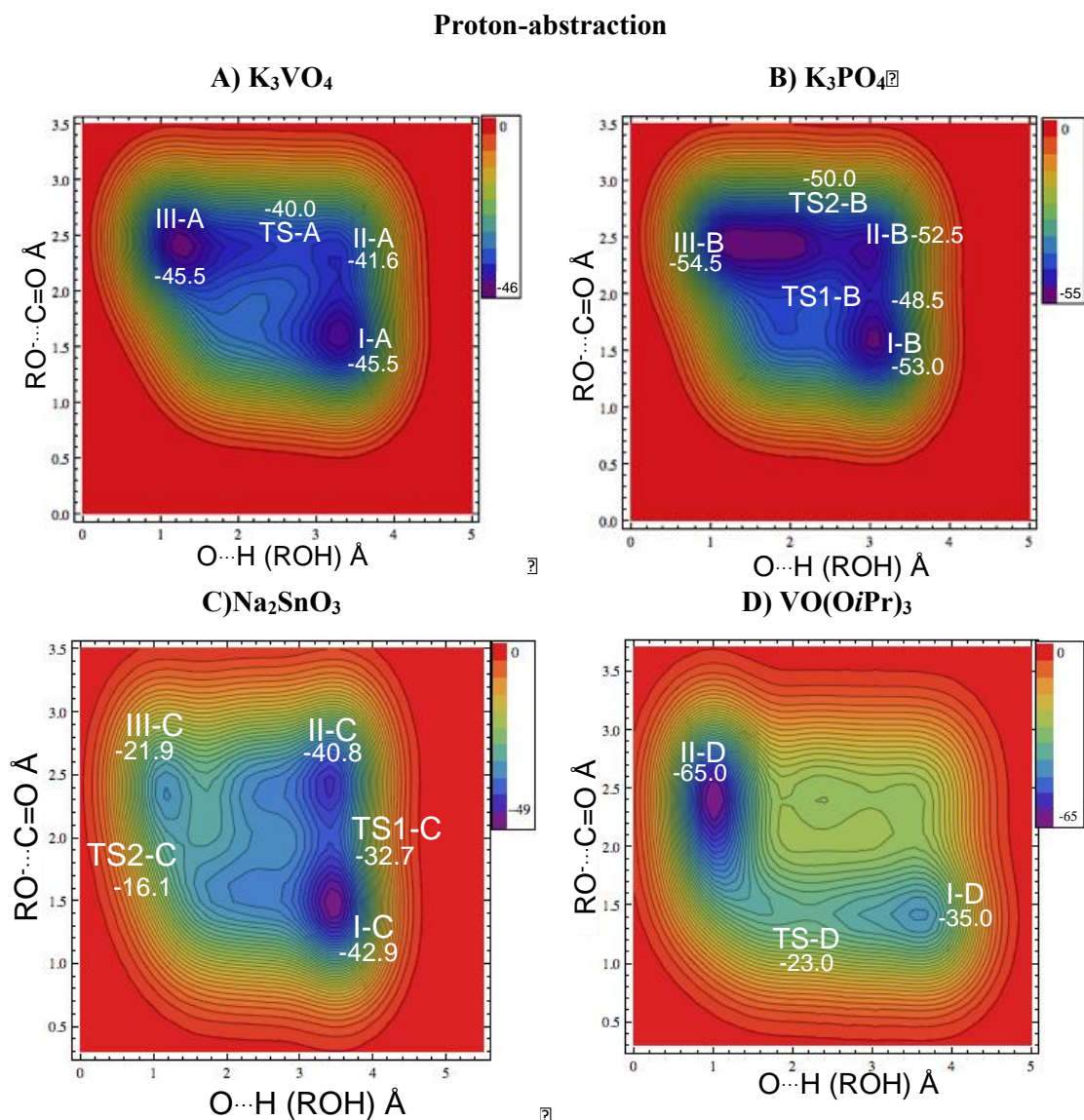
Variations of the CVs alongside the time evolution for ring opening step are depicted in **Figure S2** and the highlighted regions in each plot indicate the RO-C(C=O) bond formation (producing the product-complex with the longer chain, **Scheme 5**). For the ring-opening step, CV1 is the RO<sup>-</sup>...C(C=O) distance, in which the RO<sup>-</sup> is the alkoxide generated from the first cEC and the C=O is from the second cEC ring. CV2 is the distance between the ethereal O and C inside the second cEC (**Scheme 5**). The starting structure has been singled out with the red box (INT) in **Scheme 5**. Multiple transitions between the intermediate and product molecular complexes indicate the convergence of the FES, which are built upon these CVs.



**Figure S2.** Variation of the two CVs alongside the time evolution for the ring-opening step; the gray highlighted regions show product-complex formation (RO<sup>-</sup>...C=O(snd cEC) is ca. 1.4 Å).

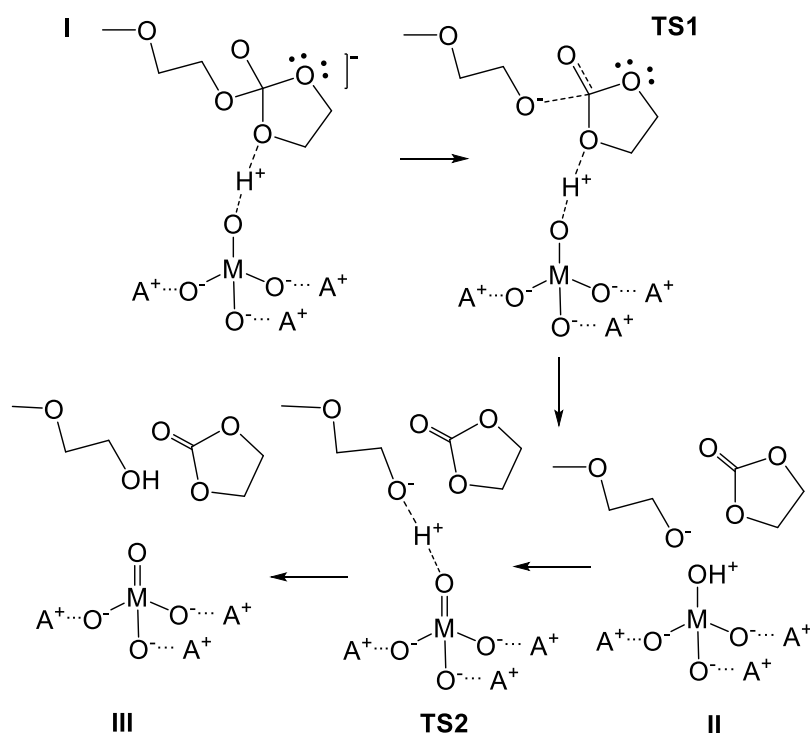
### The calculated FES for each step of the reaction

The FESs in **Figures S3 (A-D)** show position of the intermediates and transition states with related energies (kcal/mol) for the molecular systems including  $\text{K}_3\text{VO}_4$ ,  $\text{K}_3\text{PO}_4$ ,  $\text{Na}_2\text{SnO}_3$ , and  $\text{VO}(\text{O}i\text{Pr})_3$  in the proton-abstraction step. In case of the  $\text{K}_3\text{VO}_4$  and  $\text{K}_3\text{PO}_4$  within the molecular cluster the patterns of the FES are rather similar, in which starting from the intermediate state (**I-A** and **I-B**), first the CV2 increases and then CV1 decreases (RO-H bond formation).



**Figure S3.** Calculated FESs for the proton-abstraction step in molecular systems with  $\text{K}_3\text{VO}_4$ ,  $\text{K}_3\text{PO}_4$ ,  $\text{Na}_2\text{SO}_3$  and  $(\text{O}i\text{Pr})_3\text{VO}$  catalyts.

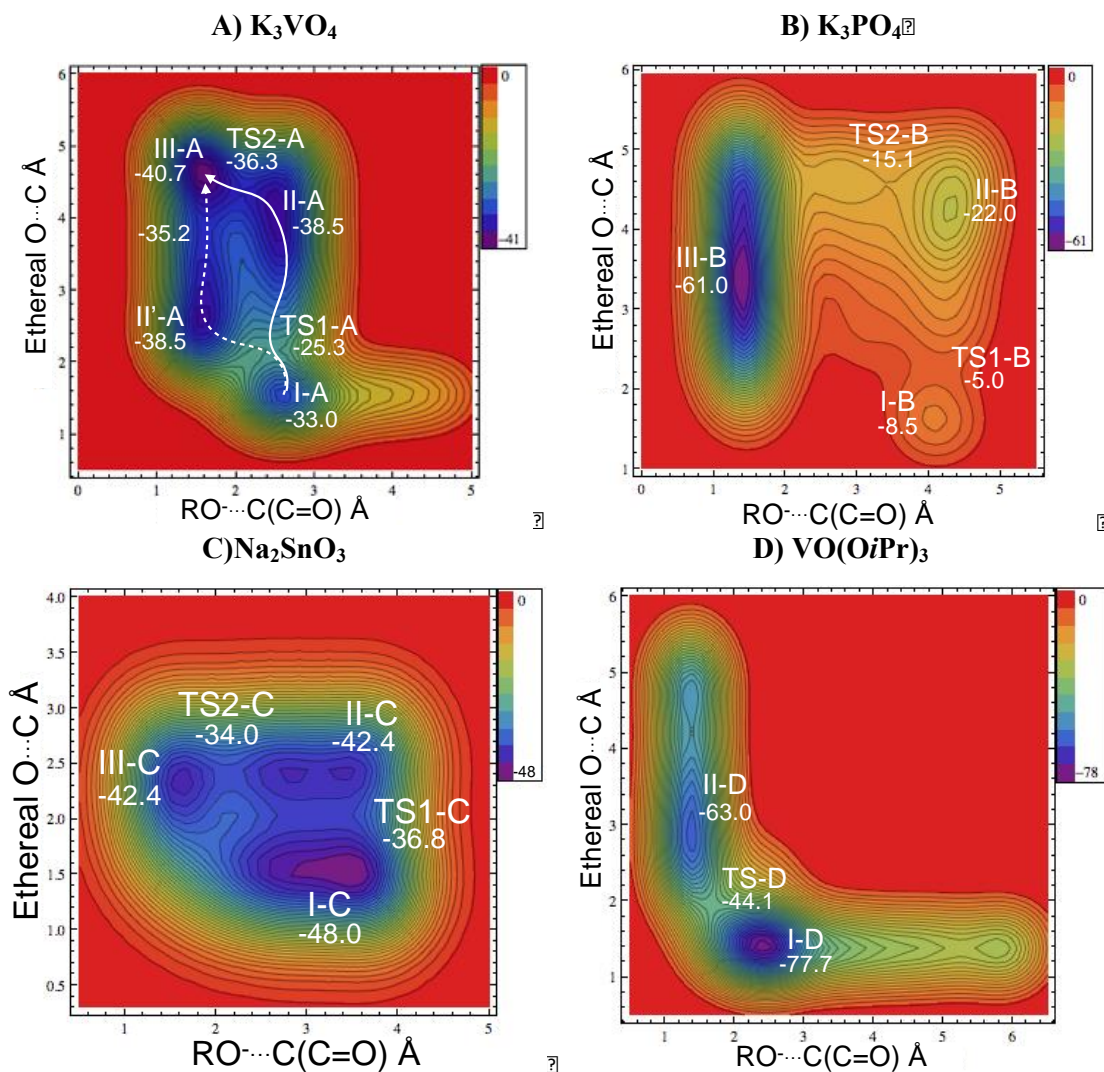
The higher barrier of conversion of the intermediate **II-C** to the ROH (**III-C**) in case of  $\text{Na}_2\text{SO}_3$  in **Figure S3** indicates higher stabilization of the  $\text{RO}^-$  attached to the  $\text{SnO}_3^{2-}$  anion.



**Scheme S1.** Various states in the FES depicted in **S3** (for simplicity only the reactive molecules are shown and the rest of the cluster is omitted).

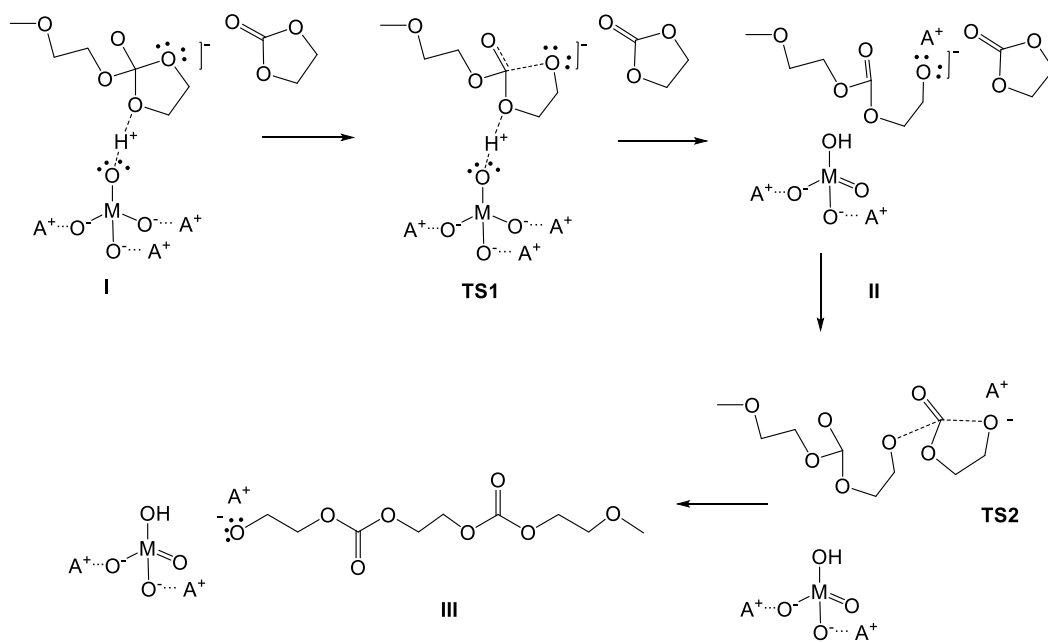
FESs for ring-opening step have been depicted in **Figure S4(A-D)**. The FES for  $K_3VO_4$  (**Figure S4-A**) identifies two pathways with rather similar energies. The first pathway starts from **I-A** and passes throughout the **TS1-A**, intermediate **II-A** and **TS2-A** to the product state **III-A**. The **TS1-A** corresponds to the rate-determining-step with a barrier of 7.7 kcal/mol, which correlates to the C-O(etheral) bond cleavage. The second pathway, which is depicted with dotted line, identifies an additional stable state (**II'-A**). Transition from the intermediate **I-A** to the product **III-A** is an exergonic process with a  $\Delta G$  of 7.7 kcal/mol. The FES of the ring-opening for the  $K_3PO_4$ , which is shown in **Figure S4-B**, indicates barriers of 3.5 and 6.9 kcal/mol for the ring-opening and RO-C bond formation.

## Ring-opening of the cEC



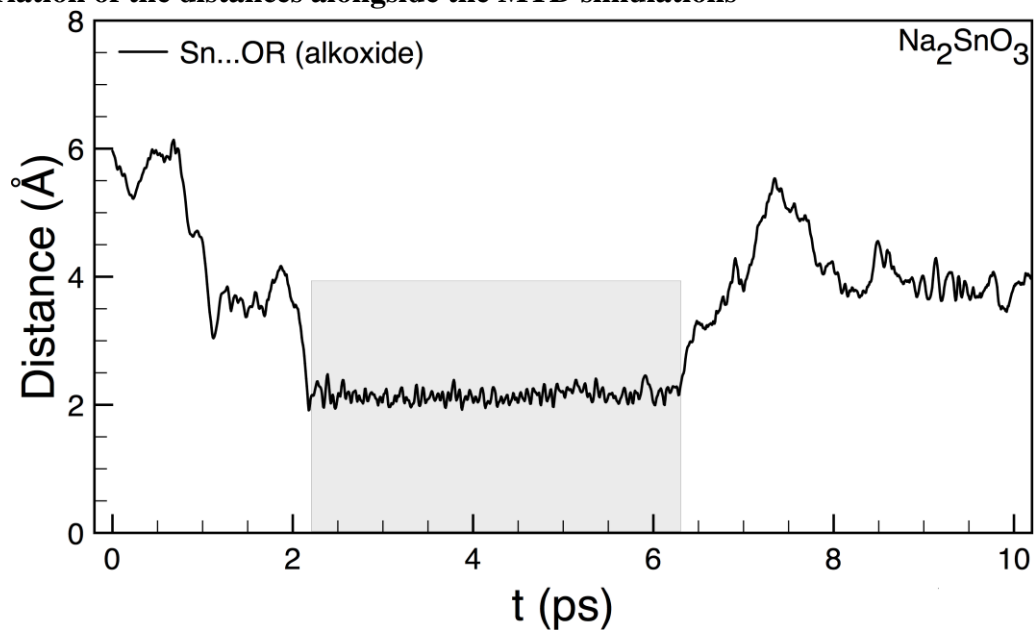
**Figure S4.** Calculated FESs for the ring-opening step in molecular systems with  $K_3VO_4$ ,  $K_3PO_4$ ,  $Na_2SO_3$  and  $(OiPr)_3VO$  catalysts.

In **Figure S4-C** starting from the intermediate state **I-C** and passing through the TS area (**TS1-C**, 11.2 kcal/mol), there is a rather wide flat surface (intermediate **II-C**) with  $RO\cdots C(C=O)$  and ethereal  $O\cdots C$  distance at ca. 3.5 and 2.5 Å. This flat area corresponds to the complexation of the  $RO^-$  to the Sn center (**Figure 2**) that a stable molecular complex is formed with 5.6 kcal/mol higher  $\Delta G$  than the initial state **I-C**. This state then passes through a barrier (**TS2-C**, 8.4 kcal/mol) and the  $RO\cdots C(C=O)$  bond is formed.



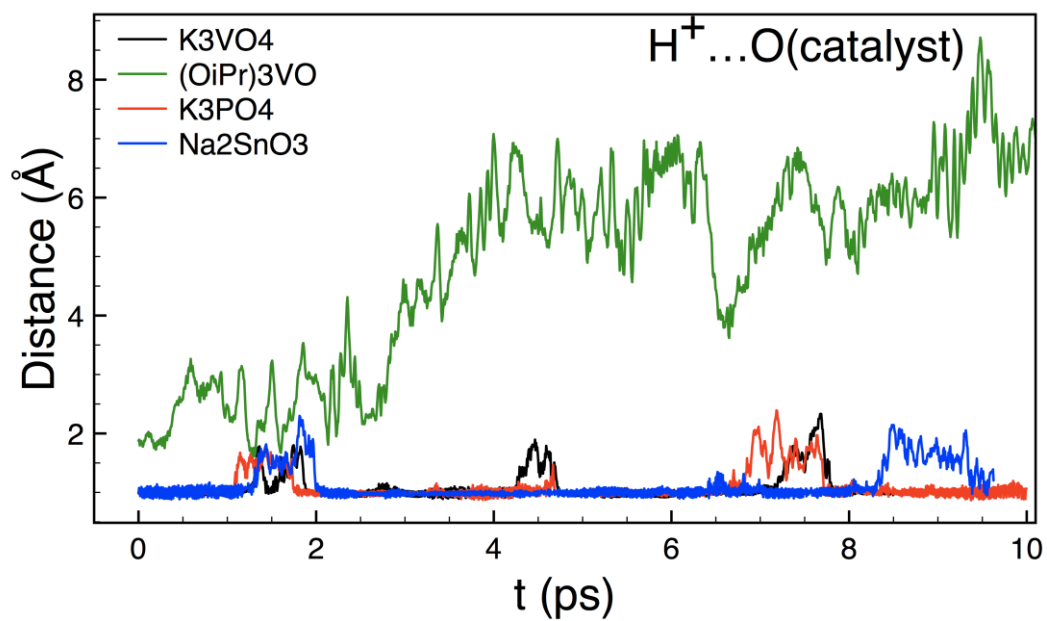
**Scheme S2.** Various states in the FES depicted in **S4** (for simplicity only the reactive molecules are shown and the rest of the cluster is omitted).

#### Variation of the distances alongside the MTD simulations



**Figure S5.** A similar behavior (to the ring opening step) of complexation of the  $\text{RO}^-$  to the Sn center can be detected in proton abstraction step.

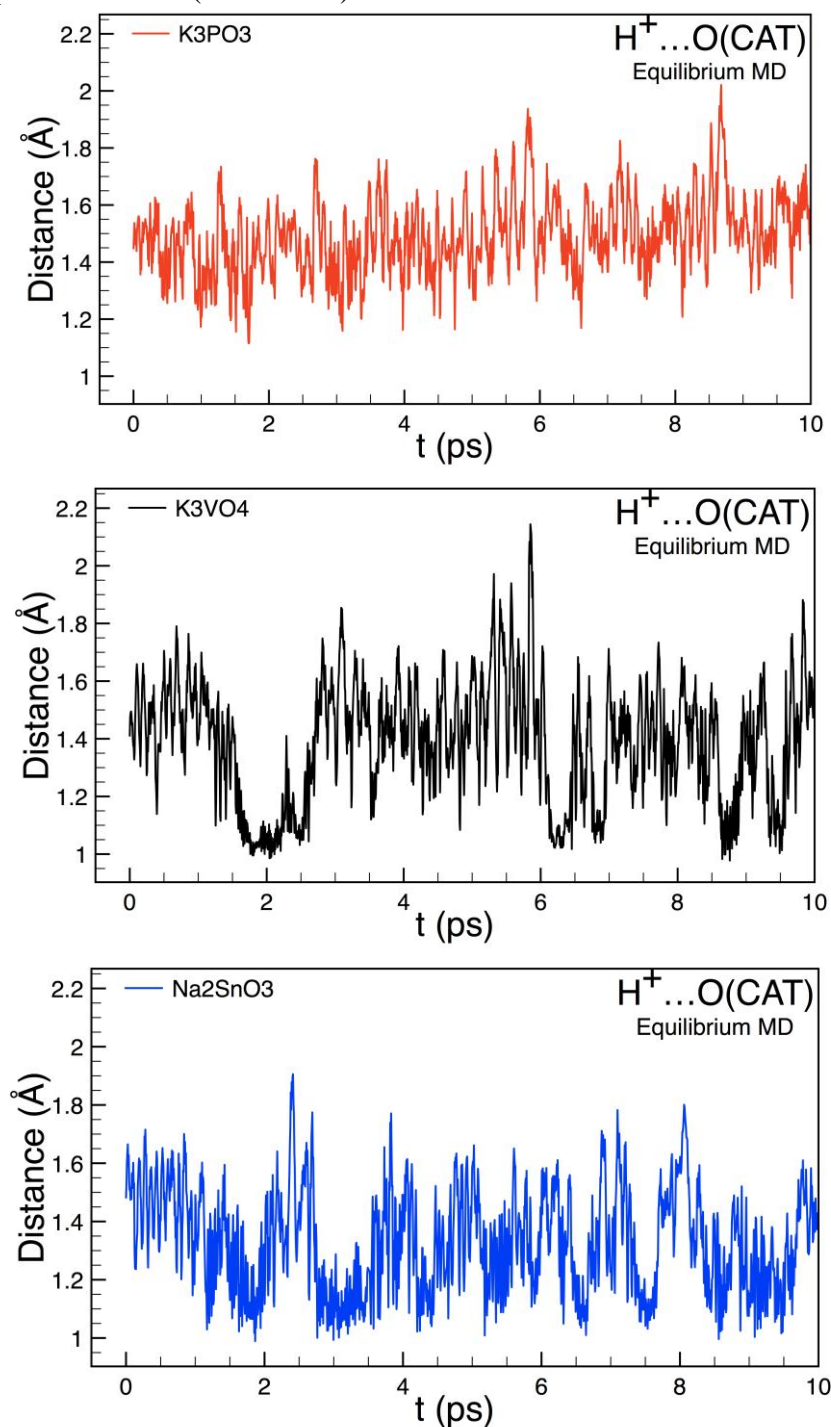




**Figure S6.** H<sup>+</sup>...O(catalyst) distances (Å) vs. simulation time (ps) in the proton abstraction step. The critical H<sup>+</sup>...O(catalyst) distances indicate the role of Brønsted basicity and availability of the anionic oxygen of the catalyst.

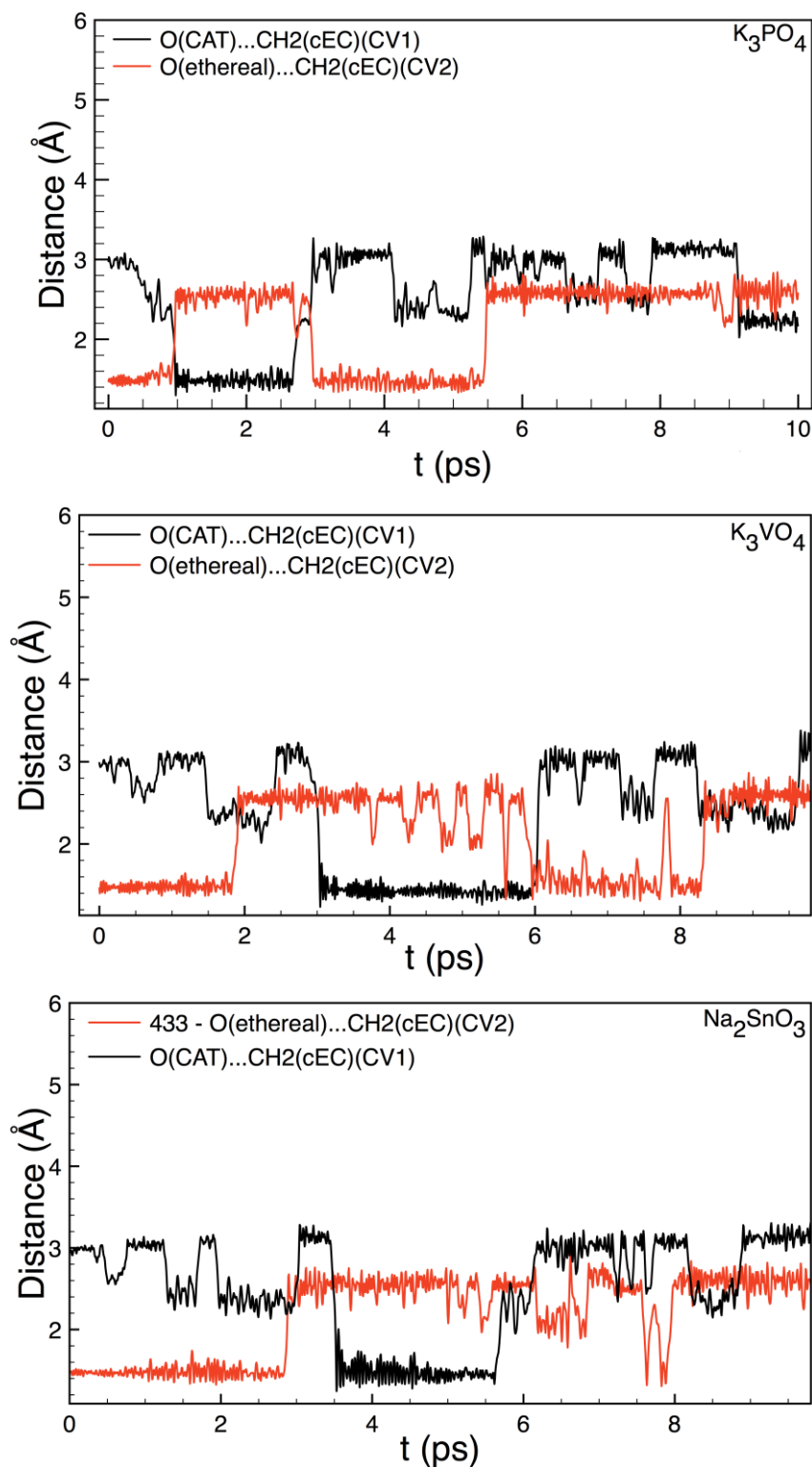
### Unbiased equilibrium DFT-MD simulations

Unbiased equilibrium DFT-MD simulations were performed in order to detect the proton exchange between the oxygen of the catalyst-anions and RO<sup>-</sup> from ROH. By probing the distances between the proton and the two oxygen atoms it is observed that in case of stronger Brønsted basic catalysts, such as K<sub>3</sub>VO<sub>4</sub> and Na<sub>2</sub>SnO<sub>3</sub>, proton exchange occurs between the catalyst-oxygen and alcohol oxygen, which is not the case for K<sub>3</sub>PO<sub>4</sub>. The corresponding behavior is shown in **Figure S7**. As can be seen in Figure S7 the average distance between catalyst and proton never approaches to a complete proton transfer (ca. at 1.0Å).

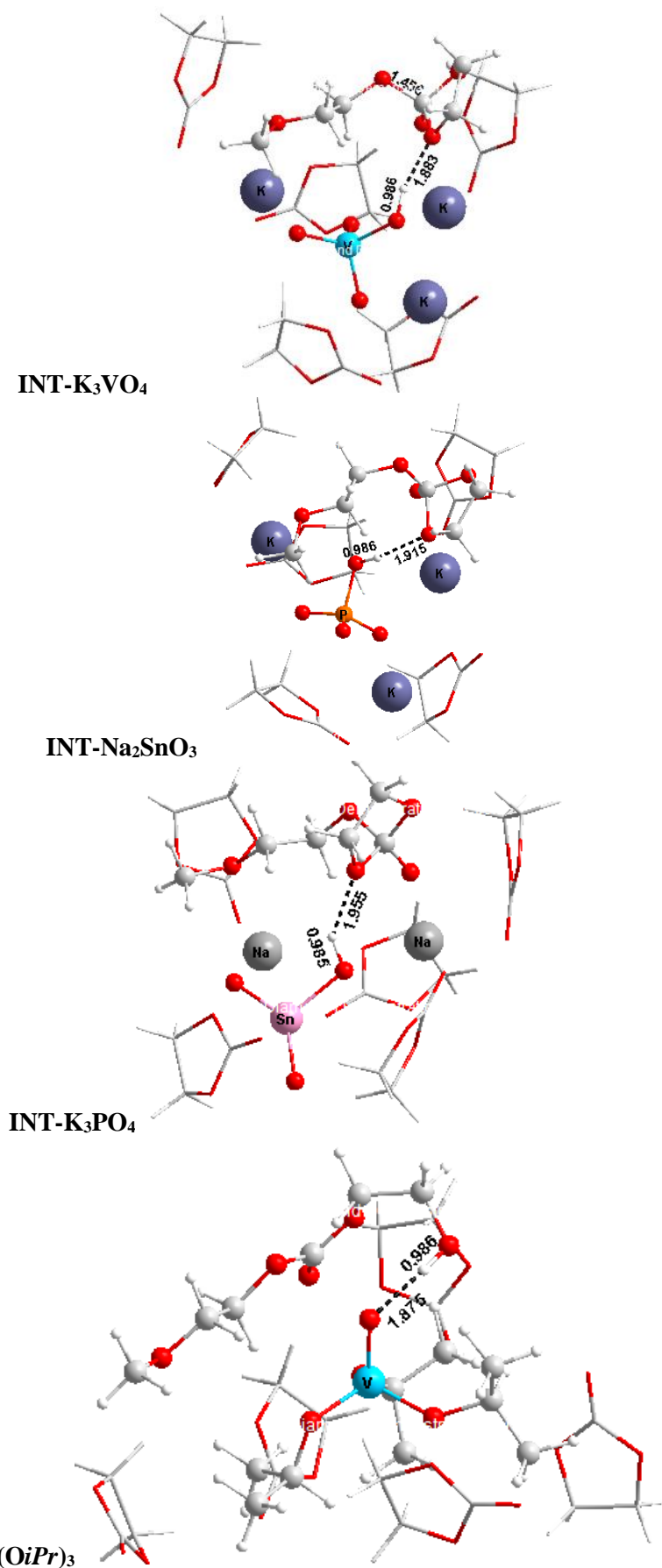


**Figure S7.** Unbiased equilibrium DFT-MD simulations were performed in order to detect the proton exchange between the oxygen of the catalyst-anions and RO<sup>-</sup> from ROH in order to prob the Brønsted basicity of the catalyst anion.

**Variation of the CVs for the CO<sub>2</sub> release mechanism through the nucleophilic attack by the catalyst anion**



**Figure S8.** Variation of the two CVs alongside the time evolution for the CO<sub>2</sub>-release Mech. I.



**Figure S9.** The intermediate structures of all molecular systems with four catalysts. The transferred proton from the ROH has been singled out with light blue. As can be

seen the proton is on the catalyst oxygen except in case of the VO(O*iPr*)<sub>3</sub>. The distances are in Å.

