Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

First Principles Studies on the Selectivity of Dimethoxymethane and Methyl Formate in Methanol Oxidation over V_2O_5/TiO_2-based Catalysts

Na Li,[a,b] Shibin Wang,[a,c] Yuhan Sun,[a,c] Shenggang Li[a,c,*]

[a] *CAS Key Laboratory of Low-Carbon Conversion Science and Engineering, Shanghai Advanced Research Institute, Chinese Academy of Sciences, 100 Haike Road, Shanghai 201210, China*

[b] *Department of Chemistry, Shanghai University, 99 Shangda Road, Shanghai 200444, China*

[c] *School of Physical Science and Technology, ShanghaiTech University, 100 Haike Road, Shanghai 201210, China*

*E-mail: lisg@sari.ac.cn

This supplementary information is divided into three sections, briefly summarized below.

Section 1: Complete list for reference 27.

Section 2: Additional figures:

Figure S1. Potential Energy Surface for the Formation of HCHO on V_4O_{10}.

Figure S2. Potential Energy Surface for the Formation of $HCOOCH_3$ on V_4O_{10}.

Figure S3. Potential Energy Surface for the Formation of DMM Initiated by CH_3OH Chemisorption on V_4O_{10}.

Figure S4. Potential Energy Surface for the Formation of DMM Initiated by Hemiacetal Chemisorption on V_4O_{10}.

Figure S5. Structures of the Stationary States on the Potential Energy Surfaces for Figures 1, 4, 7, S1 to S4.

Figure S6. Potential Energy Surface and Reaction Network for the Formation of HCHO, $HCOOCH_3$ and DMM over the $VTi_3O_7(OH)_3$ Cluster Model Calculated at the PBE Level.

Figure S7. Potential Energy Surface and Reaction Network for the Formation of HCHO, $HCOOCH_3$ and DMM over the $VTi_3O_6(SO_4)(OH)_3$ Cluster Model Calculated at the PBE Level.

Figure S8. Potential Energy Surface and Reaction Network for the Formation of HCHO, $HCOOCH_3$ and DMM over the V_4O_{10} Cluster Model Calculated at the PBE Level.

Section 3: Additional tables.

Table S1. Free Energy Barriers and Tunneling Cofficients of the Rate Determining Step at Different Temperatures for the Formation of Formyldehyde, Methyl Formate, and Dimethoxymethane over the $VTi_3O_7(OH)_3$ Cluster Model.

Table S2. Free Energy Barriers and Tunneling Cofficients of the Rate Determining Step at Different Temperatures for the Formation of Formyldehyde, Methyl Formate, and Dimethoxymethane over the $VTi_3O_6(SO_4)(OH)_3$ Cluster Model.

Table S3. Cartesian or Fractional Coordinates of the Molecular Cluster and Periodic Slab Models.

Table S4. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 1a.

Table S5. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 1b.

Table S6. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 4a.

Table S7. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 4b.

Table S8. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 7.

Section 1.

Complete List for Ref. 27

Ref. 27: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr. J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2009.

Section 2.

Figure S1. Potential Energy Surface (E_{0K}, eV) for the Formation of HCHO on the Cluster Model V_4O_{10} (B3LYP).

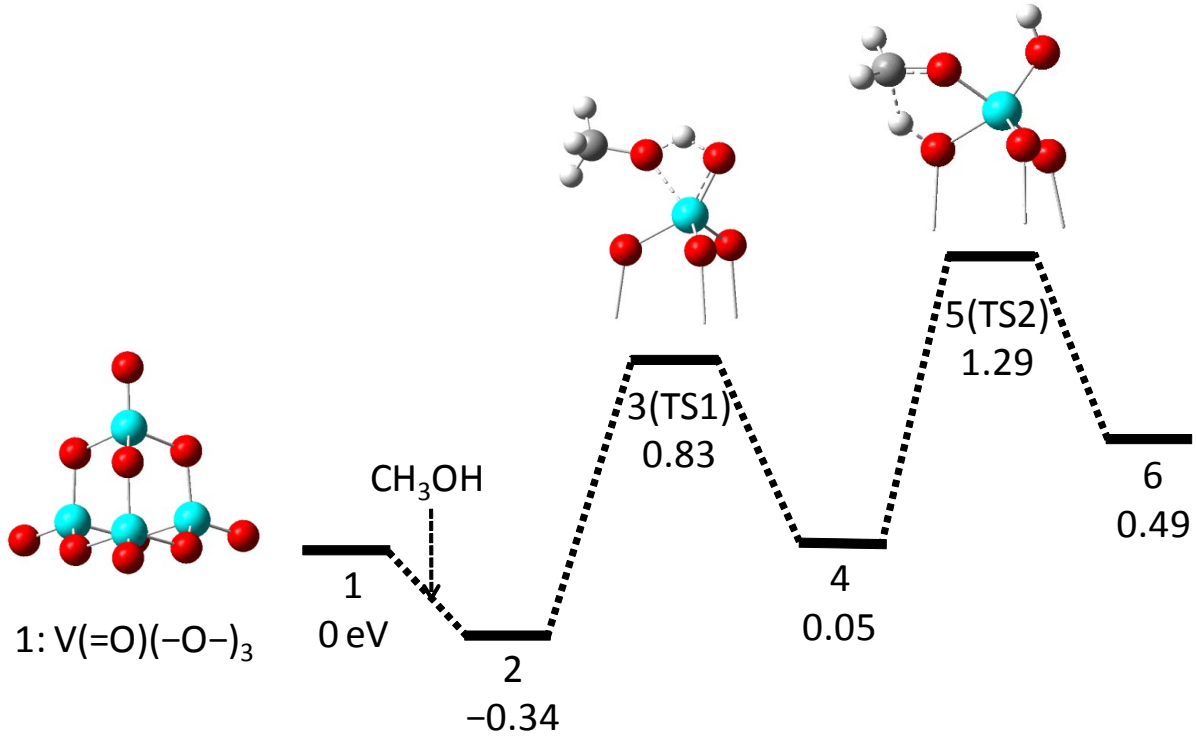


Figure S2. Potential Energy Surface (E_{0K}, eV) for the Formation of $HCOOCH_3$ via the Hemiacetal Mechanism Calculated with the Cluster Model V_4O_{10} (B3LYP).

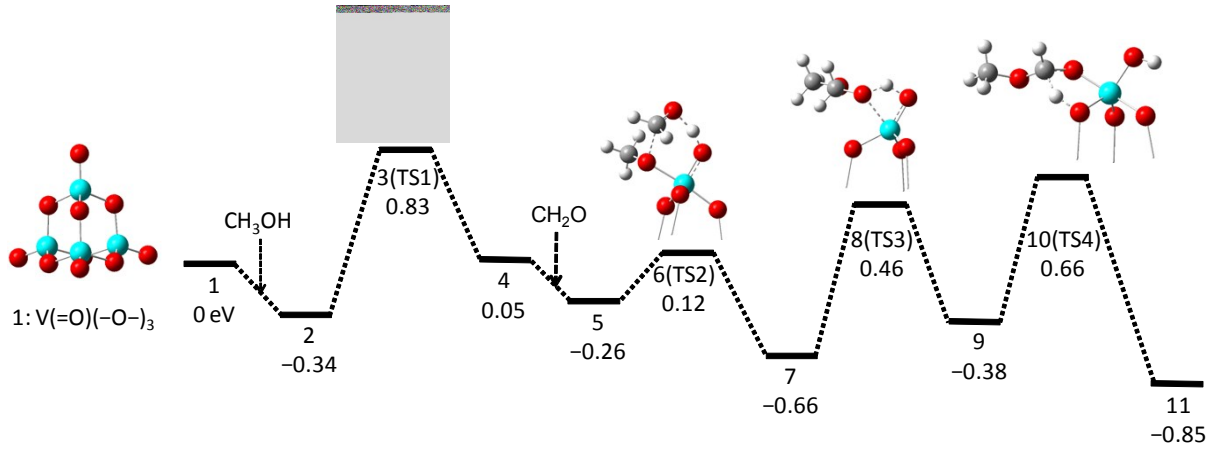


Figure S3. Potential Energy Surface (E_{0K}, eV) for the Formation of DMM via the Pathway Initiated by CH_3OH Chemisorption with the Cluster Model V_4O_{10} (B3LYP).

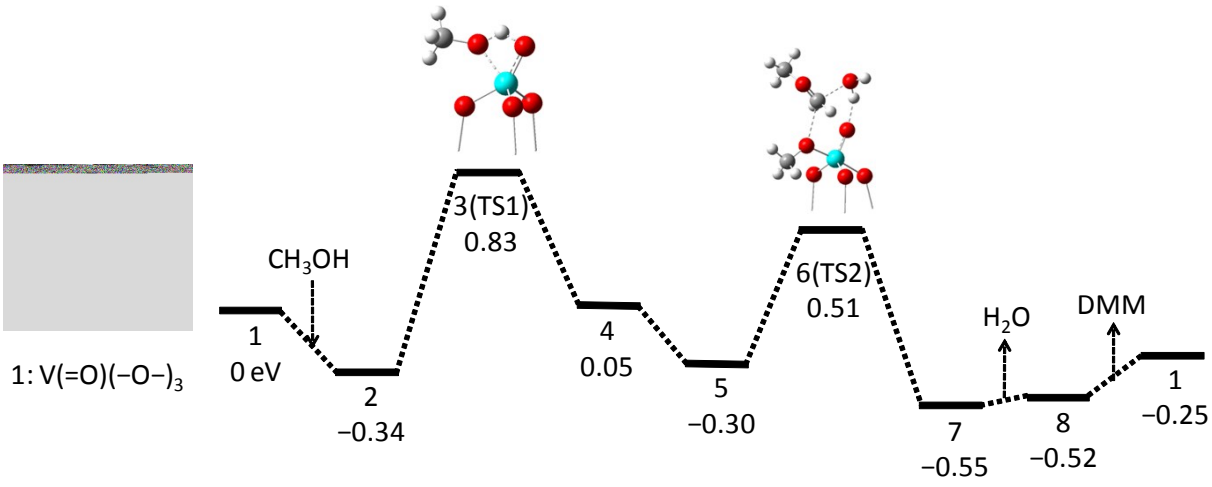


Figure S4. Potential Energy Surface (E_{0K}, eV) for the Formation of DMM via the Pathway Initiated by Hemiacetal Chemisorption with the Cluster Model V_4O_{10} (B3LYP).

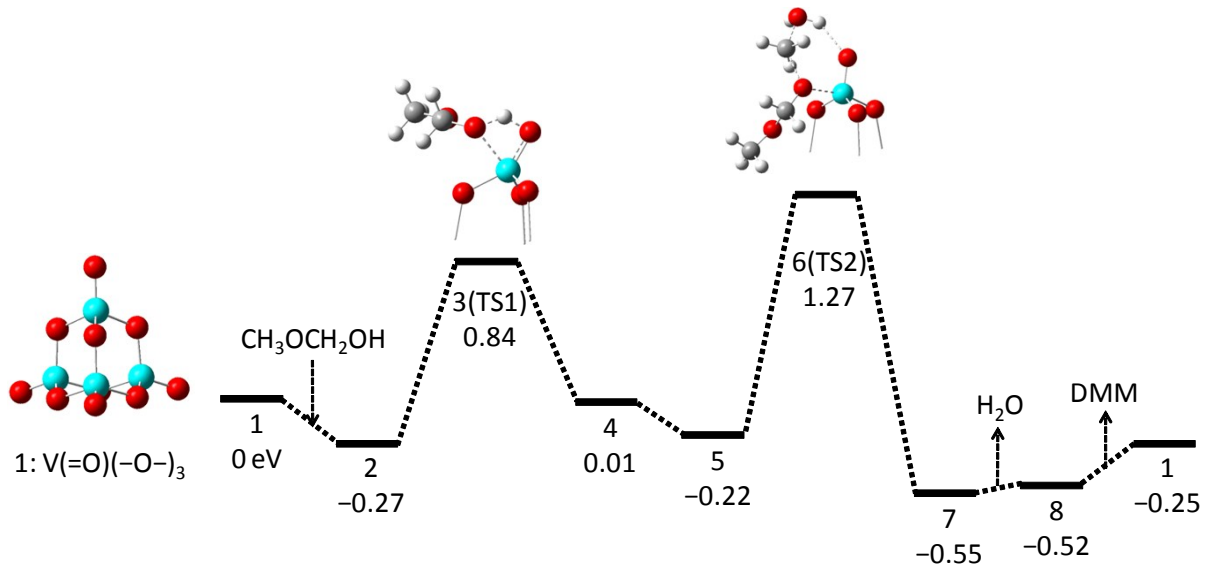


Figure S5. Structures of the Stationary States on the Potential Energy Surfaces for Figures 1, 4, 7, S1 to S4.

Figure 1a: 1a-8a

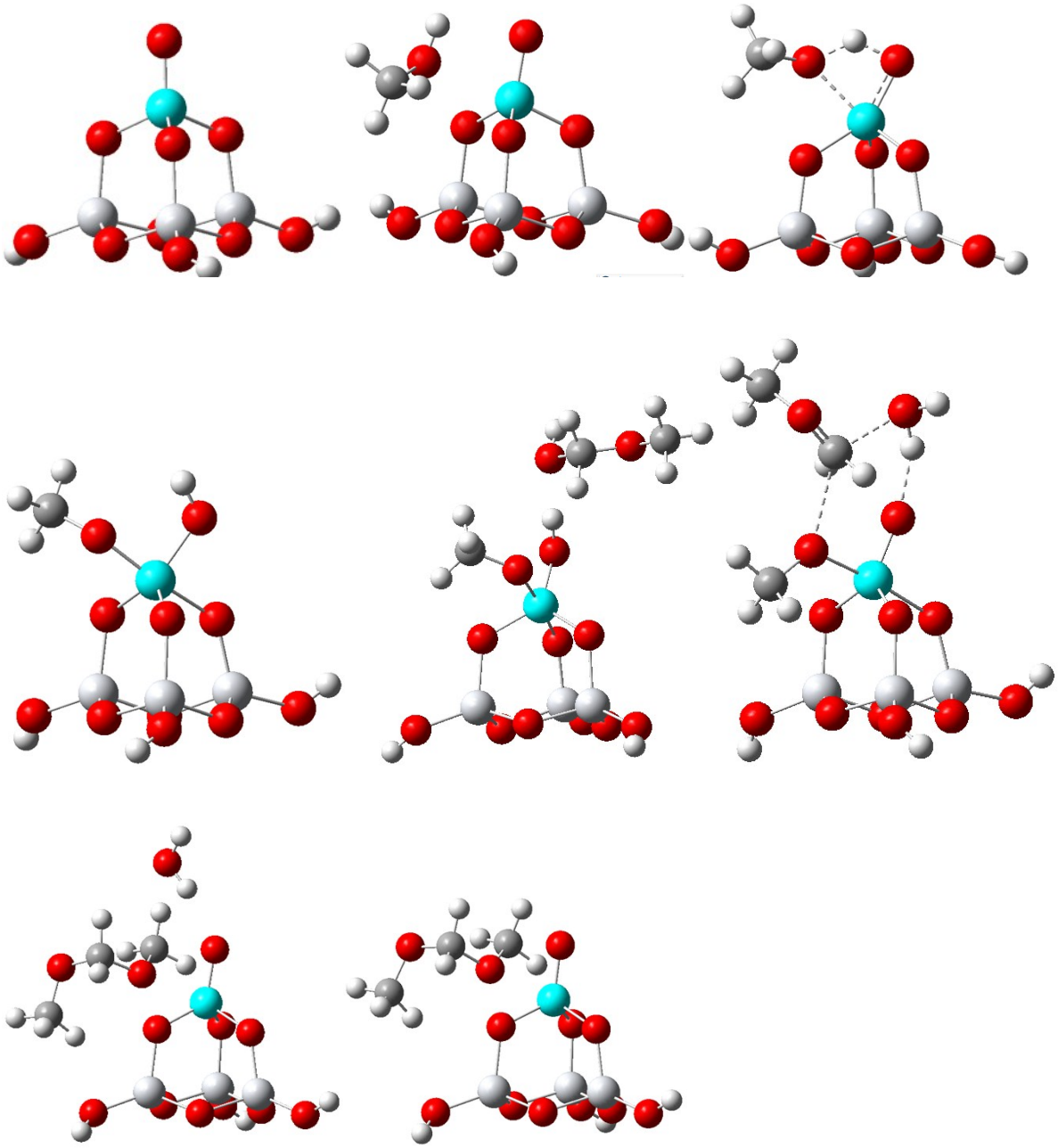
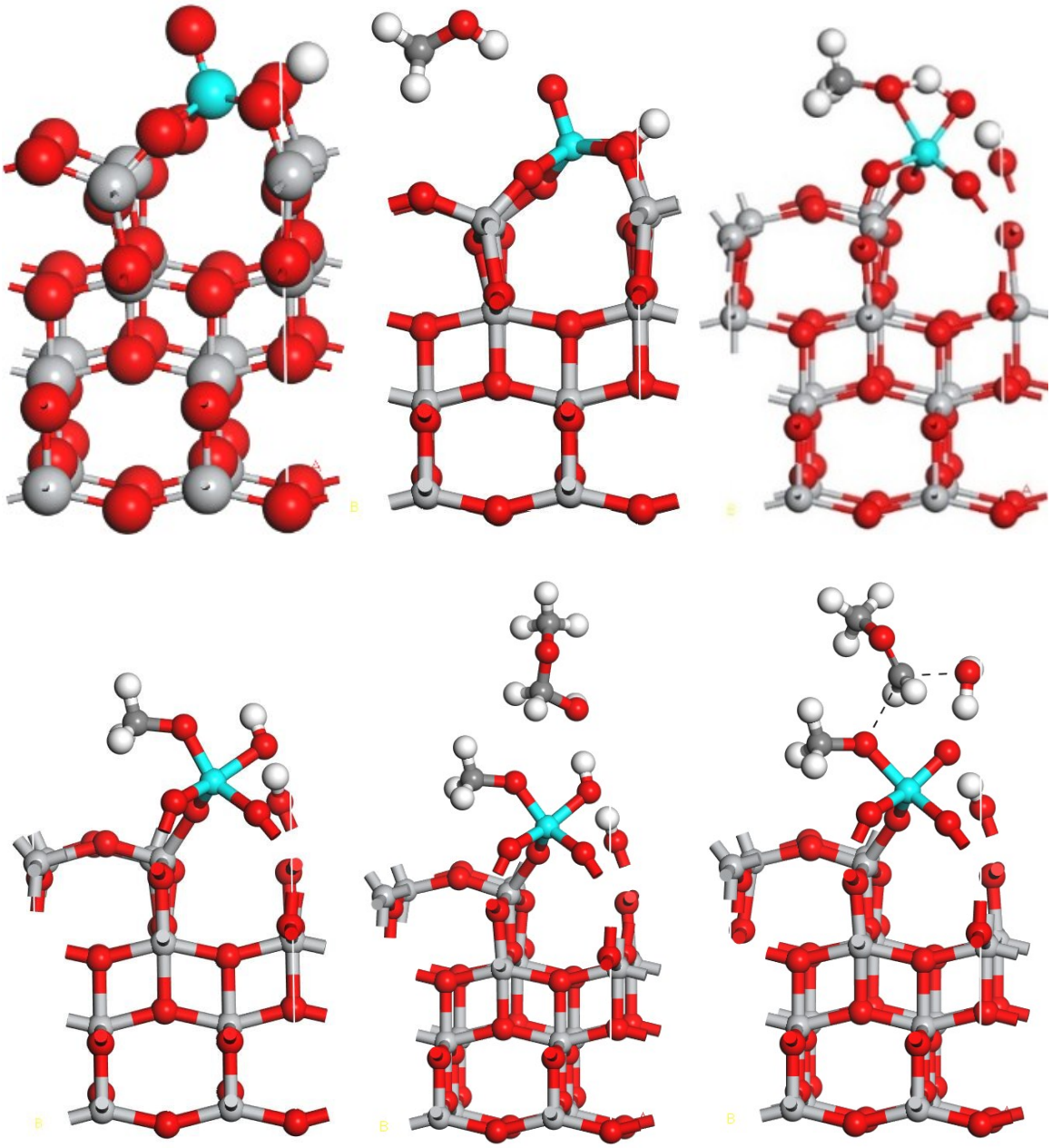


