Supporting Information for:
"On the role of Ti(IV) as a Lewis acid in the chemistry of titanium zeolites: Formation, structure, reactivity, and aging of Ti-peroxo oxidizing intermediates. A first-principles study."
by
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	Ti-Cl	ν_3	ν_1	ν_4	ν_2
BP/PW/60	2.177	501	387	159	139
BP/PW/90	2.155	492	384	155	132
BP/PW/110	2.152	495	386	151	132
BLYP/PW/60	2.178	517	390	142	119
PBE/PW/60	2.172	519	395	143	104
B3LYP/PW/60	2.178	521	402	143	104
B3LYP/PW/90	2.157	516	396	152	113
B3LYP/PW/110	2.156	513	396	152	113
B3LYP/6-31g(d,p)	2.178	497	381	139	118
B3LYP/6-311g(d,p)	2.172	503	391	142	119
B3LYP/6-311+g(d,p)	2.180	495	384	137	115
MP2/6-31g(d,p)	2.172	512	388	137	122
MP2/6-311g(d,p)	2.147	533	410	145	124
MP2/6-311+g(d,p)	2.157	520	400	139	122
MP2/6-311++g(3df,2p)	2.167				
MP2/SBKP[a]	2.171	521	396	142	124
exp[b,c]	2.170	501	389	137	121

Table S1. Ti-Cl bond distances and harmonic frequencies calculated for $TiCl_4$ at different levels of theory. The experimental values of the Ti-Cl bond distance[b] and raman frequencies in diluted $TiCl_4$[c] are reported for comparison. Modes ν_1 and ν_2 are raman active, modes ν_3 and ν_4 are both IR and raman active. Calculations with planewaves basis set (PW) were performed using norm-conserving nonlocal pseudopotentials as described in the manuscript, with p-nonlocality for Cl.
Distances in Å, frequencies in cm^{-1}.

[a]Webb, P.W.; Gordon, M. S. *J. Am. Chem. Soc.* **1999**, *121*, 2552-2560.
[b]Morito, Y.; Uehara, H. *J. Chem. Phys.* **1966**, *45*, 4543-4550.
[c]Griffiths, J.E. *J. Chem. Phys.* **1968**, *49*, 642-647.

	E(EE)	E(AA)	ΔE
BP/PW/60	-29.719318	-29.759732	25.4
BP/PW/110	-29.802958	-29.843667	25.5
BP/PW/160	-29.804429	-29.845131	25.5
BP/6-311g(d,p)	-153.830375	-153.873486	27.1
BP/6-311+g(d,p)	-153.836142	-153.878525	26.6
B3LYP/6-311g(d,p)	-153.830129	-153.876861	29.3
B3LYP/6-311+g(d,p)	-153.836040	-153.882148	28.9
MP2/6-311g(d,p)	-153.397525	-153.442579	28.3
MP2/6-311+g(d,p)	-153.405466	-153.449434	27.6
CCD/6-311g(d,p)	-153.4173327	-153.461915	28.0
CCD/6-311+g(d,p)	-153.424157	-153.467926	27.5

Table S2. Absolute energies and energy difference ΔE between the optimized structures of ethylene epoxide (EE) and acetaldehyde (AA) at different levels of theory. Both systems have the same stoichiometry (C_2H_4O). Calculations with the Becke-Perdew functional (BP), planewaves basis set (PW) and the same norm-conserving pseudopotentials adopted for the calculations in the manuscript were performed with different cutoffs (60 Ry, 110 Ry and 160 Ry). BP, B3LYP, MP2 and CCD calculations were performed with localized basis sets. Absolute energies in hartrees. ΔE = E(EE)-E(AA) in kcal/mol. Bond distances obtained for optimized geometries at the levels of theory here adopted differ by a maximum of $\sim$ 2.0%.

	ΔE
BP/PW/60	-21.2
BP/PW/90	-22.0
BP/PW/110	-22.0

Table S3. Energy difference ΔE between the optimized structures of the hydrated Ti site in Ti-off (System Ti-L) and the hydrolyzed Ti site in Ti-off (system Ti-H) as a function of basis set. Both systems have the same stoichiometry $[TiSi_{17}O_{36}](H_2O)$. Calculations were performed by using the Becke and Perdew functional (BP), norm-conserving pseudopotentials as described in the manuscript and planewaves basis set (PW) with cutoffs of 60 Ry, 90 Ry and 110 Ry. ΔE = E(Ti-L)-E(Ti-H) in kcal/mol. Ti-O distances calculated with BP/PW/60 differ by a maximum of -1.4% from those calculated with BP/PW/110.

	ΔE
BP/PW/60	-16.6
BP/PW/90	-15.9
BP/PW/110	-15.6

Table S4. Energy difference ΔE between the optimized structures of the hydrated Ti peroxo site in Ti-off (System W1) and the Ti hydroperoxo site in Ti-off (system HP) as a function of basis set. Both systems have the same stoichiometry $[TiSi_{17}O_{37}](H_2O)$. Calculations were performed by using the Becke and Perdew functional (BP), norm-conserving pseudopotentials as described in the manuscript and planewaves basis set (PW) with cutoffs of 60 Ry, 90 Ry and 110 Ry. ΔE = E(HP)-E(W1) in kcal/mol. Ti-O distances calculated with BP/PW/60 differ by a maximum of -1.4% from those calculated with BP/PW/110.

