

Supporting Information

First-Principles Study on Unidirectional Proton Transfer on Anatase TiO₂ (101) Surface Induced by External Electric Fields

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S1. Electronic Polarization Directly Induced by External Electric Field

Our approach assumes that electronic polarization directly induced by the electric fields (EFs) can be neglected. To confirm this assumption, we evaluated the electronic polarization of two water molecules (within the system used in this study) directly induced by an external EF. The energy change due to the electrostatic interaction between the external EF ($\varepsilon = 10^9$ V/m) and the induced dipole moment $\Delta\mu$, which corresponds to $\Omega\mathbf{P}$, is given as

$$\begin{aligned}\Delta\mu\varepsilon &= 2 \cdot 4\pi\varepsilon_0\alpha\varepsilon^2 \\ &= 2 \cdot 4\pi \cdot (8.854 \cdot 10^{-12} \text{ C}^2 \cdot \text{J}^{-1} \cdot \text{m}^{-1}) \cdot (1.45 \cdot 10^{-30} \text{ m}^3) \cdot (10^9 \text{ V} \cdot \text{m}^{-1})^2 \\ &= 3.226 \cdot 10^{-22} \text{ J} = 2.01 \cdot 10^{-3} \text{ eV}\end{aligned}$$

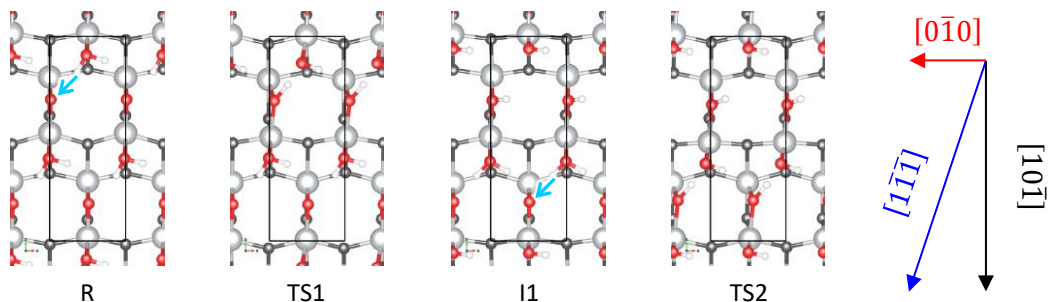
where the polarizability of the water molecule α ($1.45 \cdot 10^{-30} \text{ m}^3$) and the vacuum permittivity ε_0 ($8.854 \cdot 10^{-12} \text{ C}^2 \cdot \text{J}^{-1} \cdot \text{m}^{-1}$) were taken from the literature.^{S1} The polarization \mathbf{P} represents the dipole moment per unit volume,^{S2} and the change in \mathbf{P} of two water molecules directly induced by the external EF, \mathbf{P}_{EF} , is given by $2 \cdot 4\pi\varepsilon_0\alpha \cdot \varepsilon^2 = \Omega\mathbf{P}_{\text{EF}}$.^{S3} The resultant energy change calculated for the water molecules ($2.01 \cdot 10^{-3}$ eV) is 45 times smaller than, for example, the activation energy change for the R→TS1 transition (0.09 eV) discussed in the main manuscript. The large difference in the energy change was solely attributed to the amount of polarization. In other words, the polarization induced by an external EF contributes much less to the energy profile than the polarization due to the chemical reactions discussed in the main manuscript.

References

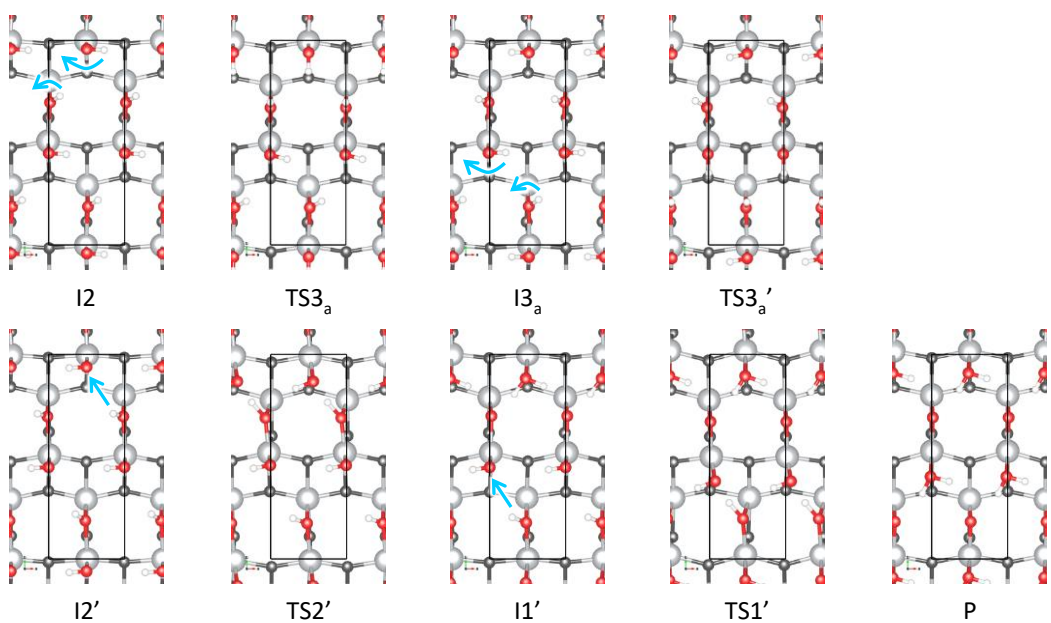
- S1. *CRC Handbook of Chemistry and Physics*, ed. W. M. Haynes, CRC Press, Boca Raton, FL, 2014.
- S2. J. D. Jackson, *Classical Electrodynamics*, 3rd ed., Wiley, 1999.
- S3. C. J. F. Böttcher, *Theory of Electronic Polarization*, 2nd ed., Elsevier, Amsterdam, 1973.