Figure 1a: 1b-8b



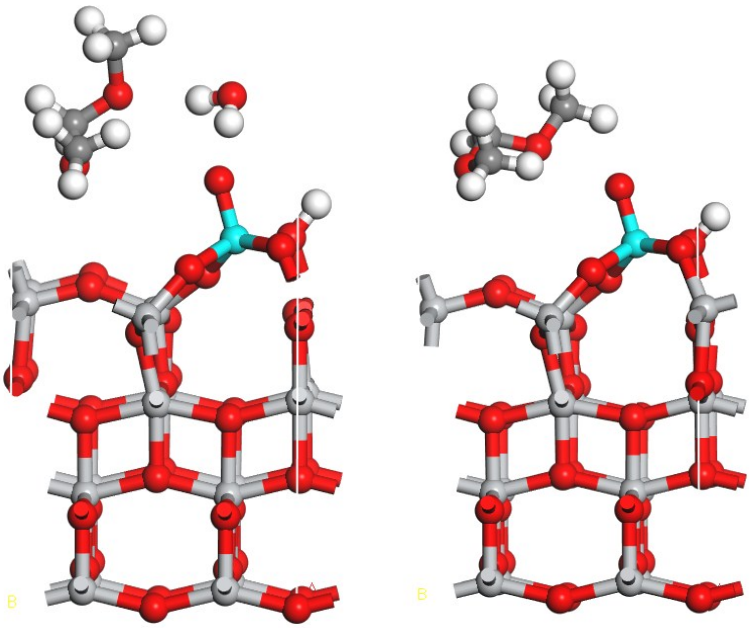


Figure 1b: 9a-13a

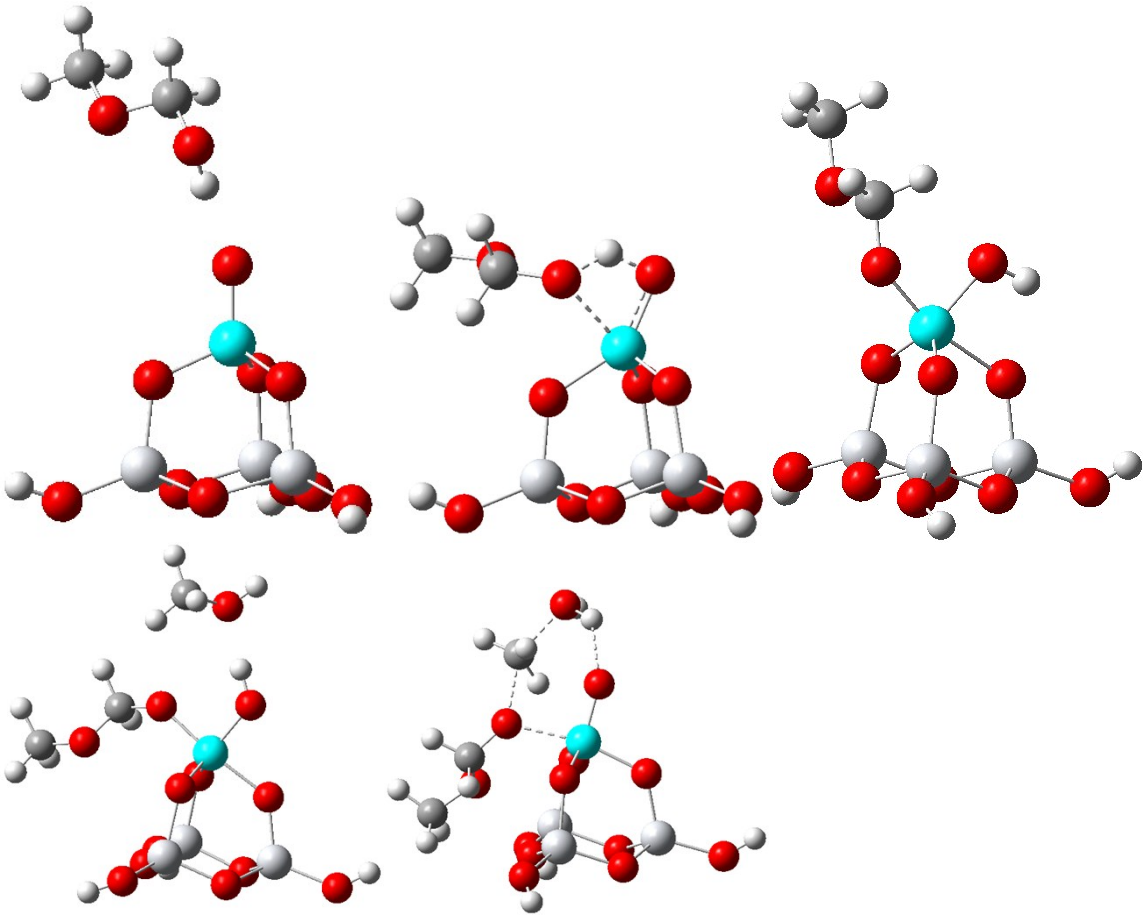


Figure 1b: 9b-13b

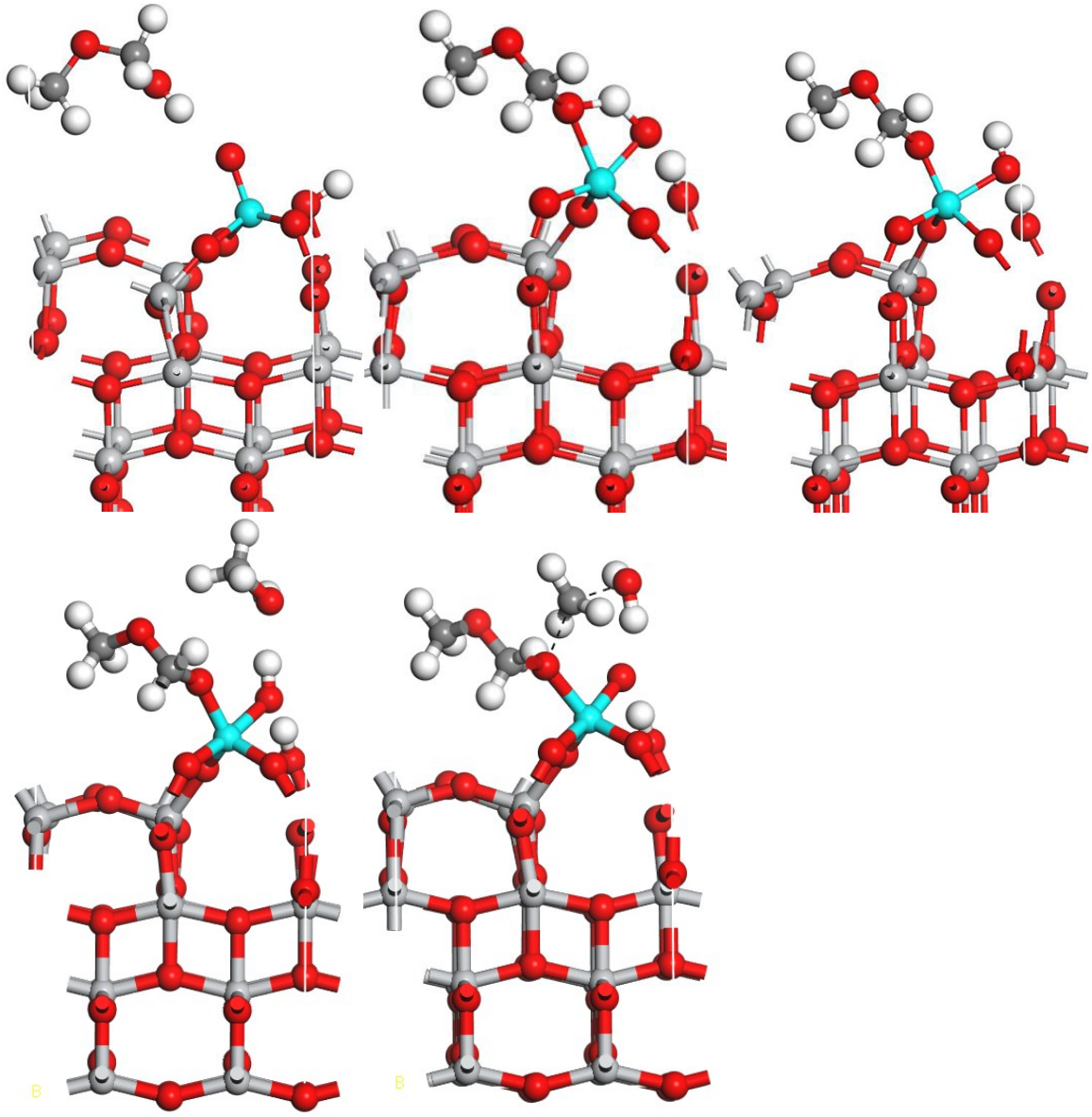


Figure 4a: 1-8

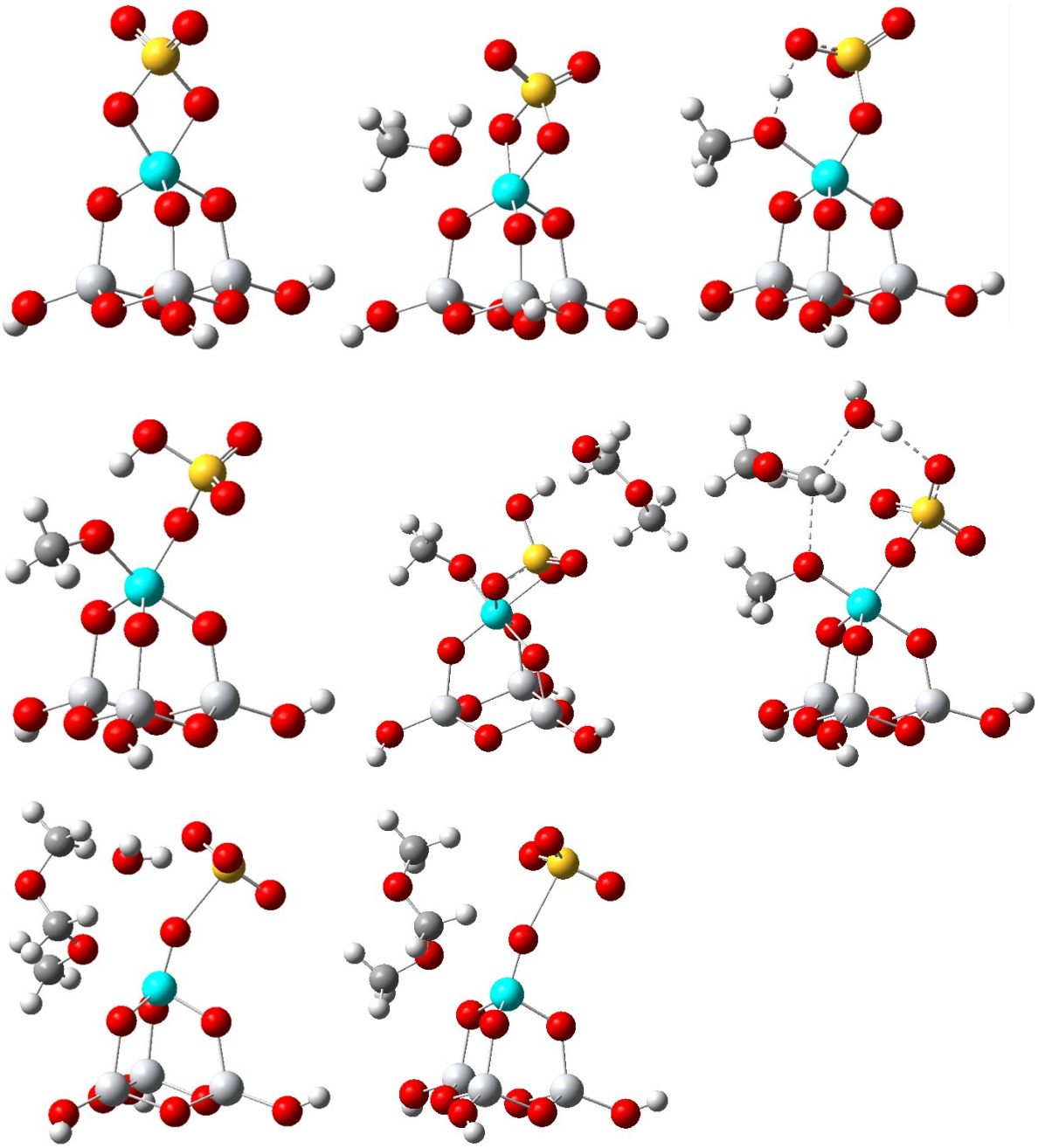


Figure 4b: 9-13

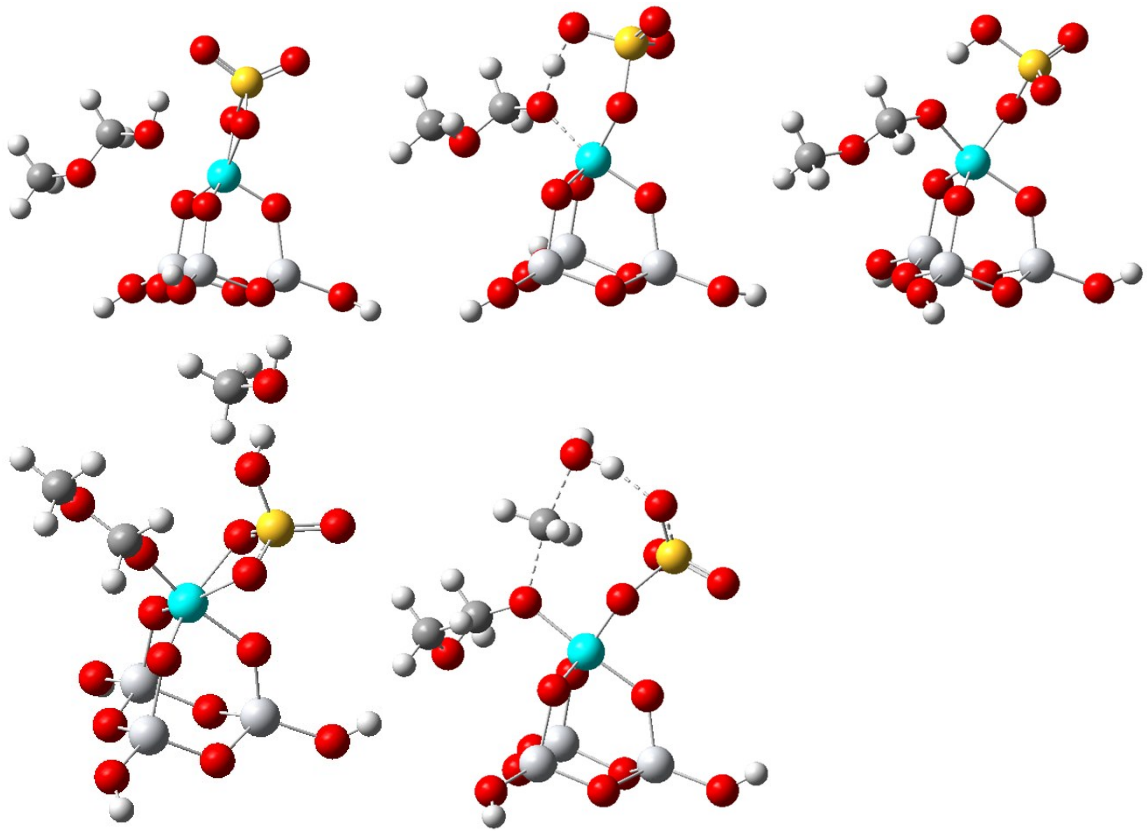


Figure 7: 1a-4a

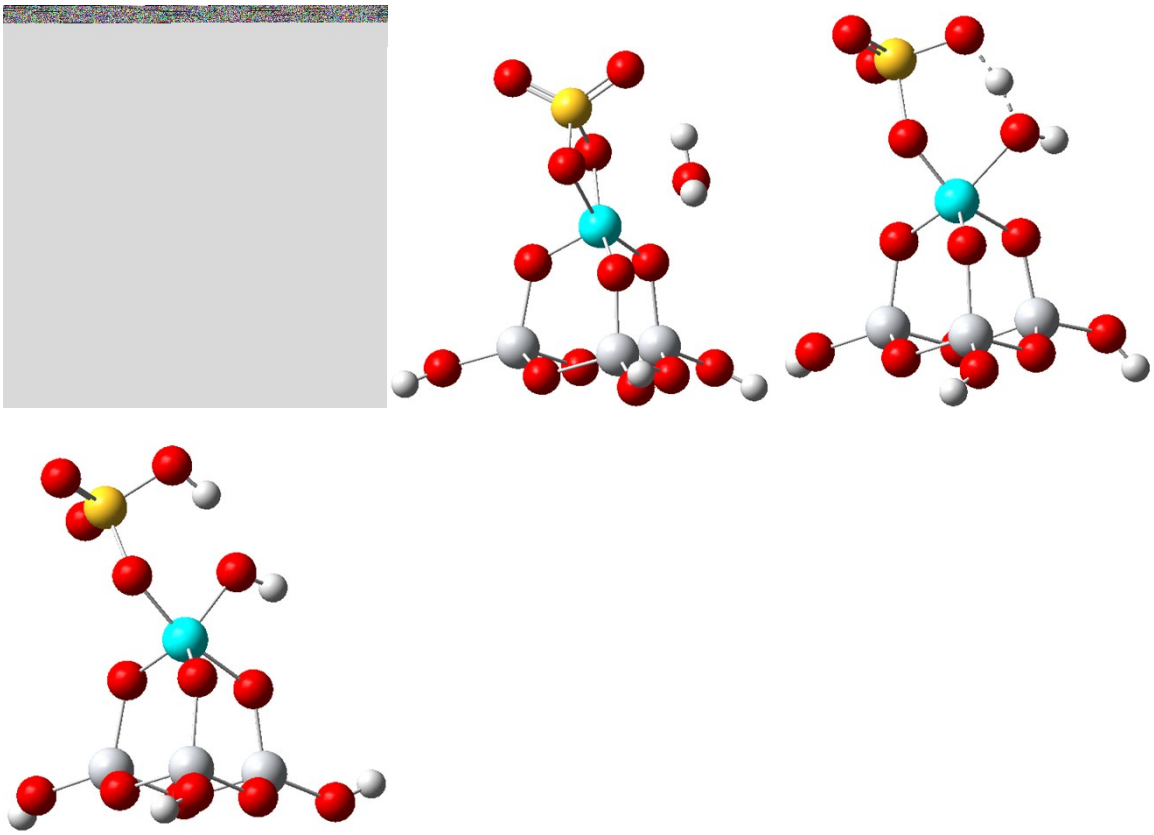


Figure 7: 1b-4b

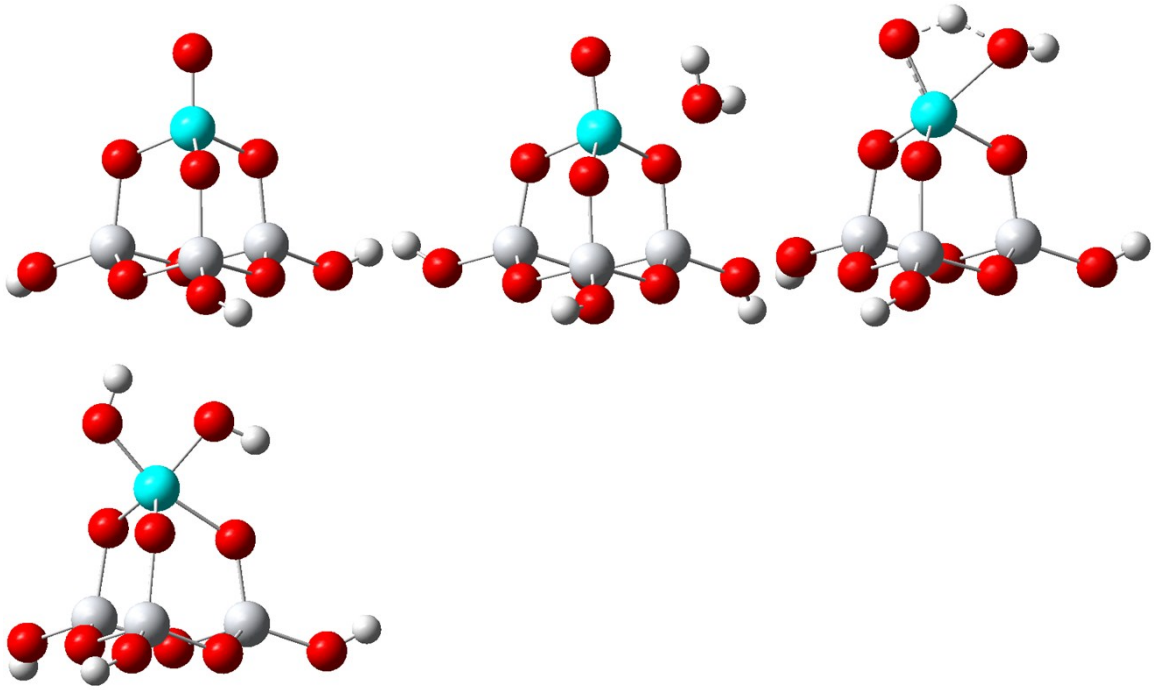


Figure S1: 1-6

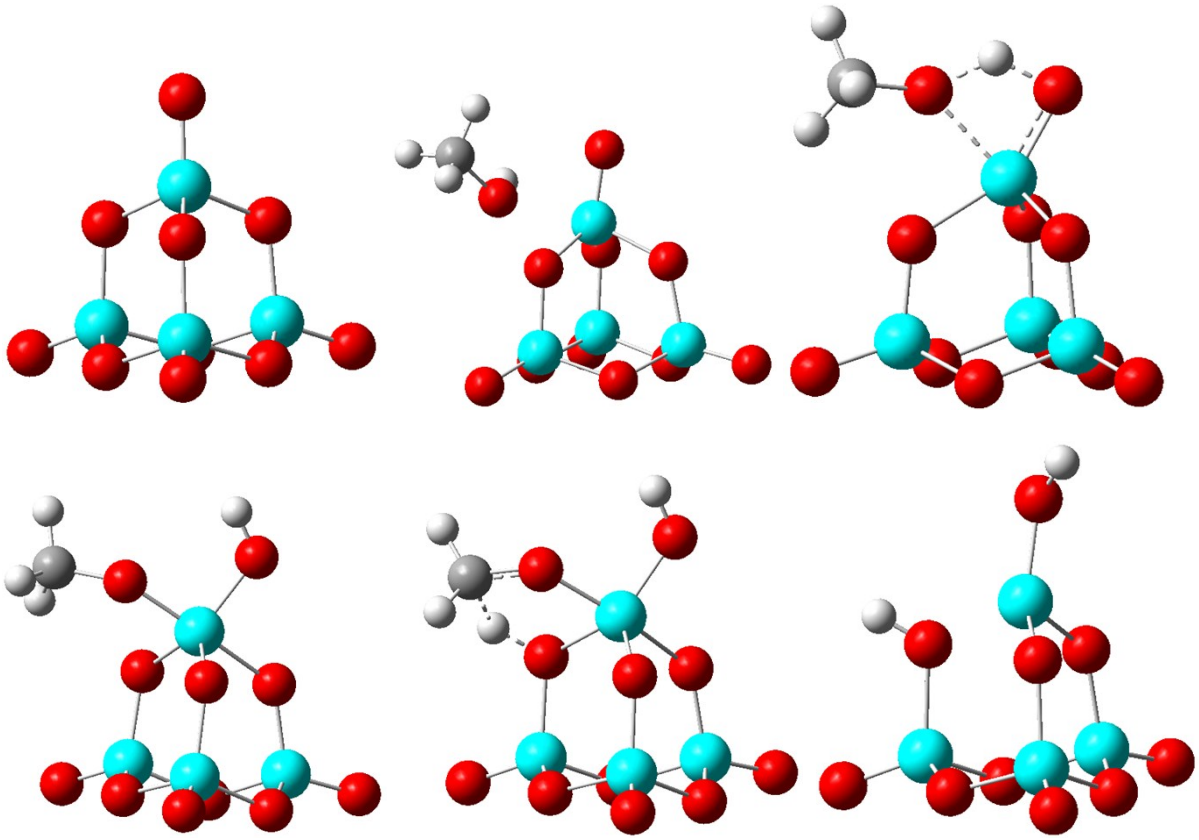
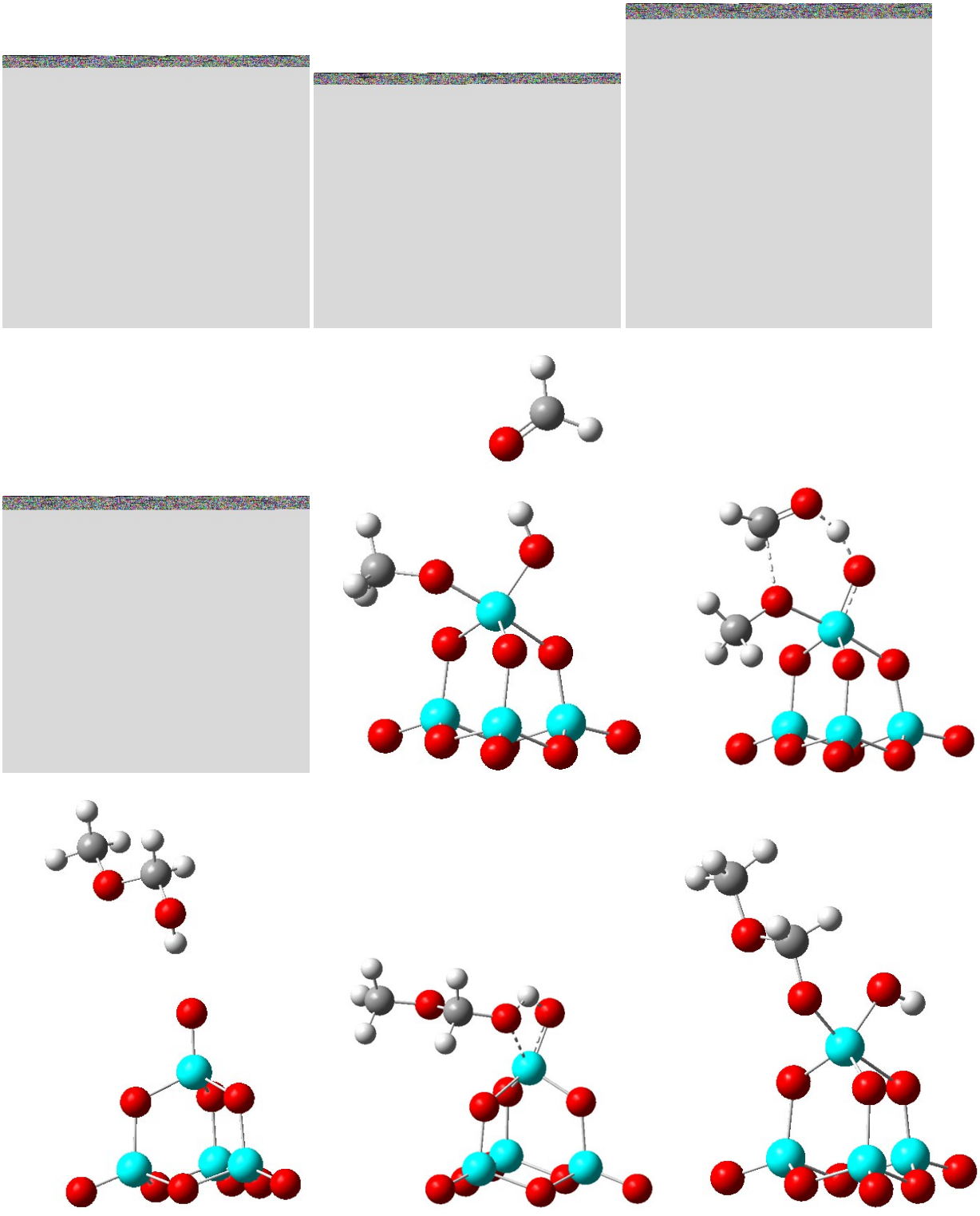