**Table S1.** The values of Mulliken atomic charges of the optimized structures of the catalysts (K<sub>3</sub>VO<sub>4</sub>, Na<sub>2</sub>SnO<sub>3</sub>, K<sub>3</sub>PO<sub>4</sub> and VO(O*iPr*)<sub>3</sub>). As can be seen VO(O*iPr*)<sub>3</sub> has the smallest negative charges on the oxygen atoms, which means the lowest basicity.

Mulliken charges <sup>a</sup>	K <sub>3</sub> VO <sub>4</sub>	Na <sub>2</sub> SnO <sub>3</sub>	K <sub>3</sub> PO <sub>4</sub>	VO(O <i>iPr</i> ) <sub>3</sub>
O <sup>1</sup>	-0.796471	-0.868219	-0.809788	<b>-0.445676(V=O)</b>
O <sup>2</sup>	-0.884282	-0.925263	-0.809733	-0.550291
O <sup>3</sup>	-0.796470	-0.868856	-0.718107	-0.527690
O <sup>4</sup>	-0.883341		-0.718198	-0.555806
<b>Average</b>	<b>-0.840141</b>	<b>-0.887446</b>	<b>-0.763956</b>	<b>-0.519866</b>

<sup>a</sup> Optimized catalyst structures at BLYP-D3 6-311g\* level of theory

**Table S2.** The activation free energies ( $\Delta G^\ddagger$ ) with various cations for the PO<sub>4</sub><sup>3-</sup>, VO<sub>4</sub><sup>3-</sup>, SnO<sub>3</sub><sup>2-</sup> anions.

Catalyst	$\Delta G^\ddagger$ H <sup>+</sup> abstraction [kcal/mol]	$\Delta G^\ddagger$ cEC opening [kcal/mol]	Exp. conversion [%]	Exp. CO <sub>2</sub> content [%]
H <sub>3</sub> PO <sub>4</sub>	22.3	50.0	4.0	3.0
Li <sub>3</sub> PO <sub>4</sub>	12.8	39.1	26.0	5.0
Na <sub>3</sub> PO <sub>4</sub>	7.6	5.2	82.0	11.0
K <sub>3</sub> PO <sub>4</sub>	4.2	4.0	100.0	15.0
Na <sub>2</sub> SnO <sub>3</sub>	6.2	11.2	99.8	26.0
K <sub>2</sub> SnO <sub>3</sub>	6.5	10.8	100.0	22.0
Na <sub>3</sub> VO <sub>4</sub>	4.8	4.5	99.8	26.0
K <sub>3</sub> VO <sub>4</sub>	5.8	7.7	100.0	25.0

**Table S3.** Average bond distances (Å) for the optimized catalyst structures at BLYP-D3 6-311g\* level of theory (obtained by Gaussian) .

Average Bond distances <sup>a</sup>	K <sub>3</sub> VO <sub>4</sub>	Na <sub>2</sub> SnO <sub>3</sub>	K <sub>3</sub> PO <sub>4</sub>	VO(O <i>iPr</i> ) <sub>3</sub>
M-O	1.7445	1.9816	1.5995	1.7447
O <sup>+</sup> cation/O( <i>iPr</i> ) <sub>3</sub>	2.4807	2.2392	2.4791	1.4523

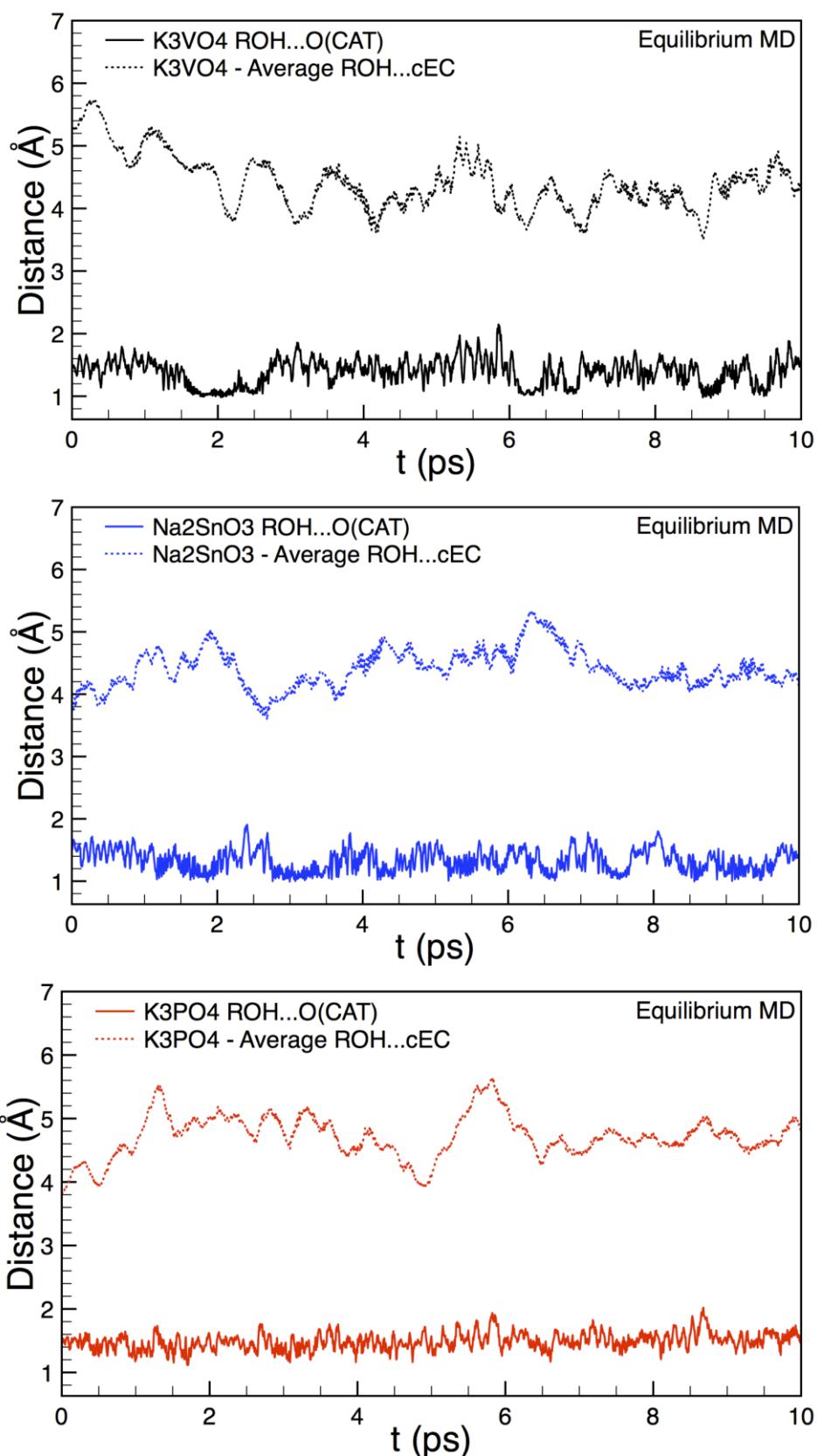
**Table S4.** Average bond distances (Å) for the optimized catalyst structures at PBE-D3 DZVP-MOLOPT-GTH level of theory (obtained by CP2K).

Average Bond distances <sup>a</sup>	K <sub>3</sub> VO <sub>4</sub>	Na <sub>2</sub> SnO <sub>3</sub>	K <sub>3</sub> PO <sub>4</sub>	VO(O <i>iPr</i> ) <sub>3</sub>
M-O	1.7340	1.9390	1.5708	1.7361
O <sup>+</sup> cation/O( <i>iPr</i> ) <sub>3</sub>	2.6166	2.2705	2.6035	1.4583

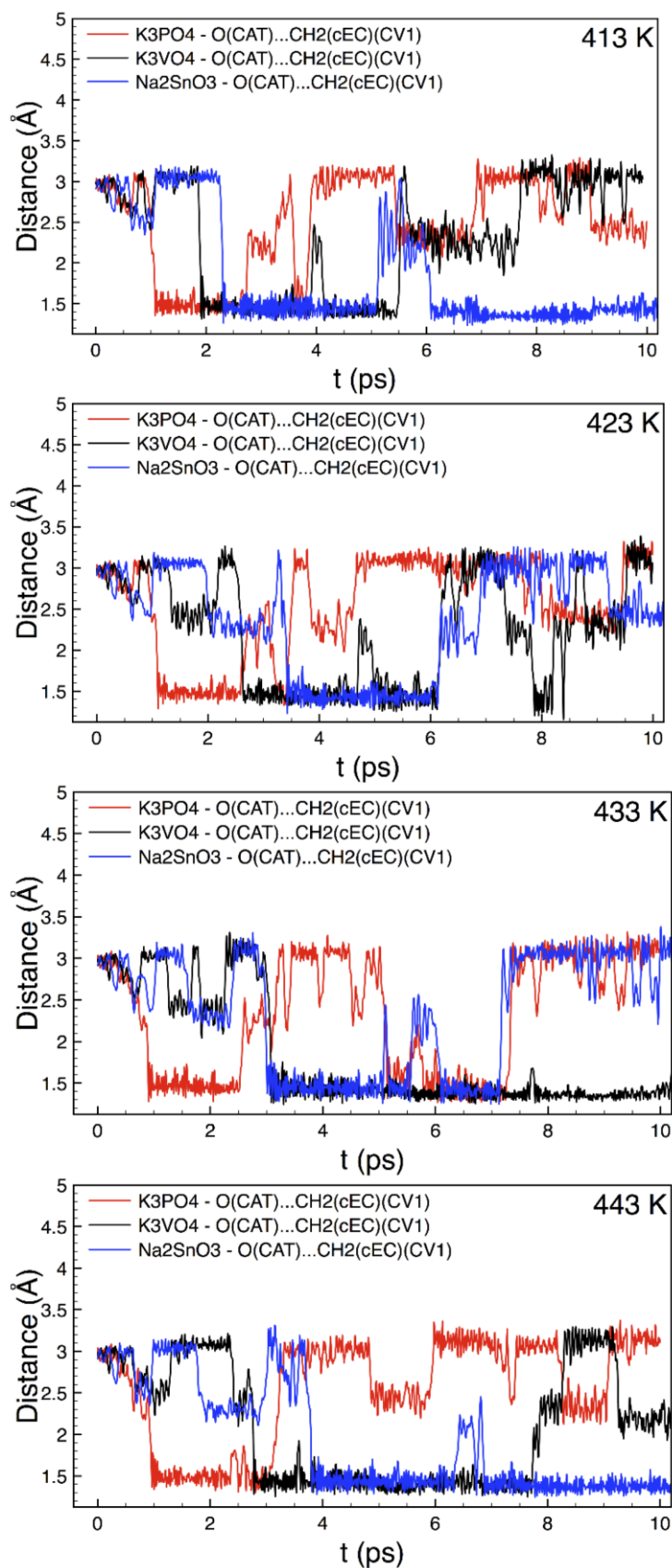
**Table S5.** The effect of M-O bond length on the performance of the catalyst anion to maintain CO<sub>2</sub> in the polymer.

anion	M-O dist. [Å]	X <sub>exp.</sub> [%]	CO <sub>2;exp.</sub> [wt.-%]
(CO <sub>3</sub> ) <sup>2-</sup>	1.27	100	15
(SO <sub>4</sub> ) <sup>2-</sup>	1.50	90	15
(PO <sub>4</sub> ) <sup>3-</sup>	1.55	100	15
(WO <sub>4</sub> ) <sup>2-</sup>	1.75	99.8	25
(VO <sub>4</sub> ) <sup>3-</sup>	1.76	100	25
(SnO <sub>3</sub> ) <sup>2-</sup>	1.90	99.8	26

The nucleophilicity or basicity of the catalyst anions are correlated to the structural parameters (M-O bond distances) that affect the catalyst performance. Hence, M-O bond distance correlates to the nucleophilicity/basicity that determines the catalyst performance, they are correlated. The original data set that we have considered for the current study consists of 30 different catalysts and the trends and conclusions are obtained for the data set is systematically examined for all the 30 molecular systems (some of them are listed in the Table S5). Due to the confidentiality reasons, we only show a few of the observed results that confirms the M-O bond distance-reactivity relationship. As can be seen in the Table S5, the anions such as CO<sub>3</sub><sup>2-</sup>, SO<sub>4</sub><sup>2-</sup> and PO<sub>4</sub><sup>3-</sup> with the M-O bond lengths smaller than 1.55 Å are prone to less CO<sub>2</sub> content than the anions with longer M-O bond length. Also, please see the variation of the catalyst-H<sup>+</sup> distances shown in Figure 3 and 4, that the weaker basicity is observed in movement of proton from anion to the cEC. As another proof of weaker basicity of phosphate anion, Figure S7 shows an equilibrium MD simulation without any bias. The average distance between O(CAT)...H<sup>+</sup> is 1.4 Å for K<sub>3</sub>PO<sub>4</sub>, however, in case of Na<sub>2</sub>SnO<sub>3</sub> and K<sub>3</sub>VO<sub>4</sub> the proton leaves ROH and bounds to the catalyst at certain time intervals. In conclusion and according to our analysis softer anions perform better than harder anions in aspect of CO<sub>2</sub> content.



**Figure S10.** The variation of average H-bond distances between ROH and surrounding cEC monomers ( $\text{H}\cdots\text{O}(\text{cEC})$ ) in the first solvation shell in comparison to the  $\text{ROH}\cdots\text{O}(\text{CAT-anion})$  alongside an unbiased MD simulations.

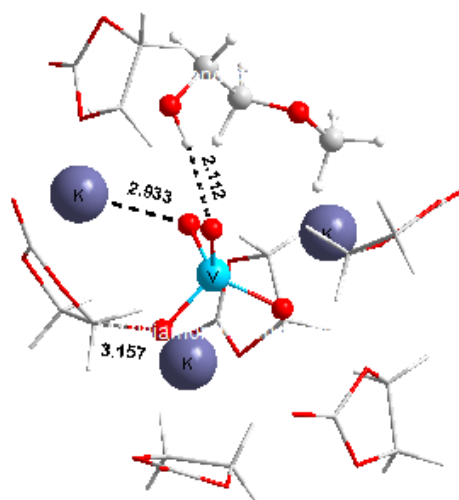


**Figure S11.** Variation of the O-(Cat)...CH<sub>2</sub> distance between the oxygen of the catalyst anion with the carbon of the CH<sub>2</sub> group connected to the ethereal oxygen (CV1) for the K<sub>3</sub>PO<sub>4</sub> (red), K<sub>3</sub>VO<sub>4</sub> (black) and Na<sub>2</sub>SnO<sub>3</sub> (blue) at 413, 423, 433 and 443 K.

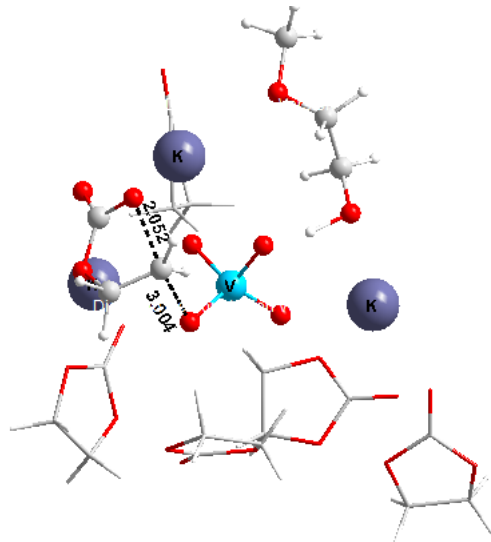


The molecular structures of various states related to Figure 5 in the main text:  
 $K_3VO_4$ , important distances are shown in Å

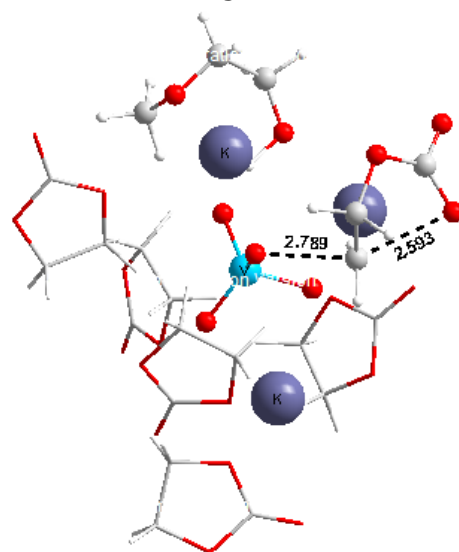
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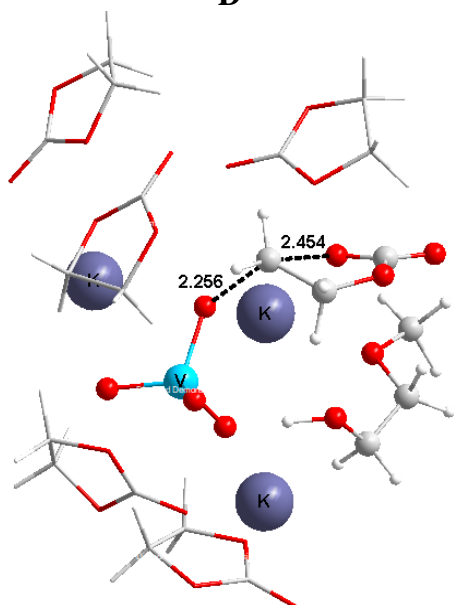
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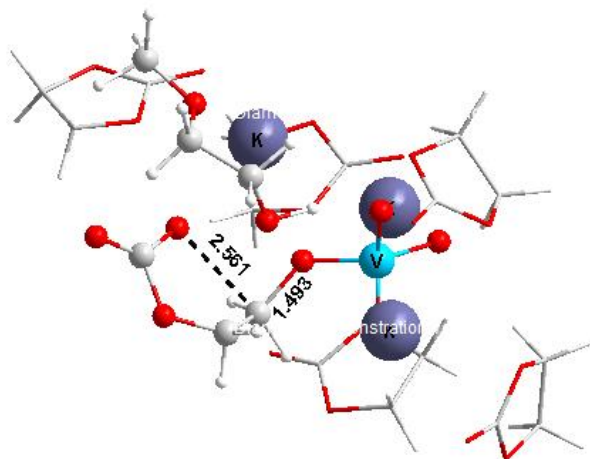
C



D

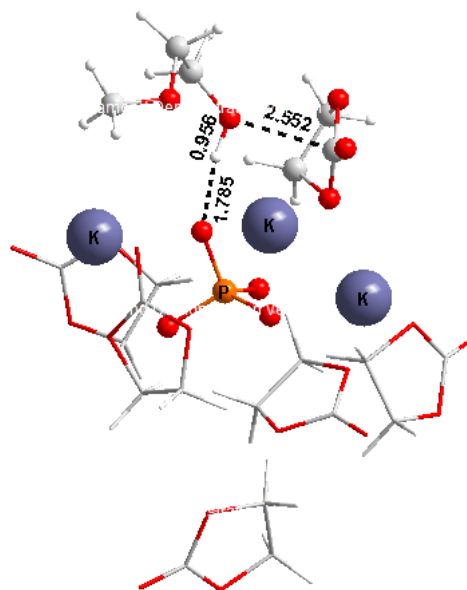


E

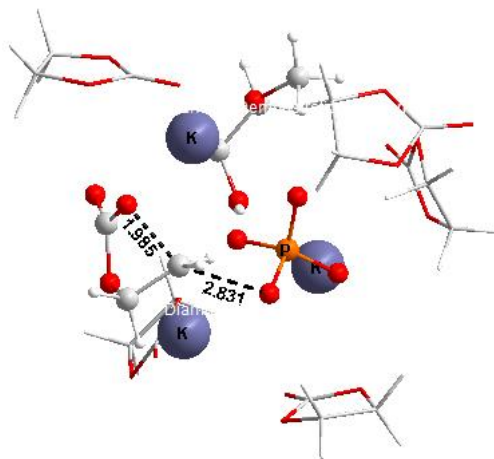


$K_3PO_4$

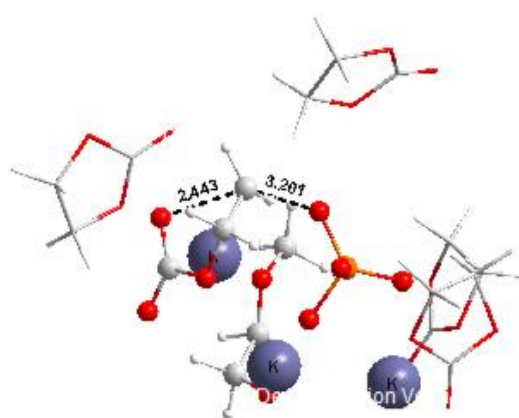
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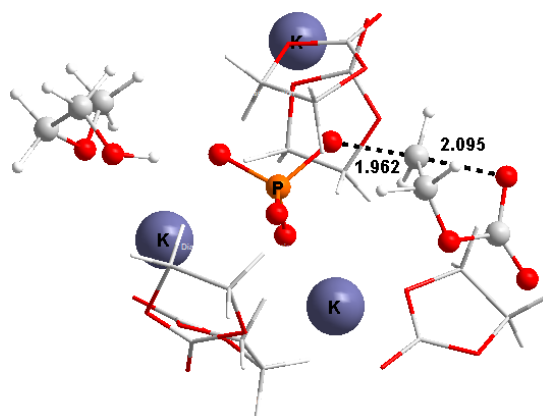
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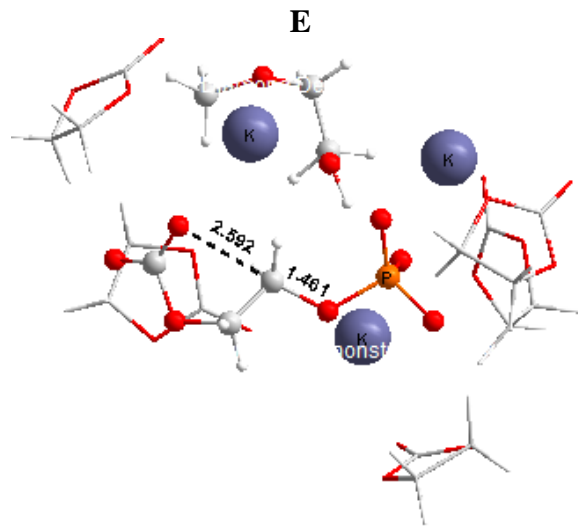


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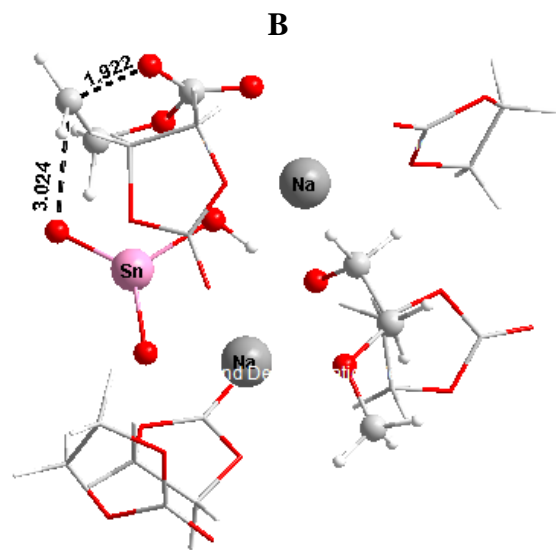
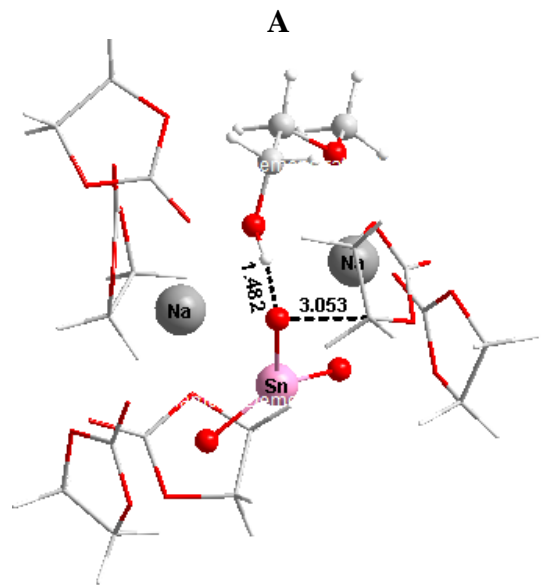


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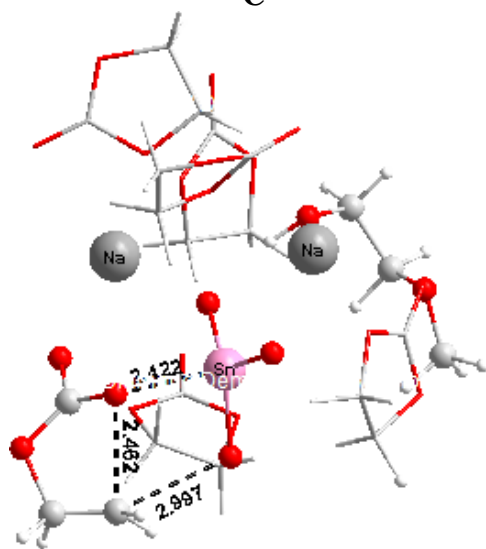




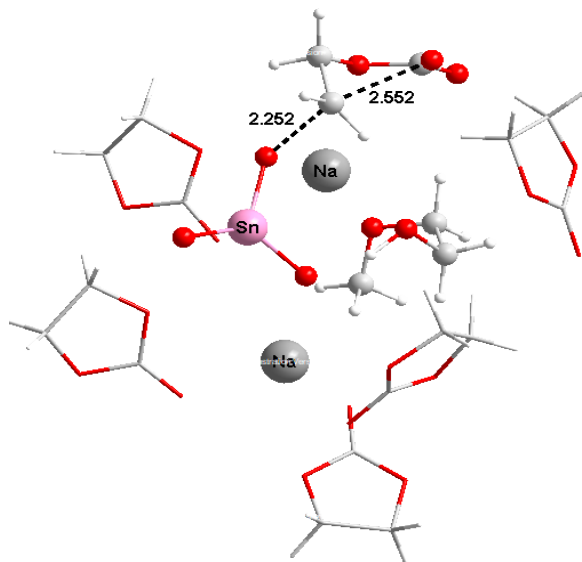
$\text{Na}_2\text{SnO}_3$



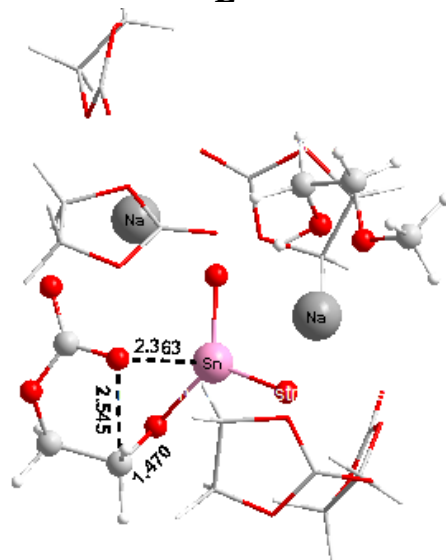
C



D

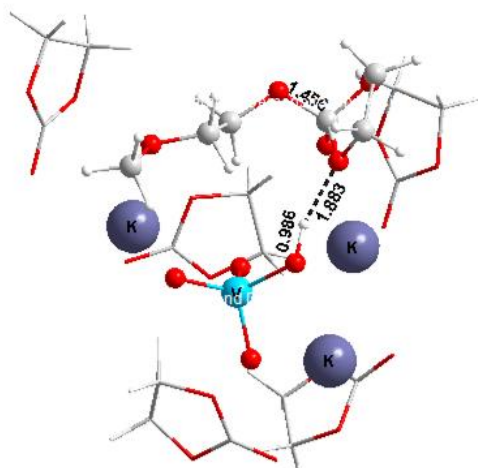


E

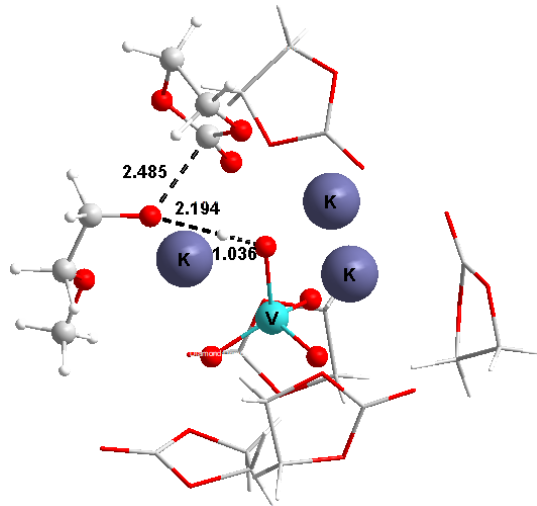


The molecular structures of various states related to Figure S3 in the SI:  
 $K_3VO_4$ , important distances are shown in Å