S2. Geometrical Structures

(a) Structures in common to both pathways



(b) Structures specific to the $[0\bar{1}0]$ pathway



(c) Structures specific to the $[1\bar{1}\bar{1}]$ pathway

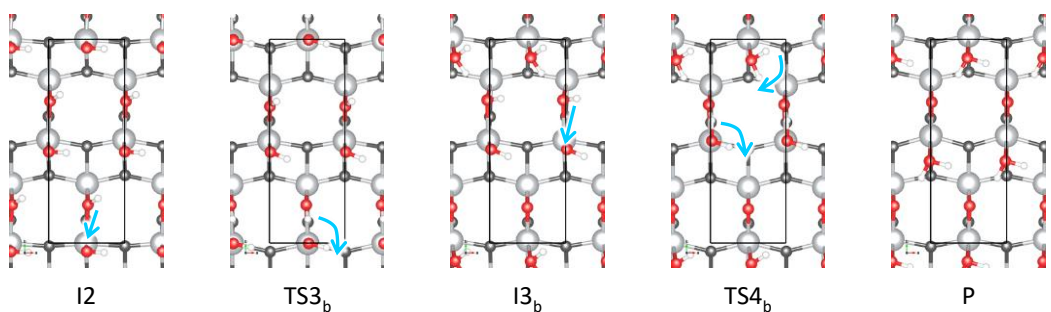


Figure S2: Geometrical structures (a) common to both pathways and specific to the (b) $[0\bar{1}0]$ and (c) $[1\bar{1}\bar{1}]$ pathways. The direction of the PT toward the next state is indicated by the cyan arrow.

S3 Dependence of the Energy Profile on the Direction of Applied Electric Field

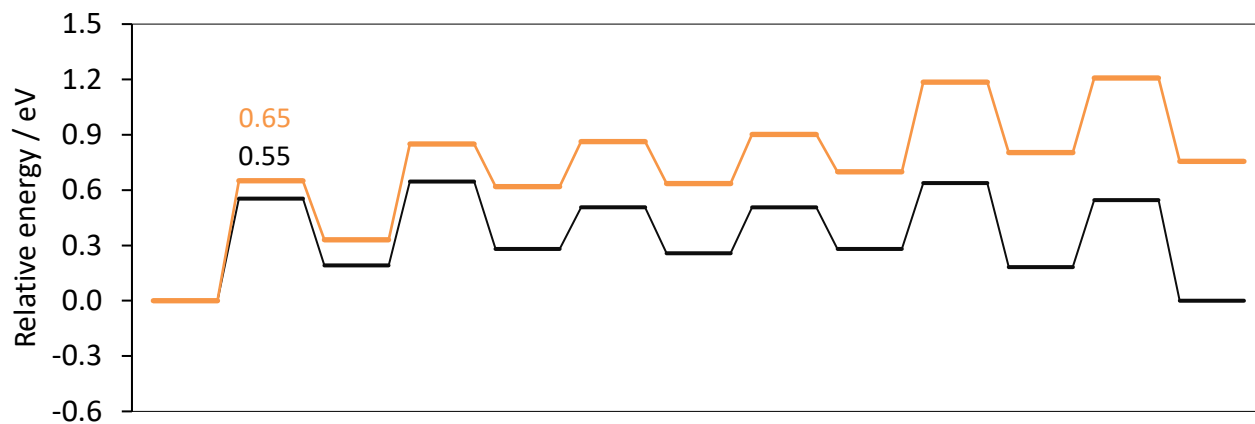


Figure S3: Energy diagram of the PT toward the $[0\bar{1}0]$ direction without an EF (black line, the same as that of Figure 1 in the main manuscript) and under an 10^9 V/m EF along the $[010]$ direction (orange line).

S4 Cartesian Coordinates of Optimized Structures

R, P			
O	1.9409371054	1.8630676675	12.9543715864
O	0.0521204870	7.0827602708	12.9515024412
Ti	1.8938721217	0.1733927351	12.2076530749
Ti	0.0027374889	5.3918362629	12.2038052356
O	1.8947465134	4.8513296547	12.2497364931
O	0.0038298568	10.0618734886	12.2516528536
O	0.0068196274	3.3840763389	11.4222918270
O	1.8981894867	8.5995325841	11.4107232403
Ti	1.8885952558	2.9930315453	11.3885951786
Ti	-0.0016481269	8.2099141816	11.3809548154
O	1.8880995129	1.0606080386	10.5985031789
O	-0.0110210099	6.2756770994	10.5948811316
O	1.8967762433	3.2493586307	9.4043123360
O	0.0063741789	8.4632846115	9.3997700210
Ti	0.0006866699	6.6379874266	8.6510297939
Ti	1.8916565005	1.4247468621	8.6558946681
O	1.8895842446	6.2193400733	8.5421548557
O	-0.0012058175	1.0052889987	8.5462416847
O	-0.0000188353	4.7382275985	7.9311846782
O	1.8909142687	9.9549026705	7.9304916228
Ti	1.8904501221	4.3479173362	7.8101702938
Ti	-0.0003005495	9.5649110464	7.8093358230
O	1.8884188481	2.4654175466	7.0602968496
O	-0.0024284270	7.6799956898	7.0584856668
O	1.8908630000	4.6368580000	5.8721510000
O	0.0000000000	9.8512340000	5.8721320000
Ti	0.0000000000	7.9793790000	5.1437830000
Ti	1.8908630000	2.7649550000	5.1437830000
O	1.8908630000	7.5869150000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	6.1075240000	4.4154330000
O	1.8908630000	0.8930530000	4.4154150000
Ti	1.8908630000	5.7150320000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	1.8908630000	3.8431630000	3.5343580000
O	0.0000000000	9.0575120000	3.5343290000
O	1.8908630000	6.0081940000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	9.3507150000	1.6194540000
Ti	1.8908630000	4.1362920000	1.6194540000
O	1.8908630000	8.9582510000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	7.4788600000	0.8911050000
O	1.8908630000	2.2643890000	0.8910870000
Ti	1.8908630000	7.0863680000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	1.8908630000	5.2144990000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	1.8309068966	9.3080879301	14.1464620156
H	2.7474148702	9.0309828082	14.3363333603
H	1.3885456598	8.4764046340	13.8522028055
O	-0.0586088843	4.1196581074	14.1577980942
H	0.8620095640	3.8804112592	14.3762327909
H	-0.4640964295	3.2704343178	13.8631045107