Figure S2: 1-11



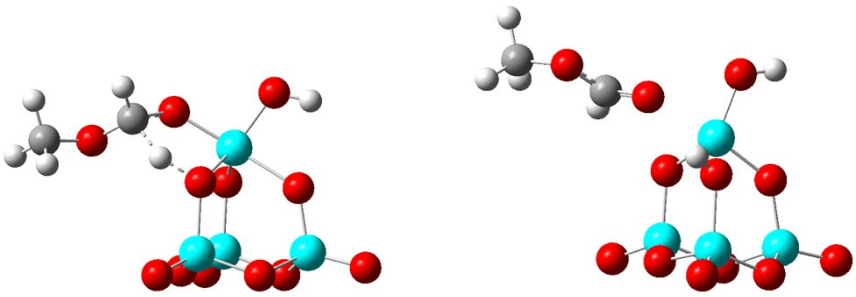


Figure S3: 1-8

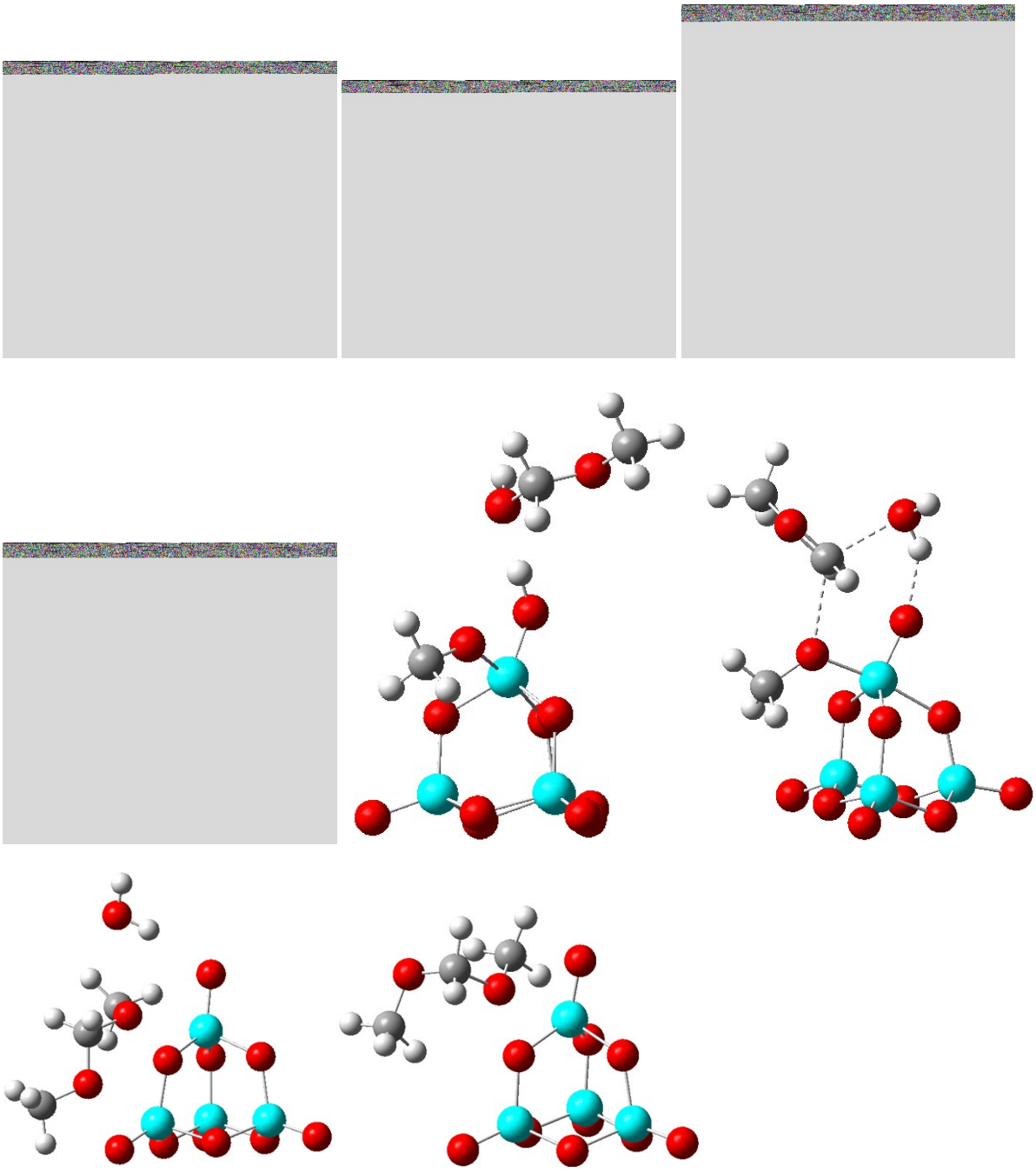


Figure S4: 1-8

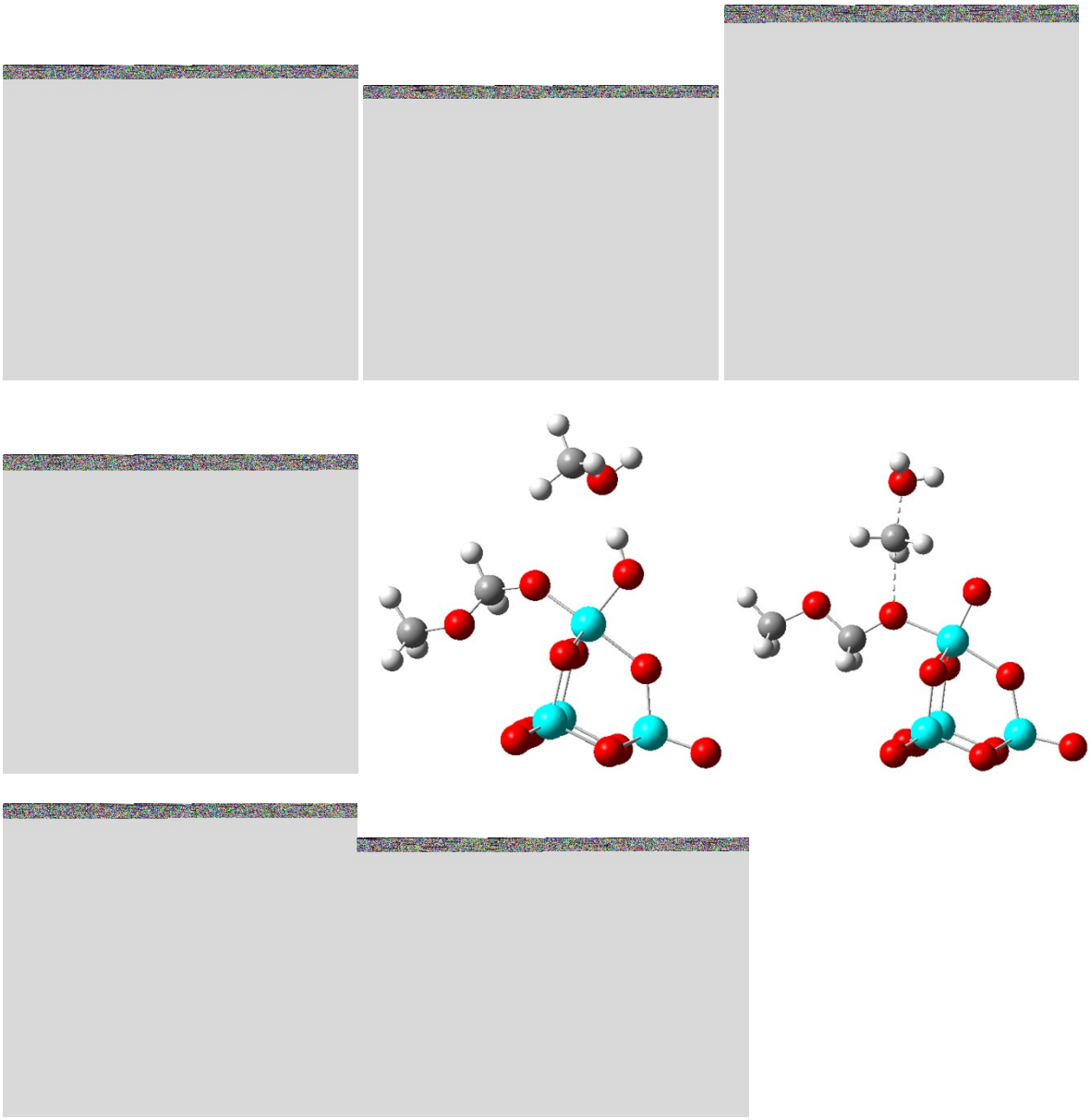
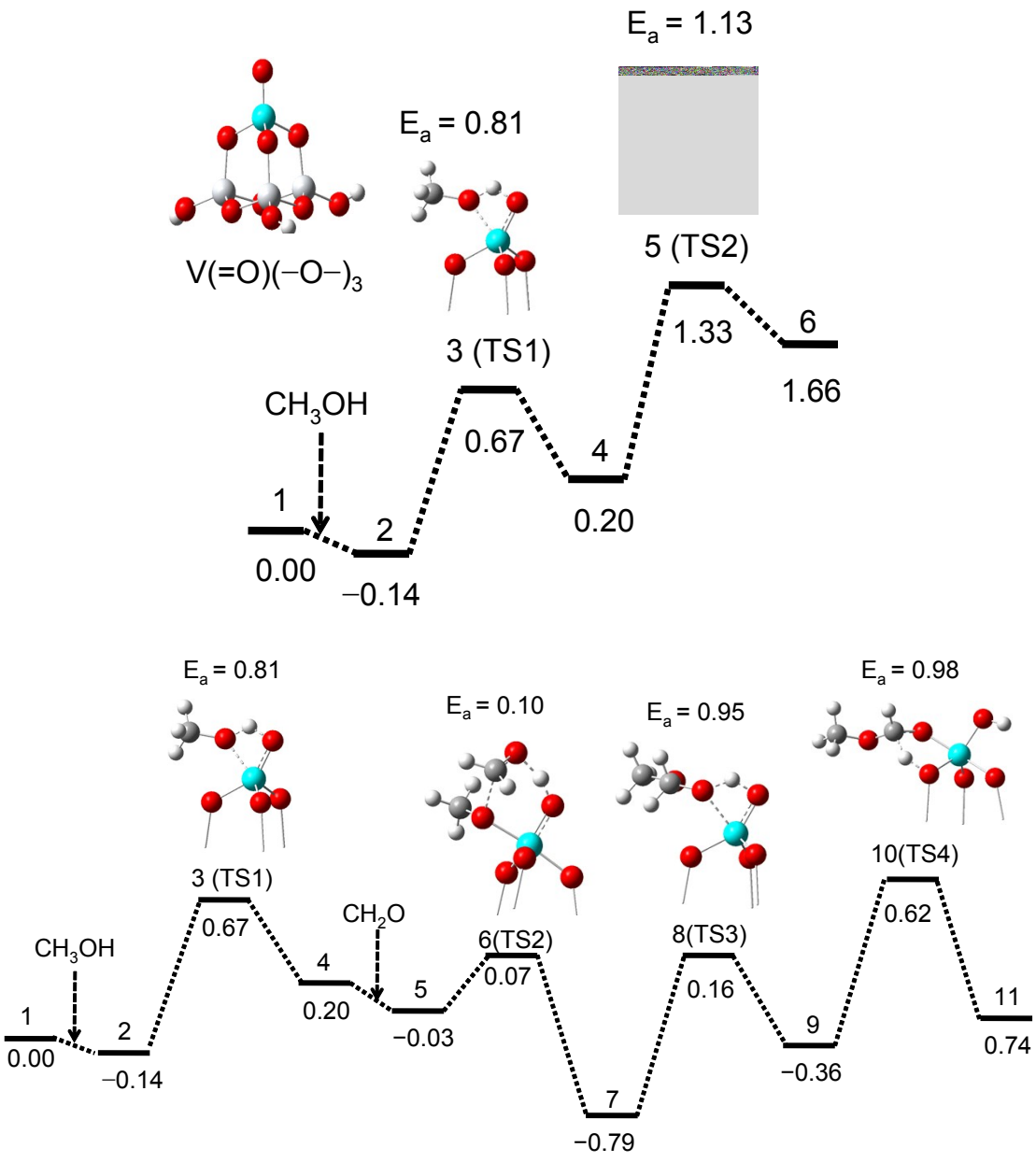


Figure S6. Potential Energy Surface and Reaction Network (E_{0K}, eV) for the Formation of FA, MF, and DMM with the $VTi_3O_7(OH)_3$ Cluster Model Calculated at the PBE Level.



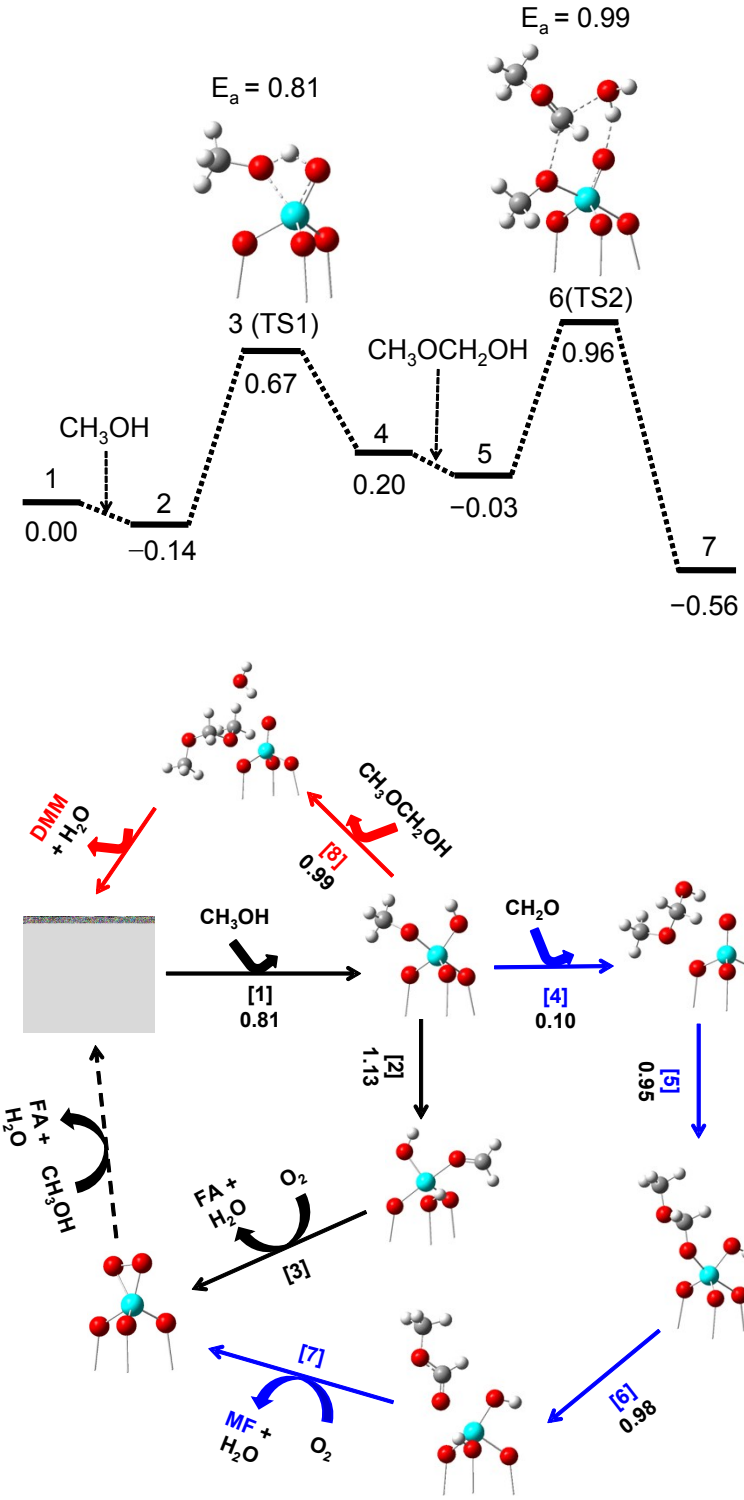
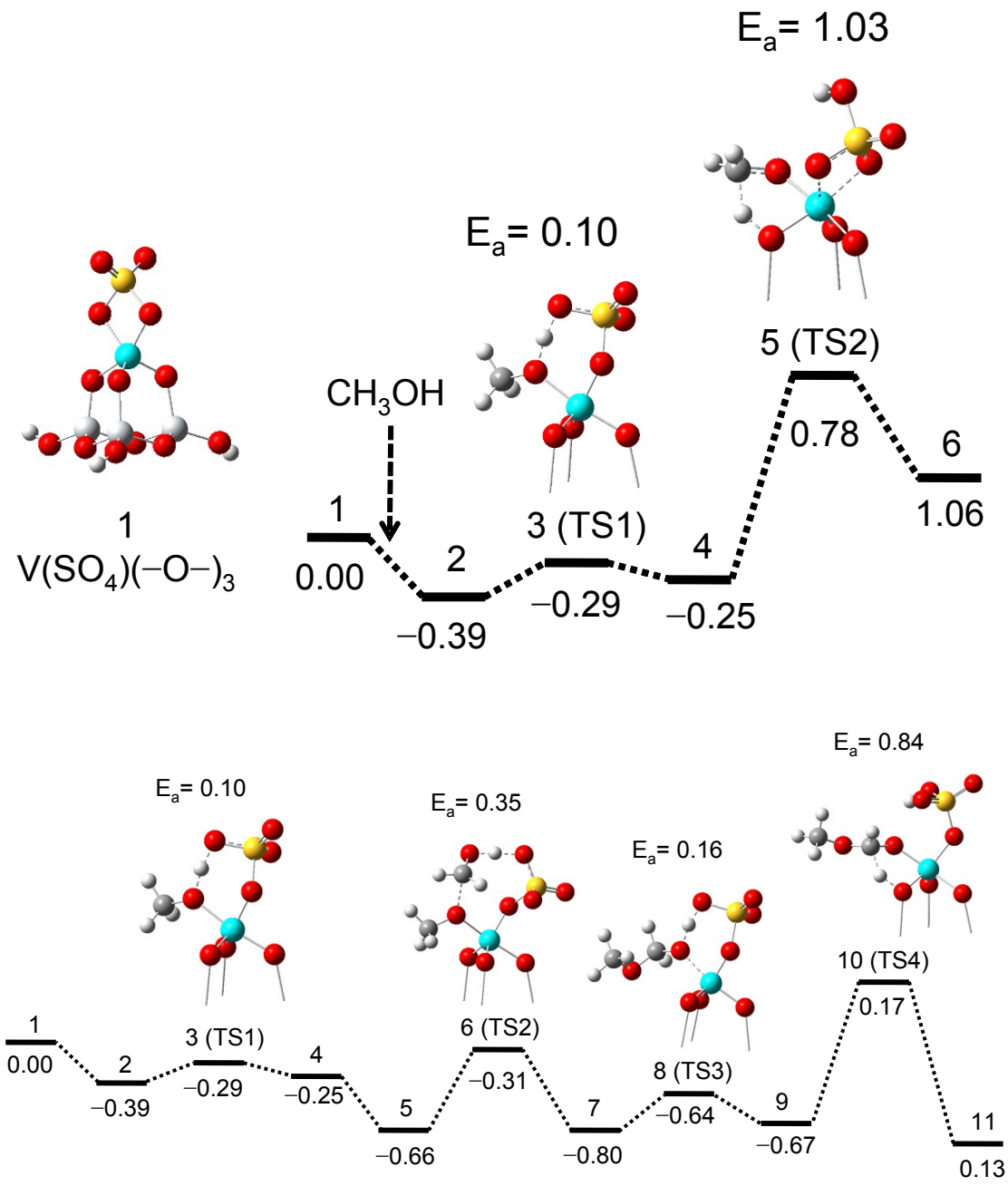
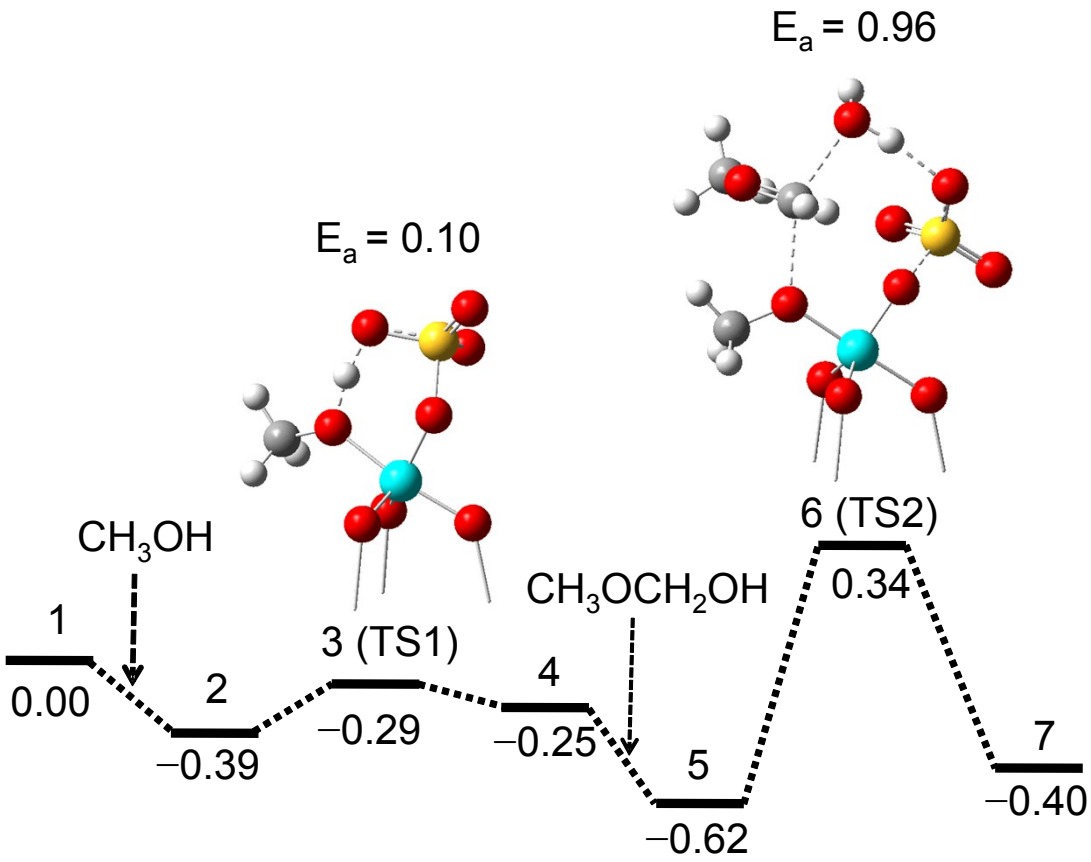

E_a = 0.99
E_a = 0.81
6(TS2)
3 (TS1)
CH3OCH2OH
0.96
0.67
CH3OH
4
5
1
0.20
−0.03
2
0.00
−0.14
7
−0.56
DMM + H2O
CH3OCH2OH
[8]
0.99
CH3OH
[1]
0.81
CH2O
[4]
0.10
[2]
1.13
[5]
0.95
FA + H2O
CH3OH
FA + H2O
O2
[3]
[7]
MF + H2O
O2
[6]
0.98

Figure S7. Potential Energy Surface and Reaction Network (E_{0K}, eV) for the Formation of FA, MF, and DMM with the $VTi_3O_6(SO_4)(OH)_3$ Cluster Model Calculated at the PBE Level.