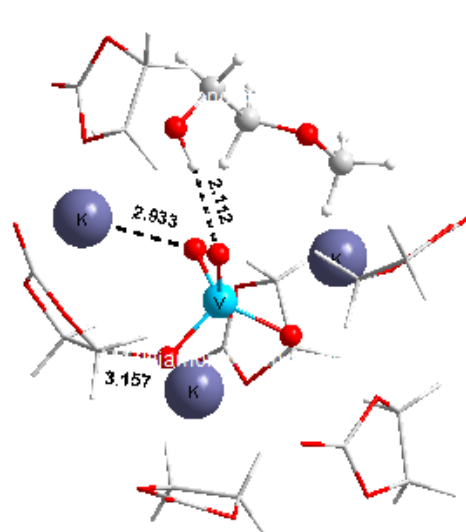
I-A



TS-A

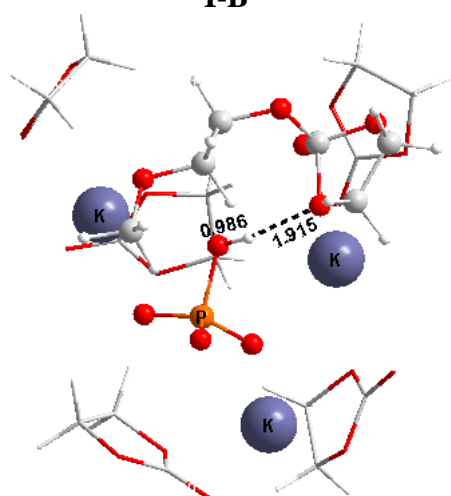


III-A

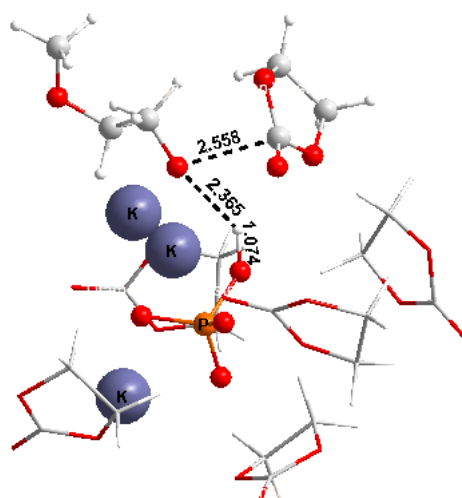


$K_3PO_4$

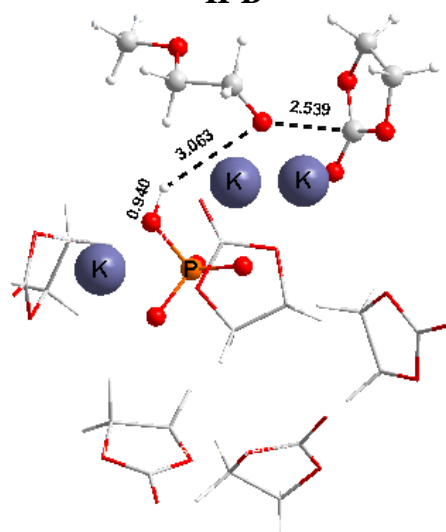
**I-B**



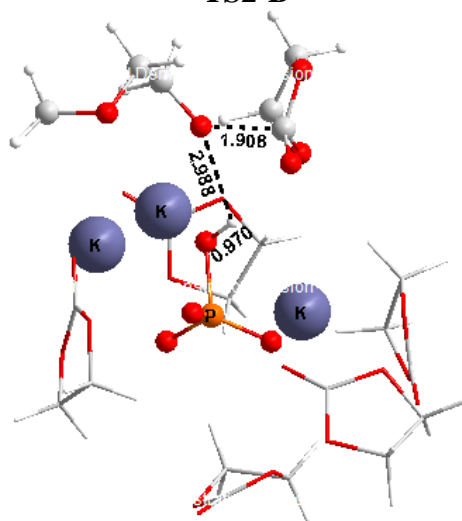
**TS1-B**



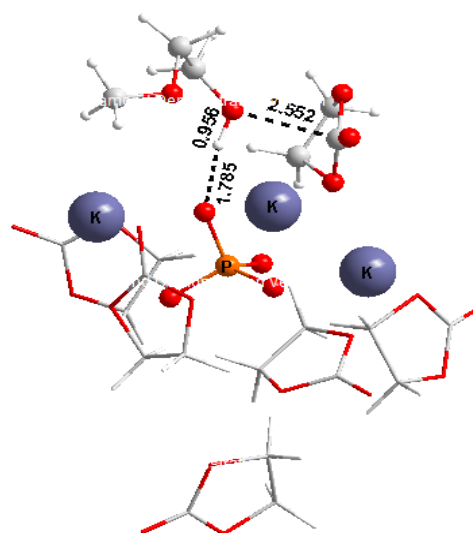
**II-B**



**TS2-B**

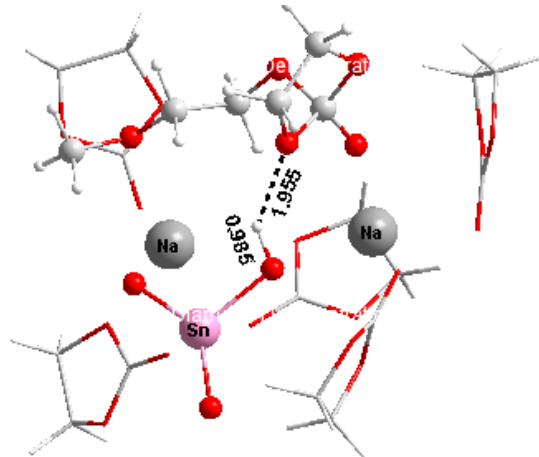


**III-B**



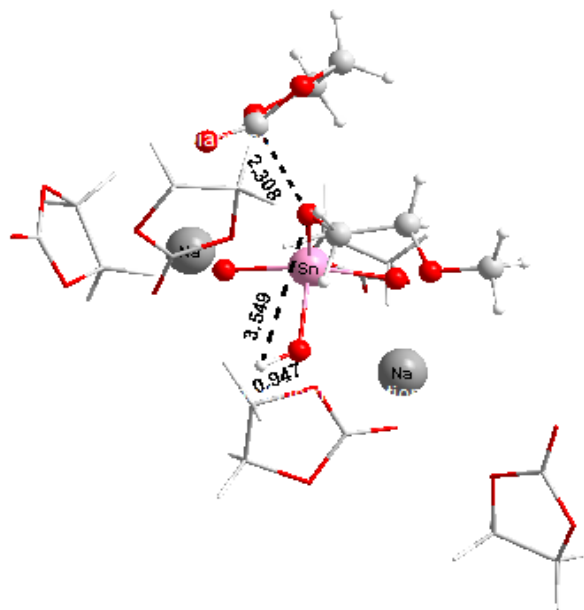
$\text{Na}_2\text{SnO}_3$

**I-C**

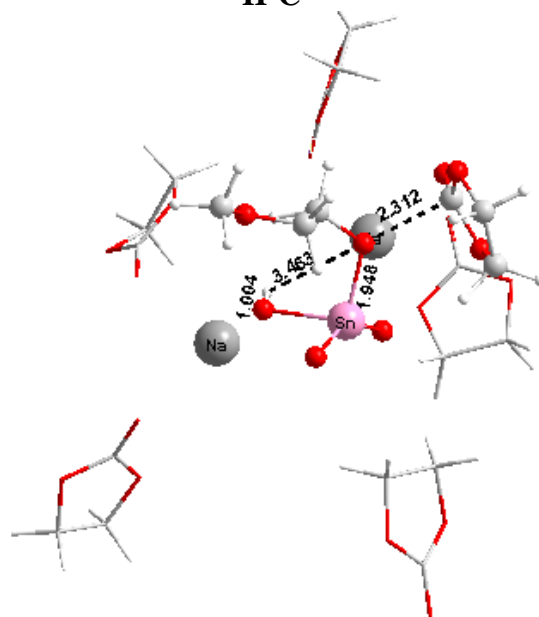




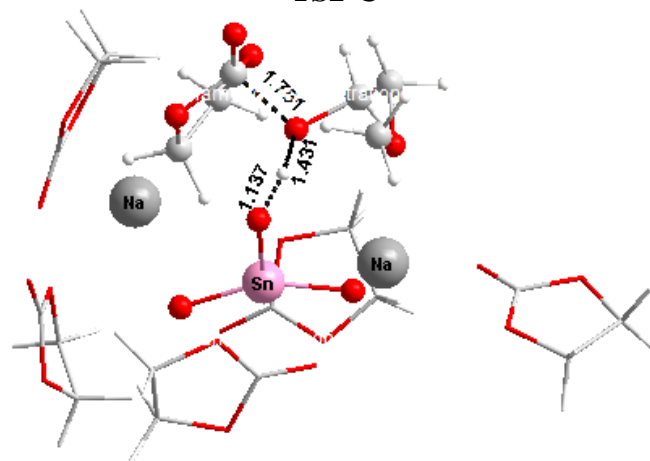
TS1-C



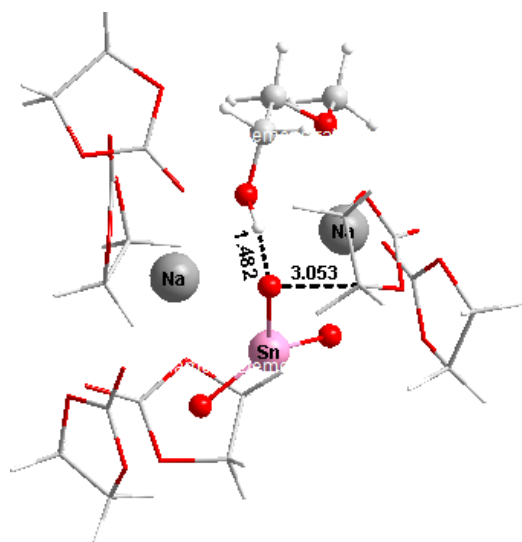
II-C



TS2-C

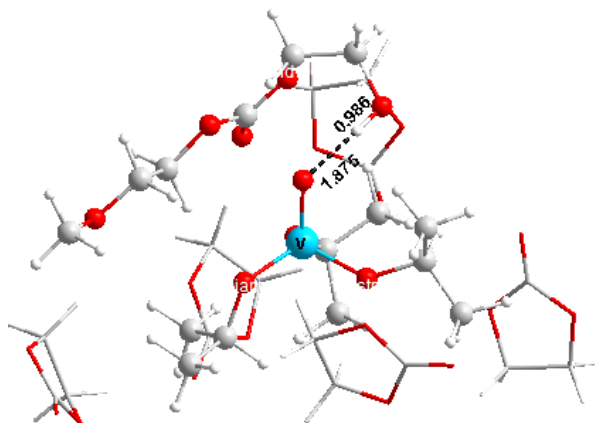


### III-C

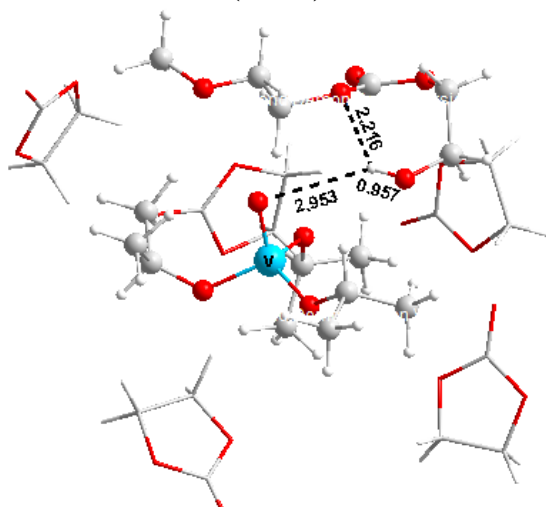


$\text{VO}(\text{O}i\text{Pr})_3$

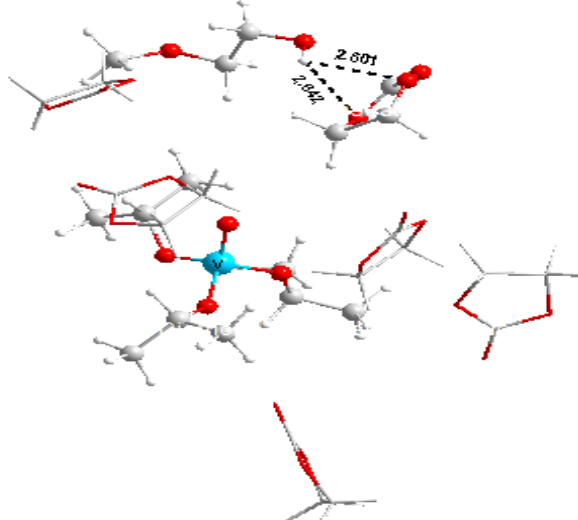
### (I-D)



### (TS-D)

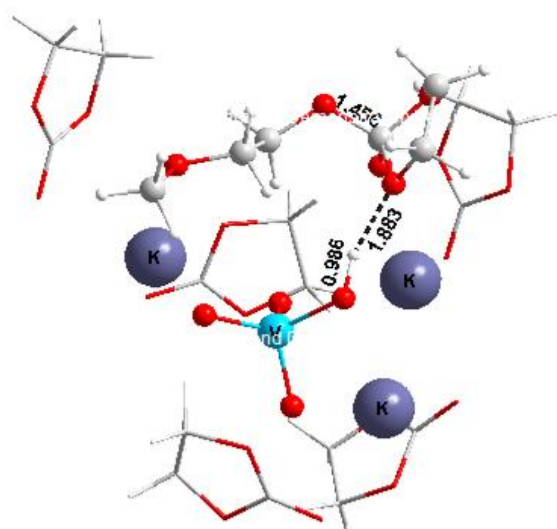


(II-D)

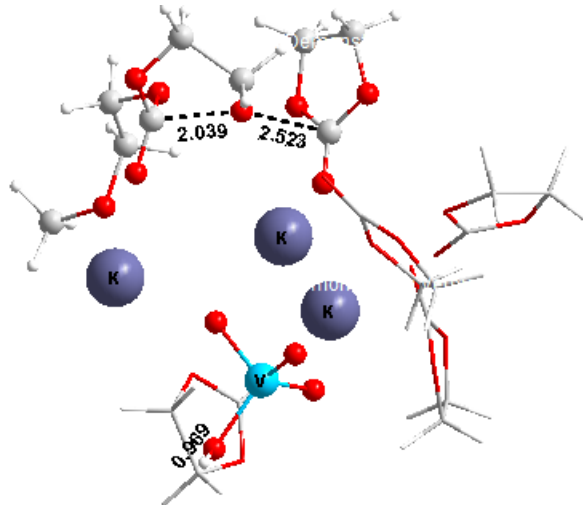


The molecular structures of various states related to Figure S4 in the SI:  
 $\text{K}_3\text{VO}_4$ , important distances are shown in Å

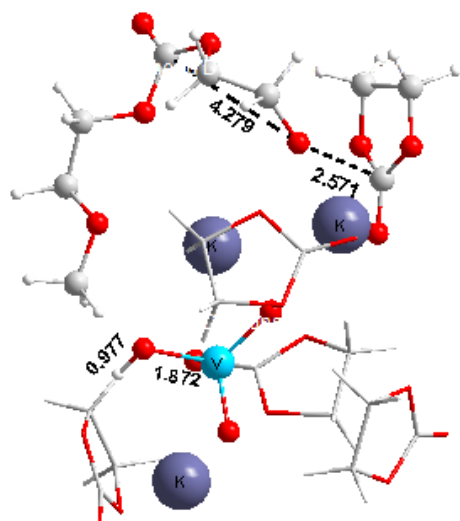
I-A



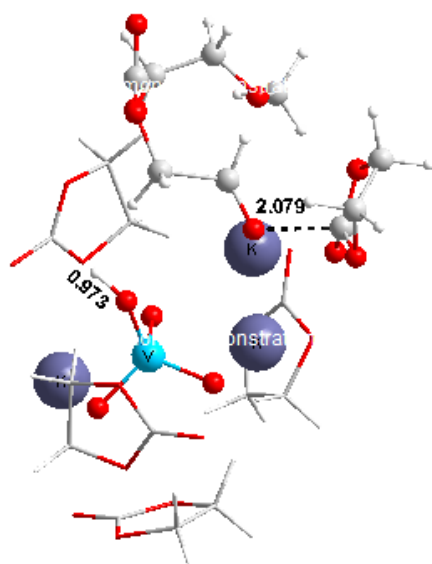
TS1-A



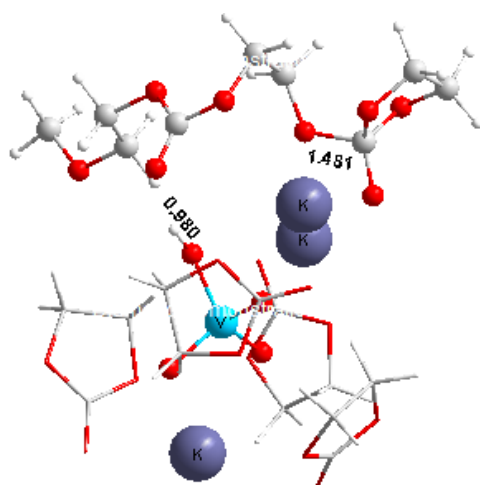
**II-A**



**TS2-A**

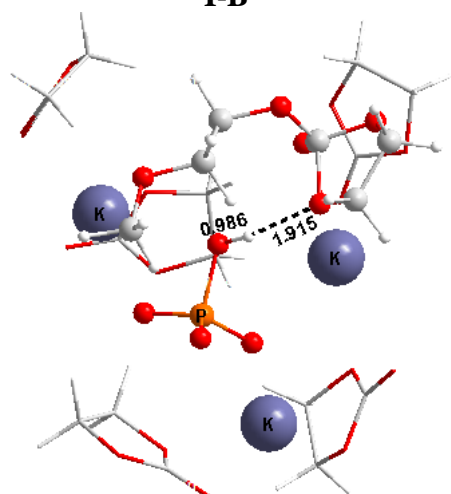


**III-A**

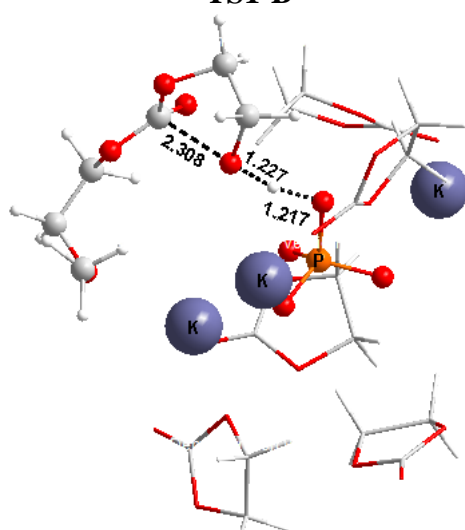




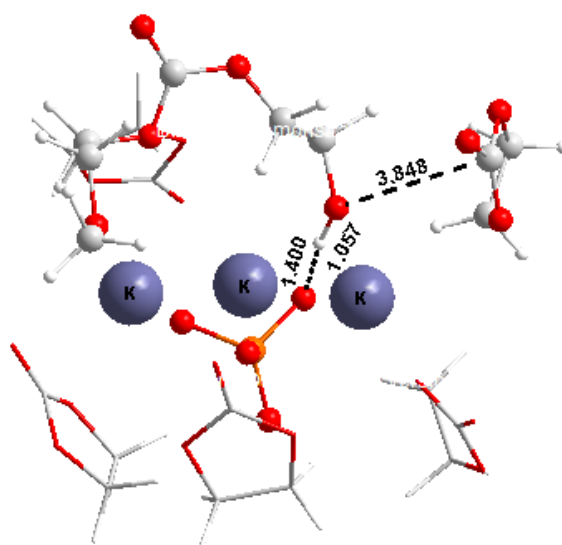
**I-B**



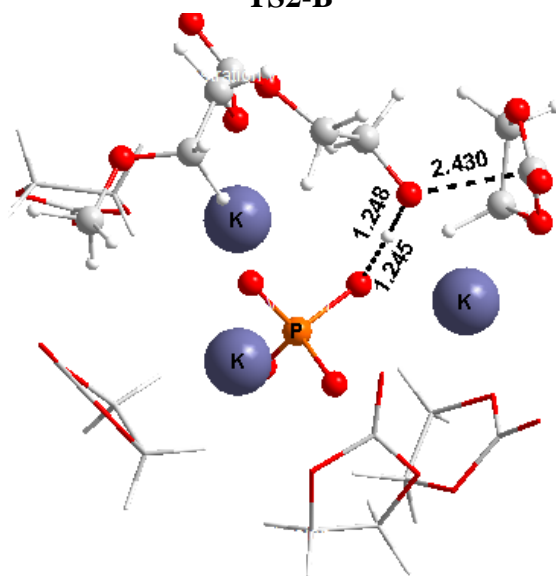
**TS1-B**



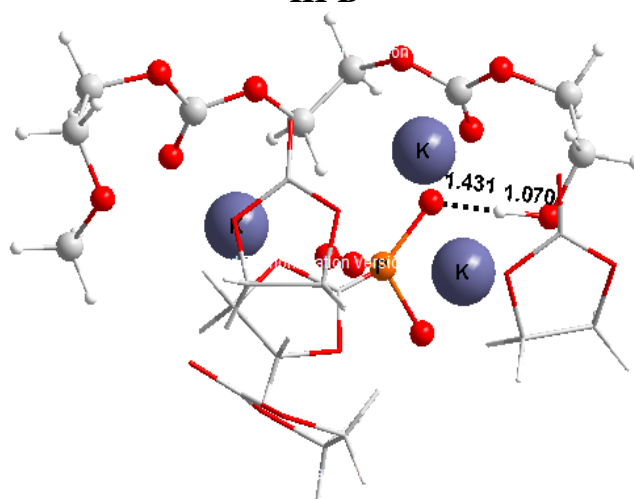
**II-B**



**TS2-B**

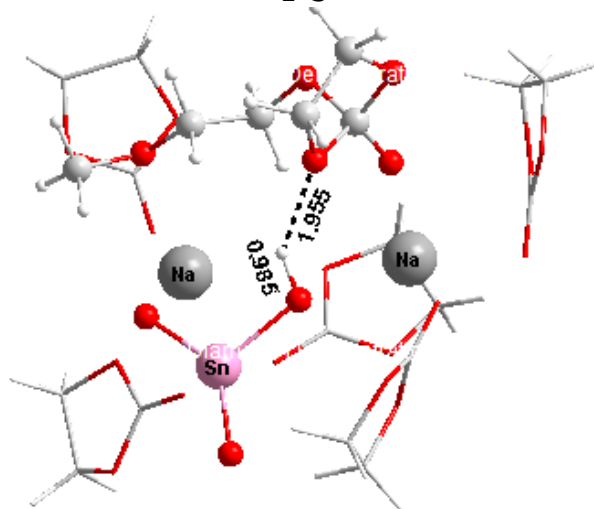


**III-B**

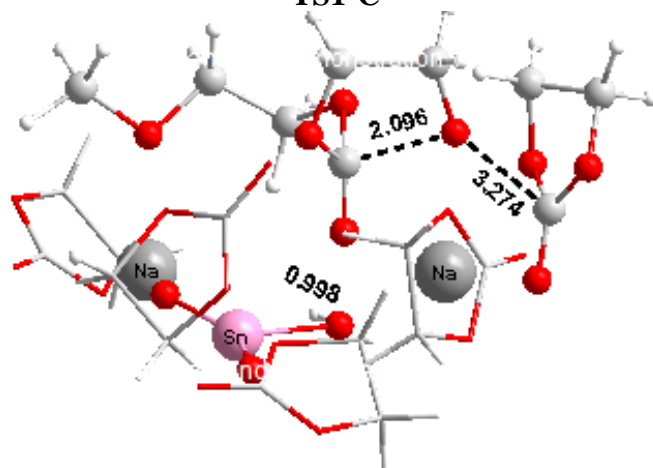


$\text{Na}_2\text{SnO}_3$

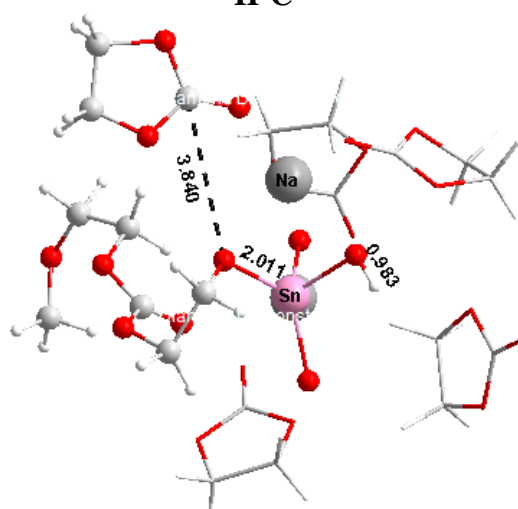
**I-C**



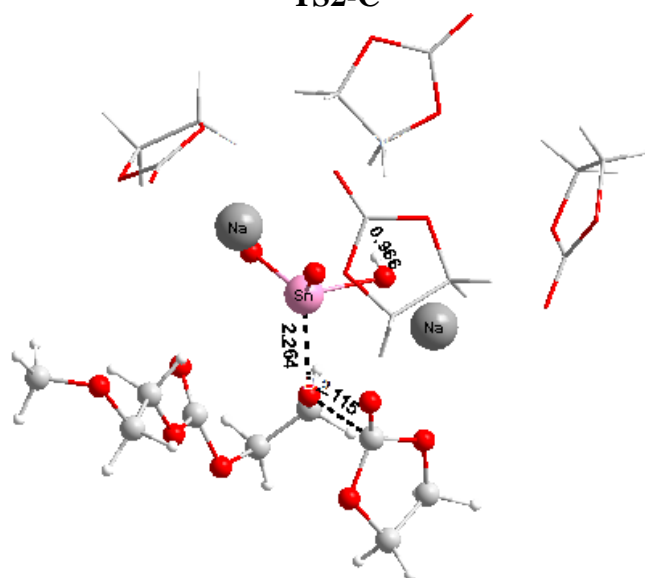
TS1-C



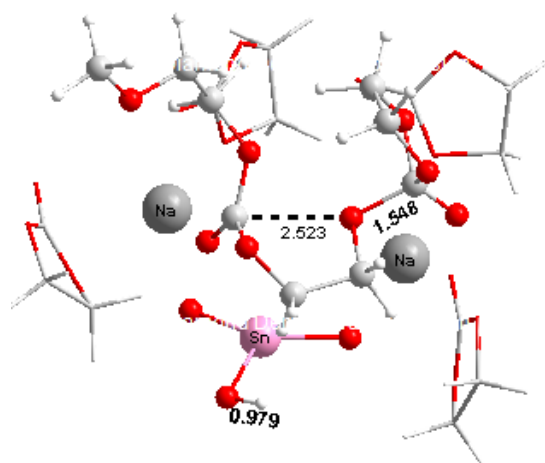
II-C



TS2-C

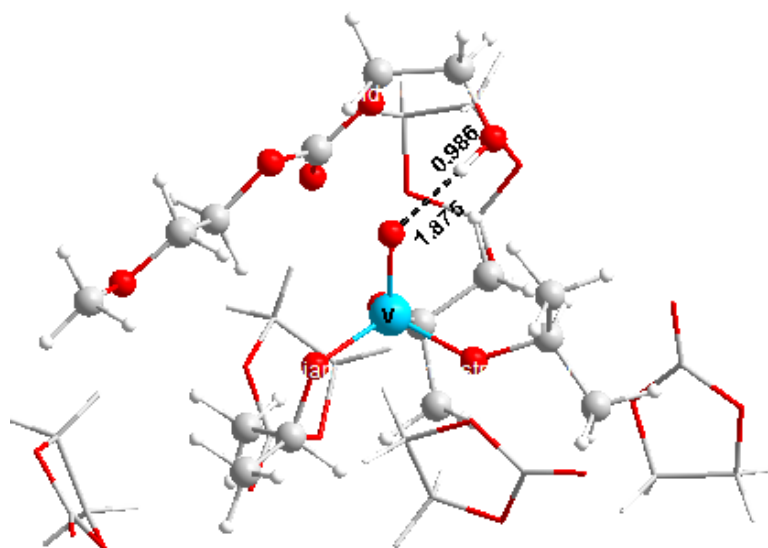


III-C

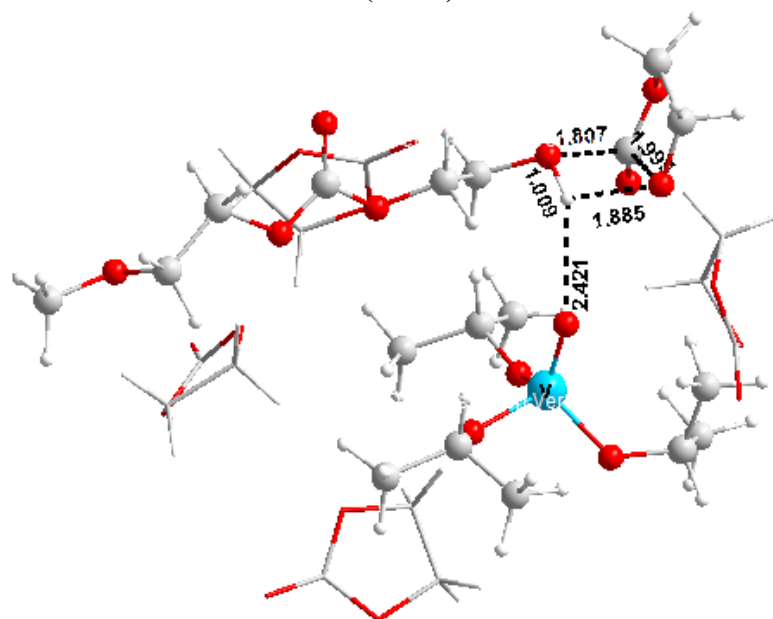


VO(O*i*Pr)<sub>3</sub>

(I-D)

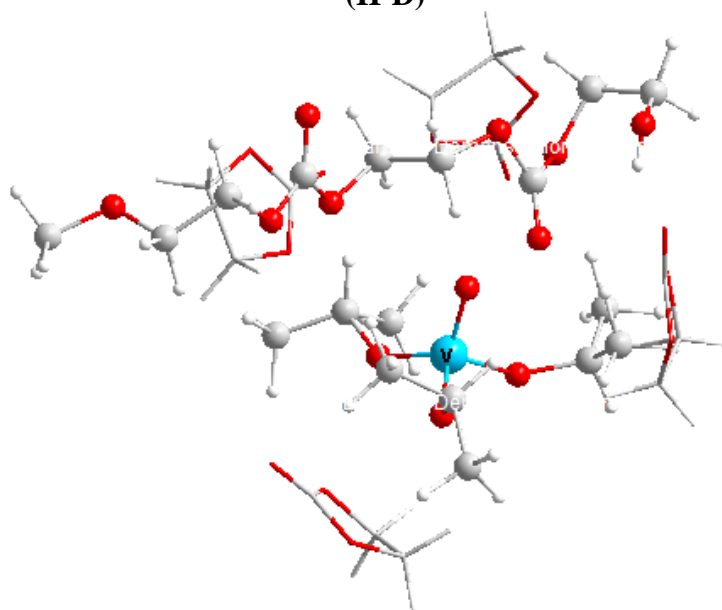


(TS-D)





(II-D)



**Cartesian coordinates (in Å) related to the intermediate structure (INT) defined in Schemes 4 and 5 in the main text**

<b>K<sub>3</sub>VO<sub>4</sub></b>			O	-4.266354	-2.210696	0.782214
V	-0.643754	-0.667850	H	-2.672907	-1.753834	4.335093
O	-3.065752	3.240710	C	-4.068881	-2.545105	1.943338
O	-1.009517	4.091291	O	-3.659796	-3.776776	2.309537
O	-1.122761	-2.276195	C	-3.344658	-3.773842	3.738094
O	-2.801731	4.174016	H	-2.287390	-4.053849	3.833697
C	-1.978773	3.881116	H	-4.297802	-2.215477	5.015930
C	-1.581618	2.387713	C	-3.603610	-2.315739	4.172011
O	-1.895963	2.082189	O	-0.999018	-0.444104	0.406556
C	-2.276394	3.429578	K	-1.532134	-3.046853	0.028677
H	-2.573229	4.061012	O	0.973506	-0.432189	2.678653
H	-0.508268	2.233141	K	0.683194	1.523293	4.396022
H	-1.090400	4.532116	O	4.293359	4.255142	3.800840
H	-2.164551	1.723801	H	4.530392	6.318261	3.871702
C	0.989659	2.813524	H	2.107660	6.636064	3.846795
C	-0.261903	3.489754	C	2.452215	5.668516	3.459265
H	0.746279	1.812215	O	3.215180	2.732871	5.107857
H	1.396038	3.426749	H	4.293133	5.611849	2.230191
H	-0.887445	2.771545	C	3.227532	3.786396	4.508454
H	0.038969	4.287118	H	1.904823	5.397686	2.545192
C	3.047378	1.829204	C	3.975647	5.574349	3.281016
O	1.966698	2.696388	O	2.175259	4.654696	4.462529
H	3.782180	1.842338	H	-1.098465	0.479950	0.076097
H	3.528607	2.196617	O	1.192524	-3.984615	1.421954
H	2.674236	0.799791	H	2.993612	-3.796187	2.434707
H	-3.739200	3.974714	H	1.853810	-4.215321	4.557135
O	-3.219443	1.354920	C	1.216342	-3.800408	3.765928
O	-1.043503	1.622944	O	-0.577957	-5.394470	1.280008
H	-3.893816	0.976441	H	1.958400	-2.285085	2.368314
C	-1.998334	1.938841	C	0.241327	-4.795326	1.956102
O	-1.952821	2.937350	H	0.584339	-2.980238	4.134243
C	-3.265460	3.063226	C	1.978496	-3.380837	2.498407
H	-3.114712	3.144505	O	0.329866	-4.866470	3.305431
H	-5.025369	1.930722	O	-1.607147	0.416233	3.130490
C	-3.980747	1.781144	K	-3.688058	0.692773	1.235486
H	-4.006628	-4.507485	C	-5.883537	4.287395	-0.041234
O	-4.249482	-1.722030	H	-5.090396	4.245421	-0.800649