TS1			
O	-1.8454644106	1.8231327436	13.0043408001
O	0.2376132255	-3.2180240684	12.9559937126
Ti	-1.9339098484	0.0717798720	12.3724456799
Ti	0.0737481203	-5.0254179289	12.2007288238
O	-1.8508550141	4.9013815004	12.2881255585
O	-0.0498964257	-0.3739805251	12.2041907017
O	0.0321799150	3.4295749362	11.4918572472
O	-1.8971735680	-1.7760762504	11.2319649109
Ti	1.9024310585	2.9328270253	11.4329656282
Ti	-0.0528953922	-2.1469848734	11.2444951922
O	1.8508582998	1.0865587224	10.6603260459
O	-0.0370491745	-4.1284497204	10.6121251752
O	-1.8701597268	3.2501914860	9.4442067915
O	0.0045781994	-1.9830343710	9.3349170357
Ti	-0.0041934470	-3.8294050270	8.6096936052
Ti	-1.8968439619	1.4094317737	8.7517525752
O	1.8825614348	-4.2363567270	8.5489808250
O	-0.0099208330	0.9951590935	8.5816289188
O	-0.0033601245	4.7094327107	7.9265169740
O	-1.8971022400	-0.4643910125	7.9355853139
Ti	1.8857526746	4.2936529810	7.8083075004
Ti	-0.0072152044	-0.8385849588	7.7851478022
O	1.8779431763	2.4576107089	7.0806698195
O	-0.0090857651	-2.7676178250	7.0420201231
O	-1.8908370000	4.6368580000	5.8721510000
O	0.0000000000	-0.5773160000	5.8721320000
Ti	0.0000000000	-2.4491710000	5.1437830000
Ti	-1.8908370000	2.7649550000	5.1437830000
O	-1.8908370000	-2.8416350000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	-4.3210260000	4.4154330000
O	-1.8908370000	0.8930530000	4.4154150000
Ti	-1.8908370000	-4.7135180000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	-1.8908370000	3.8431630000	3.5343580000
O	0.0000000000	-1.3710380000	3.5343290000
O	-1.8908370000	-4.4203560000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	-1.0778350000	1.6194540000
Ti	-1.8908370000	4.1362920000	1.6194540000
O	-1.8908370000	-1.4702990000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	-2.9496900000	0.8911050000
O	-1.8908370000	2.2643890000	0.8910870000
Ti	-1.8908370000	-3.3421820000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	-1.8908370000	-5.2140510000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	1.6193503250	-1.3340968353	13.8843766489
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H	0.9258243998	-2.4183326035	13.4818953337
O	-0.0348914144	4.1457975178	14.1903808485
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H	-0.4713286770	3.3143999581	13.8923587571

T1			
O	1.9409371054	1.8630676675	12.9543715864
O	0.0521204870	7.0827602708	12.9515024412
Ti	1.8938721217	0.1733927351	12.2076530749
Ti	0.0027374889	5.3918362629	12.2038052356
O	1.8947465134	4.8513296547	12.2497364931
O	0.0038298568	10.0618734886	12.2516528536
O	0.0068196274	3.3840763389	11.4222918270
O	1.8981894867	8.5995325841	11.4107232403
Ti	1.8885952558	2.9930315453	11.3885951786
Ti	-0.0016481269	8.2099141816	11.3809548154
O	1.8800995129	1.0606080386	10.5985031789
O	-0.0110210099	6.2756770994	10.5948811316
O	1.8967762433	3.2493586307	9.4043123360
O	0.0063741789	8.4632846115	9.3997700210
Ti	0.0006866699	6.6379874266	8.6510297939
Ti	1.8916565005	1.4247468621	8.6558946681
O	1.8895842446	6.2193400733	8.5421548557
O	-0.0012058175	1.0052889987	8.5462416847
O	-0.0000188353	4.7382275985	7.9311846782
O	1.8909142687	9.9549026705	7.9304916228
Ti	1.8904501221	4.3479173362	7.8101702938
Ti	-0.0003005495	9.5649110464	7.8093358230
O	1.8884188481	2.4654175466	7.0602968496
O	-0.0024284270	7.6799956898	7.0584856668
O	1.8908630000	4.6368580000	5.8721510000
O	0.0000000000	9.8512340000	5.8721320000
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O	1.8309068966	9.3080879301	14.1464620156
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Ti	-1.8908370000	2.7649550000	5.1437830000
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O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	-2.9496900000	0.8911050000
O	-1.8908370000	2.2643890000	0.8910870000
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Ti	0.0000000000	1.8718830000	0.7383600000
O	-1.8908370000	-5.2140510000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	-1.8837303057	-0.5712207480	14.1931731406
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H	0.7465588564	-3.1406023675	13.7026698400
O	-0.2537414785	3.8686434761	13.8860540750
H	0.5997045971	3.5295899835	14.2167355540
H	-0.9577325250	2.8153223917	13.5013916422