E_a = 0.96
E_a = 0.10
CH_3OH
CH_3OCH_2OH
1
0.00
2
−0.39
3 (TS1)
−0.29
4
−0.25
5
−0.62
6 (TS2)
0.34
7
−0.40

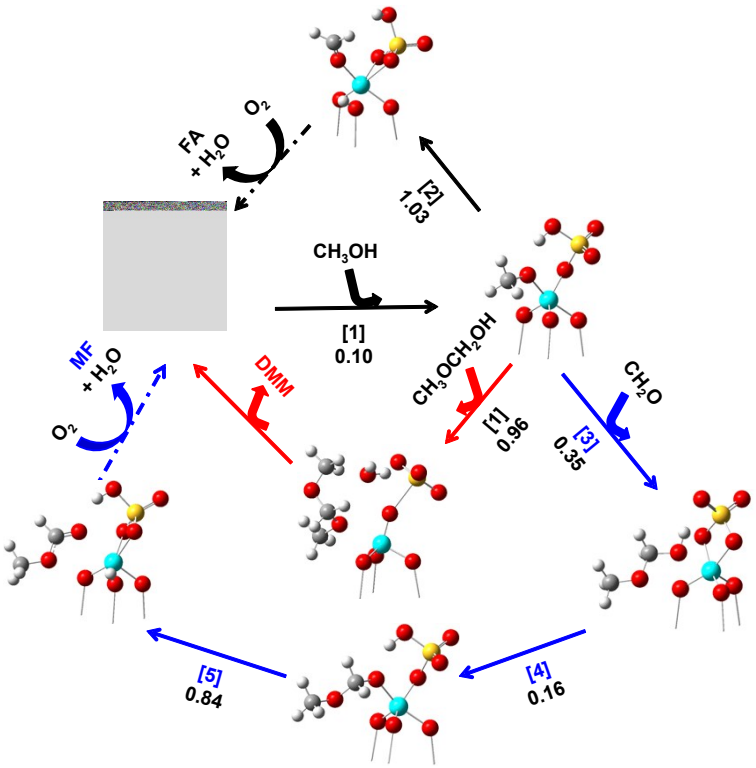
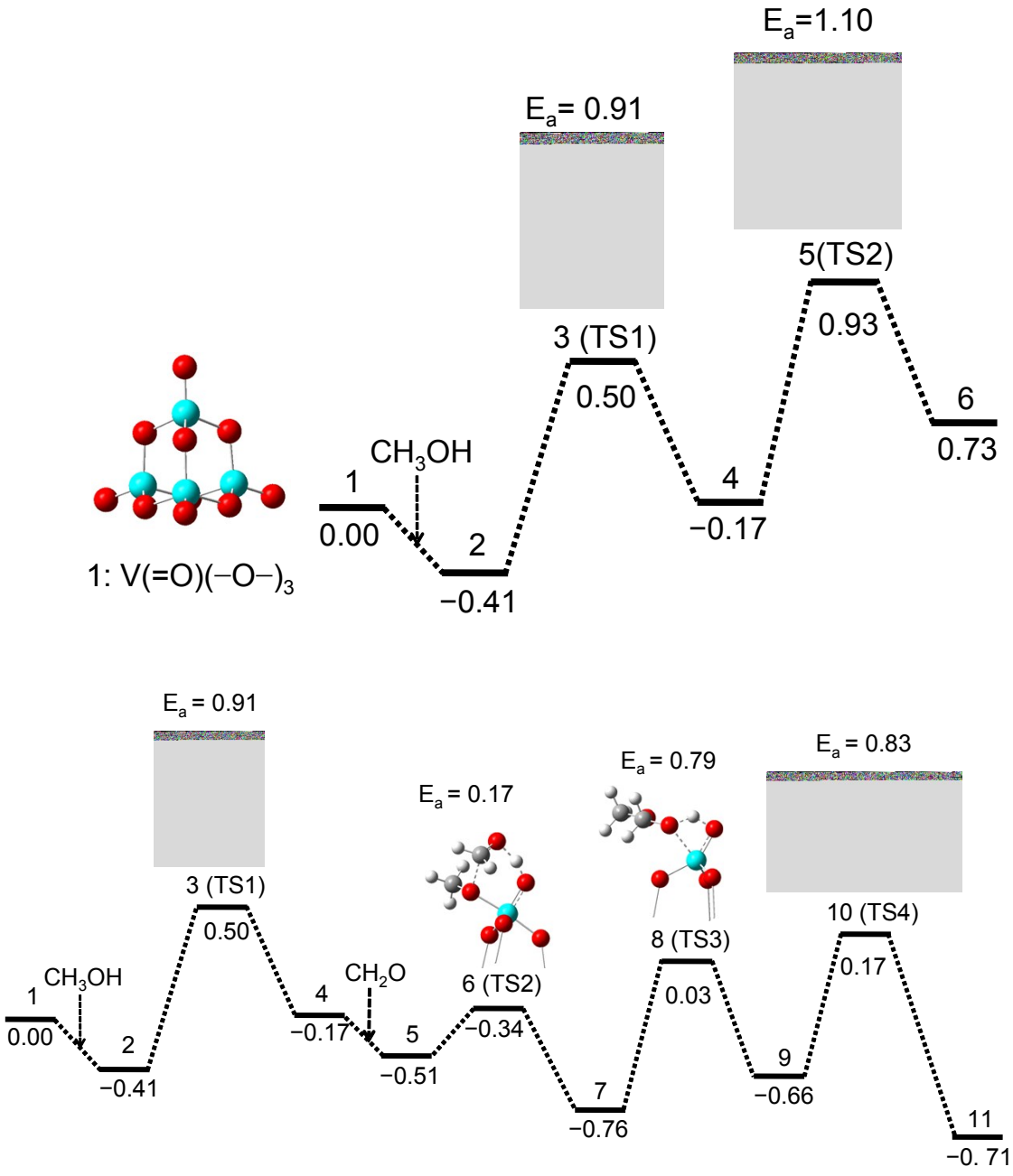
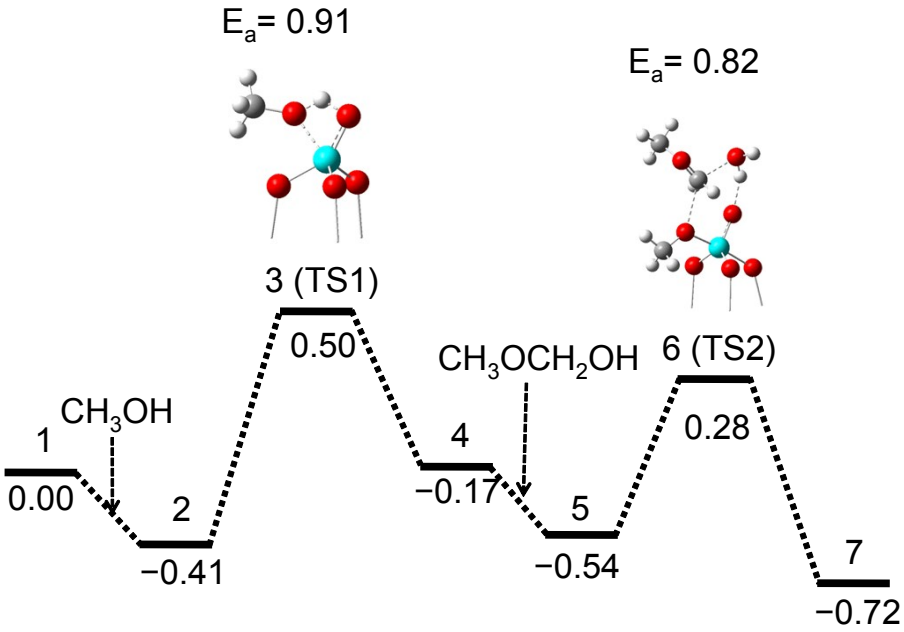
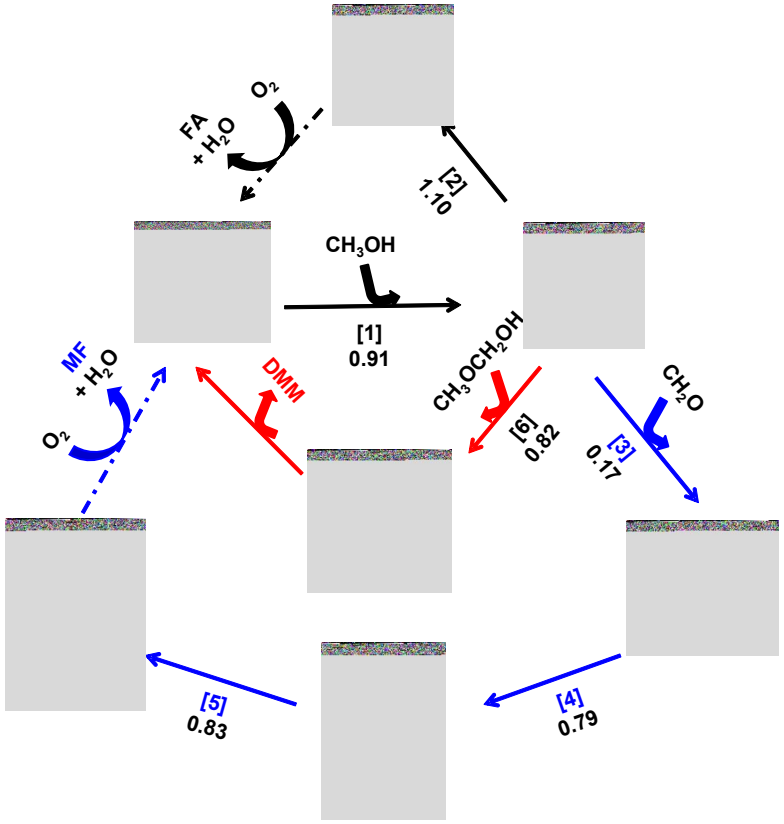

FA + H_2O
O_2
[2] 1.03
CH_3OH
[1] 0.10
MF + H_2O
O_2
DMM
CH_3OCH_2OH
[1] 0.96
CH_2O
[3] 0.35
[5] 0.84
[4] 0.16

Figure S8. Potential Energy Surface and Reaction Network (E_{0K}, eV) for the Formation of FA, MF, and DMM with the V_4O_{10} Cluster Model Calculated at the PBE Level.




Ea= 0.91
Ea= 0.82
3 (TS1)
0.50
CH3OCH2OH
6 (TS2)
CH3OH
1
0.00
2
−0.41
4
−0.17
5
−0.54
0.28
7
−0.72


O2
FA
+ H2O
[2]
1.10
CH3OH
[1]
0.91
MF
+ H2O
O2
DMM
CH3OCH2OH
[6]
0.82
CH2O
[3]
0.17
[5]
0.83
[4]
0.79

Section 3.

Table S1. Free Energy Barriers ($\Delta G^{\neq}$, eV) and Tunneling Cofficients (κ) of the Rate Determining Step (RDS) at Different Temperatures (T, °C) for the Formation of Formyldehyde (FA), Methyl Formate (MF), and Dimethoxymethane (DMM) over the $VTi_3O_7(OH)_3$ Cluster Model.

Temperature (T)	$\Delta G^{\neq}$			κ		
	FA[a]	**MF[b]**	**DMM[c]**	**FA[d]**	**MF[e]**	**DMM[f]**
100 °C	1.33	1.25	1.15	1.78	2.25	1.01
150 °C	1.34	1.26	1.17	1.60	1.98	1.01
200 °C	1.35	1.27	1.18	1.48	1.78	1.01
250 °C	1.36	1.27	1.20	1.40	1.64	1.01
300 °C	1.38	1.28	1.21	1.33	1.53	1.01

[a] Dehydrogenation of $CH_3O-(V^*)$

[b] Dehydrogenation of $CH_3OCH_2O-(V^*)$

[c] Dehydration of $CH_3O-(V^*)$ and physisorbed CH_3OCH_2OH

[d] $\nu_i = 1119\ i\ cm^{-1}$

[e] $\nu_i = 1422\ i\ cm^{-1}$

[f] $\nu_i = 148\ i\ cm^{-1}$

Table S2. Free Energy Barriers ($\Delta G^{\neq}$, eV) and Tunneling Cofficients (κ) of the Rate Determining Step (RDS) at Different Temperatures (T, °C) for the Formation of Formyldehyde (FA), Methyl Formate (MF), and Dimethoxymethane (DMM) over the $VTi_3O_6(SO_4)(OH)_3$ Cluster Model.

T	$\Delta G^{\neq}$			κ		
	FA[a]	**MF**[b]	**DMM**[c]	**FA**[d]	**MF**[e]	**DMM**[f]
100 °C	1.27	1.05	1.16	2.31	2.47	1.01
150 °C	1.28	1.06	1.18	2.02	2.15	1.01
200 °C	1.30	1.07	1.19	1.82	1.92	1.01
250 °C	1.32	1.08	1.21	1.67	1.75	1.01
300 °C	1.33	1.08	1.22	1.56	1.63	1.01

[a] Dehydrogenation of $CH_3O-(V^*)$

[b] Dehydrogenation of $CH_3OCH_2O-(V^*)$

[c] Dehydration of $CH_3O-(V^*)$ and physisorbed CH_3OCH_2OH

[d] $\nu_i = 1456\ i\ cm^{-1}$

[e] $\nu_i = 1542\ i\ cm^{-1}$

[f] $\nu_i = 147\ i\ cm^{-1}$

Table S3. Cartesian or Fractional Coordinates of the Molecular Cluster and Periodic Slab Models.

$VTi_3O_7(OH)_3$

O	-0.885132	-1.165285	1.416844
O	-1.584561	1.231879	0.000000
O	0.883324	1.068079	1.438941
O	-0.885132	-1.165285	-1.416844
O	1.567503	-1.298296	0.000000
O	-1.735127	1.312092	-3.053427
O	0.883324	1.068079	-1.438941
O	3.596272	1.032177	0.000000
V	-0.122387	-1.912423	0.000000
O	-1.735127	1.312092	3.053427
O	-0.217413	-3.485584	0.000000
TI	-0.885132	0.679062	-1.594703
TI	1.874420	0.498470	0.000000
TI	-0.885132	0.679062	1.594703
H	4.476163	0.643005	0.000000
H	-1.528074	1.609049	-3.944644
H	-1.528074	1.609049	3.944644

$VTi_3O_6(SO_4)(OH)_3$

O	-0.232613	0.001115	1.533887
O	-0.323968	-1.383329	-0.732639
O	-0.323920	1.382560	-0.734449
O	2.063483	-1.457080	0.813029
O	2.063605	1.457983	0.811270
O	2.110401	-3.046496	-1.790670
O	2.047421	-0.001070	-1.642164
O	2.110468	3.044344	-1.794197
V	-1.119518	0.000068	-0.094390
O	2.056816	0.001938	3.552290
TI	1.516721	0.001046	1.835487
TI	1.556113	1.591812	-0.899212
TI	1.555982	-1.592997	-0.897331
H	2.519773	3.897279	-1.614512
H	2.516844	-3.900605	-1.610102
H	1.642436	0.004119	4.421820
S	-3.803746	0.000021	0.018252
O	-4.531153	-1.275708	-0.003278
O	-2.619613	0.000921	1.126475
O	-4.531415	1.275570	-0.005082

O	-2.627534	-0.000702	-1.156354

$V_2Ti_2O_8(OH)_2$

O	-0.095834	-2.064198	0.005627
O	1.416330	-0.127385	-1.427913
O	-1.416103	0.004802	-1.424371
O	1.403453	-0.121036	1.440144
O	-1.429756	0.013863	1.410311
O	3.190630	1.935394	0.008058
O	0.110624	1.979651	-0.004378
O	-2.942296	2.288838	-0.028704
V	-0.056490	-1.125372	1.535199
V	-0.044923	-1.131412	-1.531473
O	-0.085925	-2.043238	-2.812673
O	-0.107005	-2.031347	2.820122
TI	-1.538925	1.168092	-0.007124
TI	1.646179	1.017895	0.003523
H	-3.896514	2.290727	0.095674
H	3.516488	2.840843	0.008069

V_4O_{10}

O	0.000000	2.016674	0.000000
O	-2.016674	0.000000	0.000000
O	0.000000	0.000000	-2.016674
O	0.000000	0.000000	2.016674
O	2.016674	0.000000	0.000000
O	-1.988639	-1.988639	1.988639
O	0.000000	-2.016674	0.000000
O	1.988639	-1.988639	-1.988639
V	-1.083915	-1.083915	1.083915
V	1.083915	1.083915	1.083915
V	-1.083915	1.083915	-1.083915
V	1.083915	-1.083915	-1.083915
O	-1.988639	1.988639	-1.988639
O	1.988639	1.988639	1.988639

V(=O)(−O−)$_3$ on anatase-TiO_2(001)

```
H  Ti  O  V
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H    Ti   O    V
1    16    35   1
Selective dynamics
Direct
  0.4050295625729172  0.9469327081002242  0.4425769305705037   T   T   T
  0.9984250385909624  0.9781673004578759  0.3414741430253860   T   T   T
```

0.2500657030223365	0.2500657030223365	0.1244398483281657	F	F	F
0.0000000000000000	0.2500657030223365	0.0197345742847261	F	F	F
0.2473354792171954	0.0008850797833775	0.2322118847263338	T	T	T
0.5049962672735714	0.9735305538266813	0.3385951567361414	T	T	T
0.7500657030223365	0.2500657030223365	0.1244398483281657	F	F	F
0.5000000000000000	0.2500657030223365	0.0197345742847261	F	F	F
0.7506732904483535	0.0014512739096848	0.2312642950064160	T	T	T
0.0000136043725922	0.5326987351428186	0.3307631229272215	T	T	T
0.2500657030223365	0.7500657030223365	0.1244398483281657	F	F	F
0.0000000000000000	0.7500657030223365	0.0197345742847261	F	F	F
0.2465697966316805	0.5020479398357910	0.2284457647536260	T	T	T
0.4943866963759455	0.5194664422686107	0.3297847915871683	T	T	T
0.7500657030223365	0.7500657030223365	0.1244398483281657	F	F	F
0.5000000000000000	0.7500657030223365	0.0197345742847261	F	F	F
0.7488538364841201	0.4970636246982189	0.2293993484982474	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2486463612770295	0.2478968938312958	0.2121813305688479	T	T	T
0.0000000000000000	0.2500657030223365	0.1047483626335719	F	F	F
0.2511525428043093	0.0080956025660348	0.3165380727697156	T	T	T
0.2500657030223365	0.0000000000000000	0.1441744226128918	F	F	F
0.0706558934484875	0.3823075327239252	0.3841574771410061	T	T	T
0.2500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.9959740888540800	0.9947853202525222	0.2525603566917952	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7483977593816761	0.2469700150698943	0.2109408387424357	T	T	T
0.5000000000000000	0.2500657030223365	0.1047483626335719	F	F	F
0.7490040424944605	0.0320680566740225	0.3241878489888118	T	T	T
0.7500657030223365	0.0000000000000000	0.1441744226128918	F	F	F
0.4236583131459670	0.3409071644419335	0.3742480902183762	T	T	T
0.7500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.5038115403762348	0.9904566805704029	0.2525306143487522	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2477972058744027	0.7529745668482773	0.2098950803364616	T	T	T
0.0000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.2482003850561259	0.5621394012462766	0.3089896456240269	T	T	T
0.2500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.9763502928378430	0.7534773024072025	0.3599073906952362	T	T	T
0.2500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.9975196665425077	0.4902850081863082	0.2464325385352192	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7495839109199427	0.7492389771759873	0.2123799655192752	T	T	T
0.5000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.7480622321128216	0.4906154038414490	0.3161337993770013	T	T	T
0.7500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.5177985489767036	0.7499039615390909	0.3576244529734796	T	T	T
0.7500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.4987309063076188	0.4882507989040044	0.2466670213055391	T	T	T
0.0729333641504356	0.0625557255940166	0.4115562661844636	T	T	T
0.2462159689272504	0.2965926131577449	0.4827465467949447	T	T	T
0.4297227421719989	0.0453355578847327	0.4168952421750090	T	T	T
0.2364803815541754	0.2357432418910989	0.4172552118390461	T	T	T

$V(SO_4)(-O-)_3$ on anatase-TiO_2(001)

```
H  S  V  O  Ti
1.00000000000000
```

```
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   28.7145000000000010
H  S  V  O  Ti
1  1   1  38  16
Selective dynamics
Direct
  0.4613558780251582  0.0691059806077034  0.3604188680508387   T   T   T
  0.2755429909572628  0.2572969761233369  0.4375959567801352   T   T   T
  0.1894055116079166  0.3012194755664336  0.3479510470533057   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.2493294433641736  0.2508492074487014  0.1713870964302237   T   T   T
  0.0000000000000000  0.2500657030223365  0.0846610597433326   F   F   F
  0.2637411004576719 -0.0097853130752336  0.2551880496697923   T   T   T
  0.2500657030223365  0.0000000000000000  0.1165264935833790   F   F   F
  0.0354101009162647  0.4599642301492397  0.3293746284261428   T   T   T
  0.2500657030223365  0.2500657030223365  0.0318654338400464   F   F   F
  0.0058468181969911  0.0062117120240995  0.2019448066979419   T   T   T
  0.5000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.7481549476488154  0.2501907413833890  0.1702224297060769   T   T   T
  0.5000000000000000  0.2500657030223365  0.0846610597433326   F   F   F
  0.7541385378527908  0.0237980199553310  0.2561416312566901   T   T   T
  0.7500657030223365  0.0000000000000000  0.1165264935833790   F   F   F
  0.3794064855516386  0.3615578905759642  0.3186235454403687   T   T   T
  0.7500657030223365  0.2500657030223365  0.0318654338400464   F   F   F
  0.5071520805757471 -0.0021719953309866  0.1999485751311829   T   T   T
  0.0000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.2489693766157608  0.7500564861376190  0.1706245596352007   T   T   T
  0.0000000000000000  0.7500657030223365  0.0846610597433326   F   F   F
  0.2346090836013719  0.5208202888322386  0.2529399455913930   T   T   T
  0.2500657030223365  0.5000000000000000  0.1165264935833790   F   F   F
  0.9750123397367910  0.7682425610204660  0.2864494465890680   T   T   T
  0.2500657030223365  0.7500657030223365  0.0318654338400464   F   F   F
  0.9878485525414883  0.5018287384312153  0.2008246484776218   T   T   T
  0.5000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.7484528224537157  0.7490683553197611  0.1718551870602716   T   T   T
  0.5000000000000000  0.7500657030223365  0.0846610597433326   F   F   F
  0.7425257379895437  0.4689496861213228  0.2591786160093958   T   T   T
  0.7500657030223365  0.5000000000000000  0.1165264935833790   F   F   F
  0.5126375834495164  0.7255996477587451  0.2865930666505898   T   T   T
  0.7500657030223365  0.7500657030223365  0.0318654338400464   F   F   F
  0.4940622593425497  0.4938226409473950  0.2028366662041064   T   T   T
  0.0681218267792470  0.1298553813219254  0.3202020358432849   T   T   T
  0.5203959988617752  0.0394961934838065  0.3303756100849408   T   T   T
  0.1781620799524705  0.4059165786318849  0.4074157494228562   T   T   T
  0.2893484161061315  0.1333063129931771  0.3926944939385725   T   T   T
  0.4470082955044785  0.3162387650395176  0.4509851715250635   T   T   T
  0.1573916773492804  0.1837618718035906  0.4709397016784919   T   T   T
  0.0068183376395772 -0.0077200212167484  0.2697594883310808   T   T   T
  0.2500657030223365  0.2500657030223365  0.1005763638579822   F   F   F
  0.0000000000000000  0.2500657030223365  0.0159501297253968   F   F   F
  0.2610690282313149  0.0003265008312072  0.1863156745991563   T   T   T
  0.5118229985765778  0.9601965219728487  0.2733984948489510   T   T   T
  0.7500657030223365  0.2500657030223365  0.1005763638579822   F   F   F
  0.5000000000000000  0.2500657030223365  0.0159501297253968   F   F   F
  0.7525259344155740  0.0006332980603238  0.1860851855736239   T   T   T
  0.9859241408204708  0.5421983232466685  0.2710298850213065   T   T   T
```

```
0.2500657030223365  0.7500657030223365  0.1005763638579822   F   F   F
0.0000000000000000  0.7500657030223365  0.0159501297253968   F   F   F
0.2378047931539811  0.5006695599481330  0.1858069247968654   T   T   T
0.4888699670032912  0.5046251014534632  0.2702160175608787   T   T   T
0.7500657030223365  0.7500657030223365  0.1005763638579822   F   F   F
0.5000000000000000  0.7500657030223365  0.0159501297253968   F   F   F
0.7431064900375658  0.4959327204354873  0.1856263142199517   T   T   T
```

Table S4. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 1a.

1a.

O	-0.885132	-1.165285	1.416844
O	-1.584561	1.231879	0.000000
O	0.883324	1.068079	1.438941
O	-0.885132	-1.165285	-1.416844
O	1.567503	-1.298296	0.000000
O	-1.735127	1.312092	-3.053427
O	0.883324	1.068079	-1.438941
O	3.596272	1.032177	0.000000
V	-0.122387	-1.912423	0.000000
O	-1.735127	1.312092	3.053427
O	-0.217413	-3.485584	0.000000
TI	-0.885132	0.679062	-1.594703
TI	1.874420	0.498470	0.000000
TI	-0.885132	0.679062	1.594703
H	4.476163	0.643005	0.000000
H	-1.528074	1.609049	-3.944644
H	-1.528074	1.609049	3.944644

2a.