H	-6.849530	4.587024	-0.470824	O	1.923965	3.588498	5.306190
O	-5.952464	2.008743	2.573685	H	4.603870	5.063061	2.419983
H	-4.373041	5.309834	1.177167	C	2.423310	4.365185	4.516481
H	-6.031381	6.054152	1.301635	H	2.270089	5.426929	1.881403
O	-5.753373	4.262195	2.311853	C	3.998266	5.449297	3.251086
C	-5.456772	5.127583	1.175798	O	1.745589	5.361288	3.885680
C	-5.914088	2.995173	1.859516	H	-1.343602	0.131953	1.978210
O	-6.044357	2.946132	0.508802	O	1.274596	-3.453986	1.909340
<b>Na<sub>2</sub>SnO<sub>3</sub></b>							
Sn	-0.343478	-1.419458	3.739257	H	3.272144	-3.819679	2.365623
O	-3.028796	2.690002	1.716006	H	2.627626	-5.299180	4.221059
O	-1.202122	3.524303	0.518538	C	1.840808	-4.639026	3.834161
O	-0.877047	-3.073951	4.444438	O	-0.322747	-4.903926	1.158816
O	-3.074536	2.848322	-0.590714	H	2.447288	-2.548244	3.364657
C	-2.323817	2.239991	-1.647705	C	0.554218	-4.626964	1.945476
C	-1.683110	0.985036	-0.994037	H	1.202951	-4.235259	4.637228
O	-1.818477	1.206573	0.416139	C	2.349218	-3.541523	2.896147
C	-2.350291	2.610701	0.635717	O	0.978894	-5.428964	2.959657
H	-3.021621	1.990994	-2.459811	Na	-3.797218	0.515598	2.109329
H	-0.621840	0.879671	-1.273810	C	-5.879637	3.965891	0.262227
H	-1.554694	2.934007	-2.022082	H	-5.218315	3.811884	-0.600526
H	-2.215159	0.056448	-1.252460	H	-6.877253	4.311257	-0.042952
C	0.918438	2.570951	1.216406	O	-5.812882	1.893666	3.040046
C	-0.286473	3.431771	1.605290	H	-4.134275	4.873920	1.236015
H	0.612470	1.521078	1.071077	H	-5.666569	5.838500	1.441311
H	1.349003	2.939550	0.267322	O	-5.512261	4.105408	2.577870
H	-0.795095	3.030803	2.499439	C	-5.227654	4.837022	1.347643
H	0.049053	4.452062	1.853753	C	-5.781765	2.815985	2.241826
C	3.024345	1.784490	2.009190	O	-6.040007	2.676026	0.922445
O	1.905587	2.660722	2.269683	<b>K<sub>3</sub>PO<sub>4</sub></b>			
H	3.770740	1.984007	2.791532	P	0.229621	-0.236090	1.999329
H	3.465955	2.002730	1.021572	O	-3.048779	2.968920	1.306796
H	2.704865	0.727785	2.065019	O	-1.671031	4.453247	0.122722
H	-2.835912	4.586864	5.087198	O	-0.924414	-1.263173	1.816612
O	-3.222839	1.423084	5.667992	O	-3.542271	3.599552	-0.864197
O	-1.028848	0.796712	5.659140	C	-2.871167	3.481258	-2.121541
H	-4.846200	2.505836	4.938938	C	-1.779169	2.386171	-1.898784
C	-1.907563	1.627220	5.470748	O	-1.812092	2.112412	-0.500480
O	-1.639232	2.882570	5.026955	C	-2.586869	3.305245	0.182323
C	-2.912752	3.553808	4.726031	H	-3.618945	3.193140	-2.874294
H	-3.052031	3.512453	3.633252	H	-0.786115	2.752387	-2.212564
H	-4.142903	3.086697	6.509286	H	-2.414918	4.441762	-2.408722
C	-3.924092	2.702518	5.502785	H	-2.000320	1.458015	-2.448781
H	-4.052184	-5.541381	2.163120	C	0.669137	3.852989	0.321771
O	-4.092996	-2.501264	3.159993	C	-0.579181	4.376403	1.041962
O	-4.729101	-1.474249	1.240858	H	0.442864	2.876541	-0.134215
H	-2.723600	-3.744944	4.102718	H	0.960036	4.543324	-0.493916
C	-4.357222	-2.476690	1.835293	H	-0.840817	3.720722	1.888703
O	-4.163976	-3.677913	1.246852	H	-0.404615	5.389939	1.438803
C	-3.525608	-4.579033	2.211168	C	2.779911	2.842446	0.731839
H	-2.475143	-4.702276	1.908322	O	1.758401	3.715979	1.257247
H	-4.484723	-4.262557	4.187150	H	3.611496	2.858026	1.451620
C	-3.683117	-3.852449	3.558208	H	3.152492	3.213180	-0.240251
O	-1.754311	-0.351319	2.731870	H	2.396885	1.809067	0.615391
O	1.280467	-0.430940	3.612544	H	-3.318368	2.032175	5.100531
Na	0.890902	1.640756	4.359549	O	-1.587344	-0.229256	5.770946
O	3.738546	4.351228	4.168553	O	0.240449	0.884699	6.574912
H	4.553333	6.226488	3.796481	H	-2.078703	-0.468551	3.770233
H	2.453456	6.979184	2.791340	C	-0.769889	0.845882	5.905243
C	2.589189	5.890419	2.826299	O	-1.238245	1.917239	5.188036
				C	-2.500937	1.554082	4.543041

H	-2.470921	1.928768	3.509899	H	-1.328060	2.733190	-2.684368
H	-3.486850	-0.385188	4.918129	H	-1.729311	0.406180	-3.185403
C	-2.504766	0.026102	4.658843	H	-0.450007	1.755936	-1.461264
H	-2.916559	-5.540689	1.852400	H	-3.250488	1.050870	-2.528190
O	-3.530627	-2.756133	1.664039	C	1.949982	3.269582	1.080642
O	-3.025253	-2.361016	-0.524521	C	0.512226	3.707472	1.328426
H	-2.056093	-2.845078	3.120220	H	2.006828	2.164449	1.059312
C	-2.894319	-3.014423	0.493544	H	2.296323	3.645786	0.099669
O	-2.084458	-4.106551	0.594382	H	0.095049	3.255069	2.239070
C	-2.241210	-4.676866	1.936102	H	0.421879	4.801604	1.393806
H	-1.244503	-4.975396	2.286487	C	4.113310	3.390088	2.006691
H	-3.580051	-3.793639	3.470275	O	2.745644	3.802442	2.139420
C	-2.837522	-3.506706	2.715969	H	4.654872	3.791335	2.873762
O	-0.507138	1.274718	1.873556	H	4.558083	3.777389	1.072877
K	0.435603	-2.567961	-0.050133	H	4.197851	2.287915	2.008012
O	1.250116	-0.325209	0.861235	H	-2.566777	5.629670	4.630021
K	1.193299	2.358701	3.824529	O	-2.827892	3.246343	6.343652
O	3.992856	5.382214	2.551025	O	-0.613563	2.840120	6.689575
H	4.635068	7.134629	1.647139	H	-4.090477	2.952061	4.708317
H	2.355131	7.969865	1.648977	C	-1.507615	3.314867	6.022082
C	2.428749	6.874749	1.610383	O	-1.313748	3.984414	4.844723
O	2.680287	4.679295	4.269861	C	-2.585647	4.553176	4.406337
H	4.063332	5.841052	0.530762	H	-2.678520	4.388680	3.324906
C	2.864274	5.402461	3.313125	H	-4.403659	4.427568	5.668918
H	1.765893	6.474477	0.830214	C	-3.619479	3.787375	5.243884
C	3.876023	6.356409	1.482874	H	-6.618346	-4.355214	4.729776
O	1.985347	6.349036	2.886855	O	-4.712279	-2.381729	3.720720
H	-0.696669	1.509916	0.935351	O	-4.740427	-2.967777	1.513314
O	2.378899	-3.091461	3.244825	H	-3.783697	-3.300105	5.337749
H	3.129737	-2.857066	5.164192	C	-4.904153	-3.250029	2.674149
H	0.880231	-3.216388	6.049592	O	-5.295016	-4.482813	3.130744
C	0.907157	-2.741056	5.060978	C	-5.532441	-4.405553	4.560117
O	0.991479	-4.389439	2.005609	H	-5.120803	-5.310799	5.026824
H	2.446126	-1.354904	4.367385	H	-5.358260	-2.501357	5.689650
C	1.236372	-3.770916	3.033721	C	-4.803784	-3.115751	4.967296
H	0.269133	-1.848197	5.015114	O	0.243795	-0.242602	0.061690
C	2.326013	-2.431749	4.548889	O	1.696950	-0.143494	2.420837
O	0.391805	-3.710392	4.089839	O	4.157448	4.046626	5.300326
O	0.782175	-0.163254	3.421876	H	3.032222	5.764059	5.610280
K	-3.131114	0.195734	0.980785	H	2.733065	4.695016	7.776119
C	-6.175481	3.234991	0.999179	C	2.460175	4.065641	6.916667
H	-5.591837	3.512958	0.110093	O	5.139733	2.088051	5.944219
H	-7.256665	3.321110	0.822825	H	2.189620	4.425180	4.748125
O	-5.106363	0.656764	3.061432	C	4.267507	2.914716	6.068823
H	-4.716005	4.446182	2.102294	H	1.398723	3.782144	6.959457
H	-6.431193	4.662815	2.686370	C	2.874892	4.677839	5.571208
O	-5.489985	2.894955	3.231577	O	3.255476	2.846963	6.984976
C	-5.692789	3.969523	2.263812	H	-1.384490	-0.305727	-0.866625
C	-5.463660	1.715212	2.571554	O	2.573738	-4.727889	1.453468
O	-5.891224	1.832589	1.288838	H	4.028277	-3.583132	2.398379
<b>VO(OiPr)<sub>3</sub></b>				H	2.691402	-3.499631	4.428940
V	0.088313	-0.391983	1.671772	C	2.117857	-3.699360	3.514230
O	-2.200930	3.826281	1.159007	O	1.565779	-6.723687	1.920223
O	-0.226439	3.226533	0.165845	H	2.676926	-2.657148	1.646889
O	-0.522780	-1.994273	2.080009	C	1.926312	-5.625846	2.264152
O	-2.200826	2.724383	-0.791373	H	1.204122	-3.087131	3.492320
C	-1.441383	2.030065	-1.843857	C	2.942418	-3.554105	2.223906
C	-2.213837	0.788798	-2.264418	O	1.730786	-5.098421	3.516600
O	-2.287614	-0.203988	-1.249814	O	-1.064685	0.806636	2.261384
C	-1.569414	3.293633	0.255250	C	-5.597213	3.127590	0.221325

H	-4.687476	2.597161	-0.097420	H	-2.479041	1.967689	3.116499
H	-6.303975	3.218126	-0.613940	H	4.042689	0.433999	3.590987
O	-6.143948	2.379707	3.551684	H	3.698237	-1.307644	3.725226
H	-4.278262	4.834276	0.670669	H	3.646821	-0.259418	5.173410
H	-6.050043	5.227414	0.754366	H	2.169775	2.137424	3.856834
O	-5.288690	4.101356	2.326509	H	1.671768	1.444278	5.430176
C	-5.280501	4.458838	0.914550	H	0.492930	1.596892	4.111202
C	-5.917569	2.893293	2.478768	H	-0.324443	-2.684257	-0.524344
O	-6.239287	2.349900	1.271769	H	-1.218958	-4.219166	-0.398558
C	1.935878	-0.017960	3.855487	H	0.353947	-4.042067	0.421099
C	1.543354	1.373616	4.340229	H	-2.094409	-3.669703	3.296795
C	3.415326	-0.313734	4.098505	H	-0.730799	-4.656800	2.703823
H	1.314678	-0.775186	4.368212	H	-2.342634	-4.824192	1.960308
C	-1.312309	-3.012816	1.383199	H	-2.071369	-0.915545	4.124091
H	-2.247147	-2.517143	1.074459	H	-3.224257	0.250546	4.820873
C	-1.632565	-4.106474	2.398921	H	-1.472112	0.565872	4.933067
C	-0.572719	-3.516639	0.150000	H	-3.333402	-0.712205	1.859035
C	-2.337578	0.886770	2.951132	H	-3.401275	0.872419	1.058818
C	-2.264477	0.154983	4.290009	H	-4.424325	0.531442	2.494459
C	-3.438619	0.367837	2.034040				

**Cartesian coordinates (in Å) related to various states in Figure 5 in the main text**

<b>K<sub>3</sub>VO<sub>4</sub></b>				O	-5.319032	1.021319	5.004481
<b>A</b>				H	-2.949385	3.177299	7.740167
V	-1.333322	0.825912	2.557013	C	-4.593630	1.854443	5.505563
O	2.249045	-4.030517	2.183470	O	-4.656294	3.194138	5.156733
O	1.187242	-1.772104	0.794900	C	-3.423120	3.823129	5.602832
O	-2.314178	0.360111	3.876230	H	-3.750538	4.808610	5.919367
O	0.077400	-4.013276	1.392260	H	-1.829908	2.656168	6.545069
C	-0.518876	-4.036918	0.045146	C	-2.891111	2.836301	6.693991
C	0.719605	-4.090765	-0.843712	O	-1.401268	-0.299777	1.307917
O	1.838233	-4.475615	-0.085437	K	0.155466	-2.267494	3.483244
C	1.491198	-4.176493	1.274879	O	0.371106	0.615646	2.991916
H	-1.062895	-4.985754	0.074152	K	-1.524129	1.820763	-0.278605
H	0.925460	-3.060332	-1.183796	O	-0.270703	4.012581	5.244793
H	-1.258489	-3.225226	-0.000061	H	-1.048889	3.617146	3.311398
H	0.670435	-4.786888	-1.725099	H	0.913562	2.332351	3.077026
C	2.396929	0.320170	0.657300	C	1.124472	3.394289	3.369066
C	2.266802	-1.111501	0.199863	O	1.364498	3.972147	6.863973
H	1.805570	0.402717	1.606385	H	-0.143953	5.185542	3.420215
H	3.491355	0.579465	0.747923	C	0.994978	3.833229	5.675425
H	2.269262	-1.281891	-0.892049	H	1.720029	4.001849	2.692653
H	3.202482	-1.588722	0.622594	C	-0.170975	4.111069	3.778707
C	1.905610	2.563329	0.120843	O	1.861722	3.424168	4.678273
O	1.801441	1.242490	-0.244381	H	0.494644	-1.160577	0.951656
H	1.520488	3.157427	-0.821368	O	1.552782	-0.672347	7.121030
H	2.940139	2.882637	0.313213	H	0.430621	0.587698	8.428397
H	1.244517	2.833064	0.996115	H	-1.334639	0.703857	6.741655
H	-5.266900	6.102712	1.140066	C	-0.315859	0.582313	6.310196
O	-4.119305	3.507773	0.616374	O	1.395115	-2.327108	5.581879
O	-5.577626	2.000174	1.556279	H	1.509805	1.444716	7.245846
H	-2.811306	4.436069	1.962290	C	0.906775	-1.351760	6.151997
C	-5.176972	3.126253	1.401877	H	-0.220096	1.212209	5.395164
O	-5.686543	4.251455	1.966741	C	0.814707	0.622989	7.378075
C	-4.808896	5.353601	1.790369	O	-0.302179	-0.793254	5.836277
H	-4.520584	5.833437	2.742847	O	-1.902140	2.394972	2.034409
H	-3.051448	5.213505	0.332333	K	-4.421713	-0.185836	2.569647
C	-3.527456	4.700378	1.194663	C	-4.349447	0.338832	-2.409693
H	-2.743379	3.799156	4.747940	H	-3.818594	-0.588709	-2.094274
O	-3.674654	1.632029	6.494279	H	-5.245714	0.448634	-1.785691

O	-2.204461	2.740707	-3.701156	O	-1.159327	0.799267	6.459270
H	-4.643493	-0.540423	-4.452134	H	0.706381	4.655820	5.735703
H	-5.782745	0.831141	-3.995465	C	-0.444211	1.689907	5.974651
O	-3.745817	1.324582	-4.504799	H	2.320630	2.781970	5.564920
C	-4.763342	0.427481	-3.898225	C	0.366248	3.710443	5.176330
C	-3.024358	1.915284	-3.547334	O	0.818927	1.360140	5.370342
O	-3.430207	1.474997	-2.292946	H	0.392346	1.668753	-0.276549
<b>B</b>				O	-0.194775	-3.088330	3.269462
V	-1.084310	1.765762	1.714720	H	-1.362880	-1.422884	3.578434
O	4.156055	-0.025092	2.496400	H	-0.806013	-1.477152	5.882115
O	0.990775	1.027908	-1.009210	C	-0.667308	-2.434998	5.474792
O	-2.656509	1.274169	1.219941	O	2.040183	-3.244952	3.437104
O	5.540850	-1.072825	3.957809	H	-2.142261	-3.013241	3.806209
C	5.292459	-2.062398	4.952302	C	0.962900	-3.016924	3.921499
C	4.032053	-1.495470	5.614654	H	-1.121793	-3.188727	6.185865
O	3.502826	-0.467972	4.672840	C	-1.224819	-2.419283	4.051015
C	4.367592	-0.480205	3.588743	O	0.755678	-2.635504	5.209148
H	5.140307	-3.044889	4.405833	O	-1.260980	3.108618	2.762728
H	4.255466	-0.952501	6.547672	K	-4.328981	2.386528	2.919505
H	6.217719	-2.088739	5.547428	C	-4.544818	-2.334779	0.846849
H	3.268702	-2.245322	5.737542	H	-4.978947	-2.791326	1.744267
C	-0.311983	1.454483	-3.060446	H	-3.649143	-2.843132	0.506269
C	0.110831	0.467690	-1.889219	O	-6.042116	-1.381517	-2.140812
H	0.073535	2.386710	-2.738849	H	-5.099174	-0.255539	1.345710
H	0.298093	1.217970	-3.974399	H	-3.329800	-0.370531	1.068839
H	-0.801169	0.283507	-1.334490	O	-4.779082	-0.511678	-0.523599
H	0.489065	-0.468822	-2.282999	C	-4.319449	-0.823262	0.866406
C	-2.220561	1.024970	-4.473234	C	-5.470088	-1.552758	-1.065570
O	-1.735271	1.520360	-3.184306	O	-5.485829	-2.583214	-0.224287
H	-2.002602	1.738400	-5.382734	<b>C</b>			
H	-3.323237	1.090011	-4.428833	V	-1.618855	1.347245	1.947674
H	-1.870841	-0.019837	-4.692616	O	3.742468	1.710216	3.117313
H	-2.724248	7.222881	2.261124	O	0.704028	0.807816	-1.074193
O	-2.890999	5.345401	0.093287	O	-2.042735	0.272824	3.146894
O	-4.695804	4.214658	0.601003	O	3.003917	0.775497	5.124514
H	-1.160743	4.745796	1.384444	C	2.629253	-0.557010	5.562733
C	-3.754919	4.973366	0.939177	C	2.968234	-1.490725	4.387168
O	-3.533957	5.333124	2.285896	O	3.068062	-0.435742	3.268674
C	-2.332187	6.157440	2.383367	C	3.325144	0.766751	3.821599
H	-2.165309	5.946495	3.483288	H	3.186232	-0.762603	6.506613
H	-1.018357	6.491855	0.539702	H	2.144577	-2.250158	4.213452
C	-1.371197	5.784154	1.400865	H	1.552412	-0.613117	5.764768
H	-4.447934	-0.610499	8.217469	H	3.932512	-1.938537	4.411020
O	-5.022827	0.513407	5.386078	C	-0.734859	0.284770	-3.156298
O	-4.798346	-1.438159	4.202615	C	0.688793	0.382464	-2.394409
H	-3.930661	1.786793	6.649188	H	-1.100759	1.274098	-3.372932
C	-4.656645	-0.829611	5.220605	H	-0.603429	-0.218685	-4.071277
O	-4.073347	-1.286988	6.378252	H	1.155359	-0.652808	-2.561561
C	-3.972698	-0.216672	7.336689	H	1.297893	1.106708	-2.913557
H	-2.920243	0.060422	7.496824	C	-1.436649	-1.668968	-1.866233
H	-5.576009	1.291860	7.251737	O	-1.706140	-0.356727	-2.336656
C	-4.686508	0.984999	6.702556	H	-2.441745	-2.155586	-1.888376
O	-0.332955	2.493548	0.362893	H	-1.174535	-1.570668	-0.786442
K	1.681215	-0.676054	1.154830	H	-0.617040	-2.209713	-2.465161
O	-0.143152	0.365846	2.129381	H	-2.455574	7.091899	0.978408
K	-3.142506	2.796295	-0.944776	O	0.020791	6.912044	0.760406
O	-0.740607	3.023792	5.957885	O	0.442772	6.403639	-1.337893
H	-0.126964	3.986789	4.171230	H	-1.173375	4.552683	1.410758
H	1.738272	2.607541	3.945343	C	-0.360787	6.482553	-0.431512
C	1.434809	2.599840	4.981043	O	-1.662980	6.171697	-0.866995

C	-2.504368	6.105745	0.444322	C	2.807183	-1.940685	-0.513675
H	-3.540739	5.681595	0.172131	H	2.467039	-4.042226	1.686749
H	-2.175661	5.566040	2.628275	H	0.067570	-2.637386	0.540074
C	-1.880169	5.373893	1.623769	H	1.705003	-2.431442	2.273224
H	-2.611428	-1.016127	6.065166	H	0.832336	-4.224254	-0.126770
O	-1.300254	-1.046767	8.859806	C	-1.204780	1.266464	-2.761368
O	0.389076	0.464067	8.404168	C	-0.057432	0.579835	-2.114753
H	-1.838410	-3.053873	8.349729	H	-1.166842	2.308023	-2.371405
C	-0.411897	-0.385502	8.057047	H	-1.219074	1.331750	-3.916071
O	-0.691710	-0.720830	6.773525	H	-0.178632	-0.533920	-2.146391
C	-1.832861	-1.581926	6.585732	H	0.830926	0.829478	-2.670009
H	-1.415070	-2.505660	6.053436	C	-3.517767	0.860731	-3.316971
H	-3.191031	-1.829451	8.346544	O	-2.534661	0.697720	-2.309050
C	-2.134220	-1.984176	8.095573	H	-4.499599	0.369102	-2.988481
O	-1.067712	0.249501	0.650491	H	-3.047968	0.423393	-4.348423
K	1.479613	2.359154	0.916133	H	-3.650492	1.950460	-3.468956
O	-0.208570	2.166150	2.590112	H	-0.066743	3.049681	1.287707
K	-2.684815	2.115982	-1.077043	O	-2.829700	2.860884	0.382338
O	-3.978394	2.695207	4.839849	O	-2.713405	4.278048	-1.294636
H	-4.987822	4.418068	4.086460	H	-2.769981	3.241237	2.757979
H	-6.221941	3.035504	2.561995	C	-2.419897	3.826294	-0.231703
C	-5.294806	2.555650	2.850743	O	-1.226284	4.572526	0.482554
O	-4.373105	0.530379	5.550168	C	-0.751227	3.859503	1.626954
H	-3.540684	3.768781	3.067970	H	-0.185906	4.560924	2.235924
C	-4.581819	1.406278	4.747282	H	-1.084722	3.049993	3.474854
H	-4.690566	2.378187	1.936827	C	-1.694957	3.072951	2.548358
C	-4.469250	3.536773	3.660536	H	-7.237003	1.218438	4.120378
O	-5.532351	1.358974	3.702571	O	-4.998696	0.776556	5.746757
H	-0.212985	0.424066	-0.402316	O	-5.109926	-1.478902	6.142713
O	0.131780	-4.415346	2.165052	H	-6.079098	2.256305	6.763343
H	0.262626	-2.780915	0.798343	C	-5.678984	-0.410366	5.910842
H	-0.013211	-1.279878	2.837986	O	-7.025339	-0.219934	5.757252
C	-0.575952	-2.229410	2.802731	C	-7.192661	1.157186	5.228382
O	0.594575	-5.187753	4.250041	H	-8.121235	1.613658	5.616893
H	-1.426851	-3.385800	1.182720	H	-5.553100	2.586723	5.058911
C	0.164021	-4.333623	3.503156	C	-5.961574	1.835963	5.731940
H	-1.621251	-1.977553	3.006355	O	0.197419	-0.447721	1.151064
C	-0.444754	-3.204228	1.581612	K	2.934785	0.733555	1.108305
O	-0.211190	-3.112624	3.971802	O	1.197260	1.039115	3.236424
O	-2.595473	2.686128	1.411244	K	-2.753880	0.301810	0.412520
K	-1.137297	1.559493	5.132133	O	-0.858399	3.396718	6.038604
C	-5.516283	-1.518302	1.317537	H	0.362816	1.938661	5.110643
H	-6.173435	-0.903032	1.974988	H	-0.489025	0.208933	6.323746
H	-5.227247	-2.417605	1.852759	C	-0.759838	1.134178	6.781792
O	-6.200862	-0.804244	-1.986825	O	-3.101188	3.538479	5.604777
H	-4.146795	0.148164	1.599666	H	0.890543	2.671115	6.757808
H	-3.263387	-1.182113	0.942307	C	-2.128621	2.918676	5.998900
O	-4.639570	-0.200904	-0.386715	H	-0.770750	1.248164	7.875158
C	-4.245881	-0.702337	0.921467	C	0.106248	2.234309	6.148792
C	-5.722317	-0.884025	-0.859205	O	-2.145313	1.579981	6.264510
O	-6.193673	-1.768277	0.086804	H	0.090506	0.385463	0.012675
<b>D</b>				O	3.612132	1.000686	5.789410
V	-0.075179	0.053453	2.779708	H	3.689709	-0.376087	7.353384
O	3.512646	-1.389146	-1.348743	H	2.780369	-2.123703	5.945926
O	0.087404	1.095196	-0.791920	C	2.616001	-1.111320	5.635314
O	-0.227011	-1.257843	3.847645	O	4.421908	0.997451	3.650312
O	3.206409	-2.382933	0.677112	H	2.182595	0.408289	7.169498
C	2.044642	-3.054145	1.386111	C	3.922123	0.432091	4.606228
C	0.994704	-3.178851	0.249691	H	1.592719	-0.967325	5.231601
O	1.485526	-2.258286	-0.761234	C	3.009370	-0.050622	6.610257

O	3.589513	-0.888209	4.559131	O	1.102198	1.152138	3.148312
O	-1.739565	0.817824	2.601073	K	-2.941960	0.268532	0.390504
K	-2.518722	-0.645384	4.572748	O	-0.879154	3.287309	6.049772
C	-5.837944	3.202708	-0.508305	H	0.643896	2.029985	5.267565
H	-5.422475	4.023311	0.000457	H	-0.680123	0.103939	6.223451
H	-5.343354	3.169867	-1.534176	C	-0.794227	1.044564	6.707744
O	-6.502684	0.227708	1.203260	O	-3.124671	3.468893	5.934672
H	-7.685524	3.936270	0.168101	H	0.849836	2.458326	6.946023
H	-7.681838	3.237072	-1.513407	C	-2.153555	2.836922	6.162927
O	-7.604205	1.803327	0.097946	H	-0.737392	0.842686	7.773885
C	-7.346130	3.071292	-0.486571	C	0.085319	2.209137	6.213769
C	-6.486151	1.247470	0.532015	O	-2.234662	1.468600	6.355862
O	-5.397990	1.990876	0.190167	H	0.035441	0.256066	-0.113239
<b>E</b>				O	3.795893	0.987208	5.835894
V	-0.108632	0.143394	2.687635	H	3.654609	-0.309490	7.340130
O	3.492373	-1.374320	-1.429582	H	2.915307	-2.052419	5.944731
O	-0.061238	1.123090	-0.713134	C	2.668520	-1.036115	5.611527
O	-0.359062	-1.046419	3.870488	O	4.560826	1.184241	3.708477
O	3.266942	-2.412153	0.538274	H	2.114043	0.588152	7.040207
C	2.084111	-2.913595	1.371927	C	3.988655	0.541879	4.568776
C	1.026043	-3.155888	0.260951	H	1.617090	-1.007191	5.325458
O	1.426334	-2.174799	-0.757281	C	3.027161	0.045923	6.620791
C	2.759923	-1.955683	-0.647127	O	3.437402	-0.683106	4.390440
H	2.512021	-3.781139	1.866930	O	-1.456303	1.373975	2.573196
H	0.003524	-2.781803	0.646674	K	-2.601799	-0.625593	4.500542
H	1.743881	-2.117965	2.137502	C	-5.895742	3.095154	-0.616549
H	0.967645	-4.208002	-0.099938	H	-5.484946	4.034631	-0.205448
C	-1.277209	1.108770	-2.953507	H	-5.531356	2.984255	-1.663216
C	-0.107785	0.679437	-2.060256	O	-6.255146	0.339066	1.271624
H	-1.320486	2.201392	-2.926679	H	-7.777924	4.022720	0.080458
H	-1.115237	0.711942	-4.026979	H	-7.978662	2.998175	-1.410032
H	-0.081433	-0.426586	-2.010084	O	-7.665191	1.994131	0.375120
H	0.827414	0.957513	-2.533538	C	-7.381039	3.128594	-0.483829
C	-3.587868	0.724788	-3.244602	C	-6.471852	1.350581	0.627335
O	-2.503368	0.595036	-2.328562	O	-5.446065	1.995054	0.126806
H	-4.583406	0.592362	-2.790409				
H	-3.611214	-0.034908	-4.178864	<b>Na<sub>2</sub>SnO<sub>3</sub></b>			
H	-3.583906	1.814897	-3.647659	<b>A</b>			
H	0.284046	2.993214	1.301181	Sn	-0.997656	-0.190095	4.615793
O	-2.917180	2.846022	0.686638	O	-2.840838	1.736699	-0.525421
O	-2.512929	4.136024	-1.333401	O	-0.799294	2.015146	2.034753
H	-2.396739	3.152467	3.051710	O	-1.837218	-1.875309	4.374974
C	-2.289118	3.741599	-0.144878	O	-1.114907	0.249961	-0.530465
O	-1.193268	4.260349	0.542277	C	-0.697524	-0.822515	0.378047
C	-0.587533	3.544947	1.628734	C	-2.016818	-1.281794	0.990827
H	-0.187300	4.353836	2.252670	O	-2.853981	-0.075299	0.857469
H	-0.618290	3.037864	3.542974	C	-2.299827	0.733800	-0.098238
C	-1.337454	2.856831	2.701957	H	-0.193052	-1.599899	-0.207404
H	-7.236470	0.759604	3.958530	H	-1.958103	-1.551813	2.057118
O	-5.023217	0.824832	5.531006	H	-0.012913	-0.382243	1.116014
O	-5.039576	-1.366529	6.295327	H	-2.501624	-2.089245	0.427818
H	-6.083696	2.303408	6.381224	C	0.571689	3.465648	0.713192
C	-5.607680	-0.359668	5.896131	C	-0.726499	3.336082	1.492556
O	-6.989756	-0.399173	5.706993	H	0.623436	2.671166	-0.054324
C	-7.252698	0.905091	5.088167	H	0.624367	4.448225	0.207488
H	-8.251022	1.285391	5.498656	H	-0.765551	4.098048	2.290457
H	-5.895153	2.520413	4.612010	H	-1.568054	3.529672	0.800537
C	-6.084498	1.783466	5.438968	C	2.943942	3.288535	0.960606
O	0.216030	-0.730544	1.246269	O	1.676382	3.324704	1.630235
K	3.008436	0.726122	1.157308	H	2.970352	2.481443	0.206930
				H	3.707693	3.081897	1.723798

H	3.157093	4.251343	0.463896	O	-0.830948	-2.156364	6.176130
H	-3.319923	5.459235	5.348226	O	-2.045567	1.175404	-2.526628
O	-1.550305	3.402458	6.542073	C	-1.379843	0.852277	-1.290292
O	0.334309	3.707168	5.300324	C	-2.470564	0.911148	-0.307813
H	-3.280137	2.442343	5.947865	O	-3.532249	1.535802	-0.999296
C	-0.868725	3.830418	5.451962	C	-3.268614	1.589299	-2.405831
O	-1.675363	4.467078	4.565259	H	-1.052299	-0.211903	-1.417364
C	-3.046652	4.435278	5.054817	H	-2.327380	1.567977	0.641827
H	-3.688650	4.082709	4.235421	H	-0.612435	1.629191	-1.307200
H	-3.498358	3.805528	7.138739	H	-2.715908	-0.138241	-0.003777
C	-2.974914	3.457542	6.239159	C	-0.604180	4.299604	2.177484
H	-4.603942	-4.761539	2.743147	C	-1.632418	3.468551	2.921124
O	-4.716910	-2.759108	4.904645	H	-0.423980	3.876318	1.144599
O	-5.132870	-0.869963	3.706231	H	-0.886648	5.384982	2.325248
H	-2.877321	-3.689219	5.059027	H	-1.657820	3.693711	4.040011
C	-4.720360	-2.018893	3.776691	H	-2.591813	3.864588	2.569428
O	-4.270974	-2.714195	2.702872	C	1.796783	4.677580	1.863800
C	-3.865420	-4.048403	3.136684	O	0.819423	4.194274	2.807359
H	-2.867071	-4.250528	2.722383	H	2.763451	4.366776	2.135281
H	-4.340096	-4.784618	5.179185	H	1.587369	5.723160	1.685781
C	-3.876514	-3.932062	4.667632	H	1.546582	4.233164	0.904280
O	-2.005542	1.438332	4.165222	H	-2.618140	2.993932	8.354385
O	0.877708	0.147816	4.829886	O	-0.253119	1.219776	7.185070
Na	1.078514	2.109520	3.609388	O	0.729807	2.892924	5.947556
O	4.082624	0.065898	5.393698	H	-2.141673	0.172068	7.629723
H	2.324955	-0.151676	6.471128	C	-0.196062	2.438066	6.571387
H	1.996862	2.211695	6.617880	O	-1.344146	3.068170	6.684545
C	3.029305	1.910881	6.394172	C	-2.369848	2.413222	7.447262
O	4.258968	0.951629	3.293001	H	-3.187184	2.162396	6.830238
H	3.843765	0.140336	7.457538	H	-1.303403	1.164833	8.958961
C	3.902319	1.022767	4.447712	C	-1.665116	1.143688	7.882583
H	3.749471	2.539040	6.938322	H	-4.143528	-4.198241	5.033149
C	3.270391	0.405804	6.560451	O	-4.732247	-1.140284	6.338336
O	3.252739	2.119108	4.967099	O	-5.387079	-0.235728	4.328378
H	-1.370004	1.932747	2.921193	H	-2.786117	-2.290931	6.914510
O	0.823850	-2.672835	2.446947	C	-4.876519	-1.099130	5.064227
H	2.634808	-3.083433	3.385027	O	-4.588281	-2.360216	4.451433
H	1.479259	-4.386134	5.113468	C	-3.702456	-3.208778	5.243795
C	0.850915	-3.681436	4.554118	H	-2.602667	-3.207297	4.872927
O	-0.797898	-3.985065	1.536312	H	-4.431659	-3.323586	7.350917
H	1.678496	-1.687387	4.076575	C	-3.751123	-2.757179	6.683011
C	-0.044672	-3.721027	2.454210	O	-1.967966	0.456793	4.510339
H	0.141655	-3.152351	5.209036	O	1.304260	0.063912	4.547501
C	1.638149	-2.713481	3.663769	Na	1.077425	2.110302	3.609132
O	0.053672	-4.447498	3.599925	O	4.978035	0.214553	3.951650
Na	-3.797380	0.890498	2.953056	H	3.502681	-0.844527	4.942248
C	-5.634284	2.853678	-1.030457	H	2.741146	1.121888	6.052645
H	-5.205389	2.045838	-1.637695	C	3.909715	1.109707	5.863764
H	-6.663092	3.077359	-1.343829	O	4.907822	2.151314	2.731746
O	-4.723769	2.993712	2.311063	H	5.065022	-0.820492	5.877743
H	-3.761194	3.931374	-1.485688	C	4.622269	1.512107	3.709824
H	-5.200149	5.017835	-1.324646	H	4.647867	1.354488	6.635976
O	-4.432473	4.257067	0.445497	C	4.382990	-0.232152	5.168356
C	-4.718147	4.096016	-0.972878	O	3.964770	2.036285	4.719236
C	-4.923355	3.195355	1.123794	H	-1.614621	1.226156	3.915768
O	-5.682389	2.389951	0.346945	O	1.331386	-0.716502	0.530464
<b>B</b>				H	3.294708	-1.522765	0.202996
Sn	-0.417199	-0.626228	5.153133	H	3.090027	-2.632072	2.433187
O	-4.018960	1.921972	-3.287308	C	2.397481	-1.810332	2.244694
O	-1.471393	2.115131	2.686327	O	-0.587257	-2.072685	0.374425