I2			
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Ti	-0.0332209611	5.1959393200	12.3700791838
O	1.9088701386	4.8651932356	12.1591422883
O	0.0185269422	10.0796209668	12.1593995477
O	0.0190404718	3.4062713262	11.4253883840
O	1.9100866492	8.6206465975	11.4258322700
Ti	1.9183307566	3.0010435205	11.2573174838
Ti	0.0277636008	8.2153022069	11.2575970607
O	1.8816078708	1.1529500268	10.6394921702
O	-0.0094479125	6.3673184960	10.6395302386
O	1.9116832954	3.2922729740	9.3921592995
O	0.0208578157	8.5066066130	9.3923721120
Ti	0.0028915455	6.5981420568	8.7207570836
Ti	1.8939461176	1.3838179291	8.7207615158
O	1.8920451934	6.2216016641	8.5517766585
O	0.0013168097	1.0072197357	8.5521448451
O	0.0032222535	4.7466311038	7.9380583696
O	1.8941721593	9.9607802239	7.9382697736
Ti	1.8915464421	4.3481736095	7.7714349825
Ti	0.0008535626	9.5624357778	7.7716098103
O	1.8872044783	2.4772291349	7.0693744492
O	-0.0037120592	7.6916691026	7.0694736560
O	1.8908630000	4.6368580000	5.8721510000
O	0.0000000000	9.8512340000	5.8721320000
Ti	0.0000000000	7.9793790000	5.1437830000
Ti	1.8908630000	2.7649550000	5.1437830000
O	1.8908630000	7.5869150000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	6.1075240000	4.4154330000
O	1.8908630000	0.8930530000	4.4154150000
Ti	1.8908630000	5.7150320000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	1.8908630000	3.8431630000	3.5343580000
O	0.0000000000	9.0575120000	3.5343290000
O	1.8908630000	6.0081940000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	9.3507150000	1.6194540000
Ti	1.8908630000	4.1362920000	1.6194540000
O	1.8908630000	8.9582510000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	7.4788600000	0.8911050000
O	1.8908630000	2.2643890000	0.8910870000
Ti	1.8908630000	7.0863680000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	1.8908630000	5.2144990000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	1.8983459393	9.8070013882	14.1347870807
H	2.7597358868	9.7591931035	14.5881330021
H	0.5588597461	7.4579864805	13.7514632416
O	0.0061060691	4.5902349756	14.1340138959
H	0.8675864225	4.5385703639	14.5867605697
H	2.4522985326	2.2446580639	13.7500349542

TS3 _a			
O	-1.8100982379	1.8701011345	12.9974106421
O	0.0013912706	-3.3691360059	12.9902183065
Ti	1.8994888737	-0.0527251089	12.3829850524
Ti	-0.0382670251	5.1338444463	12.3569259726
O	-1.8936398498	4.8178798910	12.1343136044
O	0.0176934977	-0.3551871798	12.0581449284
O	0.0042015076	3.3376774136	11.4373117270
O	-1.8742350897	-1.8624664725	11.5211653402
Ti	-1.8885870504	2.9466574209	11.2463095974
Ti	0.0193262495	-2.2283330802	11.2756504389
O	1.8586900321	1.1228213593	10.6140162725
O	0.0173409919	-4.0891750277	10.6498461476
O	-1.8717811858	3.2792458946	9.3920532656
O	0.0057890849	-1.9341150909	9.4214905721
Ti	0.0082290076	-3.8465274306	8.7421562055
Ti	-1.8939283351	1.3664587355	8.7109912182
O	-1.8825756820	-4.2142865287	8.5590663922
O	-0.0060343559	0.9994162697	8.5237424644
O	0.0077510971	4.7384095020	7.9451887937
O	-1.8936175100	-0.4965977452	7.9520418404
Ti	-1.8838074266	4.3400591328	7.7722188721
Ti	-0.0041218667	-0.8852168928	7.7714158817
O	1.8847538941	2.4762008742	7.0654421588
O	0.0028769908	-2.7416711076	7.0782535997
O	-1.8908370000	4.6368580000	5.8721510000
O	0.0000000000	-0.5773160000	5.8721320000
Ti	0.0000000000	-2.4491710000	5.1437830000
Ti	-1.8908370000	2.7649550000	5.1437830000
O	-1.8908370000	-2.8416350000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	-4.3210260000	4.4154330000
O	-1.8908370000	0.8930530000	4.4154150000
Ti	-1.8908370000	-4.7135180000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	-1.8908370000	3.8431630000	3.5343580000
O	0.0000000000	-1.3710380000	3.5343290000
O	-1.8908370000	-4.4203560000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	-1.0778350000	1.6194540000
Ti	-1.8908370000	4.1362920000	1.6194540000
O	-1.8908370000	-1.4702990000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	-2.9496900000	0.8911050000
O	-1.8908370000	2.2643890000	0.8910870000
Ti	-1.8908370000	-3.3421820000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	-1.8908370000	-5.2140510000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	-1.8672239405	-0.6139748563	14.1418158033
H	-1.8772977340	-1.5537867941	14.3847408551
H	-0.0066791009	-3.0939665122	13.9179082065
O	-0.0294193254	4.5118186353	14.1177590514
H	0.8298479488	4.2921100774	14.5217980352
H	-1.2177390342	2.1859242031	13.7044610486

I3 _a			
O	1.9484625940	1.9279217460	12.9756409435
O	-0.0574300386	7.1434322459	12.9750773673
Ti	1.9673692024	-0.0109871415	12.3609532576
Ti	-0.0755670702	5.2039793907	12.3607511960
O	1.8687272026	4.8684171606	12.1567132959
O	0.0231691028	10.0822738422	12.1570000075
O	-0.0182771673	3.4119304068	11.4179140733
O	1.9099186068	8.6264974844	11.4164451982
Ti	1.8679820911	3.0061556539	11.2583476119
Ti	0.0235742900	8.2204702941	11.2576591125
O	1.8412821407	1.1556146468	10.6423445331
O	0.0504881374	6.3698775497	10.6420725261
O	1.8995082118	3.2915723339	9.3906092445
O	-0.0083048710	8.5059452572	9.3899408845
Ti	0.0101394030	6.5997759627	8.7203364431
Ti	1.8809163588	1.3854492721	8.7209627712
O	1.9043409271	6.2209991748	8.5537501282
O	-0.0132158036	1.0068518894	8.5540607263
O	0.0090638185	4.7472278470	7.9381433320
O	1.8820067622	9.9617110753	7.9381774989
Ti	1.8992868620	4.3484542175	7.7719813015
Ti	-0.0081503103	9.5631650617	7.7719116028
O	1.8828792884	2.4763179882	7.0693318193
O	0.0081959019	7.6906404486	7.0690954455
O	1.8908630000	4.6368580000	5.8721510000
O	0.0000000000	9.8512340000	5.8721320000
Ti	0.0000000000	7.9793790000	5.1437830000
Ti	1.8908630000	2.7649550000	5.1437830000
O	1.8908630000	7.5869150000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	6.1075240000	4.4154330000
O	1.8908630000	0.8930530000	4.4154150000
Ti	1.8908630000	5.7150320000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	1.8908630000	3.8431630000	3.5343580000
O	0.0000000000	9.0575120000	3.5343290000
O	1.8908630000	6.0081940000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	9.3507150000	1.6194540000
Ti	1.8908630000	4.1362920000	1.6194540000
O	1.8908630000	8.9582510000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	7.4788600000	0.8911050000
O	1.8908630000	2.2643890000	0.8910870000
Ti	1.8908630000	7.0863680000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	1.8908630000	5.2144990000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	1.9509527358	-0.6099594916	14.1294838499
H	-2.6802497285	-0.5963925329	14.6072156806
H	-0.5432248249	-2.9435443652	13.7459032719
O	-0.0583624099	4.6077294011	14.1300962538
H	0.7906882127	4.6252014543	14.6085227315
H	-1.3492168324	2.2692198448	13.7476435980