O	-0.490860	1.647806	-0.389881
O	1.902330	0.495591	-1.475042
O	1.710583	1.050747	1.322338
O	-0.529083	-1.022930	-1.310871
O	-0.695530	-0.483744	1.456310
O	1.951386	-2.339533	-2.609858
O	1.662544	-1.666986	0.386332
O	1.588068	-1.185677	3.418719
V	-1.271779	0.079559	-0.143312
O	2.022154	3.428740	-0.617730
O	-2.850134	0.144635	-0.257017
TI	1.315581	-1.228421	-1.343909
TI	1.096927	-0.618914	1.782683
TI	1.359034	1.785024	-0.300248
H	1.196275	-1.568643	4.209778
H	2.158765	-3.271049	-2.731547
H	2.413160	4.166953	-0.140634
C	-6.496770	0.503478	-0.108075
H	-7.545966	0.218528	0.040228
H	-6.387868	0.911698	-1.127476
H	-6.245443	1.295424	0.618318
O	-5.715012	-0.667790	0.085548
H	-4.782873	-0.439712	-0.042399

3a.

O	-0.447240	-1.242442	1.319434
O	-0.215264	-1.141926	-1.431752
O	-1.337894	0.915297	-0.189833
O	2.160989	-0.884945	0.140911
O	0.904104	1.279758	1.517234
O	2.490197	-0.909986	-2.933255
O	1.175709	1.340387	-1.374785
O	-0.229125	3.743921	-0.020003
V	-1.377256	-0.984780	-0.126454
O	-2.308198	-2.381829	-0.378182
O	2.009433	-1.001102	3.202083
C	-4.171351	0.537463	-0.150974
H	-5.183130	0.367072	0.245386
H	-4.230812	0.634077	-1.246602
H	-3.774072	1.470467	0.267919
O	-3.352133	-0.553018	0.233354
H	-3.262208	-1.733932	-0.173132
TI	1.506812	-0.432126	-1.494977
TI	1.227848	-0.470415	1.664508
TI	0.078878	1.956492	-0.020990
H	-0.999069	4.310398	-0.128294
H	2.259158	-0.586939	4.034245
H	3.192656	-1.535831	-3.134770

4a.

O	1.281442	0.696626	-0.932264
O	-0.137841	-1.437412	-1.013550
O	0.715950	-0.938100	1.450012
O	-1.493416	0.941408	-1.490527
O	-0.538212	1.656151	1.111791
O	-3.006779	-1.769538	-1.948674
O	-2.093399	-0.709995	0.853908
O	-1.247646	0.084110	3.649042
V	1.476522	-0.879618	-0.100105
O	2.124143	-2.413852	-0.798520
O	0.118174	3.520666	-1.266066
C	4.141452	0.360583	-0.163417
H	4.694210	-0.245791	-0.899472
H	4.831480	0.682099	0.629139
H	3.714826	1.240436	-0.672127
O	3.101506	-0.390594	0.414974
H	3.048481	-2.575036	-0.562897
TI	-1.776718	-0.841897	-0.982028
TI	-0.840901	0.053780	1.887306
TI	-0.161946	1.823141	-0.694854
H	-0.293703	4.087739	-1.925658
H	-2.953859	-2.556976	-2.499604

H	-1.291096	0.748961	4.343188

5a.

O	-0.498428	1.710333	-0.341203
O	-0.551148	-0.535688	-1.581374
O	0.460231	-0.861875	0.837584
O	-3.027068	0.534761	-0.917771
O	-2.004267	0.372378	1.747255
O	-2.906642	-1.965727	-2.831361
O	-2.104678	-2.016204	0.209061
O	-1.180270	-2.265217	3.082549
V	0.697901	0.372883	-0.358040
O	1.881499	0.097926	-1.644604
O	-3.025097	3.105849	0.718194
C	2.113203	2.759088	0.583062
H	2.795956	3.001595	-0.245943
H	2.592339	3.021059	1.537394
H	1.179535	3.332373	0.465463
O	1.817685	1.382132	0.583592
H	2.805420	0.380494	-1.465963
C	5.156664	0.309975	-0.035598
H	4.412171	0.351323	0.774810
H	6.059979	0.883366	0.249221
O	4.538434	0.881077	-1.165677
H	5.125760	0.761711	-1.925160
TI	-2.188922	-1.077055	-1.409374
TI	-2.214382	1.530864	0.315670
TI	-1.234958	-1.253897	1.578656
H	-2.543364	-2.201411	-3.690883
H	-1.455818	-2.151524	3.997147
H	-3.825005	3.539106	0.404258
C	6.158166	-1.681556	0.730342
H	5.494711	-1.758493	1.607991
H	6.406002	-2.687472	0.376853
H	7.085950	-1.160455	1.024007
O	5.510775	-1.016129	-0.347505

6a.

O	-0.076965	-0.563985	-1.523971
O	0.698030	1.683167	-0.423244
O	-0.225187	0.134720	1.481139
O	2.728276	0.092207	-1.465049
O	1.682829	-1.764604	0.425833
O	3.391846	3.046513	-0.611027
O	2.579107	0.762484	1.406217
O	1.633303	-1.293493	3.468387
V	-0.818893	0.407674	-0.197219

O	-1.926435	1.555938	-0.493967
O	1.915192	-2.676539	-2.505973
C	-1.840864	-2.265723	0.394425
H	-2.773333	-2.850578	0.443689
H	-1.341697	-2.319228	1.377215
H	-1.179955	-2.727890	-0.357856
O	-2.134811	-0.934351	0.051026
C	-4.243265	0.283236	0.323676
O	-4.414569	2.403410	-0.113552
H	-3.447367	2.373471	-0.340178
H	-4.485063	2.987607	0.653265
H	-3.764579	0.297294	-0.646734
H	-3.699546	0.516849	1.230655
TI	1.600642	-1.298608	-1.348775
TI	1.450943	-0.572523	1.799319
TI	2.415495	1.525559	-0.300789
H	3.106348	3.935123	-0.844128
H	2.223523	-1.080884	4.197657
H	2.685330	-2.911391	-3.032382
C	-6.148641	-0.610857	-0.712123
H	-5.463894	-1.046125	-1.448055
H	-6.889043	-1.341655	-0.380693
H	-6.630313	0.292373	-1.100266
O	-5.398743	-0.237823	0.485853

7a.

O	0.111955	0.821694	1.475731
O	-0.761756	-1.817644	0.656065
O	-2.648244	0.245715	1.229625
O	0.503964	-0.170188	-1.356861
O	-1.221326	1.783703	-0.660734
O	-0.332725	-3.020256	-2.131033
O	-2.278669	-0.700717	-1.489133
O	-4.273606	1.602702	-1.011965
V	0.448631	1.220963	-0.234090
O	-1.126658	-1.030855	3.594608
O	1.388938	2.464620	-0.536847
TI	-0.709598	-1.544849	-1.152463
TI	-2.728986	0.800401	-0.522709
TI	-1.119983	-0.493826	1.868071
H	-4.548458	2.462031	-1.346191
H	-0.730164	-3.501909	-2.862769
H	-1.694523	-0.939147	4.365546
C	3.500000	-0.314382	-0.544844
H	4.276195	0.446278	-0.690631
H	2.905237	-0.463667	-1.455052
C	3.319561	-2.648148	-0.157710

H	3.970098	-3.499305	0.068769
H	2.531323	-2.580180	0.606456
H	2.856916	-2.797090	-1.147130
C	3.214634	0.653672	1.621225
H	2.423197	0.950917	2.313746
H	3.834002	-0.130743	2.073221
H	3.836744	1.519663	1.356130
O	4.151260	-1.488066	-0.155869
O	2.562556	0.138212	0.443049
O	4.224327	3.006779	-0.777573
H	4.451644	3.877584	-1.121295
H	3.252425	2.982973	-0.765020

8a.

O	-0.143444	-1.711760	0.257655
O	0.304053	0.713223	1.770791
O	2.496789	-0.885370	0.889818
O	-0.641224	0.997482	-0.948572
O	1.406339	-0.632663	-1.707685
O	-0.287559	3.535631	0.732280
O	2.019844	1.727911	-0.266102
O	4.384475	0.074479	-1.346559
V	-0.336996	-0.746219	-1.239332
O	0.736275	-1.970093	3.189075
O	-1.080851	-1.424518	-2.455713
TI	0.320486	1.871869	0.355529
TI	2.708705	0.069769	-0.667187
TI	0.852760	-1.028113	1.648255
H	4.822235	-0.225093	-2.149187
H	0.060350	4.432332	0.724762
H	1.300428	-2.547658	3.711797
C	-3.652365	0.080741	-0.973933
H	-4.086310	-0.453326	-1.830619
H	-3.068755	0.951479	-1.300672
C	-4.377566	1.377303	0.872462
H	-5.310449	1.646229	1.378719
H	-3.684245	0.926511	1.597254
H	-3.918084	2.284156	0.446263
C	-3.247001	-2.071473	-0.035760
H	-2.476870	-2.617060	0.515612
H	-4.162034	-1.995822	0.564644
H	-3.462800	-2.589014	-0.982931
O	-4.726474	0.454334	-0.160220
O	-2.718713	-0.761990	-0.298861

1b.

```
H  Ti  O  V
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H    Ti   O    V
1    16    35   1
Selective dynamics
Direct
  0.4050295625729172  0.9469327081002242  0.4425769305705037   T   T   T
  0.9984250385909624  0.9781673004578759  0.3414741430253860   T   T   T
  0.2500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
  0.2473354792171954  0.0008850797833775  0.2322118847263338   T   T   T
  0.5049962672735714  0.9735305538266813  0.3385951567361414   T   T   T
  0.7500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
  0.7506732904483535  0.0014512739096848  0.2312642950064160   T   T   T
  0.0000136043725922  0.5326987351428186  0.3307631229272215   T   T   T
  0.2500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.2465697966316805  0.5020479398357910  0.2284457647536260   T   T   T
  0.4943866963759455  0.5194664422686107  0.3297847915871683   T   T   T
  0.7500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.7488538364841201  0.4970636246982189  0.2293993484982474   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.2486463612770295  0.2478968938312958  0.2121813305688479   T   T   T
  0.0000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.2511525428043093  0.0080956025660348  0.3165380727697156   T   T   T
  0.2500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.0706558934484875  0.3823075327239252  0.3841574771410061   T   T   T
  0.2500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
  0.9959740888540800  0.9947853202525222  0.2525603566917952   T   T   T
  0.5000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.7483977593816761  0.2469700150698943  0.2109408387424357   T   T   T
  0.5000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.7490040424944605  0.0320680566740225  0.3241878489888118   T   T   T
  0.7500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.4236583131459670  0.3409071644419335  0.3742480902183762   T   T   T
  0.7500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
  0.5038115403762348  0.9904566805704029  0.2525306143487522   T   T   T
  0.0000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.2477972058744027  0.7529745668482773  0.2098950803364616   T   T   T
  0.0000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
  0.2482003850561259  0.5621394012462766  0.3089896456240269   T   T   T
  0.2500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
  0.9763502928378430  0.7534773024072025  0.3599073906952362   T   T   T
  0.2500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
  0.9975196665425077  0.4902850081863082  0.2464325385352192   T   T   T
  0.5000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.7495839109199427  0.7492389771759873  0.2123799655192752   T   T   T
  0.5000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
  0.7480622321128216  0.4906154038414490  0.3161337993770013   T   T   T
  0.7500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
  0.5177985489767036  0.7499039615390909  0.3576244529734796   T   T   T
  0.7500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
```

```
  0.4987309063076188  0.4882507989040044  0.2466670213055391   T   T   T
  0.0729333641504356  0.0625557255940166  0.4115562661844636   T   T   T
  0.2462159689272504  0.2965926131577449  0.4827465467949447   T   T   T
  0.4297227421719989  0.0453355578847327  0.4168952421750090   T   T   T
  0.2364803815541754  0.2357432418910989  0.4172552118390461   T   T   T
```

2b.

```
H  C  V  O  Ti
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H  C  V  O  Ti
5   1  1  36  16
Selective dynamics
Direct
  0.4021650417925065 -0.0555029365234857  0.4426074853221137    T   T   T
  0.2053136526824790  0.8723790692988502  0.5547977657687174   T   T   T
  0.1950218055726342  0.7747409744182425  0.4851370962237689   T   T   T
  0.3949485445177621  0.7627847514507866  0.5273587658083839   T   T   T
  0.2167545684172112  0.5026976871610860  0.5337473535513794   T   T   T
  0.2494191639992666  0.7593796805949922  0.5291658759230324   T   T   T
  0.2375688565403317  0.2350468109027780  0.4169820333737184   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.2490834818351992  0.2480040087209304  0.2122994622105073   T   T   T
  0.0000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.2510269548929346  0.0061705618490033  0.3165278254398524   T   T   T
  0.2500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.0728008949706867  0.3826985067684923  0.3844860477957941   T   T   T
  0.2500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
 -0.0040836527067209 -0.0048280321152455  0.2526516998935281   T   T   T
  0.5000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.7487378583845521  0.2471208582420143  0.2109854145747030   T   T   T
  0.5000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.7490280433217932  0.0311954981472891  0.3243410587783570   T   T   T
  0.7500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.4241233122671250  0.3373400135415947  0.3735925325233019   T   T   T
  0.7500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
  0.5039328452888746 -0.0087171717955330  0.2526023382720368   T   T   T
  0.0000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.2483172810067082  0.7529019020372598  0.2100120935072158   T   T   T
  0.0000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
  0.2487157697722905  0.5605270957006897  0.3090985625776921   T   T   T
  0.2500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
 -0.0233014323431504  0.7526774882301887  0.3599820790978591   T   T   T
  0.2500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
 -0.0021511891162714  0.4909921941293997  0.2464610656839382   T   T   T
  0.5000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.7500004232582755  0.7493155744658831  0.2125112214544458   T   T   T
  0.5000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
  0.7487522162608020  0.4888735829399775  0.3163215859139789   T   T   T
  0.7500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
  0.5179533215313981  0.7485141374390253  0.3573133921886397   T   T   T
  0.7500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
  0.4993902778698655  0.4887379951715882  0.2467278393388927   T   T   T
  0.0731701301616822  0.0632638065060983  0.4113166838186361   T   T   T
```

```
  0.2491384976448501  0.2978973064176120  0.4825986046164072   T   T   T
  0.4285017878778895  0.0428572658906787  0.4169554616401371   T   T   T
  0.1857671520580378  0.6055617977982075  0.5568934396975650   T   T   T
 -0.0016921842687242 -0.0225645436385349  0.3413324083541658   T   T   T
  0.2500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
  0.2473846155267213  0.0008818502423341  0.2321900256299738   T   T   T
  0.5047797206835437 -0.0273738292239092  0.3387648556787201   T   T   T
  0.7500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
  0.7504414043547974  0.0016056531863966  0.2312458885580972   T   T   T
  0.0005183951857772  0.5321685199906346  0.3308557586832640   T   T   T
  0.2500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.2469173075284361  0.5020879002072062  0.2284251267488694   T   T   T
  0.4953078925443935  0.5180538941929892  0.3296700900194969   T   T   T
  0.7500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.7493846808492401  0.4971747222217510  0.2292865129338474   T   T   T
```

3b.

```
H    C    V    O    Ti
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H    C    V    O    Ti
5    1     1    36    16
Selective dynamics
Direct
  0.4504435606355318  0.0761921862541749  0.4453254368864612   T   T   T
  0.1003326978082529  0.6795115616287047  0.4917797796768763   T   T   T
  0.3310223664153972  0.6450877925805090  0.5028350998338791   T   T   T
  0.1814732718409558  0.6309695446827791  0.5624032501049305   T   T   T
  0.2627024749890881  0.2877521481555224  0.5158662784343785   T   T   T
  0.1982245871041008  0.6037958174532486  0.5161454050049613   T   T   T
  0.1991862837282144  0.2921500403024724  0.4296927895006175   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.2485603607470613  0.2501377096848660  0.2120168327238278   T   T   T
  0.0000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.2627661603263470  0.9859145207559215  0.3155882232650559   T   T   T
  0.2500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.0412149297477185  0.4620808026417233  0.4083372188924411   T   T   T
  0.2500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
  0.0043278808337471  0.0044958137432496  0.2496964411849011   T   T   T
  0.5000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.7483939897999317  0.2496118192979998  0.2105092861554326   T   T   T
  0.5000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.7518100060175729  0.0220090738330343  0.3173092439129008   T   T   T
  0.7500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.3879773413390202  0.3576174786451494  0.3924997113659831   T   T   T
  0.7500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
  0.5061650744761939  0.9975149212611903  0.2476357803219697   T   T   T
  0.0000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.2487927194865720  0.7499990521641667  0.2108955776145949   T   T   T
  0.0000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
  0.2357944740290044  0.5214996808246166  0.3127130540740353   T   T   T
```

```
  0.2500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
  0.9747036668879754  0.7680936771848194  0.3556357769423483   T   T   T
  0.2500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
  0.9888007113070261  0.5008285452403233  0.2483637177149305   T   T   T
  0.5000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.7480965312662849  0.7489709813046587  0.2124940666651306   T   T   T
  0.5000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
  0.7444235843486937  0.4669572382090534  0.3205418317675769   T   T   T
  0.7500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
  0.5149619009166808  0.7231566365964199  0.3545580563231448   T   T   T
  0.7500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
  0.4950252583817632  0.4926100105481049  0.2503052704409215   T   T   T
  0.0670861033135949  0.1340785207436570  0.3938704166301749   T   T   T
  0.2913168697336401  0.1650818947398543  0.4859186835746745   T   T   T
  0.5126186873632022  0.0308959815965298  0.4103581460785986   T   T   T
  0.1706246025242174  0.4204875695208189  0.5069793236648878   T   T   T
  0.0042949391454518  0.9896822927851942  0.3330085619641528   T   T   T
  0.2500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
  0.2604895642174698  0.9997034957033880  0.2305401298521837   T   T   T
  0.5097325226311062  0.9571450279408518  0.3386636498610671   T   T   T
  0.7500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
  0.7508174743083422  0.0004056406586399  0.2301908062671155   T   T   T
  0.9888242370828801  0.5393353989782860  0.3373034840613499   T   T   T
  0.2500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.2365438271740970  0.5002537919038851  0.2299967642299117   T   T   T
  0.4910632806982917  0.5021601086192027  0.3331553663213896   T   T   T
  0.7500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.7452359855090046  0.4956614564110342  0.2299380395581540   T   T   T
```

4b.

```
H  C  V  O  Ti
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H  C  V  O  Ti
5   1  1  36  16
Selective dynamics
Direct
  0.4293542714743666  0.0550308223831451  0.4387160687326883   T   T   T
  0.0927395348932194  0.6547835057135387  0.4877850337247978   T   T   T
  0.3273643615517514  0.6478661395678884  0.4922844846032604   T   T   T
  0.1976566326485667  0.6225178687036887  0.5565533275097465   T   T   T
  0.3155166478907105  0.1379606198074796  0.5153344151772430   T   T   T
  0.2047076193723214  0.5934802213586252  0.5101921589344798   T   T   T
  0.1963511887877445  0.2986202920040668  0.4340213793048022   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.2521642752725697  0.2513836695410134  0.2117155716475665   T   T   T
  0.0000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.2665652049386935  0.9757284568623348  0.3150533799475213   T   T   T
  0.2500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
```

0.0349924756780950	0.4506109968607745	0.4085334681205950	T	T	T
0.2500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.0087904227201250	0.0105022337695857	0.2496698170464384	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7511909170064541	0.2508349245214276	0.2105410822384073	T	T	T
0.5000000000000000	0.2500657030223365	0.1047483626335719	F	F	F
0.7565933903622479	0.0089036045971582	0.3164048471962317	T	T	T
0.7500657030223365	0.0000000000000000	0.1441744226128918	F	F	F
0.3833744751231194	0.3664198981490188	0.3988191405017361	T	T	T
0.7500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.5091011636930958	0.0023110927362069	0.2469074207159920	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2514123416443468	0.7495079902039166	0.2109625478912207	T	T	T
0.0000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.2371730144147790	0.5057294885574848	0.3135054060542188	T	T	T
0.2500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.9813240105974685	0.7594036389992880	0.3558848845297859	T	T	T
0.2500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.9899554087498998	0.5051050915397113	0.2485545041347805	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7502610767320377	0.7493057751112602	0.2123338500232563	T	T	T
0.5000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.7442531305002049	0.4621092463968708	0.3207885784732554	T	T	T
0.7500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.5141591913582957	0.7162297784094491	0.3568677724749136	T	T	T
0.7500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.4965943556639374	0.4971583173887240	0.2510352501085436	T	T	T
0.0664292854830677	0.1298959964573854	0.3930572723747190	T	T	T
0.2753724903352435	0.0976730855532537	0.4776691195171523	T	T	T
0.5200673234221682	0.0396209559478606	0.4059923189325545	T	T	T
0.1993521809715020	0.4077136728375805	0.5031437296173422	T	T	T
0.0122655632555180	0.9865111421193262	0.3343777901972373	T	T	T
0.2500657030223365	0.2500657030223365	0.1244398483281657	F	F	F
0.0000000000000000	0.2500657030223365	0.0197345742847261	F	F	F
0.2624723650604537	0.0005221964987996	0.2303564349502594	T	T	T
0.5149035114632028	0.9499233239566962	0.3366435650552262	T	T	T
0.7500657030223365	0.2500657030223365	0.1244398483281657	F	F	F
0.5000000000000000	0.2500657030223365	0.0197345742847261	F	F	F
0.7562281029120541	0.0009538041971595	0.2304261253046462	T	T	T
0.9885736085408183	0.5344613772487179	0.3361724636424270	T	T	T
0.2500657030223365	0.7500657030223365	0.1244398483281657	F	F	F
0.0000000000000000	0.7500657030223365	0.0197345742847261	F	F	F
0.2395283895602205	0.5005815809874576	0.2300926335686384	T	T	T
0.4918899953251739	0.4980242919797107	0.3346108631052047	T	T	T
0.7500657030223365	0.7500657030223365	0.1244398483281657	F	F	F
0.5000000000000000	0.7500657030223365	0.0197345742847261	F	F	F
0.7454040999193481	0.4963007322939674	0.2297073062484642	T	T	T

5b.

```
H  C  V  O  Ti
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
```

```
H    C    V    O    Ti
11   3     1    38    16
Selective dynamics
Direct
  0.4432080147148774  0.0655937960954579  0.4429978511633837   T   T   T
  0.0270471187757189  0.6495006445619792  0.4769871576666950   T   T   T
  0.2533274382023177  0.7037349023741010  0.4878364531773596   T   T   T
  0.1181125665656087  0.6474874318299171  0.5484718471492924   T   T   T
  0.3108507992277976  0.1545921990496538  0.5240753506584650   T   T   T
  0.3392201822287306  0.4536796878952775  0.6225593477609882   T   T   T
  0.1385193656378649  0.3409799902891441  0.6030247588453513   T   T   T
  0.4372175127148194  0.4353152277855524  0.7162756308567819   T   T   T
  0.4520965344749734  0.1991293552667242  0.7194459066716842   T   T   T
  0.4835052683113759  0.2089897230804760  0.6050799903832662   T   T   T
  0.3074279981329323  0.3139137782063185  0.7670570494939188   T   T   T
  0.1447971540897891  0.6192569023957623  0.5027183765326904   T   T   T
  0.2623853423032826  0.3308681144184790  0.6267834387853511   T   T   T
  0.3627274575270830  0.3125046312589693  0.7234566309866726   T   T   T
  0.1978880512729014  0.2992130708734328  0.4340508774887560   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.2495406530773427  0.2508089944243659  0.2117805441357695   T   T   T
  0.0000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.2654526835532358  0.9886756365096629  0.3161659067367279   T   T   T
  0.2500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.0301588136665064  0.4447361009134032  0.4039085924013543   T   T   T
  0.2500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
  0.0068971219545486  0.0070681308457957  0.2506146438555051   T   T   T
  0.5000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.7486918430609854  0.2500615898478423  0.2105188672434549   T   T   T
  0.5000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.7545207379446633  0.0192898951421696  0.3172080354011610   T   T   T
  0.7500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.3805201298495423  0.3621690062936606  0.3946942575847582   T   T   T
  0.7500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
  0.5076342083584506 -0.0014359867246365  0.2475074632609205   T   T   T
  0.0000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.2487456433661408  0.7504173494472430  0.2108466866189606   T   T   T
  0.0000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
  0.2355538318165501  0.5211357484291562  0.3126657491960863   T   T   T
  0.2500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
  0.9781867524086406  0.7669309236316849  0.3575280576625684   T   T   T
  0.2500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
  0.9884428432481431  0.5019861439551565  0.2478937738786179   T   T   T
  0.5000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.7492321420841874  0.7492876762498226  0.2123985838476370   T   T   T
  0.5000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
  0.7410813039691213  0.4703207308648439  0.3195927319139027   T   T   T
  0.7500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
  0.5122669248203708  0.7232601752839852  0.3557542658246605   T   T   T
  0.7500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
  0.4935770907450038  0.4948678061722987  0.2501478489951909   T   T   T
  0.0670158757407947  0.1257632954085665  0.3976564806589634   T   T   T
  0.2878799714244760  0.1269287396603343  0.4830546066149946   T   T   T
  0.5226312952898733  0.0381388974354695  0.4090456097830953   T   T   T
  0.1905259148657229  0.4394619624643175  0.4973474655186431   T   T   T
  0.3580698253099226  0.1887148446039235  0.6005295821476262   T   T   T
  0.2179381894546081  0.2998594065354739  0.6844825884201847   T   T   T
```

```
  0.0097835604987322  0.9913713103148729  0.3359782485878106   T   T   T
  0.2500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
  0.2602791036304470  0.0004875380637594  0.2309471961767088   T   T   T
  0.5134444346921906  0.9578727574941707  0.3381366147831307   T   T   T
  0.7500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
  0.7543828655137865  0.0007390144112831  0.2308737437914134   T   T   T
  0.9860562870932076  0.5415836550483579  0.3351435330109336   T   T   T
  0.2500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.2371591702493600  0.5006869309726473  0.2296552071175703   T   T   T
  0.4877548988442352  0.5042675018638869  0.3334577347769760   T   T   T
  0.7500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.7432473122011196  0.4959645065196427  0.2297333704172871   T   T   T
```