H	3.230322	-0.017120	1.051643	C	-2.056977	-3.059578	6.909654
C	0.518590	-1.875888	0.893854	O	-1.667361	0.165598	2.965044
H	2.055985	-1.200503	3.109058	O	0.799307	0.310055	5.161025
C	2.697072	-0.974429	0.959836	Na	1.080952	2.106589	3.613007
O	1.229531	-2.587213	1.781036	O	4.003748	-0.289657	4.753146
Na	-3.796969	0.890894	2.946467	H	2.591742	-1.215939	5.867895
C	-6.839136	0.528593	-1.289062	H	2.846154	0.562180	7.659192
H	-6.168182	1.163174	-1.907261	C	3.638053	0.503831	6.949515
H	-7.040638	-0.473629	-1.863905	O	3.646502	1.721571	3.764710
O	-5.884065	1.551768	1.801174	H	4.286716	-1.535262	6.409989
H	-8.288932	2.093453	-1.636213	C	3.660582	1.041549	4.742568
H	-8.954212	0.874056	-0.522609	H	4.592635	0.747809	7.473207
O	-7.481212	2.050799	0.255905	C	3.549385	-0.763359	6.107296
C	-7.984873	1.353311	-0.858138	O	3.413528	1.550019	5.970363
C	-6.458722	1.264438	0.774670	H	-0.764770	1.218905	1.747487
O	-6.135771	0.255968	-0.022148	O	-4.109588	-3.196123	1.648036
<b>C</b>				H	-2.831058	-2.355893	2.971184
Sn	-0.698036	-0.641730	4.300440	H	-1.008855	-3.566926	2.296127
O	-3.484244	3.288051	-1.421981	C	-1.941240	-4.030118	1.915364
O	0.005572	1.814811	1.500887	O	-3.970176	-2.893756	-0.682197
O	-0.589336	-2.612043	4.335765	H	-3.433560	-4.040626	3.389636
O	-2.903699	1.185434	-2.170416	C	-3.492126	-3.249457	0.387806
C	-2.763178	-0.212994	-1.552997	H	-1.940202	-5.124373	1.892831
C	-3.584084	-0.028940	-0.238305	C	-3.095314	-3.372813	2.643934
O	-3.611463	1.465897	-0.043011	O	-2.153965	-3.495541	0.535026
C	-3.383871	2.128308	-1.200127	Na	-3.797378	0.889180	2.953202
H	-3.079980	-0.893740	-2.305699	C	-2.301965	3.944323	1.724635
H	-3.021747	-0.473108	0.592792	H	-1.649176	4.337221	2.559946
H	-1.714459	-0.485253	-1.230361	H	-1.725373	3.316888	1.036927
H	-4.585818	-0.301183	-0.261494	O	-5.477869	3.219110	3.151698
C	1.181301	0.188025	-0.030878	H	-2.848446	6.037817	1.506150
C	0.343861	1.509818	0.090847	H	-3.360685	5.178260	0.138800
H	0.475351	-0.676290	0.239617	O	-4.561487	4.837487	1.859227
H	1.508152	0.205430	-1.075767	C	-3.252687	5.074613	1.213867
H	1.071355	2.314169	-0.161342	C	-4.552864	3.694165	2.516789
H	-0.508311	1.565356	-0.558020	O	-3.289899	3.087559	2.420345
C	2.874247	-1.042912	1.130380	<b>D</b>			
O	2.346030	0.258822	0.832953	Sn	-1.124948	-0.214380	5.067285
H	3.949921	-0.954313	1.492268	O	-4.911665	-1.121877	1.342814
H	2.908698	-1.740744	0.284656	O	0.215398	0.519095	1.647669
H	2.399675	-1.494520	2.003690	O	-1.984335	-1.174091	6.439838
H	-0.727692	4.943044	7.993631	O	-3.478228	-2.903880	1.242416
O	-0.623604	3.718535	4.951295	C	-2.249284	-3.182307	0.461371
O	1.002303	5.025416	4.063737	C	-2.018146	-1.917178	-0.325395
H	-2.376659	3.614930	6.089832	O	-3.139403	-1.070144	-0.038699
C	0.346493	4.698228	5.030952	C	-3.920208	-1.699340	0.884107
O	0.470675	5.183189	6.310386	H	-1.475534	-3.329980	1.211895
C	-0.907514	4.917388	6.934456	H	-1.951716	-2.114762	-1.356355
H	-1.409062	5.783144	6.553054	H	-2.462036	-4.073902	-0.055317
H	-0.793763	2.731763	6.669068	H	-1.012480	-1.541803	-0.061899
C	-1.242808	3.670937	6.274055	C	0.803644	2.675797	0.814592
H	-3.580489	-3.321510	8.342991	C	0.041001	1.387505	0.492768
O	-2.476739	-0.839466	5.932306	H	1.851265	2.406055	1.121883
O	-4.304682	-0.820771	4.685905	H	0.814234	3.358875	-0.024639
H	-1.639651	-3.778868	6.104094	H	-0.986726	1.590231	0.180549
C	-3.669190	-1.297046	5.698173	H	0.601138	0.864304	-0.267451
O	-4.328964	-2.083873	6.651164	C	-1.063312	3.916378	1.641949
C	-3.381301	-3.184605	7.260438	O	0.279303	3.443475	1.965939
H	-3.806415	-4.075063	6.853402	H	-1.827155	3.046212	1.652499
H	-1.249625	-2.767615	7.523134	H	-1.069936	4.352238	0.599129

H	-1.391814	4.720098	2.344643	O	-1.117209	-2.657208	3.942590
H	0.150543	5.720973	7.819573	O	-2.435939	1.620110	-1.577456
O	0.644439	3.339622	6.244454	C	-0.993852	1.284249	-1.616370
O	-1.296250	3.303250	5.114050	C	-0.976134	-0.255955	-1.251522
H	0.685759	2.704660	8.222021	O	-2.331463	-0.576043	-0.923910
C	-0.647960	3.590903	6.099210	C	-3.147079	0.500180	-1.067640
O	-1.203481	4.231824	7.199654	H	-0.401501	1.574966	-2.556349
C	-0.075760	4.683585	8.037327	H	-0.343342	-0.381602	-0.379568
H	-0.434319	4.572073	9.077739	H	-0.491808	1.787293	-0.737158
H	1.962836	3.919642	7.741855	H	-0.642808	-0.807665	-2.143695
C	0.947618	3.624409	7.727447	C	0.166846	4.756716	2.388053
H	-4.952960	2.598457	8.908369	C	-0.901828	3.734122	2.217568
O	-3.703159	1.596856	6.155326	H	0.536095	5.055243	1.373413
O	-5.300375	2.193346	4.642632	H	-0.224775	5.593894	2.960012
H	-3.228649	0.549469	7.736225	H	-1.465569	3.414791	3.154915
C	-4.901534	2.093622	5.803799	H	-1.640576	4.207128	1.506770
O	-5.609546	2.420782	6.911508	C	2.181318	5.206645	3.426937
C	-4.999694	1.847728	8.073859	O	1.188518	4.204774	3.181962
H	-5.575333	0.968627	8.403217	H	3.162945	4.819366	3.635809
H	-2.849064	2.389963	7.882609	H	1.955282	5.855401	4.278672
C	-3.537155	1.607407	7.602633	H	2.287467	5.930039	2.556687
O	-1.699795	0.447507	3.330362	H	-5.263169	3.224984	6.423081
O	0.697177	0.254015	5.236754	O	-2.228571	3.063641	7.450268
Na	1.077302	2.107412	3.609945	O	-1.124544	3.977819	5.705025
O	4.164458	-0.913498	2.797472	H	-3.701557	1.974829	8.406169
H	1.837406	-1.124998	3.570658	C	-2.141351	3.591909	6.174070
H	2.911573	0.380089	5.860253	O	-3.400353	3.554003	5.612182
C	3.411222	-0.166736	5.069983	C	-4.321923	2.764857	6.380841
O	4.271635	1.146773	1.871530	H	-4.458366	1.735213	5.983542
H	2.186764	-1.912673	5.257509	H	-4.022220	3.849000	8.181197
C	4.122505	0.328384	2.808606	C	-3.594576	2.894576	7.750074
H	4.345340	-0.598235	5.503561	H	-2.594527	-4.022810	6.622430
C	2.323580	-1.144260	4.549315	O	-2.060849	-0.616464	5.402589
O	3.640552	0.915376	4.040998	O	-4.320784	-0.525290	4.823611
H	-0.671130	0.566670	2.159365	H	-0.323562	-3.819816	5.768501
O	2.801465	-1.755926	-1.020914	C	-3.264387	-1.078620	5.424003
H	4.535643	-2.654705	-0.462511	O	-3.315479	-2.157528	6.141583
H	3.259998	-4.191214	1.079059	C	-2.581126	-3.337456	5.744504
C	2.732243	-3.320736	0.822525	H	-3.186213	-3.829978	4.896731
O	0.723671	-2.213255	-1.811097	H	-0.858728	-2.081221	5.974432
H	3.943794	-1.395726	0.761600	C	-1.050580	-2.952238	5.381228
C	1.654689	-2.414608	-1.045774	O	-1.779685	0.492204	2.436325
H	2.435506	-2.808388	1.733081	O	1.145651	-0.097526	3.584898
C	3.664989	-2.191408	0.055548	Na	1.078238	2.107647	3.606140
O	1.588783	-3.419206	-0.093350	O	2.968164	-0.794569	6.502181
Na	-3.796387	0.890945	2.952071	H	1.141451	-1.596140	5.997781
C	-7.217268	0.836521	0.769075	H	0.150083	0.600458	5.982386
H	-7.276758	-0.172396	1.275328	C	1.076397	0.571711	6.602263
H	-8.164435	1.384553	1.018709	O	4.360391	0.737349	5.501890
O	-4.172471	2.354673	1.008433	H	1.432433	-1.405792	7.749700
H	-6.581450	-0.140321	-1.150620	C	3.264656	0.376715	5.912000
H	-7.377407	1.508466	-1.419932	H	0.820058	1.029963	7.649813
O	-5.488449	1.486508	-0.687089	C	1.609172	-0.939759	6.775817
C	-6.812249	0.863159	-0.763692	O	2.171753	1.131482	5.886444
C	-5.202743	1.848593	0.599573	H	-0.904140	1.824860	1.977051
O	-6.204690	1.586862	1.448824	O	2.392385	-1.706228	0.505096
<b>E</b>				H	3.953201	-2.167480	1.761525
Sn	-0.682107	-0.690834	3.484422	H	3.160881	-4.444103	1.929355
O	-4.309826	0.532116	-0.807071	C	2.415536	-3.700449	1.584311
O	-0.394310	2.582359	1.526439	O	1.471382	-2.524896	-1.492237

H	2.367810	-1.668691	2.545444	H	-5.304789	-1.438232	1.886561
C	1.947319	-2.740850	-0.389580	C	-4.363800	-0.930626	2.071560
H	1.415587	-3.907169	2.047677	O	-0.507224	0.947644	0.203082
C	2.844369	-2.240176	1.731493	K	-0.444232	-1.272040	-0.930891
O	2.143592	-3.934049	0.144130	O	-0.485746	-0.888142	1.841195
Na	-3.800023	0.891801	2.957032	K	-0.540806	3.382911	3.524571
C	-7.060128	1.777252	0.973900	O	-3.290227	4.382052	3.755989
H	-6.817774	1.010787	0.271128	H	-4.801035	3.137066	3.104126
H	-8.127798	1.804732	1.361618	H	-5.364514	3.334344	5.443733
O	-5.174746	3.274363	3.537104	C	-4.354701	2.951978	5.252179
H	-5.866628	3.302226	-0.195794	O	-1.745332	5.132763	5.301274
H	-7.452956	3.769649	-0.124437	H	-3.209845	2.275227	3.453561
O	-6.447057	3.891547	1.762070	C	-2.781230	4.563039	5.024843
C	-6.734229	3.181515	0.428306	H	-4.229743	1.923637	5.655831
C	-5.896943	3.010784	2.600808	C	-3.936187	3.052574	3.777971
O	-6.061841	1.730619	2.081267	O	-3.436190	3.812598	5.936771
<b>K<sub>3</sub>PO<sub>4</sub></b>				H	0.341136	2.012944	-0.950943
<b>A</b>				O	2.963866	-3.183118	1.747946
P	-0.522448	0.679323	1.745070	H	1.081872	-2.378145	2.396993
O	-0.820470	4.848807	0.024107	H	1.817855	-0.093808	1.885669
O	0.568270	2.735455	-1.535106	C	2.539624	-0.916030	1.828449
O	-1.707577	1.432773	2.406469	O	3.075876	-3.452840	-0.505173
O	0.775062	3.742380	1.428595	H	2.454786	-2.372719	3.555068
C	2.128454	3.237410	0.852251	C	2.983608	-2.701910	0.458764
C	2.599683	4.530731	0.241815	H	3.544344	-0.524516	2.196290
O	1.407345	5.043255	-0.366695	C	2.167509	-2.258091	2.522254
C	0.334049	4.481548	0.311728	O	2.791871	-1.379931	0.396822
H	2.667715	2.825508	1.689526	O	0.711595	1.245853	2.500588
H	3.404608	4.459736	-0.526350	K	-2.444156	2.602962	0.233872
H	1.986138	2.470230	0.053032	C	-2.551461	-1.295507	7.249008
H	2.980686	5.249986	0.962767	H	-2.894560	-0.819572	8.177940
C	-0.331626	2.647246	-3.942116	H	-1.467353	-1.360028	7.086730
C	0.813347	2.500809	-2.902015	O	-3.987530	-4.164765	5.929954
H	-0.604033	3.727269	-3.968866	H	-3.960349	-0.054903	6.034437
H	-0.091781	2.301255	-4.989821	H	-2.419100	-0.264988	5.251679
H	1.364372	1.596990	-3.162546	O	-3.619800	-1.946771	5.253806
H	1.650182	3.217170	-3.206906	C	-3.132902	-0.769019	5.881121
C	-1.887986	0.850821	-4.016616	C	-3.574979	-3.041680	6.121335
O	-1.482716	2.004797	-3.321566	O	-2.938042	-2.713073	7.273004
H	-1.285244	-0.019176	-3.740674	<b>B</b>			
H	-1.885531	0.882282	-5.114023	P	-0.505454	1.574841	2.999408
H	-2.953679	0.693604	-3.705708	O	3.102648	-2.426528	3.044575
H	2.352526	1.309090	3.941231	O	-0.597374	-2.216510	1.783703
O	0.070181	-0.006383	5.558192	O	0.472738	2.214291	2.056085
O	-1.037471	1.835538	6.311448	O	2.776164	-1.182320	4.875969
H	1.892224	-0.889096	6.057570	C	3.014681	0.209471	5.288823
C	-0.041472	1.321585	5.810987	C	3.202382	0.895198	3.967119
O	1.079949	2.016532	5.395869	O	3.737808	-0.232441	3.065057
C	2.143543	1.088007	5.007560	C	3.177545	-1.347503	3.599695
H	2.950586	1.276466	5.725575	H	2.148927	0.579848	5.811585
H	1.350480	-0.944758	4.368879	H	3.882501	1.804089	3.955526
C	1.499376	-0.289413	5.247962	H	3.819039	0.267497	6.021943
H	-3.359301	-2.903919	2.392766	H	2.200621	1.235318	3.579866
O	-4.078259	-0.057014	0.952979	C	1.276076	-2.307243	0.225114
O	-2.981007	-0.273706	-1.019557	C	-0.188985	-2.710257	0.559062
H	-4.358004	-0.273358	2.967491	H	2.011434	-2.490772	1.042345
C	-3.284809	-0.750943	0.069209	H	1.617951	-2.970992	-0.659024
O	-2.847635	-1.899998	0.578065	H	-0.762473	-2.577573	-0.342066
C	-3.155382	-1.863524	2.076753	H	-0.136586	-3.888759	0.754413
H	-2.165131	-1.503920	2.429425	C	2.360696	0.027118	0.042031

O	1.206835	-0.921314	-0.064975	O	-1.032382	2.643388	-3.546273
H	2.867520	0.276863	-0.844007	C			
H	3.156914	-0.295158	0.728606	P	-0.593185	1.595378	2.989324
H	1.867578	0.830377	0.563794	O	2.661099	-2.639987	3.114022
H	-4.944900	4.251713	0.515246	O	-0.833207	-2.140006	1.020747
O	-2.957436	3.434266	-0.563739	O	0.024479	2.640066	2.000451
O	-3.349033	1.308088	-0.978316	O	2.317176	-1.016071	4.676581
H	-2.171105	3.276189	1.764835	C	2.984871	0.269075	5.024082
C	-3.598666	2.343665	-0.378936	C	3.811223	0.466046	3.768256
O	-4.434510	2.327523	0.823652	O	4.030070	-0.829389	3.185168
C	-4.387812	3.647246	1.231606	C	3.017963	-1.609774	3.674216
H	-4.818889	3.789767	2.257504	H	2.067137	1.016732	5.019382
H	-2.536522	5.015574	1.532161	H	4.795439	0.934670	3.907253
C	-2.900209	3.985593	1.342774	H	3.463595	0.137024	5.926706
H	-5.014246	-5.935678	3.995494	H	3.263399	1.208662	3.114364
O	-3.173931	-3.480893	2.923289	C	1.419716	-1.801332	-0.254402
O	-4.540270	-1.783813	3.445438	C	-0.128709	-2.183551	-0.154432
H	-2.822738	-5.441813	2.072457	H	2.033535	-2.354931	0.440064
C	-4.316092	-2.952670	3.351349	H	1.652577	-2.207169	-1.289222
O	-5.260571	-3.914024	3.723705	H	-0.699575	-1.671375	-0.957284
C	-4.769450	-5.171636	3.258113	H	-0.012645	-3.347088	-0.389745
H	-5.418802	-5.378730	2.341013	C	3.110306	-0.222587	-0.291656
H	-2.668430	-5.163486	3.905128	O	1.676231	-0.426735	-0.267277
C	-3.226542	-4.935531	3.048608	H	3.665817	-0.616268	-1.148331
O	-1.281883	0.378344	2.181279	H	3.530421	-0.785909	0.585093
K	-3.717943	0.750071	3.099269	H	3.243032	0.882870	-0.183585
O	-1.546258	2.643153	3.435981	H	-4.700936	4.502710	0.682352
K	-0.094225	-1.331127	4.161680	O	-2.853419	3.164737	-0.942782
O	3.688696	4.247226	1.090209	O	-3.818412	1.072310	-0.841502
H	2.843124	5.140925	-0.489445	H	-1.759616	3.660305	1.476450
H	1.707911	6.731466	1.182526	C	-3.543170	2.216901	-0.400535
C	1.798678	5.637372	1.463347	O	-4.186811	2.505935	0.861791
O	4.826968	4.790813	3.019169	C	-4.057446	3.850778	1.271629
H	1.924080	3.800065	0.218628	H	-4.506908	3.840794	2.281631
C	3.845904	4.846823	2.333087	H	-2.409600	5.197246	0.597379
H	0.876030	5.140642	1.863187	C	-2.598176	4.295270	1.207886
C	2.508694	4.677795	0.442712	H	-3.532271	-5.569406	4.756093
O	2.769563	5.628731	2.567472	O	-3.554103	-3.284696	3.048519
H	-0.732909	-1.252052	1.846791	O	-5.026026	-1.816697	4.086942
O	-1.165864	0.048918	7.003303	H	-4.301459	-4.715670	1.820478
H	-1.280350	1.350252	8.490775	C	-4.581170	-2.954083	3.898249
H	-3.014674	2.551098	7.401796	O	-5.086869	-4.110800	4.451234
C	-2.416878	1.936549	6.711463	C	-4.283151	-5.275914	3.930540
O	-2.636566	-1.422678	6.144320	H	-5.000418	-6.083058	3.662428
H	-0.201100	1.779843	7.164152	H	-2.633658	-5.006802	2.568003
C	-2.328578	-0.328650	6.445320	C	-3.701407	-4.647934	2.672373
H	-2.303064	2.481499	5.754829	O	-1.176795	0.304672	2.271417
C	-1.220823	1.392668	7.460823	K	-3.864725	0.308617	2.550128
O	-3.173553	0.797913	6.322182	O	-1.927164	2.289521	3.454431
O	0.122734	1.102845	4.290232	K	-0.308544	-1.418750	4.145691
K	-0.605328	1.217400	-0.573542	O	3.114145	4.001056	1.480463
C	-2.088782	2.623753	-4.518661	H	2.297771	4.829780	-0.223999
H	-1.650440	2.319000	-5.516480	H	1.965569	6.796031	1.015895
H	-2.723825	1.829727	-4.104524	C	1.854311	5.892769	1.625944
O	-0.175343	4.198650	-2.170296	O	4.785665	4.504129	2.953633
H	-2.804927	4.553139	-5.524599	H	1.129549	3.911076	0.836545
H	-3.759368	3.939616	-4.018405	C	3.724917	4.809386	2.413569
O	-1.878888	4.764548	-3.606203	H	0.983243	5.835356	2.324550
C	-2.724429	3.975477	-4.545132	C	1.985244	4.604920	0.799381
C	-0.914192	3.900242	-3.031225				

O	2.897635	5.869458	2.598540	O	-3.638301	0.552326	-0.848603
H	-0.879347	-1.215869	1.437344	O	-3.115038	-1.328795	-2.025738
O	-1.180786	1.044015	7.257959	H	-3.312479	1.845479	0.734921
H	-0.761080	3.073318	7.488873	C	-3.310962	-0.787183	-0.954590
H	-3.167799	2.589595	7.167630	O	-3.041633	-1.295798	0.222200
C	-2.562773	2.504390	6.207974	C	-3.308100	-0.331656	1.285613
O	-2.056896	-0.825870	6.377632	H	-2.351630	-0.155247	1.778404
H	-0.471952	2.445441	5.774258	H	-4.869811	1.134043	0.753826
C	-2.044627	0.369616	6.456578	C	-3.816707	0.888498	0.589906
H	-2.757098	3.250943	5.419123	O	-0.091544	2.308405	0.691822
C	-1.112765	2.427628	6.648965	K	-0.526660	0.217846	-1.631148
O	-2.751151	1.208476	5.698242	O	-0.144794	-0.230613	0.753451
O	0.371038	1.014690	4.069924	K	0.387473	0.157379	4.486050
K	-0.613660	1.200266	-0.506369	O	-5.271898	2.889332	4.567892
C	-2.200842	1.934430	-3.570927	H	-4.337223	2.405952	6.437240
H	-1.889978	1.261435	-4.365672	H	-2.082906	2.494390	5.429760
H	-2.848304	1.392768	-2.821746	C	-2.986113	2.471575	4.766085
O	0.160901	3.947884	-1.976200	O	-5.104680	4.811833	3.362676
H	-2.971884	3.708067	-4.817118	H	-4.650033	1.094956	5.323032
H	-3.552970	3.711849	-3.207920	C	-4.595574	3.907301	4.007329
O	-1.550675	4.280437	-3.450590	H	-2.691041	1.826538	3.929261
C	-2.649386	3.362374	-3.840344	C	-4.272592	2.120363	5.385336
C	-0.767263	3.502186	-2.642896	O	-3.259095	3.829919	4.216772
O	-0.901840	2.193633	-2.862417	H	0.817467	3.766945	0.600509
<b>D</b>				O	3.384433	-1.335148	-0.592560
P	0.139593	1.082256	1.617642	H	3.788041	-0.129342	1.165589
O	0.490003	3.661515	5.454353	H	2.473168	1.583809	0.108715
O	1.175588	4.660120	0.423791	C	3.129093	1.027691	-0.595438
O	-1.056766	1.108929	2.656962	O	1.437779	-1.754883	-1.847380
O	2.284668	2.212003	4.889252	H	5.044406	-0.090857	-0.239890
C	3.451194	2.401232	3.929929	C	2.222336	-0.978286	-1.303842
C	2.995024	3.664257	3.199649	H	3.616130	1.724998	-1.267602
O	2.134648	4.362580	4.134510	C	3.960701	-0.113673	0.025172
C	1.591731	3.444900	4.897412	O	2.131382	0.355080	-1.446627
H	4.303100	2.473014	4.609620	O	1.504996	1.155327	2.290962
H	2.437912	3.274086	2.330768	K	-1.335231	3.844554	2.365823
H	3.431545	1.527048	3.243430	C	-3.894764	-2.637979	3.802720
H	3.697797	4.456416	2.893603	H	-4.973036	-2.452345	3.610928
C	-0.492712	6.124746	-0.439474	H	-3.460182	-3.142068	2.935672
C	0.710108	5.262456	-0.755618	O	-1.986327	-0.634200	5.865261
H	-0.116701	6.872436	0.350152	H	-4.455769	-3.750973	5.670421
H	-0.839990	6.711084	-1.338269	H	-3.173571	-4.551066	4.713935
H	0.401541	4.486171	-1.500594	O	-2.691088	-2.791161	5.826104
H	1.414456	5.915621	-1.255945	C	-3.594570	-3.563723	5.051294
C	-2.540400	4.867577	-0.983328	C	-2.601580	-1.529798	5.316035
O	-1.601191	5.356335	0.076528	O	-3.312187	-1.363937	4.140906
H	-2.055727	3.954480	-1.414574	<b>E</b>			
H	-2.707979	5.444909	-1.841583	P	1.013443	0.738390	1.484180
H	-3.468883	4.703200	-0.473082	O	0.958545	4.588825	4.423115
H	1.465213	-1.271267	2.096172	O	-1.314648	1.357614	4.075186
O	-0.486545	-4.051864	2.063008	O	1.105192	-0.128171	2.698664
O	-0.756896	-4.193657	4.407232	O	0.790422	5.071674	2.195278
H	-0.439562	-2.509042	0.376294	C	1.852351	5.229502	1.108272
C	-0.392244	-3.681600	3.322705	C	2.978432	4.214964	1.499515
O	0.565393	-2.594248	3.397726	O	2.609147	3.960211	2.948320
C	0.930246	-2.239847	2.138036	C	1.365279	4.450392	3.247590
H	1.561711	-2.989912	1.786257	H	1.350361	4.960606	0.144086
H	-1.135192	-1.675040	1.852351	H	4.012758	4.666653	1.515924
C	-0.248691	-2.097533	1.347115	H	2.182813	6.252635	1.248091
H	-4.069155	-0.783810	1.943177	H	2.982054	3.260952	0.986214

C	-2.529707	2.138625	5.912539	H	-5.454584	-3.327501	2.587294
C	-2.056194	2.494571	4.488176	O	-3.989242	-2.541877	6.180082
H	-1.675116	2.060565	6.503867	H	-4.622005	-5.982183	4.001210
H	-3.273237	2.861094	6.257045	H	-3.983032	-4.931179	2.652882
H	-2.942942	2.627728	3.789592	O	-3.738796	-4.162514	4.683517
H	-1.516176	3.515121	4.636794	C	-4.472342	-4.907240	3.671561
C	-4.511039	0.750600	5.355325	C	-4.475339	-3.209904	5.291033
O	-3.102440	0.803846	5.891687	O	-5.746952	-3.228346	4.713268
H	-4.901918	-0.313454	5.573269	<b>Cartesian coordinates (in Å) related to</b>			
H	-4.543734	1.119471	4.321860	<b>Figure S3 in the SI</b>			
H	-5.090178	1.446018	5.983983	<b>K<sub>3</sub>VO<sub>4</sub></b>			
H	-1.366542	-2.404216	-0.343849	<b>TS-A</b>			
O	-2.972657	-2.313864	1.882233	V	-0.484144	0.315058	3.026688
O	-5.004294	-1.503063	1.070400	O	-2.340705	1.219329	-0.697880
H	-2.149126	0.074593	1.327772	O	0.583565	1.095821	-0.386149
C	-3.768860	-1.791019	1.027969	O	-0.227961	-0.787263	4.393842
O	-3.200885	-1.453928	-0.245498	O	-1.142765	0.829018	-2.648654
C	-1.776177	-1.404617	-0.177429	C	-0.926758	-0.529826	-3.281751
H	-1.612168	-0.830161	-1.072466	C	-0.552355	-1.354886	-1.905038
H	-0.986155	-1.115764	1.823884	O	-1.499292	-0.766860	-1.075513
C	-1.298188	-0.548186	0.989773	C	-1.620354	0.595491	-1.419276
H	-7.436698	0.871903	0.054449	H	-1.825030	-0.860426	-3.785048
O	-4.866840	1.791602	1.812528	H	0.371582	-0.957251	-1.625184
O	-3.518190	2.592988	0.171517	H	-0.087961	-0.395783	-4.000517
H	-6.351010	0.797510	2.667092	H	-0.569647	-2.418326	-1.974518
C	-4.590695	2.145478	0.528618	C	2.083457	2.990769	-0.297458
O	-5.631132	1.962634	-0.320281	C	1.602990	1.744094	-1.069451
C	-6.403855	0.926850	0.378445	H	2.616616	2.663425	0.627175
H	-5.922408	-0.027870	0.266547	H	2.895731	3.514457	-0.873426
H	-6.847466	2.320302	2.046856	H	1.259266	2.033728	-2.119560
C	-6.351718	1.423023	1.792371	H	2.560112	1.191187	-1.188174
O	0.510145	2.100193	2.041495	C	1.418290	4.998498	0.810548
K	-1.097810	3.647150	0.367145	O	1.041778	3.839378	0.018801
O	-0.147059	0.202253	0.493249	H	2.160488	4.706317	1.630762
K	1.654145	1.631408	4.468266	H	0.464077	5.385664	1.182702
O	4.013449	-0.395754	3.372440	H	1.831526	5.709181	0.140569
H	3.773190	-2.162823	2.268649	H	-3.598692	3.492740	5.214790
H	6.041803	-1.481099	1.734097	O	-3.449614	4.109730	2.259764
C	5.252611	-0.791517	1.420971	O	-2.194468	5.961477	2.443711
O	5.120015	1.362059	4.108779	H	-5.183924	3.030722	2.639852
H	3.097607	-0.665469	1.436680	C	-2.949136	5.181406	2.957163
C	4.919193	0.547728	3.255040	O	-3.467539	5.310059	4.274526
H	5.258872	-0.660367	0.335915	C	-4.199872	4.080641	4.527339
C	3.893643	-1.100825	2.012501	H	-5.194922	4.339168	4.883539
O	5.488542	0.539014	2.060948	H	-3.648249	2.339926	3.166374
H	-0.781396	1.512283	3.200115	C	-4.221915	3.267593	3.134671
O	2.263590	3.600467	-1.959045	H	-3.906310	-3.600893	6.885120
H	3.887139	2.579232	-2.574477	O	-3.844057	-1.733728	4.858982
H	2.560180	1.416626	-4.113401	O	-3.794263	-3.066556	2.925706
C	2.088612	1.500118	-3.062365	H	-1.923309	-1.550042	5.647917
O	0.024006	4.027721	-2.014813	C	-3.679621	-2.874057	4.124784
H	2.950899	1.876521	-1.021296	O	-3.190679	-3.874036	4.919354
C	0.967954	3.352872	-2.323858	C	-3.035953	-3.331024	6.281953
H	1.937796	0.468395	-2.655691	H	-2.114829	-3.826012	6.691305
C	2.946948	2.328078	-2.090228	H	-3.273587	-1.172602	6.769042
O	0.840209	2.189860	-3.060061	C	-2.924423	-1.855786	5.956235
O	2.265229	0.941956	0.566439	O	-0.327802	-0.961596	1.599105
K	-2.162720	-1.038475	4.319528	K	-0.619533	-2.866849	3.187205
C	-5.732269	-3.926332	3.455535	O	0.713396	1.485235	3.116824
H	-6.609905	-4.524673	3.381275	K	-1.062387	2.872413	0.691786