TS3 _a '			
O	-1.9022187922	1.8561236576	12.9846305899
O	-0.0727749101	-3.3546073104	13.0116843762
Ti	-1.8462175082	-0.0753938571	12.3553574860
Ti	-0.0094783558	5.1567550889	12.4001884806
O	1.8697797709	4.8594213874	12.0732377249
O	0.0081792969	-0.3960526297	12.1369612590
O	-0.0193444404	3.3595984969	11.5084232085
O	-1.8893409369	-1.8814120040	11.4493572504
Ti	1.8705209457	2.9929256579	11.2730407168
Ti	0.0036049977	-2.2729518962	11.2527462101
O	1.8756445865	1.1287606951	10.6503976819
O	0.0304576983	-4.0916653287	10.6199733612
O	-1.8980340010	3.2828892607	9.4181161486
O	-0.0140635796	-1.9324204039	9.3990758400
Ti	0.0024426645	-3.8447485446	8.7161476346
Ti	1.8842975014	1.3707368060	8.7412100480
O	-1.8852446035	-4.2127380207	8.5300147186
O	-0.0066927428	1.0017971010	8.5598492059
O	0.0022619454	4.7235006089	7.9488786959
O	1.8849284358	-0.4750725140	7.9464614542
Ti	-1.8875792962	4.3325049754	7.7712391175
Ti	-0.0050649597	-0.8741906426	7.7739292505
O	1.8887562117	2.4744240377	7.0776591945
O	0.0055292544	-2.7357814955	7.0681205222
O	-1.8908370000	4.6368580000	5.8721510000
O	0.0000000000	-0.5773160000	5.8721320000
Ti	0.0000000000	-2.4491710000	5.1437830000
Ti	-1.8908370000	2.7649550000	5.1437830000
O	-1.8908370000	-2.8416350000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	-4.3210260000	4.4154330000
O	-1.8908370000	0.8930530000	4.4154150000
Ti	-1.8908370000	-4.7135180000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	-1.8908370000	3.8431630000	3.5343580000
O	0.0000000000	-1.3710380000	3.5343290000
O	-1.8908370000	-4.4203560000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	-1.0778350000	1.6194540000
Ti	-1.8908370000	4.1362920000	1.6194540000
O	-1.8908370000	-1.4702990000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	-2.9496900000	0.8911050000
O	-1.8908370000	2.2643890000	0.8910870000
Ti	-1.8908370000	-3.3421820000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	-1.8908370000	-5.2140510000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	-1.8435926673	-0.6743405681	14.1256278346
H	1.0797794907	-0.8482546722	14.5532466166
H	-0.6541099324	-3.0256933111	13.7217780854
O	-0.0320801534	4.5438373822	14.1418362614
H	0.0141571539	3.5949080720	14.3442215689
H	-1.8592869796	2.1416601240	13.9083235002

I2'			
O	1.8248238796	1.9175854853	12.9784077195
O	-0.0670186763	7.1326241537	12.9782461540
Ti	1.9247260662	-0.0184489612	12.3694110268
Ti	0.0332746228	5.1962668572	12.3698922657
O	1.8730902782	4.8656345571	12.1585244169
O	-0.0171664661	10.0794630100	12.1582213089
O	-0.0185870198	3.4060217962	11.4261431566
O	1.8725174428	8.6201602293	11.4251996872
Ti	1.8641152405	3.0009780123	11.2575577576
Ti	-0.0263895227	8.2151332024	11.2570493684
O	1.9011957590	1.1530821902	10.6393546545
O	0.0102032757	6.3672248814	10.6391984837
O	1.8701743699	3.2924848018	9.3924779977
O	-0.0206516650	8.5067128538	9.3920222800
Ti	-0.0029536074	6.5982510301	8.7206318581
Ti	1.8880584998	1.3840882014	8.7207360600
O	1.8898381727	6.2216447055	8.5519770790
O	-0.0009286079	1.0074424988	8.5519640290
O	-0.0031018362	4.7465356110	7.9384705717
O	1.88781444818	9.9611503136	7.9379710736
Ti	1.8902505283	4.3482369064	7.7716103902
Ti	-0.0004892949	9.5626171647	7.7714656479
O	1.8949067461	2.4775526122	7.0694507478
O	0.0040215256	7.6917560230	7.0692831614
O	1.8908630000	4.6368580000	5.8721510000
O	0.0000000000	9.8512340000	5.8721320000
Ti	0.0000000000	7.9793790000	5.1437830000
Ti	1.8908630000	2.7649550000	5.1437830000
O	1.8908630000	7.5869150000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	6.1075240000	4.4154330000
O	1.8908630000	0.8930530000	4.4154150000
Ti	1.8908630000	5.7150320000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	1.8908630000	3.8431630000	3.5343580000
O	0.0000000000	9.0575120000	3.5343290000
O	1.8908630000	6.0081940000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	9.3507150000	1.6194540000
Ti	1.8908630000	4.1362920000	1.6194540000
O	1.8908630000	8.9582510000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	7.4788600000	0.8911050000
O	1.8908630000	2.2643890000	0.8910870000
Ti	1.8908630000	7.0863680000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	1.8908630000	5.2144990000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	1.8861217588	-0.6246254666	14.1332217006
H	-2.7568950652	-0.6770409751	14.5861840965
H	-0.5615903372	-2.9688616587	13.7491270205
O	-0.0062778871	4.5918896384	14.1341512871
H	-0.8673839330	4.5430121129	14.5879415666
H	-2.4495859557	2.2436655282	13.7508408369