6b.

```
H    C    V    O    Ti
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H    C    V    O    Ti
11    3    1    38    16
Selective dynamics
Direct
0.4395049565388563  0.0812053530658588  0.4395813728211900   T   T   T
0.0100434072980788  0.6675281816756945  0.4688701727717807   T   T   T
0.2263329681867447  0.7506775231827362  0.4807232902129701   T   T   T
0.0917506836203556  0.6902471760302957  0.5410027494749023   T   T   T
0.3147029279287948  0.0904579715253240  0.5437989977228838   T   T   T
0.3636764986162366  0.3739994810030441  0.5600099823806735   T   T   T
0.1332580082495948  0.2809316303106158  0.5659428482590558   T   T   T
0.4416267414713140  0.5776384843107136  0.6245007705761347   T   T   T
0.4377066979798013  0.4403235226342915  0.6883006661165397   T   T   T
0.4665419634155161  0.0831078567395890  0.5918391495258902   T   T   T
0.2951226300912965  0.6280336297948785  0.6831120362030456   T   T   T
0.1274362394450551  0.6557666421291205  0.4962022802081251   T   T   T
0.2479771889404020  0.3410631319363125  0.5851187074474775   T   T   T
0.3600065608491087  0.5227177203501884  0.6590781841686706   T   T   T
0.2026784092024074  0.3101767746061431  0.4351281495298493   T   T   T
0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
0.2514060753895943  0.2506029457431030  0.2116195810102063   T   T   T
0.0000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
0.2687601802326979  0.9881546844494806  0.3157611718267574   T   T   T
0.2500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
0.0184695147582308  0.4479896750608612  0.4056994376965251   T   T   T
0.2500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
0.0089669515797396  0.0074037763242091  0.2503530335163142   T   T   T
0.5000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
0.7500319670667197  0.2500952073993247  0.2104285345889425   T   T   T
0.5000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
0.7557853310511998  0.0206167640193195  0.3171933431263717   T   T   T
0.7500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
```

```
0.3897898501336686  0.3683401692144280  0.3963243333004063   T   T   T
0.7500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
0.5098431158399928  0.9977842374755503  0.2475159689462719   T   T   T
0.0000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
0.2500666820698779  0.7503127005582872  0.2107208996366177   T   T   T
0.0000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
0.2359449386849757  0.5214627106218637  0.3131942403107653   T   T   T
0.2500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
0.9820089986030991  0.7710405613621090  0.3586399191219168   T   T   T
0.2500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
0.9896271239606870  0.5011965598068480  0.2480551580192527   T   T   T
0.5000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
0.7511614929240253  0.7494147175016540  0.2122371096699207   T   T   T
0.5000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
0.7417019268397282  0.4739873666481297  0.3192963854058581   T   T   T
0.7500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
0.5146722841214761  0.7260995560766837  0.3557796812682734   T   T   T
0.7500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
0.4939236994049914  0.4945783662772584  0.2503320047057513   T   T   T
0.0742333717943739  0.1388880194250839  0.3937695804735676   T   T   T
0.2742388509312398  0.1585162967765870  0.4844772714593224   T   T   T
0.5227133670543513  0.0397892986793806  0.4095944580388309   T   T   T
0.1962011000869223  0.4828543243571404  0.4953827445437893   T   T   T
0.3387703595456081  0.0825334365172938  0.5885180943539281   T   T   T
0.2199313621231341  0.4162081012725787  0.6345537974949917   T   T   T
0.0129586528754157  0.9953892629174254  0.3357409134244305   T   T   T
0.2500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
0.0000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
0.2621375867958188  0.0001832590014063  0.2307916439519893   T   T   T
0.5154222508419564  0.9592951162419188  0.3376236679151066   T   T   T
0.7500657030223365  0.2500657030223365  0.1244398483281657   F   F   F
0.5000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
0.7567427149240940  0.0010837252587946  0.2308713810562561   T   T   T
0.9868870861156976  0.5436420226036044  0.3368507853533446   T   T   T
0.2500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
0.0000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
0.2372805568735017  0.5004647768627382  0.2301006681158873   T   T   T
0.4887921167572270  0.5063469676946193  0.3336511823461985   T   T   T
0.7500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
0.5000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
0.7451175841696421  0.4963965054560400  0.2302887603506052   T   T   T
```

7b.

```
H  C  V  O Ti
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H    C    V    O    Ti
11    3    1    38    16
Selective dynamics
Direct
  0.4157134099805411  0.9446996011384649  0.4465635762411307   T   T   T
  0.4998727236057400  0.9202260965979557  0.5704432325982350   T   T   T
  0.6508769795479507  0.8208945930146049  0.5195866342508287   T   T   T
  0.1991108226242252  0.6460514191601648  0.5371287181409806   T   T   T
```

0.1334340086443155	0.7910374303044883	0.4801999034209056	T	T	T
0.1866852044584557	0.8804976675829861	0.5495090365733234	T	T	T
0.3298055191580112	0.7133599256739949	0.6334378683473049	T	T	T
0.4670662595030275	0.5302914877134479	0.6510684212410697	T	T	T
0.5486732218203950	0.7505433989445317	0.6596520563922871	T	T	T
0.4042038210743834	0.2567062458262913	0.5470611290071730	T	T	T
0.5589065498003966	0.3628650588684044	0.5698831771830632	T	T	T
0.5258770532875892	0.8051843800910971	0.5426961309127655	T	T	T
0.2183938444126130	0.7766864742943658	0.5180157585597287	T	T	T
0.4656780291292176	0.6636530817937561	0.6331796327100923	T	T	T
0.2368844694703072	0.2291552453520042	0.4169315259707995	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2478050119542513	0.2478340261050729	0.2121747978097319	T	T	T
0.0000000000000000	0.2500657030223365	0.1047483626335719	F	F	F
0.2501594123483850	0.0032774489861455	0.3164272044428263	T	T	T
0.2500657030223365	0.0000000000000000	0.1441744226128918	F	F	F
0.0730075151583083	0.3811520571897721	0.3853382392336090	T	T	T
0.2500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.9955386635252788	0.9935319560219187	0.2524611469563400	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7489674598660078	0.2468953804399731	0.2108584486738304	T	T	T
0.5000000000000000	0.2500657030223365	0.1047483626335719	F	F	F
0.7484009355855530	0.0283298287516269	0.3239604926178954	T	T	T
0.7500657030223365	0.0000000000000000	0.1441744226128918	F	F	F
0.4217614154802011	0.3377537554747185	0.3744238001390859	T	T	T
0.7500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.5029603218190027	0.9922523157148502	0.2523280042192863	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2485314998381681	0.7526590800392969	0.2099086590420199	T	T	T
0.0000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.2479306570375606	0.5587502386345633	0.3091860818912198	T	T	T
0.2500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.9748968550923225	0.7491791303360834	0.3603205152833729	T	T	T
0.2500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.9973779867489501	0.4909401338434417	0.2464365960671256	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7485799634769914	0.7489761739657564	0.2124075511973217	T	T	T
0.5000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.7484857011706356	0.4850767685241472	0.3162450159318449	T	T	T
0.7500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.5198640940024598	0.7455267581356131	0.3567708081902051	T	T	T
0.7500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.4987555992244629	0.4875010873648470	0.2466685455809124	T	T	T
0.0694228099473621	0.0608612214545005	0.4104377760729216	T	T	T
0.2463266364711945	0.2844997957723536	0.4834866899878348	T	T	T
0.4264269906791397	0.0391040528642109	0.4159900820379396	T	T	T
0.3967586718554137	0.7950629012772429	0.4978212285620980	T	T	T
0.5341600240031310	0.6494673243333627	0.5756363792973884	T	T	T
0.4997400897470818	0.2502653942730336	0.5753422091367452	T	T	T
0.9962095583815737	0.9734040729803949	0.3403970313919988	T	T	T
0.2500657030223365	0.2500657030223365	0.1244398483281657	F	F	F
0.0000000000000000	0.2500657030223365	0.0197345742847261	F	F	F
0.2489491819471495	0.0006340138030620	0.2321322905181231	T	T	T
0.5025953312099956	0.9698089120692915	0.3394083334804566	T	T	T
0.7500657030223365	0.2500657030223365	0.1244398483281657	F	F	F
0.5000000000000000	0.2500657030223365	0.0197345742847261	F	F	F
0.7496849984451134	0.0013566235707526	0.2314114217669029	T	T	T

```
  0.0002683944245111  0.5288644255072877  0.3311393088121622   T   T   T
  0.2500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.2462874258829721  0.5019425632099742  0.2284715095059447   T   T   T
  0.4947086747757997  0.5155556216755647  0.3298245692798588   T   T   T
  0.7500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.7488558659434525  0.4968719959607403  0.2294329280741809   T   T   T
```

8b.

```
H  C  V  O Ti
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H    C    V    O    Ti
9     3    1    37    16
Selective dynamics
Direct
  0.4140322778745627 -0.0418108703607602  0.4478729169542369    T   T   T
  0.4766604300039000  0.7922872128603055  0.5883612235649394   T   T   T
  0.6299946722647738  0.8664791422602761  0.5334361637306719   T   T   T
  0.2210275866932856  0.6144496301209025  0.5094141377070072   T   T   T
  0.1206397844255024  0.8167894403913967  0.4859838889062486   T   T   T
  0.1698390306988939  0.7845704485210226  0.5610201398622436   T   T   T
  0.5468808309169294  0.5169082549398204  0.6152361003559853   T   T   T
  0.6381533277854853  0.3706439436179938  0.5624032081513270   T   T   T
  0.7634397991106293  0.5554273677489633  0.5869320539463309   T   T   T
  0.5165329619122877  0.7801124385771862  0.5424375803214456   T   T   T
  0.2126602193414935  0.7568776027595733  0.5165261102740654   T   T   T
  0.6300820643742419  0.5080759073025480  0.5762559626805904   T   T   T
  0.2369551651190142  0.2345476945987791  0.4175270803160103   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.2483413813970331  0.2480992031826898  0.2120661151779093   T   T   T
  0.0000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.2503938520318539  0.0077998114326211  0.3166260457614478   T   T   T
  0.2500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.0716876994277461  0.3845719387376294  0.3850548323240633   T   T   T
  0.2500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
 -0.0043170826424884 -0.0055658702000258  0.2526018562949807   T   T   T
  0.5000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.7489123302379762  0.2469774174874075  0.2108738361283257   T   T   T
  0.5000000000000000  0.2500657030223365  0.1047483626335719   F   F   F
  0.7484545610777693  0.0311632173754259  0.3241187524045552   T   T   T
  0.7500657030223365  0.0000000000000000  0.1441744226128918   F   F   F
  0.4216468700952286  0.3455744811327501  0.3752760869795754   T   T   T
  0.7500657030223365  0.2500657030223365  0.0394260599793199   F   F   F
  0.5031159932061937 -0.0080064945787928  0.2525526435058978   T   T   T
  0.0000000000000000  0.5000000000000000  0.0000000000000000   F   F   F
  0.2485002387096787  0.7530105686183352  0.2097960935111774   T   T   T
  0.0000000000000000  0.7500657030223365  0.1047483626335719   F   F   F
  0.2481089202709719  0.5631530270149055  0.3089778632929778   T   T   T
  0.2500657030223365  0.5000000000000000  0.1441744226128918   F   F   F
  0.9758171160445163  0.7531926568832126  0.3604682074851532   T   T   T
  0.2500657030223365  0.7500657030223365  0.0394260599793199   F   F   F
  0.9977270307844344  0.4906354958533155  0.2464688700246580   T   T   T
```

0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7490774419965783	0.7492499609800749	0.2123588397734187	T	T	T
0.5000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.7485935461390869	0.4899231118944185	0.3161793345984025	T	T	T
0.7500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.5188020520557559	0.7497606453271145	0.3577383601823598	T	T	T
0.7500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.4988392143545009	0.4877707090597447	0.2468352748459533	T	T	T
0.0696889590464441	0.0645206075498250	0.4111593491302232	T	T	T
0.2448909116202402	0.2917509672209847	0.4836167529674152	T	T	T
0.4275797940112857	0.0469553218009044	0.4160464478609889	T	T	T
0.3806642727068201	0.8394993570323410	0.5063547360856770	T	T	T
0.5549313665572380	0.6029188950193437	0.5294807116925783	T	T	T
-0.0030084075497352	-0.0225847298398045	0.3410084480995734	T	T	T
0.2500657030223365	0.2500657030223365	0.1244398483281657	F	F	F
0.0000000000000000	0.2500657030223365	0.0197345742847261	F	F	F
0.2484411153648836	0.0013319272713757	0.2322603958607950	T	T	T
0.5028837518272909	0.9731826743113224	0.3394922444486609	T	T	T
0.7500657030223365	0.2500657030223365	0.1244398483281657	F	F	F
0.5000000000000000	0.2500657030223365	0.0197345742847261	F	F	F
0.7499301452299485	0.0012892334870616	0.2315724421606438	T	T	T
0.0006298909776093	0.5327397067781473	0.3310061363195186	T	T	T
0.2500657030223365	0.7500657030223365	0.1244398483281657	F	F	F
0.0000000000000000	0.7500657030223365	0.0197345742847261	F	F	F
0.2468777018720854	0.5024962022517848	0.2285474434759684	T	T	T
0.4947603810969187	0.5202885594968670	0.3300744456179429	T	T	T
0.7500657030223365	0.7500657030223365	0.1244398483281657	F	F	F
0.5000000000000000	0.7500657030223365	0.0197345742847261	F	F	F
0.7489992516391200	0.4968091189120507	0.2296073277129398	T	T	T

Table S5. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 1b.

9a.

O	-0.303261	-1.777328	-0.348311
O	-2.702345	-0.446705	-1.193070
O	-2.102676	-0.732005	1.593987
O	-0.121023	0.752681	-1.586456
O	0.442292	0.481086	1.170572
O	-2.612710	2.246108	-2.639320
O	-1.922139	1.844616	0.336925
O	-1.383887	1.678733	3.355671
V	0.678713	-0.308952	-0.419169
O	-3.010567	-3.228824	0.027550
O	2.198621	-0.590289	-0.768698
TI	-1.911491	1.193300	-1.357480
TI	-1.242146	0.882424	1.747559
TI	-2.116940	-1.665603	0.034430
H	-0.819376	1.940059	4.090029
H	-2.859539	3.166049	-2.774746
H	-3.253472	-3.935195	0.633865
C	5.848162	-0.788118	-0.381216
H	6.801133	-1.326165	-0.237221
H	5.734669	-0.520289	-1.451463
C	6.839892	1.323225	-0.036797
H	6.691997	1.622434	-1.090716
H	6.757193	2.210786	0.600736
H	7.855789	0.900526	0.068213
O	5.847464	0.408342	0.389879
O	4.836123	-1.628348	0.057281
H	3.978423	-1.250147	-0.196990

10a.

O	0.507587	-1.918327	-0.152235
O	2.558171	-0.152811	0.851524
O	1.641851	0.105964	-1.837383
O	-0.184185	-0.004950	1.712991
O	-0.989879	0.289797	-0.815891
O	1.893791	1.877956	3.052660
O	0.932438	2.099640	0.162395
O	-0.144465	2.492605	-2.729318
V	-0.855463	-1.076315	0.508767
O	3.429849	-2.272667	-1.170462
O	-1.674881	-2.203758	1.469003
TI	1.355306	1.041378	1.545895
TI	0.299415	1.328248	-1.411275
TI	2.145650	-1.123196	-0.635603
H	-0.942730	2.700540	-3.224318

H	1.937056	2.783989	3.373974
H	3.889738	-2.475586	-1.991165
C	-3.705877	-0.644831	-0.693304
H	-3.358193	0.038431	-1.487643
H	-4.596456	-1.202053	-1.042192
C	-5.013299	1.090603	0.236132
H	-5.962135	0.645441	-0.111157
H	-5.187152	1.603140	1.188372
H	-4.670505	1.825811	-0.513254
O	-4.029677	0.097188	0.473178
O	-2.708622	-1.552255	-0.375312
H	-2.582918	-2.127648	0.741181

11a.

O	0.179348	-1.532138	0.735020
O	-2.540329	-1.137193	-0.051896
O	-1.387180	0.660815	1.831533
O	-0.330021	-0.541435	-1.671133
O	0.804727	1.152401	-0.007543
O	-3.009683	-0.279820	-3.038276
O	-1.888504	1.620192	-0.806786
O	-0.721381	3.584017	1.199476
V	1.156146	-0.527504	-0.287459
O	-2.092189	-2.163401	2.773219
O	2.056162	-1.156648	-1.727195
TI	-2.002235	-0.108004	-1.531953
TI	-0.817577	1.882875	0.593839
TI	-1.530510	-1.111267	1.413432
H	-1.040541	4.438207	0.891586
H	-2.821968	-0.564095	-3.938011
H	-2.799796	-2.805227	2.890548
C	4.040134	-0.775272	0.247043
H	4.537869	-1.318434	1.072467
H	4.134492	-1.340669	-0.699150
C	5.955553	0.490591	-0.231513
H	6.118839	-0.014291	-1.199378
H	6.281817	1.532905	-0.308808
H	6.554463	-0.018827	0.543787
O	4.577449	0.518939	0.111969
O	2.692473	-0.658279	0.562755
H	1.449472	-1.207788	-2.480824

12a.

O	0.252874	0.271302	-1.512493
O	-0.566457	-1.868005	-0.372008
O	0.445427	-0.315891	1.466489
O	-2.513727	-0.212637	-1.406835

O	-1.391228	1.668859	0.398486
O	-3.149281	-2.813879	-0.398370
O	-2.340229	-0.764972	1.455316
O	-1.292560	1.155868	3.158282
V	-2.239867	-1.540802	-0.199504
V	-1.308867	1.087453	-1.306222
V	0.993289	-0.728639	-0.158750
V	-1.148653	0.506451	1.733820
O	1.995946	-2.117696	-0.328247
O	-1.541806	2.224752	-2.371449
C	2.519650	1.749959	-0.562783
H	3.602972	1.965280	-0.619268
H	2.051315	1.908545	-1.554427
O	2.357883	0.415546	-0.208787
H	2.993008	-2.060784	-0.454254
C	5.314449	-1.737587	0.630182
H	4.878073	-0.801080	0.990626
H	5.188421	-2.516799	1.394385
H	6.381175	-1.586460	0.418643
O	4.605888	-2.072457	-0.580866
H	4.946941	-2.901917	-0.938075
C	1.999466	3.937580	0.134577
H	1.479531	4.456474	0.945693
H	3.052474	4.265008	0.108454
H	1.517896	4.187538	-0.825256
O	1.899901	2.544444	0.416318

13a.

O	-0.325526	-0.624540	1.389762
O	1.202355	-1.739882	-0.418008
O	-0.029301	0.177041	-1.716247
O	2.487393	-0.337914	1.586643
O	0.930746	1.753615	0.453454
O	3.925761	-2.030467	-0.228232
O	2.761077	0.388889	-1.238947
O	1.301846	2.570093	-2.225824
V	-0.608242	-0.989132	-0.408316
O	-1.326144	-2.346505	-0.812037
O	0.767904	1.162625	3.217836
C	-2.394919	1.310243	0.005950
H	-1.867437	1.942873	-0.734746
H	-2.011363	1.539628	1.020438
O	-2.226383	-0.027168	-0.295475
C	-4.071478	-1.429224	-0.051452
O	-5.296387	-2.593773	0.051194
H	-4.916474	-3.443367	0.336439
H	-5.700355	-2.739361	-0.821213

H	-4.644808	-0.571416	-0.392275
H	-3.777565	-1.404962	0.993983
H	-3.373260	-1.903824	-0.736201
C	-4.082844	2.944244	0.241388
H	-3.603295	3.615691	-0.489685
H	-5.170073	3.058357	0.175356
H	-3.749976	3.222724	1.255215
O	-3.789911	1.579412	-0.042621
V	1.247002	1.316371	-1.266316
V	2.716750	-1.020340	-0.086270
V	0.950690	0.531390	1.780266

9b.