O	0.449626	3.897437	4.207953	O	-5.577626	2.000174	1.556279
H	-0.385586	4.067214	6.043286	H	-2.811306	4.436069	1.962290
H	0.719463	2.126500	6.895686	C	-5.176972	3.126253	1.401877
C	0.701995	2.236831	5.786899	O	-5.686543	4.251455	1.966741
O	2.708827	4.185496	3.679168	C	-4.808896	5.353601	1.790369
H	-1.174039	2.809125	4.994300	H	-4.520584	5.833437	2.742847
C	1.771273	3.716433	4.358364	H	-3.051448	5.213505	0.332333
H	0.635724	1.216917	5.274323	C	-3.527456	4.700378	1.194663
C	-0.231614	3.277776	5.301796	H	-2.743379	3.799156	4.747940
O	1.978258	2.906102	5.471933	O	-3.674654	1.632029	6.494279
H	0.375715	-0.673273	0.895537	O	-5.319032	1.021319	5.004481
O	1.614943	-3.032177	4.991019	H	-2.949385	3.177299	7.740167
H	3.636330	-2.575546	4.705606	C	-4.593630	1.854443	5.505563
H	3.401721	-1.571439	7.003766	O	-4.656294	3.194138	5.156733
C	2.616086	-1.303386	6.301338	C	-3.423120	3.823129	5.602832
O	-0.146491	-3.459712	6.310435	H	-3.750538	4.808610	5.919367
H	2.399394	-1.286499	4.121322	H	-1.829908	2.656168	6.545069
C	0.864730	-2.817939	6.082647	C	-2.891111	2.836301	6.693991
H	2.633345	-0.203870	6.204296	O	-1.401268	-0.299777	1.307917
C	2.667043	-2.030269	4.919785	K	0.155466	-2.267494	3.483244
O	1.277136	-1.754964	6.835178	O	0.371106	0.615646	2.991916
O	-2.154452	0.872354	2.989817	K	-1.524129	1.820763	-0.278605
K	-3.181203	-0.284615	1.260365	O	-0.270703	4.012581	5.244793
C	-6.167699	2.109367	-2.594601	H	-1.048889	3.617146	3.311398
H	-5.923613	1.451883	-3.468727	H	0.913562	2.332351	3.077026
H	-7.147231	2.550638	-2.794039	C	1.124472	3.394289	3.369066
O	-5.634477	1.261602	0.739944	O	1.364498	3.972147	6.863973
H	-4.060530	2.996042	-2.719963	H	-0.143953	5.185542	3.420215
H	-5.405114	4.188530	-2.184860	C	0.994978	3.833229	5.675425
O	-4.828221	2.824881	-0.804059	H	1.720029	4.001849	2.692653
C	-5.077647	3.141663	-2.226719	C	-0.170975	4.111069	3.778707
C	-5.546381	1.708586	-0.393046	O	1.861722	3.424168	4.678273
O	-6.206496	1.149659	-1.489537	H	0.494644	-1.160577	0.951656
<b>III-A</b>				O	1.552782	-0.672347	7.121030
V	-1.333322	0.825912	2.557013	H	0.430621	0.587698	8.428397
O	2.249045	-4.030517	2.183470	H	-1.334639	0.703857	6.741655
O	1.187242	-1.772104	0.794900	C	-0.315859	0.582313	6.310196
O	-2.314178	0.360111	3.876230	O	1.395115	-2.327108	5.581879
O	0.077400	-4.013276	1.392260	H	1.509805	1.444716	7.245846
C	-0.518876	-4.036918	0.045146	C	0.906775	-1.351760	6.151997
C	0.719605	-4.090765	-0.843712	H	-0.220096	1.212209	5.395164
O	1.838233	-4.475615	-0.085437	C	0.814707	0.622989	7.378075
C	1.491198	-4.176493	1.274879	O	-0.302179	-0.793254	5.836277
H	-1.062895	-4.985754	0.074152	O	-1.902140	2.394972	2.034409
H	0.925460	-3.060332	-1.183796	K	-4.421713	-0.185836	2.569647
H	-1.258489	-3.225226	-0.000061	C	-4.349447	0.338832	-2.409693
H	0.670435	-4.786888	-1.725099	H	-3.818594	-0.588709	-2.094274
C	2.396929	0.320170	0.657300	H	-5.245714	0.448634	-1.785691
C	2.266802	-1.111501	0.199863	O	-2.204461	2.740707	-3.701156
H	1.805570	0.402717	1.606385	H	-4.643493	-0.540423	-4.452134
H	3.491355	0.579465	0.747923	H	-5.782745	0.831141	-3.995465
H	2.269262	-1.281891	-0.892049	O	-3.745817	1.324582	-4.504799
H	3.202482	-1.588722	0.622594	C	-4.763342	0.427481	-3.898225
C	1.905610	2.563329	0.120843	C	-3.024358	1.915284	-3.547334
O	1.801441	1.242490	-0.244381	O	-3.430207	1.474997	-2.292946
H	1.520488	3.157427	-0.821368	<b>K<sub>3</sub>PO<sub>4</sub></b>			
H	2.940139	2.882637	0.313213	<b>TS1-B</b>			
H	1.244517	2.833064	0.996115	P	-0.094525	-0.330306	1.445357
H	-5.266900	6.102712	1.140066	O	-0.503218	4.349000	2.563517
O	-4.119305	3.507773	0.616374	O	-0.785389	3.195124	-0.029594

O	-0.729897	-0.663065	0.060134	O	0.817200	-1.620468	-3.173656
O	1.615127	4.055637	1.952310	H	4.022364	-2.102232	-0.326454
C	2.604921	4.773143	1.261965	C	1.655162	-1.395236	-2.330112
C	1.700342	5.615255	0.272013	H	3.889405	0.243333	-1.388035
O	0.379273	5.738863	0.904393	C	3.039190	-1.630675	-0.524775
C	0.340653	4.621289	1.771513	O	1.916698	-0.059141	-1.883520
H	3.086487	5.338456	2.084458	O	-0.948099	0.352048	2.562844
H	1.467501	4.989468	-0.602079	K	-0.257210	1.350787	-1.280300
H	3.267889	4.098534	0.746819	C	-0.551213	-2.379119	4.442655
H	2.024525	6.625107	-0.014836	H	-0.037518	-3.292414	4.764156
C	-3.039958	4.291174	-0.556551	H	-0.487202	-2.253053	3.351883
C	-1.464079	4.197109	-0.733252	O	-3.269427	-2.069595	6.593626
H	-3.387023	3.276702	-0.248925	H	0.768109	-1.096103	5.803854
H	-3.307217	4.936389	0.265670	H	-0.340697	-0.213130	4.657805
H	-1.370560	4.055313	-1.827942	O	-1.147483	-1.196813	6.351916
H	-0.945821	5.195211	-0.524580	C	-0.160903	-1.107357	5.261891
C	-4.245822	6.004111	-1.778524	C	-2.241368	-1.945176	5.958276
O	-3.825976	4.669346	-1.719276	O	-1.916536	-2.561921	4.785352
H	-3.433973	6.708289	-1.622167	<b>II-B</b>			
H	-4.896838	6.067101	-0.910863	P	0.207523	0.342212	2.104109
H	-4.846232	6.241584	-2.679046	O	0.921946	4.902812	0.908184
H	-0.474581	4.751786	5.020443	O	0.741640	3.058767	-1.007709
O	1.185057	2.050514	5.824755	O	-1.095734	1.217714	1.906850
O	0.965437	2.179111	8.068894	O	1.454803	5.829191	-1.167892
H	1.560774	2.922390	3.939837	C	0.619761	6.147036	-2.337440
C	0.880901	2.638793	6.977222	C	-0.833863	6.140066	-1.834069
O	0.413830	3.972431	6.766113	O	-0.828198	5.721002	-0.443750
C	0.449835	4.270748	5.343527	C	0.577751	5.441497	-0.147623
H	1.279241	4.982864	5.133950	H	0.950219	7.145300	-2.641552
H	-0.122612	2.363497	4.327133	H	-1.420525	5.396090	-2.393267
C	0.752964	2.874364	4.702328	H	0.807611	5.395842	-3.139976
H	-3.842561	-2.408774	2.649000	H	-1.345917	7.088738	-1.949066
O	-4.319345	-2.336778	-0.164639	C	1.973562	1.387538	-2.256390
O	-3.100278	-4.170548	-0.829380	C	0.811281	2.417297	-2.173362
H	-3.209074	-0.612628	0.194169	H	2.097416	1.030919	-1.205321
C	-3.312171	-3.286057	-0.034603	H	1.717752	0.480771	-2.872224
O	-2.604247	-3.102804	1.112539	H	1.095550	2.998549	-3.154655
C	-3.192870	-1.982720	1.870639	H	-0.119428	1.830644	-2.365803
H	-2.414943	-1.397360	2.344188	C	4.317894	1.180032	-2.749819
H	-4.804601	-0.751590	1.063266	O	3.124462	2.044123	-2.681221
C	-3.908540	-1.241042	0.722947	H	4.530260	0.682727	-1.784242
O	1.072325	0.765646	1.191014	H	5.151917	1.929250	-2.944424
K	-0.215649	-2.947217	-0.216520	H	4.158864	0.349449	-3.500109
O	0.537879	-1.625201	1.825340	H	0.447270	-0.085156	5.346349
K	-2.563227	2.093632	1.758366	O	-0.281947	-3.007440	6.171311
O	-2.696165	1.690010	6.202815	O	-2.385384	-2.580634	6.919450
H	-2.954277	1.075763	8.215181	H	1.763944	-2.576312	6.122901
H	-3.354872	3.443224	8.855606	C	-1.280898	-2.205168	6.576471
C	-2.874356	3.244221	7.887124	O	-0.902346	-0.879874	6.661499
O	-4.280469	2.480330	4.776329	C	0.464303	-0.759051	6.171903
H	-1.313906	1.743083	7.818851	H	1.069473	-0.280867	6.972197
C	-3.731270	2.556272	5.848277	H	0.828265	-2.054827	4.633873
H	-2.110387	4.010234	7.691898	C	0.812111	-2.188861	5.729168
C	-2.420976	1.844634	7.630826	H	-4.386755	-1.112564	2.971959
O	-4.010505	3.371336	6.928796	O	-3.703112	1.119166	0.703864
H	0.839255	1.787870	0.956619	O	-2.396681	-0.218133	-0.632103
O	2.444597	-2.278315	-1.691440	H	-4.357097	1.773731	2.623370
H	2.315066	-1.840726	0.324607	C	-3.063249	-0.056099	0.366079
H	2.732107	0.559612	-0.068307	O	-3.295972	-1.023510	1.286802
C	2.997575	-0.093047	-0.888097	C	-3.733457	-0.379951	2.501339



H	-2.860736	-0.158432	3.133394	C	-3.028178	2.170912	-3.748419
H	-5.474676	0.672461	1.741291	O	-2.960130	3.299125	-2.754121
C	-4.433948	0.872073	1.965872	H	-2.082405	1.558485	-3.654610
O	0.572385	-0.411652	0.704691	H	-3.053830	2.667446	-4.719731
K	-0.868109	-2.586800	1.003017	H	-3.985543	1.600037	-3.747451
O	-0.008427	-0.900730	2.988199	H	2.646227	2.200974	3.467921
K	2.336592	2.759072	0.982508	O	2.148642	0.681333	6.348497
O	-2.948354	4.263648	2.973595	O	0.175149	1.709686	6.934269
H	-1.307290	3.039051	3.432200	H	4.008162	0.559115	5.373071
H	-1.902091	3.212663	5.889474	C	1.157692	1.612409	6.197786
C	-2.172521	4.121132	5.292379	O	1.394566	2.418340	5.149115
O	-5.006500	4.976225	3.498488	C	2.699135	2.124600	4.586339
H	-1.004098	4.762025	3.559486	H	3.514042	2.783235	4.983789
C	-3.941051	4.561841	3.864827	H	2.555322	-0.087954	4.390917
H	-1.673141	5.006105	5.773485	C	2.941041	0.656904	5.107356
C	-1.759764	3.995431	3.741242	H	-4.847996	-3.206655	0.768365
O	-3.578975	4.488492	5.226006	O	-4.100631	-0.313831	0.336564
H	0.814045	0.169235	0.006185	O	-2.264315	-0.651468	-0.974864
O	2.831487	-2.692732	0.988744	H	-4.551141	-0.619387	2.383019
H	4.225150	-1.150555	1.034468	C	-3.048991	-1.017356	-0.134759
H	4.857619	-2.664832	2.916407	O	-2.980632	-2.257654	0.398697
C	3.874904	-2.177146	2.982339	C	-4.150159	-2.490817	1.216103
O	1.281224	-4.142715	1.851250	H	-3.748551	-2.880961	2.154266
H	2.662913	-0.730445	1.790777	H	-5.790677	-1.029157	1.159118
C	2.230723	-3.402369	1.982561	C	-4.734719	-1.070625	1.406228
H	3.773084	-1.460030	3.767424	O	0.592716	0.359949	0.839174
C	3.455175	-1.530970	1.672233	K	0.245020	-1.621200	-0.901160
O	2.831064	-3.159695	3.183874	O	-0.174559	-1.844368	1.822808
O	1.479947	1.022212	2.522990	K	-1.343968	2.222741	3.617676
K	-1.500843	3.031635	-0.025959	O	-5.417927	2.946059	6.253660
C	-4.861806	-1.482718	5.745220	H	-5.989004	4.478590	7.468117
H	-4.842273	-2.492337	6.243147	H	-3.574522	5.199288	7.802051
H	-3.939610	-1.360471	5.186913	C	-3.776554	4.199830	7.390010
O	-7.260863	0.344976	4.107507	O	-4.239190	2.738519	4.303938
H	-5.698301	-0.714561	7.584248	H	-5.390959	2.986394	8.337394
H	-4.148380	0.131165	6.927900	C	-4.421286	3.291456	5.376029
O	-5.879725	0.546755	5.926116	H	-3.019954	3.489477	7.746528
C	-5.112578	-0.327381	6.725662	C	-5.225399	3.727997	7.474393
C	-6.478528	-0.142809	4.903629	O	-3.592277	4.215999	5.955925
O	-6.084532	-1.457549	4.896287	H	0.508810	1.319184	0.959603
<b>TS2-B</b>				O	3.082011	-2.740593	0.748482
P	-0.319718	-0.341434	2.150728	H	2.227913	-2.124570	2.545550
O	-0.724526	4.467462	1.003203	H	2.901188	0.102158	1.680479
O	-0.511655	3.254943	-1.074568	C	3.699171	-0.670356	1.680208
O	-1.686553	0.249470	1.840384	O	3.118187	-2.014672	-1.371555
O	1.376354	3.436746	0.930452	H	4.027372	-2.619777	2.574988
C	2.135237	3.176429	-0.262884	C	3.432894	-1.892645	-0.200723
C	2.293602	4.609408	-0.717353	H	4.602639	-0.337705	2.151893
O	1.075450	5.287523	-0.383106	C	3.247891	-2.069790	2.039693
C	0.278279	4.314880	0.300712	O	4.113177	-0.837287	0.289574
H	3.139752	2.690898	-0.197421	O	0.216412	-0.024475	3.533593
H	2.472395	4.831845	-1.773131	K	-2.671551	2.311071	-0.257733
H	1.534529	2.448443	-0.869169	C	-1.511809	-2.244991	4.904061
H	3.091323	5.139431	-0.156230	H	-1.010389	-3.190966	5.161423
C	-1.716239	3.998102	-3.001549	H	-1.305845	-1.830082	3.935007
C	-0.438240	3.303245	-2.465792	O	-4.838364	-1.398512	5.281372
H	-1.821452	4.961925	-2.437723	H	-1.506427	-1.613744	7.075515
H	-1.509777	4.095446	-4.106199	H	-0.665209	-0.455173	5.967113
H	-0.306034	2.296673	-2.934801	O	-2.798223	-0.496383	5.771220
H	0.448392	3.763655	-2.837854	C	-1.475116	-1.195352	6.078078

C	-3.618507	-1.519081	5.369141	O	-3.436190	3.812598	5.936771
O	-2.906741	-2.628909	5.036561	H	0.341136	2.012944	-0.950943
<b>III-B</b>				O	2.963866	-3.183118	1.747946
P	-0.522448	0.679323	1.745070	H	1.081872	-2.378145	2.396993
O	-0.820470	4.848807	0.024107	H	1.817855	-0.093808	1.885669
O	0.568270	2.735455	-1.535106	C	2.539624	-0.916030	1.828449
O	-1.707577	1.432773	2.406469	O	3.075876	-3.452840	-0.505173
O	0.775062	3.742380	1.428595	H	2.454786	-2.372719	3.555068
C	2.128454	3.237410	0.852251	C	2.983608	-2.701910	0.458764
C	2.599683	4.530731	0.241815	H	3.544344	-0.524516	2.196290
O	1.407345	5.043255	-0.366695	C	2.167509	-2.258091	2.522254
C	0.334049	4.481548	0.311728	O	2.791871	-1.379931	0.396822
H	2.667715	2.825508	1.689526	O	0.711595	1.245853	2.500588
H	3.404608	4.459736	-0.526350	K	-2.444156	2.602962	0.233872
H	1.986138	2.470230	0.053032	C	-2.551461	-1.295507	7.249008
H	2.980686	5.249986	0.962767	H	-2.894560	-0.819572	8.177940
C	-0.331626	2.647246	-3.942116	H	-1.467353	-1.360028	7.086730
C	0.813347	2.500809	-2.902015	O	-3.987530	-4.164765	5.929954
H	-0.604033	3.727269	-3.968866	H	-3.960349	-0.054903	6.034437
H	-0.091781	2.301255	-4.989821	H	-2.419100	-0.264988	5.251679
H	1.364372	1.596990	-3.162546	O	-3.619800	-1.946771	5.253806
H	1.650182	3.217170	-3.206906	C	-3.132902	-0.769019	5.881121
C	-1.887986	0.850821	-4.016616	C	-3.574979	-3.041680	6.121335
O	-1.482716	2.004797	-3.321566	O	-2.938042	-2.713073	7.273004
H	-1.285244	-0.019176	-3.740674	<b>Na<sub>2</sub>SnO<sub>3</sub></b>			
H	-1.885531	0.882282	-5.114023	<b>TS1-C</b>			
H	-2.953679	0.693604	-3.705708	Sn	-0.954670	-0.075590	2.396139
H	2.352526	1.309090	3.941231	O	-3.849565	0.924168	-0.458527
O	0.070181	-0.006383	5.558192	O	-1.474682	1.169880	1.000759
O	-1.037471	1.835538	6.311448	O	-2.507785	-1.196690	2.787663
H	1.892224	-0.889096	6.057570	O	-2.004711	1.314905	-1.925875
C	-0.041472	1.321585	5.810987	C	-0.947108	0.462198	-2.389887
O	1.079949	2.016532	5.395869	C	-1.129542	-0.871730	-1.602408
C	2.143543	1.088007	5.007560	O	-2.383044	-0.741916	-0.862943
H	2.950586	1.276466	5.725575	C	-2.715178	0.615269	-0.864500
H	1.350480	-0.944758	4.368879	H	-1.140833	0.268920	-3.422036
C	1.499376	-0.289413	5.247962	H	-0.401215	-1.049793	-0.788615
H	-3.359301	-2.903919	2.392766	H	-0.010061	0.971892	-2.182046
O	-4.078259	-0.057014	0.952979	H	-1.322954	-1.793705	-2.133813
O	-2.981007	-0.273706	-1.019557	C	0.258678	2.836748	0.807490
H	-4.358004	-0.273358	2.967491	C	-1.134397	2.479124	1.192571
C	-3.284809	-0.750943	0.069209	H	0.865105	1.931874	0.910357
O	-2.847635	-1.899998	0.578065	H	0.353974	3.067156	-0.286570
C	-3.155382	-1.863524	2.076753	H	-1.420810	2.809725	2.238110
H	-2.165131	-1.503920	2.429425	H	-1.792582	3.092483	0.615757
H	-5.304789	-1.438232	1.886561	C	1.705142	4.652666	1.354262
C	-4.363800	-0.930626	2.071560	O	0.610141	3.854264	1.666480
O	-0.507224	0.947644	0.203082	H	2.600877	4.056686	1.288311
K	-0.444232	-1.272040	-0.930891	H	1.800296	5.331122	2.168044
O	-0.485746	-0.888142	1.841195	H	1.699451	5.303353	0.437072
K	-0.540806	3.382911	3.524571	H	-3.231131	5.470740	4.990986
O	-3.290227	4.382052	3.755989	O	-1.601177	4.182504	6.584893
H	-4.801035	3.137066	3.104126	O	0.257377	3.837662	5.264937
H	-5.364514	3.334344	5.443733	H	-2.975739	2.666996	6.323240
C	-4.354701	2.951978	5.252179	C	-0.913915	4.145433	5.435124
O	-1.745332	5.132763	5.301274	O	-1.773597	4.386748	4.380322
H	-3.209845	2.275227	3.453561	C	-3.126209	4.391497	4.866941
C	-2.781230	4.563039	5.024843	H	-3.732986	4.045608	4.040259
H	-4.229743	1.923637	5.655831	H	-3.592366	4.308739	7.028577
C	-3.936187	3.052574	3.777971	C	-2.964747	3.784981	6.242225

H	-5.601841	-4.760538	2.104197	C	-1.132931	2.514322	1.180218
O	-5.712108	-2.110896	3.529894	H	0.909988	1.898961	0.951708
O	-7.310017	-1.091656	2.329679	H	0.382740	3.080111	-0.226592
H	-3.657315	-2.641785	3.229986	H	-1.213258	2.898687	2.244946
C	-6.491694	-1.959676	2.457093	H	-1.903744	3.095360	0.616671
O	-6.237277	-2.883742	1.439190	C	1.727185	4.650427	1.360702
C	-5.220022	-3.737566	1.961000	O	0.618565	3.864256	1.675508
H	-4.424478	-3.856250	1.214327	H	2.703796	4.069348	1.275519
H	-4.683300	-3.822012	4.093594	H	1.769535	5.305123	2.265077
C	-4.662610	-3.115128	3.239410	H	1.556331	5.184544	0.428680
O	-1.301365	1.108332	4.114720	H	-3.316509	5.403127	4.995464
O	0.936804	0.105380	2.504442	O	-1.617765	4.201579	6.593648
Na	0.892437	1.641694	4.356210	O	0.244235	3.859797	5.269966
O	4.989318	1.983405	7.521156	H	-3.029458	2.709944	6.295866
H	5.913879	0.337574	8.391555	C	-0.911852	4.146667	5.407795
H	3.993591	-0.934262	8.051932	O	-1.762493	4.369997	4.380485
C	3.776351	0.131614	8.115193	C	-3.153551	4.387771	4.848735
O	4.325619	2.049196	5.305705	H	-3.803832	4.018384	4.050186
H	5.042264	1.426871	9.549305	H	-3.637397	4.242856	6.979848
C	4.268462	1.583806	6.418054	C	-2.980668	3.768016	6.239276
H	2.920248	0.357930	8.727137	H	-5.610560	-4.763520	2.162997
C	5.020484	0.932829	8.517379	O	-5.702037	-2.109292	3.538736
O	3.467317	0.600617	6.752226	O	-7.306675	-1.082189	2.336043
H	-2.152667	1.302508	4.481441	H	-3.658592	-2.629290	3.180899
O	0.435760	-5.094383	3.003405	C	-6.484262	-1.976397	2.447847
H	0.344088	-4.174813	1.207661	O	-6.225256	-2.881663	1.459270
H	2.254009	-2.512303	1.912518	C	-5.206484	-3.754870	1.963040
C	1.644990	-3.070497	2.682794	H	-4.466938	-3.991326	1.203104
O	2.153672	-6.357170	3.903114	H	-4.641924	-3.863603	4.103854
H	-0.615497	-3.351939	2.514829	C	-4.644565	-3.128434	3.238244
C	1.749487	-5.335235	3.388958	O	-1.288507	1.117089	4.138750
H	1.509923	-2.312789	3.482282	O	0.935961	0.113062	2.504272
C	0.367901	-3.826479	2.264951	Na	0.890823	1.641214	4.360459
O	2.429546	-4.138326	3.255247	O	4.976727	1.975911	7.504394
Na	-3.799500	0.515402	2.110471	H	5.938389	0.361387	8.440848
C	-5.504799	4.586190	-0.011666	H	3.948903	-0.901496	8.111643
H	-5.951780	4.111217	-0.827763	C	3.767601	0.153488	8.112338
H	-5.816881	5.629368	-0.080623	O	4.335292	2.049762	5.278991
O	-5.073058	2.579540	2.786761	H	4.928082	1.451215	9.517941
H	-3.682759	3.724821	-0.828833	C	4.291833	1.602097	6.402022
H	-3.420574	5.250153	0.135387	H	2.880648	0.346732	8.739484
O	-3.797728	3.565435	1.251181	C	5.004323	0.955973	8.489072
C	-4.017566	4.349529	-0.005507	O	3.483907	0.598802	6.757228
C	-4.984053	3.324262	1.805457	H	-2.270374	1.137208	4.347665
O	-6.044691	3.933092	1.178012	O	0.434369	-5.117524	3.014495
<b>II-C</b>				H	0.407937	-4.199041	1.214694
Sn	-0.962362	-0.077859	2.398965	H	2.237936	-2.557839	1.974735
O	-3.856314	0.881185	-0.483459	C	1.630384	-3.076410	2.701045
O	-1.468952	1.155317	0.979053	O	2.155920	-6.355782	3.901597
O	-2.515096	-1.196116	2.764749	H	-0.604639	-3.393078	2.522570
O	-2.005511	1.311261	-1.919731	C	1.757338	-5.316600	3.386993
C	-0.968764	0.453079	-2.393367	H	1.527097	-2.303572	3.532567
C	-1.127070	-0.859351	-1.606807	C	0.364608	-3.838541	2.255625
O	-2.338135	-0.703483	-0.850231	O	2.437550	-4.155923	3.292018
C	-2.696242	0.618848	-0.905002	Na	-3.798062	0.516047	2.105320
H	-1.273445	0.274165	-3.424304	C	-5.514398	4.591054	-0.022808
H	-0.332341	-0.936356	-0.843233	H	-6.028204	4.111703	-0.904850
H	-0.023494	0.938986	-2.225477	H	-5.784633	5.668291	-0.025951
H	-1.330021	-1.795738	-2.163151	O	-5.042645	2.594194	2.785778
C	0.282273	2.810289	0.819293	H	-3.663207	3.736605	-0.848409

H	-3.456640	5.281710	0.088140	H	-2.925697	-2.529844	4.252311
O	-3.814645	3.581168	1.255042	C	-3.479455	-1.367860	5.896544
C	-4.020756	4.348898	0.012883	O	-1.319736	-2.310456	5.714427
C	-5.009928	3.335660	1.833265	H	-1.188526	2.174947	2.507328
O	-6.049189	3.929862	1.194223	O	2.077012	-2.217328	0.339710
<b>TS2-C</b>				H	2.870518	-0.526756	1.240992
Sn	-0.530089	-0.382440	2.332175	H	1.793476	0.925019	-0.423549
O	-2.672514	4.086445	0.623294	C	2.042203	-0.085373	-0.786277
O	-0.790479	2.644109	1.215048	O	0.391934	-3.129406	-0.868979
O	-1.804779	-1.625305	1.872287	H	3.795213	-1.239164	-0.089054
O	-1.435059	2.955662	-1.068546	C	1.059567	-2.171841	-0.551357
C	-1.486179	1.608675	-1.617276	H	2.600925	-0.043199	-1.714232
C	-2.249591	0.715101	-0.608278	C	2.802495	-0.973311	0.236001
O	-2.925303	1.772010	0.157441	O	0.818710	-0.859714	-0.984919
C	-2.153515	3.041329	0.190808	Na	-3.797570	0.515240	2.110582
H	-1.988478	1.495575	-2.614789	C	-5.722472	3.621839	2.219815
H	-1.524059	0.051439	0.000220	H	-4.625753	3.816787	2.095189
H	-0.391641	1.447391	-1.741426	H	-6.299629	4.053892	1.386344
H	-3.023614	0.021652	-0.995393	O	-6.385614	0.592002	3.767122
C	0.301712	4.631460	2.179808	H	-5.753155	4.589139	4.222496
C	0.268128	3.632917	1.033313	H	-7.300818	4.604527	3.329147
H	1.401156	4.930916	2.191454	O	-6.842932	2.783526	4.179440
H	-0.405868	5.458879	2.156199	C	-6.419171	4.035266	3.604774
H	-0.064420	4.193757	0.145737	C	-6.393272	1.766392	3.438971
H	1.175468	3.054526	0.854608	O	-5.821615	2.186546	2.215114
C	-0.439852	4.477113	4.543849	<b>III-C</b>			
O	0.369283	3.921677	3.551991	Sn	-0.997656	-0.190095	4.615793
H	-1.495228	4.271485	4.306988	O	-2.840838	1.736699	-0.525421
H	-0.364894	5.570377	4.781977	O	-0.799294	2.015146	2.034753
H	-0.116297	4.033954	5.479589	O	-1.837218	-1.875309	4.374974
H	3.244831	3.393733	10.106564	O	-1.114907	0.249961	-0.530465
O	3.969816	3.681677	7.036491	C	-0.697524	-0.822515	0.378047
O	2.175638	2.894042	6.049449	C	-2.016818	-1.281794	0.990827
H	5.572956	3.135589	8.329726	O	-2.853981	-0.075299	0.857469
C	2.759475	3.066138	7.076893	C	-2.299827	0.733800	-0.098238
O	2.365554	2.737037	8.324502	H	-0.193052	-1.599899	-0.207404
C	3.522840	2.838061	9.187061	H	-1.958103	-1.551813	2.057118
H	3.780593	1.777515	9.462988	H	-0.012913	-0.382243	1.116014
H	4.771521	4.580482	8.705732	H	-2.501624	-2.089245	0.427818
C	4.611474	3.589109	8.399655	C	0.571689	3.465648	0.713192
H	-3.883201	-4.483471	-0.412600	C	-0.726499	3.336082	1.492556
O	-4.150191	-3.788657	2.399832	H	0.623436	2.671166	-0.054324
O	-5.296532	-1.781047	2.208919	H	0.624367	4.448225	0.207488
H	-2.054200	-3.808751	2.038402	H	-0.765551	4.098048	2.290457
C	-4.537764	-2.653662	1.741999	H	-1.568054	3.529672	0.800537
O	-4.063588	-2.600223	0.501846	C	2.943942	3.288535	0.960606
C	-3.298731	-3.822817	0.255949	O	1.676382	3.324704	1.630235
H	-2.379014	-3.570732	-0.292712	H	2.970352	2.481443	0.206930
H	-2.961158	-5.403193	1.735408	H	3.707693	3.081897	1.723798
C	-2.979319	-4.330763	1.638876	H	3.157093	4.251343	0.463896
O	-1.552374	1.326964	3.172420	H	-3.319923	5.459235	5.348226
O	1.246841	0.089205	2.635325	O	-1.550305	3.402458	6.542073
Na	0.891677	1.641742	4.357403	O	0.334309	3.707168	5.300324
O	-2.409453	-0.360342	5.867044	H	-3.280137	2.442343	5.947865
H	-3.856611	-1.532558	6.940533	C	-0.868725	3.830418	5.451962
H	-3.063514	-3.574744	5.815525	O	-1.675363	4.467078	4.565259
C	-2.721267	-2.616706	5.356200	C	-3.046652	4.435278	5.054817
O	-0.145220	-0.382347	5.748017	H	-3.688650	4.082709	4.235421
H	-4.312243	-1.028187	5.277471	H	-3.498358	3.805528	7.138739
C	-1.193281	-0.944204	5.749762	C	-2.974914	3.457542	6.239159