TS2'			
O	1.8143498538	1.7836174380	13.0649714234
O	-0.2626700064	-3.1779701594	12.9312767469
Ti	-1.8166617108	-0.0776109646	12.2519659954
Ti	-0.0908255882	5.3204320686	12.4592451777
O	1.8395453467	4.9120298299	12.1829960758
O	0.0431392360	-0.3987209329	12.2045369274
O	-0.0439049782	3.3761540295	11.5686160475
O	1.9023554291	-1.7549671493	11.2063569703
Ti	1.8393506593	3.0194688269	11.3445910213
Ti	0.0368494846	-2.2658891848	11.2032953663
O	-1.8397350322	1.1224168587	10.6754140266
O	0.0462560191	-4.0790947701	10.5970472950
O	1.8598284687	3.2820128560	9.4638878479
O	-0.0195691022	-1.9520876860	9.3193039260
Ti	0.0011721695	-3.8407132731	8.6701418962
Ti	1.9042951502	1.3890221940	8.7442594109
O	1.8992422377	-4.2223656415	8.5060933829
O	0.0139882182	1.0019013706	8.5982146805
O	0.0019032530	4.6995449017	7.9504034269
O	1.8990193804	-0.4411261195	7.9273880767
Ti	1.8957118132	4.3213702848	7.7859756585
Ti	0.0125469418	-0.8551721728	7.7692388188
O	-1.8750658311	2.4686454372	7.0938851042
O	0.0156276326	-2.7484678077	7.0406040375
O	-1.8908370000	4.6368580000	5.8721510000
O	0.0000000000	-0.5773160000	5.8721320000
Ti	0.0000000000	-2.4491710000	5.1437830000
Ti	-1.8908370000	2.7649550000	5.1437830000
O	-1.8908370000	-2.8416350000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	-4.3210260000	4.4154330000
O	-1.8908370000	0.8930530000	4.4154150000
Ti	-1.8908370000	-4.7135180000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	-1.8908370000	3.8431630000	3.5343580000
O	0.0000000000	-1.3710380000	3.5343290000
O	-1.8908370000	-4.4203560000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	-1.0778350000	1.6194540000
Ti	-1.8908370000	4.1362920000	1.6194540000
O	-1.8908370000	-1.4702990000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	-2.9496900000	0.8911050000
O	-1.8908370000	2.2643890000	0.8910870000
Ti	-1.8908370000	-3.3421820000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	-1.8908370000	-5.2140510000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	2.1187094939	-1.3514992922	13.8714271820
H	1.2559113308	-1.7026039483	14.1641860150
H	-0.9429331360	-2.4021185896	13.4850007865
O	-0.0237491011	4.6894473226	14.1936708725
H	-0.8536678324	4.5368168154	14.6815592591
H	1.1097591507	2.0312182358	13.6913099465

T1'			
O	1.8222290666	1.8169828157	13.0131311100
O	0.0826884615	7.1572260319	12.9566566553
Ti	1.8950229825	0.0138281709	12.0991348808
Ti	0.0574171259	5.3199695967	12.4765822444
O	1.9000169606	4.8839840203	12.1656526439
O	-0.0205393406	10.0583388457	12.2330369820
O	0.0095377376	3.3550651473	11.5091111157
O	1.8773013308	8.6267409312	11.3467220832
Ti	1.8477795641	3.0721724481	11.3157851674
Ti	-0.0196868283	8.1042856761	11.3380168434
O	1.9264153485	1.0922326436	10.6172826861
O	-0.0424979752	6.3158236730	10.6090464102
O	1.8841507130	3.2741357353	9.4260434761
O	0.0083110006	8.4791775921	9.3774413968
Ti	-0.0100299696	6.6177295864	8.7155692098
Ti	1.9028046226	1.3990539581	8.6474787141
O	1.8793880635	6.2212400643	8.5253741952
O	0.0113113131	1.0060793031	8.5617229360
O	-0.0078339184	4.7257934318	7.9483954214
O	1.8990176504	9.9690589633	7.9243479399
Ti	1.8813998718	4.3676342008	7.7916794239
Ti	0.0083301076	9.5367696850	7.7926057331
O	1.8967342768	2.4728012020	7.0736707259
O	-0.0067923220	7.6840232253	7.0546862947
O	1.8908630000	4.6368580000	5.8721510000
O	0.0000000000	9.8512340000	5.8721320000
Ti	0.0000000000	7.9793790000	5.1437830000
Ti	1.8908630000	2.7649550000	5.1437830000
O	1.8908630000	7.5869150000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	6.1075240000	4.4154330000
O	1.8908630000	0.8930530000	4.4154150000
Ti	1.8908630000	5.7150320000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	1.8908630000	3.8431630000	3.5343580000
O	0.0000000000	9.0575120000	3.5343290000
O	1.8908630000	6.0081940000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	9.3507150000	1.6194540000
Ti	1.8908630000	4.1362920000	1.6194540000
O	1.8908630000	8.9582510000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	7.4788600000	0.8911050000
O	1.8908630000	2.2643890000	0.8910870000
Ti	1.8908630000	7.0863680000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	1.8908630000	5.2144990000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	-1.9863649826	-1.1976898056	14.0789039513
H	1.2343986552	-1.9781940168	13.8292267331
H	-1.1011026289	-1.5904206238	14.2094766452
O	-0.0024754097	4.5843759682	14.1767808096
H	-0.8419083336	4.4715208642	14.6571872141
H	1.1274563508	2.0824392198	13.6440970713