H	C	V	O	Ti					
7	2	1	37	16					
0.4072540496275542	0.9494463927116361	0.4435765019482227	T	T	T
0.1124379915006042	0.6178596383985910	0.5860238623292873	T	T	T
0.2631306411938065	0.5725249519173392	0.6447023568453600	T	T	T
0.3317124595724339	0.8906551525140273	0.5286657254618967	T	T	T
0.2789023570110959	0.0615631122175192	0.5788279677255791	T	T	T
0.1083657136406157	0.9203615402714107	0.5518798356338921	T	T	T
0.3134538596271420	0.4863780762981528	0.5363536156311273	T	T	T
0.2480290154676000	0.6369953771686920	0.6024822849732505	T	T	T
0.2473596391369980	0.9271609298266832	0.5654938784672887	T	T	T
0.2363543277120983	0.2361101104602688	0.4166872234836852	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2486936638958877	0.2480014280052110	0.2122707203590207	T	T	T
0.0000000000000000	0.2500657030223365	0.1047483626335719	F	F	F
0.2512386064966802	0.0084865903180752	0.3165738545952608	T	T	T
0.2500657030223365	0.0000000000000000	0.1441744226128918	F	F	F
0.0710386133966093	0.3810885599376082	0.3832353082705204	T	T	T
0.2500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.9962864336629239	0.9944186997236772	0.2526651824749753	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7491303934910685	0.2470733147054924	0.2110249642060648	T	T	T
0.5000000000000000	0.2500657030223365	0.1047483626335719	F	F	F
0.7494251663654291	0.0322687818877406	0.3242555660477364	T	T	T
0.7500657030223365	0.0000000000000000	0.1441744226128918	F	F	F
0.4225056609072779	0.3396388715975699	0.3734057562111707	T	T	T
0.7500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.5040312615389198	0.9912120380809022	0.2525599901939688	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2486962193054395	0.7531160510443666	0.2099135808716932	T	T	T
0.0000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.2483049459170699	0.5629943175371196	0.3089008784954769	T	T	T
0.2500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.9767517589053524	0.7540202516797568	0.3599557249158141	T	T	T
0.2500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.9977723140454466	0.4912430414639144	0.2463235914817296	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7495402028554269	0.7493665077309756	0.2124320561302004	T	T	T
0.5000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.7482575878211541	0.4914306683725946	0.3161200737362147	T	T	T
0.7500657030223365	0.5000000000000000	0.1441744226128918	F	F	F

0.5178582482198629 0.7503306806823835 0.3574138629502549 T T T
0.7500657030223365 0.7500657030223365 0.0394260599793199 F F F
0.4989358502141477 0.4883551382870146 0.2466542102772746 T T T
0.0737401857268485 0.0631897085390925 0.4117130179574774 T T T
0.2451210124235534 0.3015912803635725 0.4821353552117983 T T T
0.4296915914313232 0.0462263956496241 0.4168826376998860 T T T
0.3719356532479078 0.5690242661459941 0.5623751361383972 T T T
0.2808687293781596 0.8157218165777841 0.6135437971084349 T T T
0.9983848282167299 0.9784561539757093 0.3413529721431997 T T T
0.2500657030223365 0.2500657030223365 0.1244398483281657 F F F
0.0000000000000000 0.2500657030223365 0.0197345742847261 F F F
0.2482404317881556 0.0009013301423860 0.2322046476055812 T T T
0.5048464385091255 0.9741907940088668 0.3387431224283884 T T T
0.7500657030223365 0.2500657030223365 0.1244398483281657 F F F
0.5000000000000000 0.2500657030223365 0.0197345742847261 F F F
0.7511884488233027 0.0015870010718147 0.2312232686876483 T T T
0.0000642054251092 0.5335809415034328 0.3304216860061630 T T T
0.2500657030223365 0.7500657030223365 0.1244398483281657 F F F
0.0000000000000000 0.7500657030223365 0.0197345742847261 F F F
0.2469318442130784 0.5019967656580890 0.2283339187970452 T T T
0.4944599247681063 0.5200148330757944 0.3296223600694200 T T T
0.7500657030223365 0.7500657030223365 0.1244398483281657 F F F
0.5000000000000000 0.7500657030223365 0.0197345742847261 F F F
0.7489528300144958 0.4972104083096551 0.2292337091112489 T T T

10b.
H C V O Ti
7 2 1 37 16
0.4448150018940255 0.0700771859940646 0.4431605276588422 T T T
0.2258109990871621 0.2462281147340082 0.5170233876783257 T T T
0.9368857084765324 0.5450261365108247 0.5047352297260309 T T T
0.9310586519946097 0.3737077658773746 0.5593737190843568 T T T
0.2761060928527378 0.7153444815553156 0.5396006367746747 T T T
0.1737397977383773 0.8286653153963266 0.5984104762600848 T T T
0.0637751749244401 0.8135246082035682 0.5300495554953681 T T T
0.0121335135775032 0.4746927006413740 0.5382313359543076 T T T
0.1502084065148259 0.7447061157982472 0.5608407323510132 T T T
0.1964624248923570 0.2923398979830610 0.4296517399415027 T T T
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.2497115835160720 0.2503718704820641 0.2120553332788757 T T T
0.0000000000000000 0.2500657030223365 0.1047483626335719 F F F
0.2646372661568470 0.9793999579223061 0.3150439474348135 T T T
0.2500657030223365 0.0000000000000000 0.1441744226128918 F F F
0.0407003175012666 0.4662847535685735 0.4111924542617045 T T T
0.2500657030223365 0.2500657030223365 0.0394260599793199 F F F
0.0061751746376436 0.0042482036900914 0.2487656976474464 T T T
0.5000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.7502775105715590 0.2499442826649860 0.2105640621258104 T T T
0.5000000000000000 0.2500657030223365 0.1047483626335719 F F F
0.7537456783877607 0.0172322288253686 0.3165533360221534 T T T
0.7500657030223365 0.0000000000000000 0.1441744226128918 F F F
0.3884640155822651 0.3616813128195185 0.3951387935145010 T T T
0.7500657030223365 0.2500657030223365 0.0394260599793199 F F F
0.5075588395859759 0.9996112878297926 0.2470833009197353 T T T
0.0000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.2511734578161768 0.7493483302406315 0.2109612198473357 T T T
0.0000000000000000 0.7500657030223365 0.1047483626335719 F F F

```
0.2363148511449771 0.5155786527596811 0.3134329076838068 T T T
0.2500657030223365 0.5000000000000000 0.1441744226128918 F F F
0.9765031958010085 0.7656014392983689 0.3551730841832552 T T T
0.2500657030223365 0.7500657030223365 0.0394260599793199 F F F
0.9895079983533931 0.5022600299082339 0.2489309521693525 T T T
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.7483337924297483 0.7487805256619938 0.2124548887607267 T T T
0.5000000000000000 0.7500657030223365 0.1047483626335719 F F F
0.7456860927779168 0.4643958386971648 0.3214637535012667 T T T
0.7500657030223365 0.5000000000000000 0.1441744226128918 F F F
0.5160787568554229 0.7212085075185728 0.3555099707073239 T T T
0.7500657030223365 0.7500657030223365 0.0394260599793199 F F F
0.4963004007765383 0.4928656972687832 0.2511900662879874 T T T
0.0677679886472804 0.1439509040065096 0.3886636156604245 T T T
0.2803056635013609 0.1449992936231303 0.4821737177329372 T T T
0.5168618745560875 0.0350354843680142 0.4087457595014871 T T T
0.1589979227816817 0.3930882997368049 0.5107397765817033 T T T
0.0681164075388178 0.5878413050706687 0.5820173663404155 T T T
0.0063499522582017 0.9870749583481617 0.3313494936123478 T T T
0.2500657030223365 0.2500657030223365 0.1244398483281657 F F F
0.0000000000000000 0.2500657030223365 0.0197345742847261 F F F
0.2628788693186404 0.9995789957195231 0.2300738616096644 T T T
0.5115894478484619 0.9542150612887432 0.3379529431465013 T T T
0.7500657030223365 0.2500657030223365 0.1244398483281657 F F F
0.5000000000000000 0.2500657030223365 0.0197345742847261 F F F
0.7519639601564678 0.0001703636457900 0.2297390270322491 T T T
0.9897913435087705 0.5363949936610745 0.3384567537348319 T T T
0.2500657030223365 0.7500657030223365 0.1244398483281657 F F F
0.0000000000000000 0.7500657030223365 0.0197345742847261 F F F
0.2379540511472530 0.5001139991545965 0.2304317712527579 T T T
0.4923101308420341 0.5002178481427361 0.3344126171730023 T T T
0.7500657030223365 0.7500657030223365 0.1244398483281657 F F F
0.5000000000000000 0.7500657030223365 0.0197345742847261 F F F
0.7463376143518191 0.4955238987830740 0.2302372255029244 T T T

11b.
H  C  V  O  Ti
7   2  1  37  16
0.4334908525958421 0.0662897789258249 0.4364869775117292 T T T
0.3300008209787030 0.1286027891499131 0.5128949511585421 T T T
-0.0602042316463123 0.5372589519360907 0.5016235421850357 T T T
-0.0625256521675356 0.3598932389495196 0.5544564509742188 T T T
0.2788258393547176 0.7100661594646671 0.5394812805522321 T T T
0.1687005057594376 0.8160073040008236 0.5984347456563651 T T T
0.0648882476421471 0.8030231247039342 0.5289260965613340 T T T
0.0165846211122870 0.4650308638090376 0.5346823662713296 T T T
0.1507547510182849 0.7346138283693814 0.5599160557449313 T T T
0.1872501643344063 0.2962799451280108 0.4348786835032390 T T T
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.2504759275613017 0.2519675217441401 0.2117412040700761 T T T
0.0000000000000000 0.2500657030223365 0.1047483626335719 F F F
0.2645646088415152 0.9710923562377047 0.3145033692979186 T T T
0.2500657030223365 0.0000000000000000 0.1441744226128918 F F F
0.0211382124587753 0.4456131153015811 0.4087394596428854 T T T
0.2500657030223365 0.2500657030223365 0.0394260599793199 F F F
0.0083518152433333 0.0109744683101973 0.2493008341231170 T T T
0.5000000000000000 0.0000000000000000 0.0000000000000000 F F F
```

```
0.7490842149827821 0.2513566690332424 0.2107635898350539 T T T
0.5000000000000000 0.2500657030223365 0.1047483626335719 F F F
0.7582282905394482 0.0019495485285728 0.3155917969465986 T T T
0.7500657030223365 0.0000000000000000 0.1441744226128918 F F F
0.3752920547778764 0.3763467198473375 0.4032458283975053 T T T
0.7500657030223365 0.2500657030223365 0.0394260599793199 F F F
0.5080179555675897 0.0056752350460075 0.2471656718874160 T T T
0.0000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.2498624147002004 0.7493912688919828 0.2110472090820155 T T T
0.0000000000000000 0.7500657030223365 0.1047483626335719 F F F
0.2338955388339448 0.5011677416703987 0.3144053422240213 T T T
0.2500657030223365 0.5000000000000000 0.1441744226128918 F F F
0.9821756289444952 0.7590970682439891 0.3569584940458336 T T T
0.2500657030223365 0.7500657030223365 0.0394260599793199 F F F
0.9870612116018856 0.5060816258763279 0.2490918808573031 T T T
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.7469382463866208 0.7493888770274011 0.2122857479928072 T T T
0.5000000000000000 0.7500657030223365 0.1047483626335719 F F F
0.7398289530531669 0.4638077099380590 0.3212229397126151 T T T
0.7500657030223365 0.5000000000000000 0.1441744226128918 F F F
0.5095728854336212 0.7168581462365998 0.3593175325157328 T T T
0.7500657030223365 0.7500657030223365 0.0394260599793199 F F F
0.4930913985992944 0.4994727439654486 0.2523926499361987 T T T
0.0676711198032780 0.1304194708514886 0.3926752969176712 T T T
0.2933325467021621 0.0938274389342423 0.4743379520572033 T T T
0.5244034575919447 0.0575734406943011 0.4014603208153944 T T T
0.1631696720343508 0.3887258462792099 0.5055639018988910 T T T
0.0712268143926099 0.5738166977439142 0.5792853074331309 T T T
0.0127245227950224 0.9835718080618854 0.3336610780559772 T T T
0.2500657030223365 0.2500657030223365 0.1244398483281657 F F F
0.0000000000000000 0.2500657030223365 0.0197345742847261 F F F
0.2609884684878350 0.0013503024911155 0.2300304720523672 T T T
0.5142237781005918 0.9490000047301909 0.3357042121360994 T T T
0.7500657030223365 0.2500657030223365 0.1244398483281657 F F F
0.5000000000000000 0.2500657030223365 0.0197345742847261 F F F
0.7550330013627753 0.0010975152334593 0.2302448841011727 T T T
0.9843839912616859 0.5333546334455239 0.3368186887518334 T T T
0.2500657030223365 0.7500657030223365 0.1244398483281657 F F F
0.0000000000000000 0.7500657030223365 0.0197345742847261 F F F
0.2380517358512945 0.5011897881523203 0.2305120234698437 T T T
0.4864940338034922 0.4990043156162471 0.3367157089886639 T T T
0.7500657030223365 0.7500657030223365 0.1244398483281657 F F F
0.5000000000000000 0.7500657030223365 0.0197345742847261 F F F
0.7422069767882843 0.4965682488731708 0.2303335653741686 T T T

12b.
H  C  V  O  Ti
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H    C    V    O    Ti
11    3    1    38    16
Selective dynamics
Direct
  0.4580458529892471  0.0820530338412541  0.4424825530273220   T   T   T
  0.3249085870409275  0.1438778789360236  0.5240842124461560   T   T   T
```

0.9334610059690405	0.5727521852687064	0.4802597241897950	T	T	T
0.8768869207303014	0.4145930153458571	0.5359254611516291	T	T	T
0.2624881574647581	0.7130984162433573	0.5292706905301993	T	T	T
0.1547395575720640	0.8435289925431048	0.5827780400058903	T	T	T
0.0693768227481605	0.8352724497979231	0.5105107522009649	T	T	T
0.1243453198944139	0.2397867335920384	0.6282305921268864	T	T	T
0.2981684401279041	0.3956203360829251	0.6267006218075597	T	T	T
0.2914660513737021	0.2299924215024187	0.6823588203649853	T	T	T
0.4820513737139186	0.1472690680147563	0.6071599176361245	T	T	T
-0.0193386052273182	0.5011328388229486	0.5187943003315424	T	T	T
0.1342072702176828	0.7595893627892097	0.5450139558433859	T	T	T
0.2646431632747310	0.2585048807478480	0.6366899201511764	T	T	T
0.1884301278494643	0.2917653031511568	0.4350224489275814	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2486361783108264	0.2504162448237625	0.2117422685224576	T	T	T
0.0000000000000000	0.2500657030223365	0.1047483626335719	F	F	F
0.2648549030669976	0.9957466565623271	0.3164237227666790	T	T	T
0.2500657030223365	0.0000000000000000	0.1441744226128918	F	F	F
0.0267995869159319	0.4401085439526579	0.4008566173689856	T	T	T
0.2500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.0077176236668707	0.0027623667786154	0.2503690642838619	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.7482398329321267	0.2497710924426510	0.2106215660055966	T	T	T
0.5000000000000000	0.2500657030223365	0.1047483626335719	F	F	F
0.7572908579615122	0.0207662894612395	0.3165046670193215	T	T	T
0.7500657030223365	0.0000000000000000	0.1441744226128918	F	F	F
0.3717801246240715	0.3731332092190416	0.3972308793827693	T	T	T
0.7500657030223365	0.2500657030223365	0.0394260599793199	F	F	F
0.5079068540463978	-0.0024271956241664	0.2475500605335876	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.2495933782801948	0.7503665974561082	0.2107994945841546	T	T	T
0.0000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.2341102773575057	0.5276307958031614	0.3126741365657664	T	T	T
0.2500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.9788699538899190	0.7703756597872601	0.3581349334476187	T	T	T
0.2500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.9873514300699981	0.4998382484526796	0.2478572362186623	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.7480090156037807	0.7487582353605002	0.2124496789275990	T	T	T
0.5000000000000000	0.7500657030223365	0.1047483626335719	F	F	F
0.7378294673549539	0.4769488588340195	0.3194592925831818	T	T	T
0.7500657030223365	0.5000000000000000	0.1441744226128918	F	F	F
0.5085952005482469	0.7275711646709271	0.3576677565727322	T	T	T
0.7500657030223365	0.7500657030223365	0.0394260599793199	F	F	F
0.4910180652967795	0.4923956173806043	0.2510441367999021	T	T	T
0.0668756185621962	0.1195469005950333	0.4010570705732812	T	T	T
0.3190429183704568	0.1377419165043005	0.4814238112782888	T	T	T
0.5327225765594967	0.0541409837845746	0.4062187891029386	T	T	T
0.1270852354101026	0.3964093061512032	0.5024203348781086	T	T	T
0.0257698077944205	0.6156219399590609	0.5635241680484024	T	T	T
0.3567253541479584	0.1368511911116509	0.5997873460569052	T	T	T
0.0092935645286818	0.9912083955504711	0.3354608388413417	T	T	T
0.2500657030223365	0.2500657030223365	0.1244398483281657	F	F	F
0.0000000000000000	0.2500657030223365	0.0197345742847261	F	F	F
0.2608413106382083	0.0004967121496656	0.2307568525641060	T	T	T
0.5138740943980925	0.9608113987831087	0.3378221856239631	T	T	T
0.7500657030223365	0.2500657030223365	0.1244398483281657	F	F	F

```
  0.5000000000000000  0.2500657030223365  0.0197345742847261   F   F   F
  0.7545444625344768  0.0002626920739187  0.2305416868784076   T   T   T
  0.9828843363863465  0.5442176249348805  0.3341241229407658   T   T   T
  0.2500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.0000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.2377641228990954  0.5005546742168626  0.2296039318926089   T   T   T
  0.4808219751769184  0.5077810022028577  0.3355347921141571   T   T   T
  0.7500657030223365  0.7500657030223365  0.1244398483281657   F   F   F
  0.5000000000000000  0.7500657030223365  0.0197345742847261   F   F   F
  0.7402453057152145  0.4956270688650486  0.2303490118716199   T   T   T

13b.
H    C    V    O    Ti
1.00000000000000
7.6100000000000003    0.0000000000000000    0.0000000000000000
0.0000000000000000    7.6100000000000003    0.0000000000000000
0.0000000000000000    0.0000000000000000   23.2079999999999984
H    C    V    O    Ti
11    3    1    38    16
Selective dynamics
Direct
  0.4574114726783446  0.0974974298047047  0.4404253744574629   T   T   T
  0.3736130362305332  0.1213055464473284  0.5539435666069379   T   T   T
  0.9399828736840168  0.6236413873775126  0.4659402004802155   T   T   T
  0.8565589735375227  0.4673761466838781  0.5181346852440143   T   T   T
  0.2326781516046245  0.7821700970290797  0.5285070282353287   T   T   T
  0.0931665820401900  0.9073897488584922  0.5752170334762694   T   T   T
  0.0420877883596834  0.8877381120499612  0.4996754745182814   T   T   T
  0.1408976316133561  0.2507222661366363  0.5622476152787644   T   T   T
  0.3415677717569928  0.3905641924296425  0.5490451766200605   T   T   T
  0.2063441071062133  0.4218729069062117  0.6152434459815155   T   T   T
  0.4973494131302265  0.1783008707019225  0.6065167541232058   T   T   T
  0.9678354486743913  0.5529401938477921  0.5063134218001274   T   T   T
  0.0958228194719340  0.8198502660669833  0.5377146825937140   T   T   T
  0.2345563862424060  0.3479867155529621  0.5759368060803343   T   T   T
  0.1957578300538736  0.2944394454792724  0.4357333003821820   T   T   T
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.2461543482588582  0.2494631435986060  0.2116876586736949   T   T   T
  0.0000000000000000  0.2500657030223364  0.1047483626335719   F   F   F
  0.2643513453671919  1.0028846530276514  0.3169451348704705   T   T   T
  0.2500657030223364  0.0000000000000000  0.1441744226128918   F   F   F
  0.0169019211623425  0.4301393453699575  0.3959664908931512   T   T   T
  0.2500657030223364  0.2500657030223364  0.0394260599793199   F   F   F
  0.0064400643620653 -0.0000303727318692  0.2514912698597210   T   T   T
  0.4999999999999911  0.0000000000000000  0.0000000000000000   F   F   F
  0.7454029694538887  0.2488973279998048  0.2106779869921923   T   T   T
  0.4999999999999911  0.2500657030223364  0.1047483626335719   F   F   F
  0.7561585368255898  0.0253558955542912  0.3173180362442430   T   T   T
  0.7500657030223350  0.0000000000000000  0.1441744226128918   F   F   F
  0.3731332933314770  0.3768186554541247  0.3953396110197092   T   T   T
  0.7500657030223350  0.2500657030223364  0.0394260599793199   F   F   F
  0.5067966633556923  0.9947414503149151  0.2483648470900444   T   T   T
  0.0000000000000000  0.4999999999999911  0.0000000000000000   F   F   F
  0.2463002816872559  0.7511389044901395  0.2103958032438399   T   T   T
  0.0000000000000000  0.7500657030223350  0.1047483626335719   F   F   F
  0.2327303319326332  0.5413524727713519  0.3114731448044459   T   T   T
  0.2500657030223364  0.4999999999999911  0.1441744226128918   F   F   F
```

0.9788336684510327	0.7751504433038993	0.3610232548884672	T	T	T
0.2500657030223364	0.7500657030223350	0.0394260599793199	F	F	F
0.9855997051578070	0.4952948554478519	0.2472517035946910	T	T	T
0.4999999999999911	0.4999999999999911	0.0000000000000000	F	F	F
0.7474692361048901	0.7489909700758648	0.2123829654195555	T	T	T
0.4999999999999911	0.7500657030223350	0.1047483626335719	F	F	F
0.7331789680856922	0.4872287823329301	0.3179696608839698	T	T	T
0.7500657030223350	0.4999999999999911	0.1441744226128918	F	F	F
0.5071428136351541	0.7343267043972187	0.3574786644364688	T	T	T
0.7500657030223350	0.7500657030223350	0.0394260599793199	F	F	F
0.4874195265871009	0.4906809984794088	0.2499833684331026	T	T	T
0.0746358734809898	0.1163460916807302	0.4037627546616108	T	T	T
0.3085455655097633	0.1688584837200593	0.4847766577704535	T	T	T
0.5333912411211246	0.0572241572857247	0.4078425937953557	T	T	T
0.1223326777022029	0.4502844342479432	0.4985771325290303	T	T	T
0.9904366620954643	0.6698255858905782	0.5526647868822573	T	T	T
0.3770762295770865	0.1431582167097337	0.5974566580182435	T	T	T
0.0090252891737704	0.9944297861030978	0.3374766341262712	T	T	T
0.2500657030223364	0.2500657030223364	0.1244398483281657	F	F	F
0.0000000000000000	0.2500657030223364	0.0197345742847261	F	F	F
0.2575841221795992	0.9999400395924894	0.2310584498601402	T	T	T
0.5128521454456401	0.9662393711562373	0.3378711871234195	T	T	T
0.7500657030223350	0.2500657030223364	0.1244398483281657	F	F	F
0.4999999999999911	0.2500657030223364	0.0197345742847261	F	F	F
0.7536339822901713	0.0002854996763065	0.2309396706642860	T	T	T
0.9806033088621448	0.5490065401269418	0.3334863521639996	T	T	T
0.2500657030223364	0.7500657030223350	0.1244398483281657	F	F	F
0.0000000000000000	0.7500657030223350	0.0197345742847261	F	F	F
0.2338133003411992	0.5001107597423650	0.2291544675791310	T	T	T
0.4769456001583055	0.5149709452286623	0.3339654424191787	T	T	T
0.7500657030223350	0.7500657030223350	0.1244398483281657	F	F	F
0.4999999999999911	0.7500657030223350	0.0197345742847261	F	F	F
0.7378368699613225	0.4957041497475055	0.2303111934123589	T	T	T

Table S6. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 4a.

1.

O	-0.232613	0.001115	1.533887
O	-0.323968	-1.383329	-0.732639
O	-0.323920	1.382560	-0.734449
O	2.063483	-1.457080	0.813029
O	2.063605	1.457983	0.811270
O	2.110401	-3.046496	-1.790670
O	2.047421	-0.001070	-1.642164
O	2.110468	3.044344	-1.794197
V	-1.119518	0.000068	-0.094390
O	2.056816	0.001938	3.552290
TI	1.516721	0.001046	1.835487
TI	1.556113	1.591812	-0.899212
TI	1.555982	-1.592997	-0.897331
H	2.519773	3.897279	-1.614512
H	2.516844	-3.900605	-1.610102
H	1.642436	0.004119	4.421820
S	-3.803746	0.000021	0.018252
O	-4.531153	-1.275708	-0.003278
O	-2.619613	0.000921	1.126475
O	-4.531415	1.275570	-0.005082
O	-2.627534	-0.000702	-1.156354

2.