H	-4.603942	-4.761539	2.743147	C	1.880576	2.935461	0.151125
O	-4.716910	-2.759108	4.904645	C	0.525668	2.839883	0.840134
O	-5.132870	-0.869963	3.706231	H	1.961441	2.030227	-0.489708
H	-2.877321	-3.689219	5.059027	H	1.956001	3.848643	-0.435224
C	-4.720360	-2.018893	3.776691	H	0.413432	1.894369	1.389575
O	-4.270974	-2.714195	2.702872	H	0.185770	3.693017	1.439198
C	-3.865420	-4.048403	3.136684	C	3.325476	4.067691	1.754786
H	-2.867071	-4.250528	2.722383	O	2.984318	2.841115	1.020312
H	-4.340096	-4.784618	5.179185	H	4.132666	3.989700	2.450925
C	-3.876514	-3.932062	4.667632	H	2.464601	4.477498	2.349905
O	-2.005542	1.438332	4.165222	H	3.623534	4.817347	1.029863
O	0.877708	0.147816	4.829886	H	-3.988904	5.187688	4.384596
Na	1.078514	2.109520	3.609388	O	-2.846802	2.912974	6.359186
O	4.082624	0.065898	5.393698	O	-0.714034	3.431506	6.278226
H	2.324955	-0.151676	6.471128	H	-4.649560	2.554359	5.432588
H	1.996862	2.211695	6.617880	C	-1.792969	3.556276	5.797921
C	3.029305	1.910881	6.394172	O	-2.149338	4.292947	4.723891
O	4.258968	0.951629	3.293001	C	-3.562173	4.178009	4.415624
H	3.843765	0.140336	7.457538	H	-3.681780	3.712606	3.451125
C	3.902319	1.022767	4.447712	H	-4.543917	4.142383	6.326704
H	3.749471	2.539040	6.938322	C	-4.053404	3.428731	5.651807
C	3.270391	0.405804	6.560451	H	-7.444914	-4.091280	2.939937
O	3.252739	2.119108	4.967099	O	-5.283144	-2.247779	2.907974
H	-1.370004	1.932747	2.921193	O	-5.450697	-1.359826	0.813874
O	0.823850	-2.672835	2.446947	H	-4.409619	-4.067885	3.346270
H	2.634808	-3.083433	3.385027	C	-5.684865	-2.257393	1.616723
H	1.479259	-4.386134	5.113468	O	-6.304482	-3.468417	1.301879
C	0.850915	-3.681436	4.554118	C	-6.468866	-4.267935	2.524894
O	-0.797898	-3.985065	1.536312	H	-6.316889	-5.366082	2.264618
H	1.678496	-1.687387	4.076575	H	-5.728581	-3.517403	4.460618
C	-0.044672	-3.721027	2.454210	C	-5.382583	-3.609502	3.421458
H	0.141655	-3.152351	5.209036	O	1.638099	0.127195	1.399194
C	1.638149	-2.713481	3.663769	O	1.348804	-0.779184	3.976641
O	0.053672	-4.447498	3.599925	O	2.734026	5.513141	4.946902
Na	-3.797380	0.890498	2.953056	H	1.444367	6.596495	6.251881
C	-5.634284	2.853678	-1.030457	H	2.230792	5.061610	7.975280
H	-5.205389	2.045838	-1.637695	C	2.172194	4.592931	7.000252
H	-6.663092	3.077359	-1.343829	O	4.842407	4.601048	4.811193
O	-4.723769	2.993712	2.311063	H	0.817310	5.150593	5.472377
H	-3.761194	3.931374	-1.485688	C	3.749424	4.749059	5.361070
H	-5.200149	5.017835	-1.324646	H	1.578868	3.654447	7.044692
O	-4.432473	4.257067	0.445497	C	1.689129	5.528978	5.907298
C	-4.718147	4.096016	-0.972878	O	3.547590	4.278695	6.628205
C	-4.923355	3.195355	1.123794	H	-0.574138	0.514223	-0.518423
O	-5.682389	2.389951	0.346945	O	3.593250	-5.742030	5.049500
<b>VO(OiPr)<sub>3</sub></b>				H	3.793431	-3.957238	6.115819
<b>TS-D</b>				H	1.771788	-3.168694	4.918862
V	0.627762	-0.741584	2.312048	C	2.360889	-3.879829	4.345294
O	-2.022924	4.122602	0.348631	O	2.019681	-7.317375	4.623022
O	-0.331283	2.714537	-0.408446	H	4.621397	-3.985209	4.542863
O	0.450427	-2.415931	1.656736	C	2.381133	-6.167628	4.582786
O	-2.211540	2.900542	-1.546802	H	2.511311	-3.384705	3.355623
C	-1.716321	1.867996	-2.482325	C	3.693807	-4.296213	5.051753
C	-1.958506	0.414751	-1.894737	O	1.638685	-5.117569	4.140328
O	-0.872551	-0.121720	-1.168977	O	-0.845223	0.306978	2.270165
C	-1.536129	3.286297	-0.395995	C	-6.836208	1.358920	0.784082
H	-2.347528	2.008476	-3.312961	H	-6.054568	0.538733	0.704168
H	-2.146698	-0.216145	-2.755709	H	-7.719279	1.005957	0.334803
H	-0.700786	2.065439	-2.779168	O	-6.624321	3.184861	3.766780
H	-2.925440	0.404749	-1.368145	H	-5.344603	2.801034	-0.271136

H	-7.014706	3.434014	-0.063800	H	-5.182637	5.686326	2.008302
O	-5.969647	3.436892	1.613966	O	-3.813302	6.425578	4.806618
C	-6.203683	2.789256	0.345119	O	-5.584238	6.567236	6.182681
C	-6.545470	2.747758	2.633960	H	-3.046551	7.445972	3.188656
O	-7.044294	1.547708	2.237263	C	-5.147214	6.413682	5.058965
C	2.385979	0.068433	4.474271	O	-5.869874	6.301761	3.933984
C	2.138249	1.556323	4.391869	C	-5.039965	6.444656	2.750929
C	3.710012	-0.228662	3.735373	H	-5.204579	7.421526	2.233391
H	2.468327	-0.233433	5.540532	H	-2.911901	5.662533	3.129179
C	0.635769	-2.920739	0.296268	C	-3.583854	6.504782	3.354883
H	1.111508	-2.176023	-0.346980	H	-0.863042	-8.720926	1.280088
C	-0.783275	-3.315564	-0.244269	O	-0.505840	-6.977576	-1.100760
C	1.537485	-4.157411	0.426390	O	-1.165502	-5.002814	-0.195442
C	-1.828439	0.418658	3.313123	H	-1.256019	-8.753068	-1.919050
C	-1.836620	-0.748414	4.317901	C	-1.196837	-6.221243	-0.213589
C	-3.176495	0.563667	2.592935	O	-1.905918	-7.060456	0.652913
H	-1.564234	1.324715	3.885042	C	-1.503235	-8.459238	0.436342
H	3.480014	0.038944	2.687720	H	-2.370557	-9.095971	0.547238
H	3.885840	-1.315029	3.752303	H	0.231451	-8.914904	-0.850112
H	4.598583	0.208011	4.127474	C	-0.732402	-8.438249	-0.946224
H	2.077445	1.940105	3.373391	O	-0.954640	0.941452	1.400117
H	2.897712	2.112189	4.978400	O	-2.214439	-1.381977	0.726340
H	1.206004	1.837439	4.896632	O	1.439989	-4.230193	8.312985
H	2.560133	-3.822802	0.806712	H	1.572059	-3.206054	10.095864
H	1.627179	-4.678701	-0.529203	H	-0.755809	-2.419830	9.393539
H	1.085774	-4.821489	1.153292	C	0.049538	-2.344549	8.673345
H	-1.401765	-2.397619	-0.158343	O	0.362152	-5.084821	6.470955
H	-1.173613	-4.149390	0.362644	H	2.259320	-2.253066	8.779213
H	-0.622253	-3.649614	-1.279551	C	0.510026	-4.235064	7.296674
H	-2.232556	-1.723041	3.912526	H	0.132803	-1.340102	8.271657
H	-2.489455	-0.428321	5.210041	C	1.430600	-2.953405	9.022351
H	-0.811000	-0.852598	4.770339	O	-0.306596	-3.128280	7.437801
H	-3.266518	-0.094248	1.732233	H	1.231938	5.339264	4.517461
H	-3.329122	1.565356	2.258561	O	-4.883658	2.170695	2.560709
H	-4.027127	0.285315	3.341238	H	-5.125210	2.232082	4.657403
<b>II-D</b>				H	-2.899916	2.951155	4.857958
V	-0.957690	-0.240636	0.289447	C	-3.040903	2.234602	4.018468
O	4.328739	3.866448	4.287562	O	-4.018411	3.501459	0.925029
O	1.837981	5.871767	4.049851	H	-4.600204	0.669389	4.013231
O	0.575264	-1.135308	0.247657	C	-3.894630	2.929492	1.979884
O	2.337522	3.045866	3.810964	H	-2.284224	1.441325	4.010433
C	1.113782	2.883245	4.450287	C	-4.471020	1.759867	3.893506
C	1.625854	3.046094	6.007466	O	-2.787891	3.019244	2.779860
O	2.667115	3.896145	5.971332	O	-1.130727	0.357806	-1.331155
C	3.181853	3.736788	4.568653	C	0.041729	-1.646902	3.879544
H	0.432112	3.765421	4.245539	H	-0.182044	-2.729119	3.911152
H	1.994341	2.133668	6.436634	H	-0.489907	-1.141972	3.017853
H	0.698126	1.944198	4.174819	O	0.025335	0.047072	6.956479
H	0.743059	3.377219	6.530074	H	2.202540	-2.102155	4.201552
C	1.070654	5.756194	1.748928	H	1.873851	-0.522177	3.280093
C	1.232817	6.602272	2.994673	O	1.521481	-0.507785	5.366424
H	2.092281	5.452122	1.303531	C	1.527507	-1.229834	4.076764
H	0.583685	4.741416	1.850635	C	0.297623	-0.507677	5.941723
H	1.732598	7.488683	2.702811	O	-0.602171	-1.203381	5.137631
H	0.270651	7.133037	3.174826	C	-3.547053	-1.450828	1.258895
C	-0.808480	6.805783	0.352207	C	-3.482973	-2.176233	2.598727
O	0.570690	6.576641	0.628970	C	-4.593668	-2.097710	0.304455
H	-1.369568	6.367628	-0.458883	H	-3.911450	-0.366529	1.333777
H	-1.031813	7.884923	0.185925	C	1.193257	-2.021253	-0.699025
H	-1.316200	6.571637	1.398767	H	0.403916	-2.641955	-1.144170

C	2.074318	-3.003073	0.069876	H	2.099573	-1.585623	7.769359
C	2.074759	-1.241325	-1.698172	C	1.388429	-2.013610	7.080411
C	-0.883215	1.781277	-1.610193	H	-2.344817	-3.581486	2.650590
C	-1.192036	1.991174	-3.066915	O	-4.066155	-1.824875	4.508684
C	0.541449	2.317713	-1.284542	O	-2.451389	-0.270478	4.799806
H	-1.581280	2.394809	-1.039944	H	-4.708708	-3.794887	4.583927
H	-4.303142	-3.149474	0.035727	C	-2.796506	-1.413595	4.542693
H	-4.594667	-1.486645	-0.647451	O	-1.915251	-2.437338	4.307548
H	-5.597044	-2.056334	0.719627	C	-2.627032	-3.522316	3.707074
H	-3.058665	-3.193748	2.444834	H	-2.416486	-4.449790	4.251228
H	-4.508224	-2.324133	2.933038	H	-4.706527	-3.035425	2.979594
H	-2.940377	-1.600089	3.348535	C	-4.123641	-3.162734	3.910296
H	2.590321	-0.439229	-1.179462	O	-4.455913	-1.058552	-0.770640
H	1.496405	-0.750770	-2.479825	K	-2.709882	1.981008	2.860954
H	2.802505	-1.943942	-2.137625	O	-2.581302	-1.786553	1.275275
H	1.612554	-3.467843	0.946612	K	-0.102928	-1.421301	1.777987
H	3.022768	-2.567926	0.424372	O	-0.958522	-3.319893	-1.662918
H	2.356489	-3.835316	-0.557660	H	-2.092067	-2.836977	-3.366835
H	-0.663943	1.230614	-3.645714	H	-1.717205	-0.462872	-2.989909
H	-0.988081	3.002001	-3.488015	C	-1.639437	-1.090090	-2.093366
H	-2.288446	1.862088	-3.170302	O	1.013020	-2.740664	-0.589578
H	1.295101	1.984445	-1.953308	H	-3.023798	-2.770839	-1.777085
H	0.850812	1.907600	-0.296308	C	0.043301	-2.478714	-1.292097
H	0.543687	3.396199	-1.224380	H	-2.065571	-0.620659	-1.195517
<b>Cartesian coordinates (in Å) related to</b>				C	-2.072816	-2.561819	-2.296089
<b>Figure S4 in the SI</b>				O	-0.175988	-1.224622	-1.732547
<b>K<sub>3</sub>VO<sub>4</sub></b>				H	-5.390670	-0.805048	-0.813904
<b>TS1-A</b>				O	-4.667376	1.777042	5.182904
V	-3.598373	-0.506993	0.779711	H	-5.343943	-0.167731	4.948014
O	-1.117804	4.270957	0.300429	H	-7.377184	0.564762	6.034451
O	0.989019	4.761789	1.079118	C	-6.440917	0.933277	6.493656
O	-4.422546	0.083122	2.092443	O	-5.142090	3.991694	5.353105
O	-0.843131	6.205607	1.499883	H	-4.403309	0.109216	6.471885
C	-0.566758	6.474490	2.857047	C	-5.380976	2.837422	5.633408
C	-1.094589	5.099933	3.621928	H	-6.492874	0.691980	7.572247
O	-0.471148	4.127438	2.966611	C	-5.159929	0.522388	5.779202
C	-0.450182	4.947395	1.100232	O	-6.433800	2.399693	6.402024
H	0.516641	6.483095	2.873675	O	-2.633560	0.826155	0.343023
H	-2.156035	5.090812	3.786857	K	-1.851578	2.561176	-1.271302
H	-1.011334	7.476942	3.096313	C	1.762151	3.528244	5.369562
H	-0.689759	5.137056	4.648887	H	1.150808	4.399864	5.540475
C	2.224323	3.405665	-0.734053	H	2.370981	3.136900	6.210995
C	1.739230	4.747552	-0.256192	O	-0.194045	1.494434	3.439995
H	3.234234	3.460751	-1.155913	H	2.603641	4.407500	3.426451
H	2.274477	2.683458	0.093133	H	3.566971	3.161134	4.245304
H	2.663534	5.196238	0.042003	O	1.777179	2.530748	3.261776
H	1.152549	5.381526	-0.989566	C	2.531776	3.526515	4.040978
C	1.736479	2.779609	-3.050547	C	0.712604	2.115581	3.924235
O	1.271374	2.746746	-1.650395	O	0.694248	2.528511	5.200690
H	2.610025	2.122270	-3.027332	<b>II-A</b>			
H	2.100163	3.798855	-3.374509	V	-0.160719	-1.173695	2.782407
H	0.841960	2.463784	-3.684635	O	-0.621771	6.479079	-1.962531
H	0.663371	0.063711	6.681030	O	-0.154447	4.789776	-0.628424
O	2.076485	-2.695911	6.002254	O	-1.435096	-1.441466	1.589370
O	2.144295	-2.471603	3.766950	O	-1.708924	4.431222	-2.247676
H	0.826336	-2.772642	7.632516	C	-1.334653	2.903843	-2.324774
C	1.726863	-2.111396	4.830732	C	-2.402842	1.786800	-2.102824
O	0.891042	-1.025188	4.981797	O	-3.009767	1.713215	-0.815223
C	0.468294	-0.953469	6.350410	C	-0.870793	5.315736	-1.685129
H	-0.619643	-1.094411	6.454999	H	-1.089690	2.829526	-3.375544

H	-1.723117	0.897809	-2.415092	K	-0.888060	1.967293	1.503270
H	-0.388076	2.737450	-1.807180	C	-5.822168	2.451876	-1.305862
H	-3.197382	1.923653	-2.862015	H	-5.453448	2.279450	-2.279595
C	1.794897	4.717220	0.815971	H	-6.923992	2.698828	-1.389943
C	1.288325	4.884619	-0.631748	O	-4.631227	1.732447	1.817828
H	2.920163	4.782538	0.834348	H	-4.055929	3.817805	-1.379980
H	1.479129	5.554546	1.454660	H	-5.621422	4.702629	-0.936061
H	1.521776	5.893151	-1.052442	O	-4.787651	3.597736	0.545725
H	1.754028	4.072782	-1.203481	C	-5.007482	3.761543	-0.890119
C	2.088346	3.029628	2.401176	C	-4.955877	2.275238	0.768147
O	1.411917	3.398110	1.188855	O	-5.551621	1.588157	-0.277730
H	1.789254	3.730165	3.244791				
H	3.118082	3.234081	2.192967	<b>TS2-A</b>			
H	1.834362	1.999138	2.674458	V	-1.268709	-0.733818	2.876840
H	-2.876952	-0.181921	5.268610	O	-0.770216	3.632566	-3.653287
O	-3.033522	2.998010	4.750036	O	-0.222095	2.554431	-1.686685
O	-0.896353	3.581999	5.262420	O	-2.469982	-0.075295	3.859079
H	-4.846958	2.003458	4.886192	O	-2.182392	2.174408	-2.679135
C	-1.776276	2.755034	5.187702	C	-2.887414	1.721507	-1.483874
O	-1.696855	1.458745	5.650980	C	-3.099090	2.847946	-0.278644
C	-3.076395	0.811802	5.675768	O	-4.114021	2.501703	0.587122
H	-3.546806	0.730078	6.680265	C	-1.040532	2.841806	-2.739268
H	-3.660209	1.303362	3.657276	H	-3.903970	1.487325	-1.727173
C	-3.753487	1.749225	4.671558	H	-3.261866	3.694690	-0.905161
H	-3.598530	-4.340860	2.807220	H	-2.349260	0.849904	-0.991306
O	-3.438221	-3.075850	5.532661	H	-2.122890	3.138869	0.297720
O	-5.147673	-1.602555	5.374297	C	0.615746	4.906439	-1.009170
H	-1.498804	-3.396161	4.780545	C	0.910516	3.527434	-1.445327
C	-4.336524	-2.354952	4.857372	H	1.610558	5.420671	-1.180281
O	-4.210289	-2.519793	3.559568	H	-0.110261	5.378044	-1.639664
C	-3.105303	-3.488171	3.272015	H	1.395957	3.624085	-2.422986
H	-2.460537	-2.962719	2.540919	H	1.548683	3.023022	-0.723924
H	-2.565220	-4.816818	4.963546	C	1.263709	5.664975	1.180986
C	-2.515139	-3.761758	4.649981	O	0.242266	5.103945	0.382885
O	1.532706	-1.354985	2.005266	H	1.021485	5.603355	2.203888
K	-3.389942	-0.521538	0.237905	H	1.344721	6.733630	0.873710
O	-0.049906	-2.336297	3.940107	H	2.174613	5.084279	1.055050
K	0.814521	-0.725890	5.824402	H	1.115981	-0.013067	6.269900
O	2.271563	2.823459	6.077986	O	-0.262481	2.787907	5.852346
H	2.669257	4.846791	6.147504	O	1.333989	3.805146	4.586574
H	1.962016	4.759405	8.366364	H	-0.855615	1.608426	7.391261
C	1.354519	4.115392	7.733320	C	1.009981	2.921923	5.331452
O	2.447769	0.900731	7.372443	O	1.845070	1.928591	5.757555
H	1.014689	4.395344	5.590147	C	1.107091	1.007776	6.629749
C	2.125503	2.080653	7.217042	H	1.489415	1.035395	7.633691
H	0.296477	4.347201	7.861482	H	-0.899316	0.778428	5.784318
C	1.824206	4.151545	6.259922	C	-0.326984	1.449513	6.476258
O	1.584437	2.792641	8.188595	H	-2.412697	-1.413638	7.568904
H	2.105992	-0.998917	2.711489	O	-1.909094	-3.885909	5.611767
O	-1.164386	-2.530478	-1.519764	O	0.331118	-4.011813	5.686610
H	0.841562	-2.462824	-1.897300	H	-3.348364	-2.462224	4.957139
H	0.796035	-4.696240	-0.490520	C	-0.691089	-3.404555	5.927498
C	0.230652	-3.816040	-0.149881	O	-0.718984	-2.195322	6.515829
O	-3.116524	-3.506584	-0.956947	C	-2.092576	-1.654312	6.535122
H	0.361787	-1.637651	-0.396955	H	-2.102878	-0.692593	5.945908
C	-1.918563	-3.439898	-0.808428	H	-3.710176	-3.220118	6.477317
H	0.578390	-3.558978	0.876999	C	-2.895411	-2.797052	5.888025
C	0.182447	-2.504556	-1.018742	O	-1.816188	-0.492876	1.116006
O	-1.164092	-4.221085	0.006009	K	-4.411010	0.981751	2.747231
O	0.035428	0.392097	3.460143	O	-0.939232	-2.339383	3.238117
				K	1.806797	-2.184544	3.585238



O	2.776656	0.749501	0.265537	O	2.041600	4.080846	3.472007
H	4.476974	1.887378	0.576497	H	-0.794912	2.046328	5.977802
H	4.152741	1.870867	2.980040	C	1.580995	3.406878	4.390921
C	3.304741	1.510660	2.411741	O	2.348466	2.801848	5.354651
O	2.489996	-1.430924	0.817407	C	1.449860	1.995161	6.175269
H	2.891998	2.830114	0.646889	H	1.464714	2.421525	7.200208
C	2.772011	-0.286723	1.092766	H	0.025181	1.020750	4.874012
H	2.341545	1.876719	2.789723	C	0.119538	1.940126	5.434911
C	3.425642	1.910815	0.897551	H	-3.475247	-0.430545	6.301067
O	3.241642	0.052023	2.367167	O	-1.361489	-2.875715	6.084885
H	-1.188660	-0.590288	0.379049	O	0.504831	-1.824425	6.911609
O	-4.965508	-2.292212	0.958658	H	-3.012377	-3.009220	4.972847
H	-3.800228	-3.627941	-0.072090	C	-0.633857	-1.776066	6.503864
H	-3.872249	-4.866344	1.843450	O	-1.344443	-0.633793	6.272717
C	-3.582160	-3.825975	2.070587	C	-2.695104	-0.946662	5.736348
O	-6.210348	-1.658937	2.716858	H	-2.654400	-0.617117	4.679467
H	-2.852246	-2.257417	0.667471	H	-3.280059	-2.891651	6.782158
C	-5.339144	-2.353329	2.250482	C	-2.771918	-2.488423	5.892601
H	-2.624152	-3.770708	2.595234	O	0.284919	0.697426	1.083555
C	-3.705117	-2.969231	0.788868	K	-4.203169	1.330119	3.235192
O	-4.563422	-3.222625	2.941371	O	-1.161358	-1.663039	2.074875
O	0.221641	0.122401	2.964561	K	0.699230	-3.200630	3.276387
K	-1.373853	2.681604	2.436546	O	3.987293	-2.194964	0.831262
C	-6.461688	4.276919	0.622356	H	5.267508	-0.541281	1.109209
H	-6.284552	3.558517	-0.205084	H	4.393162	-0.424256	3.350096
H	-7.534071	4.331996	0.787223	C	3.634644	-0.724654	2.602263
O	-3.674437	3.799939	2.648215	O	3.260193	-4.140937	1.734073
H	-5.685124	6.085329	-0.590133	H	3.618306	-0.207920	0.457946
H	-6.028525	6.358052	1.203279	C	3.484949	-2.963145	1.837158
O	-4.348169	5.234830	1.028352	H	2.722936	-0.103173	2.735663
C	-5.675836	5.587988	0.488494	C	4.199343	-0.811140	1.172594
C	-4.506473	4.122317	1.829478	O	3.292096	-2.179200	2.939711
O	-5.949115	3.748905	1.854795	H	0.042258	0.336378	0.213046
<b>III-A</b>				O	-5.081914	-1.003334	1.049746
V	-0.548155	-0.182616	2.555755	H	-4.558599	-1.193078	-0.953723
O	-1.725848	0.838869	-2.296746	H	-4.424366	-3.532551	-0.317984
O	-2.040553	3.097978	-2.226179	C	-3.828067	-2.830136	0.307233
O	-1.820162	0.721287	3.240352	O	-5.364860	-1.645279	3.208052
O	-3.708612	1.653401	-1.632579	H	-3.244689	-0.704714	0.115900
C	-4.576762	2.835479	-0.996517	C	-4.928389	-1.888981	2.108373
C	-5.280074	2.166135	0.265368	H	-2.739327	-2.970577	0.268122
O	-6.085588	2.954441	1.300390	C	-4.121391	-1.346977	0.044595
C	-2.429952	1.830972	-2.105486	O	-4.291956	-3.012696	1.659803
H	-3.877037	3.682269	-0.761062	O	0.616575	-0.324324	3.744196
H	-4.536942	1.506159	0.695278	K	-0.488188	3.024562	2.073136
H	-5.298358	2.997687	-1.796736	C	-5.399463	4.970993	4.097911
H	-6.047897	1.507641	-0.091188	H	-6.350199	5.513876	3.953707
C	-0.427888	4.809640	-2.320745	H	-4.979982	4.964694	5.107728
C	-0.638807	3.265353	-2.025404	O	-3.892149	3.437978	1.783197
H	-0.075758	5.037613	-3.348279	H	-4.453671	6.737333	3.197570
H	-1.335873	5.333606	-2.174518	H	-3.613690	5.273300	3.129388
H	-0.128883	2.545566	-2.663935	O	-5.222928	5.315971	1.865756
H	-0.440495	3.047782	-0.977352	C	-4.587161	5.648939	3.075135
C	0.751488	5.303060	-0.192520	C	-5.081128	3.838849	2.076120
O	0.722781	5.365707	-1.655746	O	-5.345644	3.644650	3.587641
H	1.525431	5.958413	0.133827	<b>K<sub>3</sub>PO<sub>4</sub></b>			
H	0.919242	4.301867	0.202090	<b>TS1-B</b>			
H	-0.238772	5.599434	0.243571	P	-0.612481	1.262360	2.896079
H	1.842990	0.956921	6.176497	O	1.960673	2.779149	-0.698334
O	0.240509	3.045534	4.467025	O	1.060937	1.292430	-2.237675

O	-1.501133	0.167770	2.249869	O	3.072521	-2.458639	3.084579
O	0.337463	3.378567	-2.200622	H	2.710727	1.076429	4.697619
C	-0.083855	4.462004	-1.309722	C	2.947351	-1.707891	4.078805
C	-1.339705	3.854654	-0.782942	H	1.163651	-0.331688	6.075467
O	-0.828406	2.572946	-0.337746	C	3.174139	0.251661	5.299469
C	1.128330	2.459074	-1.556913	O	2.077911	-1.864330	5.068986
H	0.728824	4.594177	-0.587899	O	-1.044234	1.594906	4.307353
H	-2.015987	3.744714	-1.703211	K	-3.395026	0.954300	0.585726
H	-0.064390	5.361712	-1.959829	C	-4.549825	5.979996	1.554998
H	-1.854259	4.414497	0.014036	H	-4.080269	6.673291	0.832667
C	1.824842	-0.965384	-2.220839	H	-5.243277	6.540612	2.239562
C	2.152181	0.460882	-1.896561	O	-5.325461	2.858342	0.202958
H	1.643330	-0.992754	-3.323926	H	-2.506619	5.348428	1.949470
H	2.652008	-1.581840	-1.941474	H	-3.674677	4.843290	3.249905
H	2.256915	0.663375	-0.796810	O	-3.886562	3.685118	1.752175
H	3.076765	0.792896	-2.438710	C	-3.531727	5.011244	2.179103
C	-0.523628	-1.132945	-2.166760	C	-4.960584	3.803982	0.917913
O	0.712187	-1.437181	-1.465700	O	-5.230979	5.104613	0.650822
H	-1.272823	-1.955937	-1.966587	<b>II-B</b>			
H	-0.304471	-0.915493	-3.207532	P	-0.596159	0.469003	3.703741
H	-0.956458	-0.246983	-1.746275	O	0.948074	3.302294	-3.029072
H	-1.971803	-2.474140	5.434803	O	0.841472	1.950637	-1.171660
O	-4.232300	-0.336146	5.986706	O	-1.108961	-0.444924	2.571345
O	-5.941563	-1.429197	4.823668	O	-0.590512	3.713299	-1.444468
H	-2.165900	0.269445	6.158007	C	-1.573677	3.051509	-0.659253
C	-4.800928	-1.284576	5.170506	C	-1.861670	3.701169	0.699472
O	-3.808001	-2.085875	4.651151	O	-2.298019	2.665146	1.569633
C	-2.525161	-1.605776	5.076824	C	0.479090	3.021052	-1.955810
H	-1.943492	-1.062662	4.255324	H	-2.548058	3.163773	-1.204863
H	-2.900266	-1.135691	7.243742	H	-2.736756	4.469932	0.592313
C	-2.859153	-0.624704	6.236141	H	-1.414255	1.966446	-0.425311
H	-5.757714	-4.543615	2.140021	H	-1.025140	4.240872	1.200250
O	-3.650985	-2.237117	1.306030	C	1.172267	0.147760	-2.717548
O	-1.810770	-3.611684	0.772356	C	1.790414	1.170967	-1.796014
H	-5.443175	-1.767271	2.161712	H	0.303963	0.613496	-3.279332
C	-2.946861	-3.421237	1.204617	H	1.926489	-0.059075	-3.505447
O	-3.694011	-4.439281	1.723532	H	2.348017	0.510584	-1.101723
C	-4.911191	-3.917901	2.350153	H	2.684917	1.719402	-1.287722
H	-4.768056	-3.845156	3.467335	C	0.350409	-2.046579	-2.923678
H	-5.604683	-2.803705	0.708767	O	0.818023	-1.029917	-1.989588
C	-5.039118	-2.607893	1.601943	H	0.666261	-1.722010	-3.981597
O	-1.066424	2.651250	2.064638	H	-0.757152	-2.076019	-2.930101
K	0.464215	-1.549730	1.454944	H	0.999354	-2.946883	-2.715567
O	0.860382	0.858384	2.838541	H	-4.808168	0.587249	7.205387
K	-0.770306	3.924021	4.634777	O	-4.203095	0.338046	4.029166
O	3.632348	3.419498	3.877938	O	-6.013622	-0.975426	3.424387
H	4.605548	3.788339	2.088913	H	-2.762684	1.293443	5.376436
H	2.664489	4.994028	1.574345	C	-5.313225	-0.492572	4.281149
C	2.386636	4.017172	1.954098	O	-5.520464	-0.567544	5.600650
O	2.169141	4.297396	5.379135	C	-4.427122	0.133822	6.289165
H	3.686020	2.239003	2.184700	H	-3.672827	-0.700995	6.511262
C	2.492408	4.031397	4.210390	H	-4.370998	2.059872	5.164145
H	1.703241	3.416491	1.324866	C	-3.865895	1.077654	5.284702
C	3.700134	3.290429	2.437700	H	-1.324582	-4.790442	3.389895
O	1.666351	4.241583	3.181950	O	-3.102522	-2.877068	1.902188
H	-0.846791	2.454095	0.883763	O	-1.813165	-2.691529	0.005181
O	3.792533	-0.601952	4.255889	H	-2.761495	-2.173518	3.810401
H	3.980495	0.709009	5.877898	C	-1.927256	-2.925613	1.176404
H	2.517225	-1.154965	6.935450	O	-0.879196	-3.427913	1.902758
C	2.200966	-0.711976	5.986231	C	-1.358379	-3.727602	3.243647