TS1'			
O	1.6587598439	2.0079496837	12.9548423883
O	0.0391729876	-3.3675540958	13.0016398302
Ti	-2.0040456832	0.1977139847	12.2036726073
Ti	0.0780334866	-5.1216137686	12.3717625110
O	-1.8260605057	4.8568952323	12.2008435531
O	-0.0671364300	-0.3033530369	12.2892740278
O	0.0165482723	3.4454722937	11.2304270711
O	1.8397311878	-1.7698390724	11.4701006134
Ti	1.9800296897	3.0758408075	11.2431447143
Ti	-0.0385650206	-2.2668244255	11.4160759676
O	-1.8623551890	1.0944739325	10.6125347444
O	0.0117950689	-4.1144996988	10.6569420724
O	1.8816134221	3.2403034052	9.3358747912
O	-0.0268834147	-1.9564398541	9.4351583832
Ti	0.0003432222	-3.8025141074	8.7437452037
Ti	-1.9029867891	1.3913608977	8.6142724498
O	1.8910381412	-4.2167665722	8.5822789437
O	-0.0018953200	0.9861910457	8.5471560647
O	-0.0008598751	4.7558406859	7.9310045914
O	-1.8966604944	-0.4956698293	7.9274103325
Ti	1.8928465163	4.3777689726	7.7842475061
Ti	-0.0066890208	-0.9108059272	7.8067310256
O	-1.8892852126	2.4510383370	7.0433627173
O	0.0033541296	-2.7536167665	7.0788683255
O	-1.8908370000	4.6368580000	5.8721510000
O	0.0000000000	-0.5773160000	5.8721320000
Ti	0.0000000000	-2.4491710000	5.1437830000
Ti	-1.8908370000	2.7649550000	5.1437830000
O	-1.8908370000	-2.8416350000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	-4.3210260000	4.4154330000
O	-1.8908370000	0.8930530000	4.4154150000
Ti	-1.8908370000	-4.7135180000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	-1.8908370000	3.8431630000	3.5343580000
O	0.0000000000	-1.3710380000	3.5343290000
O	-1.8908370000	-4.4203560000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	-1.0778350000	1.6194540000
Ti	-1.8908370000	4.1362920000	1.6194540000
O	-1.8908370000	-1.4702990000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	-2.9496900000	0.8911050000
O	-1.8908370000	2.2643890000	0.8910870000
Ti	-1.8908370000	-3.3421820000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	-1.8908370000	-5.2140510000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	1.7720932588	-1.0774354303	14.1701750927
H	1.2698400181	-1.8865148818	13.9115999177
H	-1.1003790839	-1.4094169547	14.2981809504
O	0.2691164572	3.8893186629	13.8721194027
H	-0.5875173294	3.5502956615	14.1946117872
H	0.9712180977	2.8080848869	13.4742399554

TS3 _b			
O	-1.9398576525	1.9147229182	12.9340970019
O	0.0216508024	-3.3725767659	12.9769974494
Ti	1.9179415198	-0.0187372015	12.1341624217
Ti	-0.0231239429	5.1258234369	12.3752141093
O	-1.8921186665	4.8181649529	12.1276604735
O	0.0307075558	-0.4392751363	12.1799161288
O	-0.0067410625	3.3570233530	11.4128717889
O	-1.8634537060	-1.8690683789	11.4311485632
Ti	-1.8964733533	2.9374588783	11.3799539456
Ti	0.0394057231	-2.2955673701	11.2591642221
O	1.9276004225	1.0529633770	10.6025954793
O	-0.0039256315	-4.1017948846	10.6306409876
O	-1.8990056987	3.2319426775	9.3877053232
O	0.0243489113	-1.9380633773	9.4072358066
Ti	-0.0005202325	-3.8437916411	8.7055564990
Ti	-1.8786316963	1.4037558359	8.6555227044
O	-1.8907177719	-4.2251676627	8.5546178526
O	0.0135650882	0.9980239199	8.5298600500
O	-0.0003788129	4.7283788823	7.9465991005
O	-1.8788995195	-0.4932636782	7.9284499958
Ti	-1.8913566532	4.3264094743	7.8114744202
Ti	0.0119654876	-0.8784638016	7.7728602184
O	1.9010234625	2.4564169364	7.0533147357
O	-0.0008390816	-2.7492696749	7.0735540615
O	-1.8908370000	4.6368580000	5.8721510000
O	0.0000000000	-0.5773160000	5.8721320000
Ti	0.0000000000	-2.4491710000	5.1437830000
Ti	-1.8908370000	2.7649550000	5.1437830000
O	-1.8908370000	-2.8416350000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	-4.3210260000	4.4154330000
O	-1.8908370000	0.8930530000	4.4154150000
Ti	-1.8908370000	-4.7135180000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	-1.8908370000	3.8431630000	3.5343580000
O	0.0000000000	-1.3710380000	3.5343290000
O	-1.8908370000	-4.4203560000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	-1.0778350000	1.6194540000
Ti	-1.8908370000	4.1362920000	1.6194540000
O	-1.8908370000	-1.4702990000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	-2.9496900000	0.8911050000
O	-1.8908370000	2.2643890000	0.8910870000
Ti	-1.8908370000	-3.3421820000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	-1.8908370000	-5.2140510000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	-1.8169636042	-0.0258120520	14.2059332853
H	-0.9211796580	-0.2239433127	14.5383651788
H	0.3505941958	-3.1231000346	13.8536983197
O	0.0458173687	4.5740615303	14.1290588011
H	0.8791273532	4.2225372297	14.4937552492
H	-1.8567382162	1.2092861107	13.8413526349