O	0.122668	0.203459	1.502225
O	0.071344	1.110498	-1.069125
O	0.105626	-1.481324	-0.551403
O	-2.223470	1.486579	0.571033
O	-2.192779	-1.358802	1.107867
O	-2.371497	2.594829	-2.279154
O	-2.301584	-0.391072	-1.594473
O	-2.286138	-3.410418	-1.170012
V	0.960342	-0.055435	-0.101425
O	-2.151572	0.571810	3.521759
TI	-1.633180	0.255708	1.825652
TI	-1.754178	-1.798595	-0.579208
TI	-1.782170	1.310986	-1.163898
H	-2.598569	-4.245514	-0.806740
H	-2.875581	3.413885	-2.245214
H	-1.727688	0.689877	4.378261
S	3.559131	-0.734823	-0.035104
O	4.484118	0.392182	0.255646
O	2.408467	-0.786257	1.065985
O	4.116328	-2.043635	-0.390560
O	2.472341	-0.228662	-1.176019

```
  C      2.233371    3.020394   -0.354586
  H      2.669289    2.686441   -1.305808
  H      1.236024    3.431846   -0.531786
  H      2.870151    3.792090    0.097154
  O      2.088029    1.920416    0.561542
  H      2.986771    1.606166    0.777553
3.
  O  0.00018000    1.53721800   -0.08517300
  O  0.10748100   -0.49507700    1.61312400
 O  -0.12712300   -0.78639000   -1.20095900
 O  2.43469700    1.11338600    1.23559900
 O  2.18138800    0.79501700   -1.65297100
  O  2.74065100   -1.29899500    3.08624500
  O  2.35765700   -1.49350100    0.07371500
  O  2.12216100   -1.99137500   -2.93972500
  V  -0.85395300   -0.07872600    0.24623900
 O  2.14892500    3.67671100   -0.50858600
 Ti  1.71917000    1.94176800   -0.27375400
  Ti  1.69811200   -0.93333400   -1.54508900
 Ti  2.00583500   -0.58255400    1.60903900
 H  2.42543500   -1.89100500   -3.84778900
 H  3.23596500   -0.99630100    3.85448000
 H  1.68437300    4.51556800   -0.59607200
 S  -3.99011000    0.56381300   -0.03356800
 O  -4.78874200    1.49490400    0.76908600
 O  -2.36906200    0.72507100    0.59658000
 O  -3.84324300    0.75718500   -1.48766300
 O  -4.21523700   -0.92465200    0.37027900
 C  -1.62660000   -3.00686500   -0.14657500
 H  -0.83729400   -3.42641100    0.49225200
 H  -2.52179700   -3.63748500   -0.07948700
  H  -1.27833800   -2.97195200   -1.18825000
 O  -1.95595900   -1.69700000    0.30505400
 H  -3.12482600   -1.43089300    0.33671800

4.
  O      0.167410    1.439285   -0.053277
  O      0.056137   -0.892860   -1.167731
  O     -0.168381   -0.680040    1.574531
  O     -2.065116    0.933580   -1.645967
  O     -2.307898    1.213368    1.252909
  O     -2.279655   -1.801882   -2.995847
  O     -2.519356   -1.354745    0.026612
  O     -2.894138   -1.173000    3.044300
  V      0.873561   -0.309650    0.269179
  O     -1.714144    3.788553   -0.430895
  TI    -1.478672    2.007407   -0.234504
```

TI	-2.075875	-0.519140	1.579804
TI	-1.774398	-0.826626	-1.566303
H	-3.377705	-0.812143	3.794901
H	-2.590001	-1.628630	-3.890632
H	-1.123486	4.547429	-0.486350
S	3.830824	0.570543	-0.043795
O	3.505410	0.490908	-1.481830
O	2.417037	0.577887	0.772393
O	4.695609	1.621048	0.492653
O	4.434574	-0.854532	0.473660
C	1.518294	-3.120528	-0.132630
H	0.784227	-3.528852	0.579148
H	1.068642	-3.081868	-1.136481
H	2.405005	-3.767711	-0.153163
O	1.910212	-1.818074	0.269830
H	3.673630	-1.483858	0.409299

5.

O	0.391740	0.202065	1.242100
O	1.366360	-1.688715	-0.259573
O	0.390136	0.613863	-1.404729
O	3.128488	-0.252043	1.474249
O	2.085347	2.224793	0.292182
O	4.388064	-2.428381	-0.241433
O	3.229989	0.193261	-1.353233
O	2.273474	2.771558	-2.686384
V	-0.083923	-0.716314	-0.424929
O	1.742240	1.814817	3.398615
TI	1.806435	1.055296	1.749271
TI	2.035850	1.569017	-1.356340
TI	3.144143	-1.123698	-0.077909
H	2.389561	3.726500	-2.722639
H	5.025031	-2.834362	0.355339
H	1.053537	1.822144	4.072116
S	-2.464827	-0.929398	0.973074
O	-1.270715	-1.885663	1.010647
O	-1.973964	0.154001	-0.021700
O	-3.015657	-0.435441	2.240820
O	-3.601156	-1.794501	0.196800
C	-0.972906	-3.168610	-1.720069
H	-1.290732	-3.400759	-2.745108
H	-0.018105	-3.668606	-1.493119
H	-1.739085	-3.495249	-1.004570
O	-0.793064	-1.771176	-1.620955
H	-4.449682	-1.268181	0.161423
C	-5.431142	0.819915	-0.973784
H	-6.287586	1.171193	-1.577891

O	-5.800258	-0.336671	-0.238809
H	-6.376724	-0.060124	0.487950
H	-4.602329	0.514950	-1.631417
C	-4.253892	2.844687	-0.646212
H	-4.012195	3.543507	0.160524
H	-3.322451	2.437114	-1.068655
H	-4.818751	3.377450	-1.429910
O	-5.033123	1.804551	-0.059839

6.

O	-0.784738	1.509995	-0.125357
O	-0.690879	-0.640766	-1.641601
O	-0.241200	-0.630150	1.212898
O	-3.203433	0.701288	-1.239750
O	-2.744146	0.690727	1.664042
O	-3.268819	-1.886799	-2.843135
O	-2.690500	-1.738332	0.154781
O	-2.248826	-1.912791	3.183747
V	0.331488	-0.058078	-0.353530
O	-3.051682	3.476799	0.246413
TI	-2.483377	1.755481	0.142573
TI	-2.027633	-0.943083	1.668132
TI	-2.547487	-0.936554	-1.481077
H	-2.644953	-1.733523	4.042486
H	-3.900454	-1.686569	-3.541461
H	-2.567132	4.309332	0.220967
S	2.752025	2.071827	0.160383
O	1.926643	3.259080	0.430824
O	1.666927	0.973943	-0.742029
O	3.133907	1.201213	1.317929
O	3.838705	2.230237	-0.866028
C	1.011471	-2.872736	-0.335397
O	1.464665	-1.546693	-0.473329
H	4.954693	0.951447	-0.988158
C	3.775918	-1.244777	-0.529329
O	5.478300	0.103894	-0.991971
H	6.134899	0.222631	-0.293561
H	0.565565	-3.028086	0.661531
H	0.251803	-3.099865	-1.101511
H	1.857191	-3.565110	-0.464213
H	3.489919	-0.465468	0.172405
H	3.605888	-1.180375	-1.596848
C	4.471898	-2.497219	1.329754
H	4.082951	-1.618748	1.855686
H	3.945280	-3.406354	1.632730
H	5.549632	-2.610716	1.480736
O	4.258741	-2.351924	-0.107148

7.

O	-0.616688	1.650668	-0.351140
O	-0.323499	-0.823560	-1.314557
O	-0.481308	-0.165626	1.594876
O	-2.798030	0.510334	-1.708657
O	-2.955182	1.157053	1.123033
O	-2.583588	-2.415157	-2.671234
O	-2.633871	-1.553616	0.260956
O	-2.902979	-1.068242	3.264929
V	0.307121	0.149848	0.034578
O	-3.036132	3.479259	-0.909072
TI	-2.406839	1.839683	-0.497355
TI	-2.313592	-0.442228	1.678355
TI	-2.138868	-1.157624	-1.456153
H	-3.371289	-0.736841	4.037332
H	-2.944196	-2.459384	-3.562076
H	-2.684731	4.367909	-1.024338
S	3.475757	2.169486	0.463260
O	2.573209	3.206845	0.980312
O	1.832778	0.664597	-0.030974
O	4.183648	1.276223	1.390976
O	3.929736	2.253651	-0.940516
C	0.747381	-2.908195	1.357189
O	1.384072	-1.895130	0.563566
H	4.182266	0.546361	-2.010123
C	2.210905	-2.457418	-0.488840
O	4.234988	-0.327031	-2.429223
H	4.732210	-0.183028	-3.242014
H	0.349931	-2.417531	2.248803
H	-0.066576	-3.388007	0.791541
H	1.487955	-3.660613	1.648657
H	2.537266	-1.604221	-1.094068
H	1.602903	-3.158336	-1.076595
C	4.349017	-2.364659	0.528360
H	4.014233	-1.749314	1.374467
H	5.126498	-3.058703	0.863365
H	4.739745	-1.717449	-0.269200
O	3.277677	-3.179488	0.024216

8.

O	-0.553510	1.747009	-0.243672
O	-0.339453	-0.666810	-1.448659
O	-0.240653	-0.290903	1.495907
O	-2.844297	0.685273	-1.496156
O	-2.750803	1.044797	1.381666
O	-2.703354	-2.129945	-2.762957

O	-2.503856	-1.561750	0.236078
O	-2.497073	-1.376890	3.285127
V	0.388265	0.222577	-0.087177
O	-3.049594	3.551535	-0.386796
TI	-2.357700	1.896626	-0.200965
TI	-2.053612	-0.592849	1.720667
TI	-2.160400	-0.993911	-1.469828
H	-2.887070	-1.126135	4.128119
H	-3.200643	-2.100187	-3.585941
H	-2.730039	4.450161	-0.515852
S	3.965772	2.008422	0.042992
O	3.295697	3.265042	-0.319689
O	1.912003	0.686042	-0.227024
O	4.120446	1.641127	1.458373
O	4.669635	1.230892	-0.989614
C	0.906738	-3.098114	0.783700
O	1.560381	-1.972260	0.183852
C	2.437535	-2.347972	-0.888522
H	0.448330	-2.746336	1.711628
H	0.135302	-3.501327	0.109319
H	1.641558	-3.878574	1.012625
H	2.738238	-1.401018	-1.354836
H	1.898028	-2.990528	-1.598394
C	4.493399	-2.313062	0.291454
H	4.071149	-1.954936	1.240688
H	5.335099	-2.983284	0.493226
H	4.837275	-1.451167	-0.299823
O	3.534675	-3.082263	-0.446507

Table S7. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 4b.

```
9.
  O      0.040971   -0.210426    1.504013
  O      0.185927    0.770455   -1.049067
  O     -0.261977   -1.798184   -0.600797
  O     -2.022769    1.534611    0.630891
  O     -2.521142   -1.279198    1.052631
  O     -1.912992    2.760934   -2.180810
  O     -2.414006   -0.203501   -1.598320
  O     -2.988398   -3.178317   -1.305193
  V      0.821511   -0.561388   -0.099743
  O     -2.143677    0.508938    3.540508
  TI    -1.675813    0.174132    1.834341
  TI    -2.153112   -1.729211   -0.647352
  TI    -1.582250    1.355147   -1.103886
  H     -3.474144   -3.941050   -0.974650
  H     -2.330005    3.626069   -2.117774
  H     -1.703664    0.560592    4.395523
  S      3.305284   -1.582244   -0.070595
  O      4.366013   -0.592688    0.263824
  O      2.148402   -1.519791    1.027363
  O      3.699204   -2.940913   -0.455412
  O      2.304622   -0.909553   -1.192798
  C      2.436356    2.417799   -0.109876
  H      2.283570    2.213830   -1.183939
  H      3.455413    2.811063    0.054317
  O      2.261813    1.236350    0.646848
  H      3.135601    0.814623    0.772743
  C      1.508812    4.554577   -0.362216
  H      0.735685    5.197732    0.071279
  H      2.488687    5.051308   -0.258114
  H      1.299101    4.401387   -1.434946
  O      1.471169    3.328348    0.354247

10.
  O     -0.069194    0.477222   -1.338925
  O     -0.200137   -1.752563   -0.120769
  O     -0.030685    0.371057    1.487772
  O     -2.475926   -0.930940   -1.501757
  O     -2.352105    1.448803    0.121490
  O     -2.577946   -3.726373   -0.205515
  O     -2.505313   -1.089549    1.387906
  O     -2.484102    1.369355    3.168164
  V      0.761010   -0.263762    0.115311
  O     -2.348329    1.761060   -2.957215
```

TI	-1.833761	0.786970	-1.534545
TI	-1.924206	0.602402	1.642042
TI	-2.012569	-2.020076	-0.127001
H	-2.964562	2.155606	3.446885
H	-2.713866	-4.432754	-0.844386
H	-2.003321	2.103385	-3.787396
S	3.849138	-1.216625	0.025032
O	3.722877	-1.617113	-1.388708
O	4.213248	0.289333	0.205450
O	4.532644	-2.080587	0.991707
O	2.210208	-1.126085	0.597295
C	1.907071	2.413467	-0.970759
H	2.920462	2.832470	-1.093170
H	1.466098	2.174491	-1.943547
C	1.583439	3.916090	0.831861
H	0.856405	4.666676	1.158544
H	1.722414	3.166845	1.624082
H	2.546740	4.409047	0.622567
O	2.051401	1.217816	-0.210508
O	1.051313	3.324402	-0.356102
H	3.185231	0.868207	-0.016045

11.

O	0.129427	-1.706267	0.137808
O	0.016127	0.640122	1.162625
O	-0.151950	0.345761	-1.585453
O	-2.138072	-1.108243	1.654769
O	-2.324263	-1.472301	-1.230539
O	-2.311316	1.680634	2.915835
O	-2.538394	1.126150	-0.095126
O	-2.865960	0.852068	-3.108545
V	0.842903	0.001779	-0.256400
O	-1.825925	-3.998139	0.548132
TI	-1.542424	-2.232180	0.296738
TI	-2.070604	0.248474	-1.611666
TI	-1.811397	0.648181	1.522592
H	-3.327680	0.463427	-3.859111
H	-2.633983	1.538680	3.811671
H	-1.260710	-4.771774	0.647199
S	3.770160	-0.981021	0.030243
O	3.436744	-0.931182	1.468165
O	2.363574	-0.902371	-0.795216
O	4.593989	-2.051639	-0.530483
O	4.434629	0.431403	-0.441572
C	1.649526	2.736361	0.354897
H	1.339034	2.616891	1.410411
H	2.555192	3.369277	0.302731

O	1.959801	1.487515	-0.183656
H	3.696977	1.087872	-0.364609
C	0.283676	4.625619	0.037364
H	1.146925	5.305428	-0.061699
H	-0.528751	4.980425	-0.604880
H	-0.055622	4.627910	1.087330
O	0.608771	3.312355	-0.401487

12.

O	0.572469	-1.306668	-0.715825
O	0.673652	1.286917	-0.877053
O	0.332062	0.055753	1.559477
O	3.025802	-0.224508	-1.465821
O	2.671253	-1.568317	1.119993
O	3.274026	2.801941	-1.669547
O	2.870234	1.275302	0.967366
O	2.619392	-0.017332	3.723765
V	-0.396025	0.229674	0.021806
O	2.651371	-3.347140	-1.486368
TI	2.241007	-1.756780	-0.711271
TI	2.194172	-0.086235	1.969008
TI	2.545701	1.370020	-0.837367
H	2.990840	-0.641439	4.355865
H	3.832245	2.925487	-2.444004
H	2.102095	-4.007118	-1.923164
S	-2.514876	-1.195965	-1.041238
O	-1.651730	-0.162762	-1.764420
O	-1.862245	-1.227497	0.370623
O	-2.727215	-2.505764	-1.667091
O	-3.938600	-0.436847	-0.866915
C	-2.122172	2.523185	-0.393483
H	-1.310845	3.041014	-0.945348
H	-2.834890	2.077393	-1.109398
O	-1.548664	1.510297	0.373981
H	-4.533362	-0.983370	-0.273977
C	-4.957367	-1.603517	2.244983
H	-5.362152	-0.676020	2.673339
H	-5.252058	-2.464347	2.860066
O	-5.397510	-1.784655	0.883925
H	-6.358798	-1.844585	0.848580
H	-3.865600	-1.540462	2.205621
C	-3.440030	4.447524	-0.196541
H	-4.211952	4.053077	-0.879697
H	-3.917192	5.069742	0.567556
H	-2.731868	5.065302	-0.775718
O	-2.772029	3.398906	0.491493

13.

O	0.237448	-1.631350	-0.392691
O	0.469081	0.787358	-1.398571
O	0.115056	0.186256	1.405571
O	2.734959	-0.905343	-1.430398
O	2.361219	-1.558822	1.398899
O	3.208054	1.944197	-2.379718
O	2.694738	1.140847	0.526295
O	2.308351	0.641004	3.531438
V	-0.566138	0.075428	-0.226658
O	2.233788	-3.905193	-0.654084
TI	1.909658	-2.158127	-0.303806
TI	1.923095	0.122454	1.842147
TI	2.366263	0.828568	-1.233910
H	2.631882	0.208960	4.328274
H	3.772079	1.821186	-3.150362
H	1.655788	-4.647785	-0.861416
S	-3.321185	-1.665207	-0.173108
O	-2.897937	-2.966228	-0.712649
O	-2.062986	-0.539966	-0.824763
O	-3.214020	-1.418785	1.291660
O	-4.547775	-1.060499	-0.812894
C	-0.884635	2.865111	0.822488
O	-1.496444	1.770148	0.177682
H	-5.228771	0.266844	-0.128495
C	-3.506306	1.632209	0.321363
O	-5.380298	1.186038	0.256008
H	-5.732357	1.042926	1.146025
H	-0.401958	2.531083	1.752044
H	-1.672786	3.606538	1.052713
H	-3.332704	0.894733	1.090903
H	-3.449287	1.363151	-0.720976
H	-3.653337	2.673126	0.588056
C	-0.357417	4.126502	-1.116116
H	-0.796712	3.415998	-1.829894
H	-1.106654	4.890202	-0.846915
H	0.508568	4.615564	-1.573602
O	0.121536	3.460255	0.052290

Table S8. Cartesian or fraction coordinates for the potential energy surfaces shown in Figure 7.

1a.

O	-0.232613	0.001115	1.533887
O	-0.323968	-1.383329	-0.732639
O	-0.323920	1.382560	-0.734449
O	2.063483	-1.457080	0.813029
O	2.063605	1.457983	0.811270
O	2.110401	-3.046496	-1.790670
O	2.047421	-0.001070	-1.642164
O	2.110468	3.044344	-1.794197
V	-1.119518	0.000068	-0.094390
O	2.056816	0.001938	3.552290
TI	1.516721	0.001046	1.835487
TI	1.556113	1.591812	-0.899212
TI	1.555982	-1.592997	-0.897331
H	2.519773	3.897279	-1.614512
H	2.516844	-3.900605	-1.610102
H	1.642436	0.004119	4.421820
S	-3.803746	0.000021	0.018252
O	-4.531153	-1.275708	-0.003278
O	-2.619613	0.000921	1.126475
O	-4.531415	1.275570	-0.005082
O	-2.627534	-0.000702	-1.156354

1b.

O	-0.885132	-1.165285	1.416844
O	-1.584561	1.231879	0.000000
O	0.883324	1.068079	1.438941
O	-0.885132	-1.165285	-1.416844
O	1.567503	-1.298296	0.000000
O	-1.735127	1.312092	-3.053427
O	0.883324	1.068079	-1.438941
O	3.596272	1.032177	0.000000
V	-0.122387	-1.912423	0.000000
O	-1.735127	1.312092	3.053427
O	-0.217413	-3.485584	0.000000
TI	-0.885132	0.679062	-1.594703
TI	1.874420	0.498470	0.000000
TI	-0.885132	0.679062	1.594703
H	4.476163	0.643005	0.000000
H	-1.528074	1.609049	-3.944644
H	-1.528074	1.609049	3.944644

2a.

O	0.201658	-0.772541	1.321362
O	0.296924	1.463078	-0.148042

O	0.031962	-0.841772	-1.399446
O	-1.980882	1.027233	1.479412
O	-2.255705	-1.527075	0.134766
O	-1.941214	3.658029	-0.094738
O	-2.210412	0.907852	-1.379802
O	-2.548341	-1.715765	-2.912746
V	1.033757	-0.091240	-0.186104
O	-2.076717	-1.530972	3.213696
TI	-1.551606	-0.764857	1.670198
TI	-1.834624	-0.881072	-1.490423
TI	-1.533260	1.910167	-0.020698
H	-3.040903	-2.516287	-3.120002
H	-2.178472	4.373257	0.504536
H	-1.681733	-1.875085	4.021049
S	3.686344	0.308959	-0.015949
O	4.387596	1.595345	-0.061960
O	2.567920	0.210782	1.103753
O	4.477960	-0.949189	-0.087402
O	2.531763	0.221414	-1.212128
O	1.968385	-2.244209	-0.085778
H	2.939734	-2.136920	-0.166582
H	1.825046	-2.520704	0.829326

2b.

O	-1.076289	-1.579654	-0.289368
O	-0.269150	0.103930	1.930161
O	1.647300	-1.366547	0.404487
O	-1.221894	1.424982	-0.458541
O	0.558053	-0.086831	-1.871297
O	-0.465506	3.169305	1.938164
O	1.537728	1.520394	0.251340
O	3.617987	0.052512	-1.481584
V	-1.165028	-0.143333	-1.347407
O	-0.174771	-2.930130	2.339449
O	-2.029837	-0.278135	-2.665298
TI	-0.114394	1.668266	0.990588
TI	1.970616	0.030419	-0.736074
TI	0.012200	-1.544213	1.192533
H	4.000114	0.018235	-2.363688
H	0.026798	3.841539	2.418470
H	0.009803	-3.874175	2.339823
O	-3.459332	-0.094847	-0.336095
H	-3.625032	0.856771	-0.291512
H	-4.035619	-0.423912	-1.039115

3a.

O	-0.039184	0.184689	1.631961

O	-0.309441	-1.014074	-0.823912
O	0.255333	1.496912	-0.760323
O	1.977013	-1.687288	0.780683
O	2.584386	1.094749	0.824003
O	1.580783	-3.234783	-1.862934
O	2.253860	-0.263133	-1.695774
O	2.752083	2.813403	-1.780443
V	-0.899953	0.316368	0.165734
O	2.433805	-0.336503	3.486432
TI	1.822001	-0.218733	1.802212
TI	2.031744	1.405689	-0.909526
TI	1.411227	-1.676182	-0.986474
H	3.608355	3.235557	-1.898814
H	1.795040	-3.561686	-2.742520
H	2.716389	-1.021601	4.101456
S	-4.108855	-0.189080	-0.056505
O	-4.013673	-0.529152	-1.488178
O	-2.458557	-0.384159	0.522157
O	-4.906543	-1.013660	0.856620
O	-4.253385	1.332072	0.209707
O	-1.956637	1.964720	0.103851
H	-3.116881	1.804531	0.116454
H	-1.590440	2.664621	-0.451866

3b.

O	-1.109897	-1.158837	1.034143
O	0.730126	0.976211	1.697780
O	1.655458	-1.347312	0.328117
O	-1.210763	1.321923	-0.366479
O	-0.410257	-0.859353	-1.593726
O	0.522030	3.738269	0.316828
O	1.499346	1.150797	-1.090062
O	2.463448	-1.298094	-2.651157
V	-1.707065	-0.497019	-0.444010
O	0.977983	-1.576018	3.313672
O	-2.934542	-1.478608	-1.083218
TI	0.367967	1.940865	0.162057
TI	1.406826	-0.618499	-1.354820
TI	0.623450	-0.827137	1.712054
H	3.044230	-0.962810	-3.341162
H	-0.032613	4.503455	0.136690
H	1.470355	-2.333909	3.644610
O	-3.519482	0.367674	0.011950
H	-3.611577	1.288514	-0.261686
H	-3.676865	-0.652065	-0.733423

4a.

O	0.055025	0.092540	1.620374
O	0.439909	0.469967	-1.145030
O	-0.537204	-1.745029	-0.184258
O	-1.672779	1.937660	0.202650
O	-2.687259	-0.544496	1.170685
O	-1.253253	2.516144	-2.783905
O	-2.264328	-0.127438	-1.686431
O	-3.285876	-2.923276	-0.740784
V	0.875217	-0.480171	0.232457
O	-2.177924	1.616693	3.214961
TI	-1.690430	0.866034	1.656702
TI	-2.264904	-1.475485	-0.383917
TI	-1.220624	1.297215	-1.466097
H	-3.161206	-3.867947	-0.874222
H	-1.562630	2.585262	-3.693112
H	-2.312335	2.497821	3.579231
S	3.981452	0.171017	-0.064640
O	3.837259	0.088961	-1.527891
O	2.471910	0.337595	0.576182
O	4.846235	1.167228	0.568362
O	4.379207	-1.277159	0.553463
O	1.869367	-2.032711	0.228353
H	3.584079	-1.855629	0.408918
H	1.327647	-2.796084	-0.014053

4b.

O	-1.159919	-0.540678	1.363202
O	1.534783	0.415729	1.505897
O	0.942296	-1.865527	-0.103288
O	-0.528265	1.708245	0.108470
O	-1.134609	-0.347446	-1.453189
O	2.096149	3.212484	0.234289
O	1.555066	0.594747	-1.411625
O	1.003282	-1.814217	-3.172589
V	-1.887654	0.241251	-0.001449
O	0.959570	-2.170148	2.962388
O	-3.413801	-0.656817	-0.079440
TI	1.211425	1.628195	0.127422
TI	0.647257	-0.912012	-1.649109
TI	0.623515	-1.130667	1.524203
H	1.547402	-1.661019	-3.951734
H	1.825930	4.134278	0.288053
H	1.133944	-3.101024	3.132689
O	-2.982121	1.696933	0.096421
H	-2.434117	2.492924	0.159980
H	-4.244912	-0.161720	-0.055299