H	-0.679162	-3.172337	3.937418	C	3.637051	-0.786489	-2.603301
H	-3.514740	-3.804654	3.717903	O	2.995156	0.478813	-2.878916
C	-2.772835	-3.142911	3.302830	H	3.318800	-1.702879	-3.227197
O	-1.289995	1.857067	3.647020	H	3.487125	-1.075084	-1.542796
K	1.106050	-0.322025	1.110981	H	4.739932	-0.693839	-2.756655
O	0.927286	0.742050	3.348581	H	-3.674187	-1.271449	6.905795
K	0.704821	2.998392	4.929593	O	-5.012505	0.232514	4.715365
O	4.018571	3.988951	3.276913	O	-5.680465	-1.330779	3.225245
H	4.721961	3.955012	1.316243	H	-3.283837	1.110628	5.191251
H	2.542644	4.878645	0.695513	C	-5.031678	-1.042820	4.206523
C	2.497393	4.119076	1.480189	O	-4.182317	-1.831188	4.968007
O	2.720914	4.889128	4.870406	C	-3.376881	-0.982947	5.889163
H	3.924978	2.479811	1.819851	H	-2.346596	-1.028818	5.639162
C	2.916695	4.513572	3.727422	H	-4.350210	0.876042	6.581606
H	1.759096	3.360808	1.128743	C	-3.933565	0.430676	5.676725
C	3.868133	3.572076	1.899352	H	-1.014944	-5.179532	3.035839
O	2.049430	4.799711	2.699144	O	-3.160346	-3.236781	2.314660
H	-1.783116	2.395522	2.452262	O	-2.303440	-2.174079	0.461503
O	3.297888	-0.606180	4.706388	H	-2.423043	-2.687510	4.140508
H	2.688060	-1.389091	6.547552	C	-2.216079	-2.961250	1.394209
H	2.013832	-3.463236	5.369995	O	-1.019427	-3.607429	1.735553
C	1.862594	-2.504324	4.824069	C	-1.122356	-4.081321	3.100989
O	3.887283	-0.905247	2.510204	H	-0.320083	-3.600752	3.612410
H	1.522192	-0.435038	5.617368	H	-3.102120	-4.390347	4.006133
C	3.336657	-1.279442	3.516119	C	-2.496121	-3.616842	3.554312
H	0.800987	-2.399984	4.588249	O	-2.354681	1.963891	3.541426
C	2.316785	-1.194865	5.544117	K	0.339170	-1.223682	1.556500
O	2.669241	-2.518787	3.574322	O	-0.114244	1.242019	2.507483
O	-0.817705	-0.190437	5.106748	K	-0.166029	3.979282	4.384893
K	-3.656581	0.379982	1.424269	O	4.364577	3.095528	2.355814
C	-5.304022	4.860229	1.833534	H	4.549657	3.194442	0.298391
H	-4.335035	5.315758	1.972731	H	2.179141	2.881041	0.226057
H	-6.167167	5.351951	2.363202	C	2.676464	2.219523	0.973873
O	-5.818482	2.788095	-0.952486	O	3.059929	3.600127	4.095673
H	-4.178135	3.011485	2.345294	H	4.827932	1.557401	0.944654
H	-5.755464	3.204697	3.224876	C	3.213412	3.188414	2.988743
O	-5.972333	2.619813	1.357380	H	2.361242	1.203882	0.802754
C	-5.179480	3.406829	2.302280	C	4.192924	2.451307	1.019762
C	-5.834321	3.271774	0.180320	O	2.245291	2.635126	2.234355
O	-5.561252	4.599633	0.373035	H	-2.823740	2.376324	2.464970
<b>TS2-B</b>				O	3.394587	0.641037	4.651709
P	-1.113936	0.882615	3.606076	H	2.703624	0.452619	6.614613
O	1.386307	4.303957	-1.950272	H	2.101437	-1.872772	5.767356
O	0.592214	2.143446	-1.836665	C	1.765934	-1.011497	5.154265
O	-1.747122	-0.544291	3.275149	O	4.016171	-0.202325	2.658624
O	-0.234570	3.840864	-0.502694	H	1.366956	1.044493	5.516344
C	-1.343074	3.032099	-0.157140	C	3.332726	-0.262845	3.668650
C	-2.273349	3.601793	0.925618	H	0.634113	-0.945228	5.021008
O	-3.120081	2.561881	1.267420	C	2.247973	0.403116	5.604852
C	0.612191	3.449492	-1.527256	O	2.425874	-1.244893	3.880752
H	-1.973534	2.852503	-1.018002	O	-0.622289	1.008625	5.052555
H	-2.898645	4.377773	0.490014	K	-4.147799	0.242036	1.470978
H	-1.011901	2.071497	0.253538	C	-5.241351	4.766429	2.093347
H	-1.722456	3.968796	1.780281	H	-4.386617	5.508328	2.085394
C	1.688736	0.411625	-3.263690	H	-6.171317	5.294299	2.184770
C	1.089782	1.857096	-3.230058	O	-5.492350	2.028887	-0.090086
H	1.018989	-0.153439	-2.515071	H	-4.138863	3.154084	3.394659
H	1.576796	-0.110388	-4.254317	H	-5.792407	3.803956	3.838711
H	1.828154	2.676711	-3.478230	O	-5.742467	2.525118	2.081454
H	0.217603	1.864502	-3.931306	C	-5.127668	3.515369	2.986202

C	-5.487270	2.867958	0.810935	O	3.048947	3.150501	3.745864
O	-5.233738	4.188628	0.700482	H	-3.030188	1.670802	4.193999
<b>III-B</b>				O	0.076056	-3.347268	1.453849
P	-1.124542	0.474454	2.810330	H	-1.153287	-2.495336	2.901085
O	2.514398	3.303682	0.053565	H	0.621119	-1.623819	4.076385
O	1.100304	3.608650	-1.740935	C	0.943604	-2.490883	3.470747
O	-1.558189	-0.403803	1.586328	O	1.452651	-2.208593	0.041003
O	0.326969	3.991118	0.252697	H	-0.506417	-4.166177	3.276218
C	0.478638	4.105108	1.720751	C	1.089222	-2.487053	1.173595
C	-0.421191	5.212913	2.210146	H	1.628188	-3.171771	3.993984
O	-1.831376	4.835227	2.262547	C	-0.287051	-3.174109	2.862186
C	1.423890	3.609987	-0.415335	O	1.649371	-1.978851	2.292645
H	0.242905	3.110382	2.156554	O	-1.017233	-0.333508	4.133296
H	-0.387156	6.083324	1.540634	K	-3.871777	1.002653	1.182957
H	1.526329	4.355416	1.943231	C	-4.335812	4.117699	4.663163
H	-0.094510	5.504905	3.219695	H	-3.715256	4.482832	5.492956
C	1.953393	1.808013	-3.166996	H	-5.250949	4.724046	4.582800
C	2.167302	3.228087	-2.653219	O	-1.629324	4.523406	4.529783
H	0.932270	1.709319	-3.566594	H	-5.384069	2.580005	5.695483
H	2.666063	1.619740	-3.993496	H	-5.253141	2.301378	3.955541
H	3.136648	3.347940	-2.150317	O	-3.571703	1.809915	5.105834
H	2.104058	3.937088	-3.493031	C	-4.683396	2.643465	4.842111
C	3.422980	0.529968	-1.750984	C	-2.295589	4.543427	3.499375
O	2.070041	0.794331	-2.163706	O	-3.626563	4.356204	3.401543
H	3.848157	1.377267	-1.186281	<b>Na<sub>2</sub>SnO<sub>3</sub></b>			
H	4.061789	0.303885	-2.622376	<b>TS1-C</b>			
H	3.376505	-0.356667	-1.101056	Sn	-0.680208	-1.759999	3.992083
H	-3.860727	-2.754863	4.284209	O	-2.062509	2.167978	2.532948
O	-5.857433	-0.596811	4.877001	O	-1.298568	3.558902	0.748585
O	-6.301663	0.129202	2.756494	O	-0.956253	-3.631027	4.002233
H	-4.170221	-0.250206	6.023228	O	-3.105644	1.676391	0.017756
C	-5.600175	-0.471234	3.552791	C	-2.254529	1.366925	-1.069847
O	-4.443654	-1.088040	3.198986	C	-0.718170	1.213517	-0.456288
C	-3.801606	-1.661708	4.383031	O	-0.735379	1.213880	0.933995
H	-2.751480	-1.294772	4.394864	C	-1.594145	2.171438	1.382926
H	-4.972602	-1.869099	6.262733	H	-2.565319	0.383662	-1.513013
C	-4.655187	-1.109220	5.537077	H	-0.074287	2.020239	-0.858658
H	-1.915854	-3.151314	-2.270751	H	-2.180685	2.138122	-1.869229
O	-3.462699	-1.335669	-0.701505	H	-0.333625	0.239995	-0.728864
O	-2.768274	0.666626	-1.542661	C	0.920308	4.318643	1.440256
H	-2.322804	-2.340007	0.700932	C	-0.624444	4.426878	1.640941
C	-2.586111	-0.519911	-1.343903	H	1.260005	3.859794	0.480272
O	-1.466821	-1.192241	-1.731085	H	1.269482	5.362203	1.343123
C	-1.623983	-2.602495	-1.363391	H	-0.808693	4.294154	2.779046
H	-0.658289	-2.955333	-0.978740	H	-0.971062	5.454185	1.395485
H	-3.422261	-3.386010	-0.325339	C	3.015884	3.526125	2.242055
C	-2.724457	-2.540309	-0.304912	O	1.589979	3.720507	2.616669
O	-2.218764	1.614058	3.016543	H	3.692914	3.077119	3.077352
K	0.309573	0.520185	-0.016616	H	3.510098	4.458709	1.976620
O	0.230724	1.185120	2.488430	H	2.986481	2.934628	1.323949
K	-0.729135	2.042540	5.422747	H	-3.519665	4.847389	4.830142
O	2.392717	1.407861	5.011137	O	-3.009622	1.838684	5.935407
H	3.544089	-0.030201	4.040585	O	-0.775066	1.834844	5.979796
H	4.693776	1.985874	3.243007	H	-4.857641	2.328217	5.003663
C	3.605741	1.974004	3.083552	C	-1.805031	2.403251	5.721720
O	1.785842	3.516384	5.606434	O	-1.873776	3.670024	5.234345
H	1.990785	0.488187	3.202701	C	-3.223361	3.788660	4.617211
C	2.364868	2.757100	4.851768	H	-3.271209	3.475705	3.577788
H	3.369080	2.061865	2.013559	H	-4.445758	3.195665	6.455023
C	2.885037	0.803096	3.768800	C	-4.009071	2.809205	5.529688

H	-2.712374	-4.816126	0.107089	C	-0.060717	3.166191	0.357518
O	-4.293437	-3.148276	2.164652	H	0.115961	4.775100	-1.046799
O	-4.753719	-1.388456	0.842814	H	0.289449	5.111339	0.658499
H	-2.705838	-4.079695	3.058757	H	0.379394	2.864567	1.372420
C	-4.124930	-2.398681	1.034716	H	-1.114966	3.182149	0.340417
O	-3.090553	-2.815902	0.244206	C	2.780970	3.322927	-0.658569
C	-2.549789	-4.046974	0.817230	O	2.009023	4.521790	-0.346807
H	-1.491889	-3.786869	1.095787	H	2.501368	2.502891	0.010684
H	-3.813920	-5.193167	2.232790	H	3.821142	3.487230	-0.357190
C	-3.312993	-4.227658	2.152810	H	2.778088	2.915147	-1.690292
O	-2.348803	-0.646442	3.423749	H	-2.707543	2.622595	4.611177
O	0.634611	-0.502893	4.115923	O	-0.376620	4.038111	4.507014
Na	0.891398	1.640957	4.358917	O	0.464021	3.188348	6.443923
O	3.162505	5.226231	4.948882	H	-1.804573	5.568531	4.189609
H	2.745025	7.283638	5.377414	C	-0.500628	3.554430	5.796045
H	0.735504	6.416607	6.378028	O	-1.790563	3.600689	6.180218
C	0.932872	5.914049	5.426133	C	-2.613971	3.650723	4.960784
O	2.879813	3.026577	5.532655	H	-3.611758	4.083244	5.181505
H	2.231618	6.609805	3.739177	H	-1.909107	4.117081	3.065177
C	2.393958	4.174813	5.424898	C	-1.706182	4.456493	4.086874
H	0.043355	6.079022	4.867167	H	-4.432069	-1.147158	5.432374
C	2.298194	6.409627	4.788497	O	-6.223196	-2.533027	3.806412
O	1.143307	4.480861	5.756487	O	-6.308393	-0.986447	2.082893
H	-1.998482	0.265979	3.623952	H	-7.349839	-2.393503	5.592321
O	1.631328	-4.677629	1.693970	C	-6.143106	-1.274566	3.281850
H	2.862047	-5.885015	2.755552	O	-6.007454	-0.341477	4.272870
H	1.106757	-6.882998	4.109643	C	-5.546486	-1.043277	5.496287
C	0.829663	-6.010333	3.494204	H	-5.942598	-0.523919	6.383725
O	0.378354	-5.586348	-0.011630	H	-5.802706	-3.213666	5.713199
H	2.490031	-4.334001	3.538245	C	-6.290547	-2.391042	5.262302
C	0.704834	-5.565475	1.176528	O	-2.882304	-1.098290	3.475391
H	0.046469	-5.334705	3.922037	O	-1.172299	1.305789	3.651099
C	2.081713	-5.209613	2.986589	Na	0.891218	1.641044	4.360996
O	0.265918	-6.387656	2.170540	O	3.938023	0.271197	2.298563
Na	-3.798842	0.516560	2.109579	H	3.637706	-1.256617	0.993928
C	-5.380110	3.928149	-1.044802	H	1.883468	-1.992700	2.771559
H	-5.273939	3.401195	-2.054530	C	2.918369	-1.689492	3.137582
H	-6.293268	4.600319	-1.126849	O	3.057522	1.714701	3.811096
O	-5.612538	3.355949	2.329646	H	4.921283	-1.506906	2.175307
H	-3.341122	4.213995	-0.498573	C	3.222141	0.540085	3.412626
H	-4.204775	5.809031	-0.954152	H	3.410328	-2.432053	3.775737
O	-4.885591	4.954672	0.833773	C	3.918717	-1.161902	2.066648
C	-4.265737	4.796282	-0.515784	O	2.725663	-0.557531	4.009812
C	-5.356284	3.750681	1.181029	H	-2.757787	-2.066811	3.584679
O	-5.611207	2.994314	0.033101	O	-0.635490	-3.959151	6.343806
<b>II-C</b>				H	0.889903	-2.876712	6.942081
Sn	-1.070642	-0.416693	2.697348	H	-0.572446	-1.039574	7.066151
O	0.854488	0.863597	1.067498	C	-0.683021	-1.640397	6.143708
O	0.172838	2.194988	-0.647092	O	-2.916961	-4.249213	6.389430
O	0.273081	-1.867004	2.993351	H	0.759616	-3.043315	5.133996
O	-1.825174	0.026577	0.886536	C	-1.927483	-3.554655	6.364057
C	-1.771774	-1.002504	-0.077979	H	-0.683614	-1.073168	5.194397
C	-0.270693	-1.293939	-0.612618	C	0.254348	-2.876701	6.100821
O	0.209131	0.085760	-1.027215	O	-2.035736	-2.179465	6.311720
C	0.419677	1.005311	-0.070546	Na	-3.798651	0.515714	2.109082
H	-2.039737	-1.992008	0.327084	C	-4.400812	4.658786	-1.288537
H	-0.336099	-1.800937	-1.570415	H	-5.326901	4.514629	-1.921172
H	-2.389032	-0.752995	-0.928823	H	-3.959667	5.740287	-1.222914
H	0.510901	-1.780745	0.031680	O	-3.989516	2.812881	1.756562
C	0.607869	4.419943	-0.148309	H	-3.531742	3.149778	-2.429590

H	-2.291474	4.063384	-1.824579	H	2.354837	-3.376580	5.309526
O	-3.240196	2.765719	-0.413782	C	3.415683	-2.632533	3.559983
C	-3.316150	3.660405	-1.523645	O	2.075297	-1.361873	5.042391
C	-3.975421	3.192005	0.567895	H	-2.240000	-2.061194	2.187648
O	-4.745183	4.322911	0.208572	O	-1.299652	-2.174034	7.617062
<b>TS2-C</b>				H	-0.526666	-0.404718	6.854255
Sn	-0.803910	-0.102589	1.993653	H	-2.140268	-0.297654	5.236510
O	1.655232	0.234798	-0.172744	C	-1.951555	-1.322851	5.497698
O	1.522552	2.465731	-0.705273	O	-3.396921	-2.719985	8.312404
O	0.537353	-1.472634	2.092548	H	0.127956	-1.865138	6.106495
O	-1.302112	0.821300	-0.011800	C	-2.645455	-2.254499	7.475541
C	-1.352957	-0.284273	-0.943952	H	-1.748486	-1.933977	4.588465
C	-0.362944	-0.145887	-2.061947	C	-0.763079	-1.410278	6.466588
O	0.359097	1.143590	-2.027100	O	-3.090383	-1.732290	6.274422
C	1.140956	1.152444	-0.827897	Na	-3.797699	0.516353	2.110429
H	-1.384156	-1.218426	-0.447512	C	-3.612186	2.575463	-2.346855
H	-0.730120	-0.304818	-3.057030	H	-4.235083	3.404008	-2.677507
H	-2.361713	-0.175442	-1.319698	H	-3.038987	2.141288	-3.235865
H	0.426549	-0.889828	-1.928144	O	-2.679914	2.609843	1.059223
C	2.454398	4.481138	0.366340	H	-5.397852	1.188250	-1.829991
C	2.212656	2.999078	0.481563	H	-4.096474	0.378107	-2.212531
H	2.844052	4.885311	-0.579410	O	-4.013387	1.345373	-0.350173
H	1.505481	5.078338	0.410712	C	-4.295578	1.298675	-1.710845
H	3.127576	2.505589	0.682982	C	-2.857741	2.254174	-0.035340
H	1.646362	2.814783	1.432964	O	-2.588803	2.946429	-1.267299
C	4.743182	4.662601	1.319061	<b>III-C</b>			
O	3.346757	4.896142	1.499731	Sn	-2.091919	0.122449	5.199480
H	4.925886	3.574918	1.570059	O	0.202028	-0.715019	3.660405
H	5.279690	5.271508	2.098094	O	0.593699	-0.847582	1.369387
H	4.999980	4.796019	0.258549	O	-0.710366	1.206357	5.901323
H	-4.385231	2.589181	4.145037	O	-2.023299	-1.060220	1.372133
O	-1.645050	3.613902	4.725681	C	-2.674163	-2.319693	1.893811
O	-1.041288	2.476329	6.607931	C	-1.577766	-2.937878	2.880269
H	-2.851248	5.282711	4.489558	O	-0.201614	-2.702850	2.581526
C	-1.891038	2.914934	5.846406	C	0.142978	-1.396201	2.620106
O	-3.240858	2.745722	5.999157	H	-3.682704	-2.284935	2.315868
C	-3.985579	3.347335	4.865969	H	-1.582847	-4.020460	2.846832
H	-4.883746	3.867581	5.308232	H	-2.713163	-3.120170	1.186638
H	-2.748924	4.112992	3.092500	H	-1.901186	-2.492924	3.868770
C	-2.854757	4.233826	4.202785	C	2.856390	-1.360711	0.298771
H	-6.278838	-0.970325	6.946180	C	1.840117	-0.382017	0.972903
O	-6.032391	-1.638576	3.904869	H	2.284348	-2.032099	-0.306986
O	-6.191148	0.468778	3.069302	H	3.499340	-0.744758	-0.362341
H	-7.217773	-3.039131	4.873294	H	2.300673	0.269722	1.765275
C	-6.427678	-0.344501	3.980611	H	1.582976	0.341030	0.127338
O	-6.971121	-0.073450	5.166591	C	4.712349	-2.870324	0.771482
C	-6.892921	-1.237798	6.055828	O	3.602324	-2.066203	1.309737
H	-7.902211	-1.395634	6.424730	H	5.354082	-2.168625	0.214319
H	-5.489090	-2.875883	5.409360	H	4.390803	-3.644654	0.044978
C	-6.375734	-2.367663	5.114552	H	5.223529	-3.368957	1.610048
O	-2.502851	-1.132521	2.223295	H	0.951909	6.913846	2.035876
O	-0.962119	1.361966	3.370970	O	0.092947	4.781239	3.524366
Na	0.890157	1.641456	4.358850	O	1.593553	3.246654	2.872672
O	3.711119	-1.225252	3.465542	H	-1.674944	5.278801	2.505505
H	3.211231	-2.989874	2.474648	C	0.955867	4.272385	2.617237
H	1.304346	-3.036454	3.908070	O	1.001910	4.948872	1.448616
C	2.192100	-2.687093	4.482727	C	0.208031	6.154933	1.662033
O	3.011662	0.643443	4.573693	H	-0.238307	6.405928	0.679408
H	4.301822	-3.141609	4.001933	H	-0.909319	6.602549	3.516019
C	2.887962	-0.564945	4.362160	C	-0.740377	5.781449	2.818458

H	-4.377644	2.930480	-2.617449	C	2.209137	0.416982	8.340556
O	-3.386590	2.447314	0.448913	C	2.665740	1.392790	7.153779
O	-1.255228	3.324382	0.209403	H	1.746491	-0.546831	7.968243
H	-5.155194	1.571386	-0.113700	H	3.161153	0.102359	8.847036
C	-2.320303	2.948254	-0.265676	H	2.672766	2.466638	7.429011
O	-2.597425	3.029748	-1.594175	H	3.663161	1.015065	6.748033
C	-3.909773	2.403736	-1.807251	C	1.392158	0.761067	10.626069
H	-3.694942	1.376554	-2.109499	O	1.409912	1.177868	9.222358
H	-5.130227	3.361590	-0.198995	H	0.962773	1.702321	11.013429
C	-4.573563	2.452544	-0.401164	H	2.457231	0.507679	10.820077
O	-1.886193	-1.766024	6.089065	H	0.635301	-0.083476	10.809560
O	-3.763190	0.413567	4.266324	H	-2.493006	4.986309	6.405595
Na	0.890916	1.640805	4.359665	O	-3.286955	5.270680	3.339370
O	2.097472	-0.512818	6.041231	O	-1.201946	5.112175	2.472136
H	1.050225	-2.162215	6.783137	H	-4.557854	6.169816	4.765621
H	3.417599	-3.023699	6.556060	C	-1.914040	5.335330	3.427803
C	2.981303	-2.655582	5.615952	O	-1.489223	5.507038	4.707069
O	3.741259	0.656512	5.055523	C	-2.661564	5.675917	5.576695
H	0.952345	-1.902217	5.062333	H	-2.669956	6.712089	6.000059
C	3.281515	-0.401827	5.406392	H	-4.259838	4.389411	4.955104
H	2.875722	-3.498789	4.924251	C	-3.823203	5.349866	4.678249
C	1.683046	-1.920689	5.880380	H	2.336884	-1.409842	-2.197556
O	3.818762	-1.628098	5.122561	O	4.587023	-3.640509	-1.612935
H	-2.470655	-2.366528	5.582949	O	3.394019	-5.542512	-1.768420
O	-6.057727	1.693394	2.846599	H	4.865073	-1.559991	-1.479487
H	-7.556841	0.218008	3.172567	C	3.504782	-4.353843	-1.929147
H	-7.871363	1.209192	5.455808	O	2.425799	-3.575600	-2.192837
C	-6.869337	1.366317	5.022504	C	2.861601	-2.210868	-1.696133
O	-5.474667	3.850304	3.129519	H	2.893427	-2.203859	-0.613667
H	-5.946032	-0.199400	3.823382	H	4.531908	-2.192472	-3.181733
C	-6.046094	2.868793	3.563273	C	4.268119	-2.290976	-2.071877
H	-6.113811	1.045668	5.772896	O	-0.370302	-0.372290	0.610236
C	-6.673951	0.651495	3.687430	O	-1.716199	-1.616561	2.706491
O	-6.666456	2.759670	4.765865	O	-3.631874	1.344128	8.185893
Na	-3.796396	0.516444	2.109644	H	-1.718545	1.018771	9.058108
C	-0.886733	-0.552548	-1.240514	H	-0.710775	1.042981	6.806962
H	-0.575482	-0.037541	-2.217885	C	-1.818970	0.943196	6.875807
H	0.015119	-0.425334	-0.557080	O	-4.288389	3.370550	7.215985
O	-3.959665	-0.658462	0.215578	H	-2.572453	-0.450965	8.327790
H	-1.246803	-2.471739	-2.285726	C	-3.544096	2.399529	7.233870
H	-0.595475	-2.504077	-0.608849	H	-2.259837	0.196997	6.162055
O	-2.612470	-2.122165	-0.815799	C	-2.380115	0.619150	8.253684
C	-1.288262	-2.011167	-1.278550	O	-2.439719	2.241893	6.488579
C	-2.772383	-0.865938	0.031380	H	1.042970	1.553366	0.216617
O	-1.973224	0.161811	-0.703146	O	-5.638069	-2.826435	4.745308
<b>VO(OiPr)<sub>3</sub></b>				H	-4.970385	-2.911050	2.775316
<b>TS-D</b>				H	-3.771267	-0.875829	3.136410
V	-1.828659	-0.792162	1.059067	C	-4.685500	-0.961048	3.726033
O	3.100278	2.686821	4.799780	O	-4.799748	-2.476293	6.872354
O	1.777455	1.221244	5.956232	H	-6.480795	-2.012306	3.014827
O	-2.633610	-2.027471	0.028911	C	-4.891288	-2.150988	5.704906
O	1.208125	1.908193	3.920098	H	-5.322392	-0.061347	3.706981
C	1.704892	1.922567	2.575784	C	-5.480175	-2.226544	3.433151
C	0.698860	2.704345	1.770799	O	-4.252819	-1.123061	5.129932
O	1.189409	2.534306	0.403895	O	-2.960106	0.525179	1.343452
C	2.117706	1.987936	4.913975	C	2.678745	1.779142	-2.068662
H	2.713971	2.288294	2.430060	H	3.680331	1.413101	-1.884875
H	0.536236	3.770272	2.059625	H	2.793421	1.676658	-3.171318
H	1.680182	0.861074	2.223363	O	-0.630433	2.951586	-1.287045
H	-0.375991	2.379185	1.937133	H	3.274025	3.715703	-0.990418

H	3.217517	3.775024	-2.738805	H	0.513130	5.296034	0.513961
O	1.359916	3.583685	-1.916835	O	-2.357446	5.124883	2.005383
C	2.727113	3.227440	-1.872631	O	-3.775329	5.325850	0.280625
C	0.532389	2.854762	-1.248140	H	-0.730627	5.674628	3.146686
O	1.554028	1.169622	-1.556987	C	-2.646678	5.340455	0.675555
C	-0.749942	-2.596551	3.166159	O	-1.512915	5.666704	-0.049390
C	-0.967924	-3.807855	2.277120	C	-0.368170	5.770677	0.942518
C	-0.784765	-3.039637	4.686074	H	-0.156379	6.861468	1.062412
H	0.250743	-2.233486	2.954542	H	-0.581983	4.053378	2.307468
C	-2.759145	-2.015558	-1.382851	C	-0.897099	5.102798	2.226528
H	-3.085628	-3.028583	-1.585096	H	0.523950	-4.423057	-2.093759
C	-1.428447	-1.590954	-1.919518	O	1.903610	-1.622231	-1.624780
C	-3.803440	-0.979595	-1.920908	O	4.025509	-2.179222	-1.248805
C	-3.062120	1.894549	1.841812	H	-0.128855	-1.879217	-1.375588
C	-3.518983	1.907195	3.364561	C	2.893750	-2.542432	-1.380465
C	-3.996158	2.687660	1.021893	O	2.463673	-3.830024	-1.450128
H	-2.055214	2.312849	1.843210	C	1.019328	-3.770675	-1.389399
H	0.154465	-3.617005	4.848086	H	0.722134	-3.891490	-0.358117
H	-1.686987	-3.584234	4.886466	H	0.445379	-2.294964	-3.017956
H	-0.759003	-2.144455	5.341306	C	0.698346	-2.362483	-1.969928
H	-1.660491	-4.547420	2.684320	O	-1.766266	0.872696	1.774599
H	0.025846	-4.232024	2.053665	O	-2.997899	-1.447749	2.345128
H	-1.385867	-3.531483	1.300929	O	-0.181809	3.120588	6.224761
H	-3.627090	0.026409	-1.448097	H	0.937770	1.777643	7.305840
H	-4.829477	-1.334435	-1.683634	H	-0.368434	0.112174	6.296749
H	-3.737470	-0.869137	-2.991822	C	-1.029594	0.956601	6.630633
H	-0.589521	-2.010237	-1.381391	O	-1.557136	3.643255	4.512565
H	-1.364085	-0.489680	-1.838957	H	-0.462565	2.543483	8.129353
H	-1.340468	-1.737447	-3.002751	C	-1.113128	2.833854	5.289207
H	-4.612305	1.664144	3.483302	H	-1.845398	0.589928	7.210661
H	-3.365695	2.900549	3.833213	C	-0.122154	2.085589	7.204731
H	-2.937066	1.069777	3.831550	O	-1.557375	1.582633	5.393538
H	-3.909833	2.492519	0.009218	H	2.707674	0.518279	-1.122648
H	-3.912560	3.728869	1.296022	O	-5.189996	-3.016642	4.068007
H	-5.043991	2.423937	1.394239	H	-5.321376	-2.572844	1.993999
<b>II-D</b>				H	-6.844256	-0.778662	2.425997
V	-3.265962	0.335846	2.007114	C	-6.816207	-1.523753	3.225143
O	3.961257	0.712466	5.797058	O	-4.364501	-1.672889	5.678635
O	2.901819	-1.162555	6.573748	H	-6.557342	-3.633687	2.666679
O	-4.115531	0.511969	0.472276	C	-5.155636	-1.827420	4.773797
O	1.869759	0.141978	5.096968	H	-7.835517	-1.751860	3.579191
C	1.983401	1.194586	4.038537	C	-5.965226	-2.748176	2.861940
C	2.803148	0.547836	2.922355	O	-6.095267	-0.934795	4.328042
O	2.688165	1.383315	1.647639	O	-4.298036	1.101250	3.253580
C	3.030860	-0.077332	5.825840	C	2.754187	2.354071	-1.602449
H	0.900198	1.456980	3.724312	H	3.643470	2.916755	-1.923299
H	2.412512	-0.485806	2.671579	H	2.182008	2.272335	-2.504722
H	2.411869	2.041085	4.547176	O	1.239547	-0.229015	0.784542
H	3.849382	0.571894	3.227680	H	2.572511	3.399532	0.387924
C	3.196636	-1.887005	8.860400	H	1.302822	3.790867	-0.864799
C	3.968655	-1.392081	7.619681	O	1.190772	2.009532	0.243289
H	2.322540	-2.496193	8.507975	C	1.993254	3.040066	-0.474500
H	3.855329	-2.559670	9.413405	C	1.692013	0.898464	0.868168
H	4.432399	-0.427040	7.861796	O	3.312972	1.092796	-1.209321
H	4.579600	-2.193197	7.236426	C	-1.615200	-2.129204	2.373271
C	2.424699	-1.248501	11.104465	C	-1.933856	-3.620099	2.142687
O	2.803726	-0.768239	9.769662	C	-0.993210	-1.878350	3.716969
H	2.770056	-2.294908	11.326465	H	-1.056662	-1.643895	1.556152
H	1.281215	-1.269370	11.185254	C	-3.836708	0.681196	-0.974871
H	2.910514	-0.499764	11.745512	H	-4.687289	0.153026	-1.488311



C	-2.515576	0.038262	-1.352831
C	-3.992667	2.141369	-1.449762
C	-4.573967	2.474377	3.772179
C	-5.176814	2.317763	5.134795
C	-5.538300	2.971366	2.685492
H	-3.599850	2.993786	3.780463
H	-0.068775	-2.454041	3.830530
H	-1.647920	-2.307365	4.508761
H	-0.776295	-0.866622	4.039395
H	-2.259630	-4.105389	3.071094
H	-0.999272	-4.069373	1.779798
H	-2.756917	-3.743093	1.418014
H	-3.148743	2.817429	-1.128440
H	-4.914060	2.659050	-1.222377
H	-4.007762	2.069788	-2.566670
H	-2.405097	-0.989937	-0.941601
H	-1.633033	0.675008	-1.012247
H	-2.446528	-0.083325	-2.458958
H	-5.920747	1.460649	5.171922
H	-5.765702	3.214560	5.404359
H	-4.374296	2.104196	5.824896
H	-6.274589	3.642485	3.059875
H	-6.018094	2.140008	2.202312
H	-4.900624	3.560467	2.036029