I3 _b			
O	1.8766446576	1.7884235350	12.9127057771
O	-0.1255348811	7.1902816714	13.0626728892
Ti	1.8912066532	0.1294033681	12.1524063916
Ti	-0.0693355239	5.1746631698	12.3252695170
O	1.8731657396	4.8357756207	12.1147042577
O	0.0191509124	10.0663207228	12.1554659686
O	-0.0189041489	3.3471103831	11.4745215084
O	1.8971654365	8.5500679204	11.4457388751
Ti	1.8727518027	2.9164102298	11.3979071633
Ti	0.0699507518	8.2182821712	11.2709569577
O	1.9005992182	1.0470137061	10.5528382769
O	0.0140546145	6.3558539177	10.6624778978
O	1.8798536532	3.2395874205	9.4001728240
O	-0.0015721964	8.5047109977	9.4027979628
Ti	-0.0066943536	6.6061378401	8.7305671209
Ti	1.8923166159	1.4144822246	8.6256388857
O	1.8896505820	6.2129336228	8.5788884993
O	0.0018691632	1.0122081370	8.5009107032
O	-0.0027099016	4.7452302427	7.9566937355
O	1.8918792111	9.9441916219	7.9195984271
Ti	1.8872657839	4.3465511479	7.8225020081
Ti	0.0018298652	9.5551533466	7.7705715723
O	1.8937400172	2.4771863008	7.0501258310
O	0.0005408838	7.6790136890	7.0773056498
O	1.8908630000	4.6368580000	5.8721510000
O	0.0000000000	9.8512340000	5.8721320000
Ti	0.0000000000	7.9793790000	5.1437830000
Ti	1.8908630000	2.7649550000	5.1437830000
O	1.8908630000	7.5869150000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	6.1075240000	4.4154330000
O	1.8908630000	0.8930530000	4.4154150000
Ti	1.8908630000	5.7150320000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	1.8908630000	3.8431630000	3.5343580000
O	0.0000000000	9.0575120000	3.5343290000
O	1.8908630000	6.0081940000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	9.3507150000	1.6194540000
Ti	1.8908630000	4.1362920000	1.6194540000
O	1.8908630000	8.9582510000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	7.4788600000	0.8911050000
O	1.8908630000	2.2643890000	0.8910870000
Ti	1.8908630000	7.0863680000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	1.8908630000	5.2144990000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	2.0465536883	9.3233743637	14.1405655203
H	2.5750700355	8.5447755733	13.8085921302
H	0.5553276602	7.2621292666	13.7549487599
O	0.0674547213	4.7090803150	14.1129572251
H	0.9093250103	4.3578022586	14.4566177068
H	2.6543321922	9.7958225046	14.7372984617

TS4 _b			
O	1.8976257315	1.7122753457	12.9174068992
O	-0.0887263716	-3.2824088266	12.9971256940
Ti	-1.8904724398	0.0353390000	12.1399677377
Ti	-0.0143017671	5.1344288218	12.1054616564
O	1.8959424620	4.7279745900	12.1479508641
O	0.0211447574	-0.4262094512	12.1707746655
O	0.0047945056	3.2770982885	11.4645469264
O	-1.8848585670	-1.9058243366	11.4114236637
Ti	1.8988827763	2.8112373997	11.4212453996
Ti	0.0252831405	-2.3044746914	11.4034702811
O	-1.8744213124	0.9915523544	10.5561139175
O	0.0270131106	-4.1802818667	10.6290314895
O	1.8929868083	3.2060553502	9.4088125403
O	0.0026076299	-1.9941669603	9.4002576917
Ti	0.0021818302	-3.8021050210	8.6549192328
Ti	-1.8838915360	1.4055546091	8.6192943550
O	1.8964092456	-4.2301031660	8.5585778879
O	0.0074307785	0.9889553782	8.5168541568
O	0.0035296465	4.7127481136	7.9474228519
O	-1.8849849005	-0.5068611231	7.9292739305
Ti	1.8931004461	4.3271261951	7.8256970797
Ti	0.0074286000	-0.8907948774	7.8126149916
O	-1.8851497127	2.4572443056	7.0499364356
O	0.0045673423	-2.7734121743	7.0587562297
O	-1.8908370000	4.6368580000	5.8721510000
O	0.0000000000	-0.5773160000	5.8721320000
Ti	0.0000000000	-2.4491710000	5.1437830000
Ti	-1.8908370000	2.7649550000	5.1437830000
O	-1.8908370000	-2.8416350000	4.9910730000
O	0.0000000000	2.3724150000	4.9910430000
O	0.0000000000	-4.3210260000	4.4154330000
O	-1.8908370000	0.8930530000	4.4154150000
Ti	-1.8908370000	-4.7135180000	4.2627130000
Ti	0.0000000000	0.5005470000	4.2626890000
O	-1.8908370000	3.8431630000	3.5343580000
O	0.0000000000	-1.3710380000	3.5343290000
O	-1.8908370000	-4.4203560000	2.3478220000
O	0.0000000000	0.7937220000	2.3478030000
Ti	0.0000000000	-1.0778350000	1.6194540000
Ti	-1.8908370000	4.1362920000	1.6194540000
O	-1.8908370000	-1.4702990000	1.4667440000
O	0.0000000000	3.7437510000	1.4667150000
O	0.0000000000	-2.9496900000	0.8911050000
O	-1.8908370000	2.2643890000	0.8910870000
Ti	-1.8908370000	-3.3421820000	0.7383840000
Ti	0.0000000000	1.8718830000	0.7383600000
O	-1.8908370000	-5.2140510000	0.0100290000
O	0.0000000000	0.0000000000	0.0100000000
O	-1.7331436110	-1.0463165488	14.1810548114
H	-1.3452694212	-1.9180595117	13.9178959516
H	0.0662553239	-4.0735947787	13.8453714289
O	0.0704329852	5.1389436055	14.1605495184
H	0.9388821094	4.8311470473	14.4810890504
H	-1.0105983912	-0.6016571345	14.6617697094