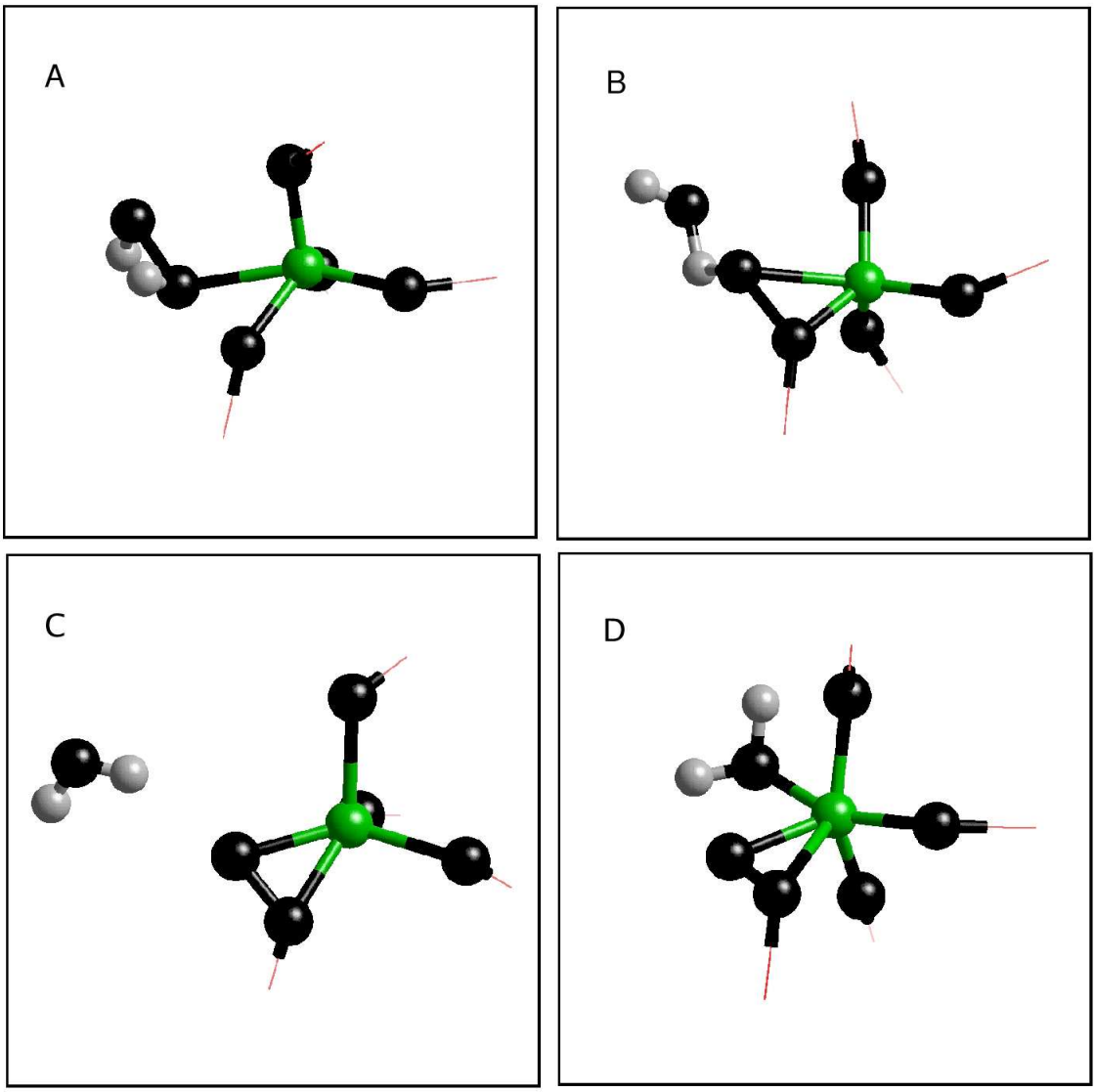

Figure S1. Ball-and-stick representation of relevant snapshots from the bluemoon simulation of the first part of the reaction in Model I. Top left Panel A: initial stage of the reaction, representing H_2O_2 molecularly linked to the Ti site; Top right panel B: a configuration taken from the transition state, showing the breaking of the O-O bond of the H_2O_2 molecule and a proton shift from one oxygen to the other in H_2O_2; Bottom left panel C: formation of the new O-O bond at the Ti site and release of a water molecule; Bottom right panel D: transient insertion of a water molecule as sixth ligand at the Ti site. Ti: green sphere, O: black spheres, H: gray spheres.

Optimized geometries for the Ti-off model systems described in the manuscript. The Cartesian coordinates of the atoms in the unit cell of Ti-off are reported in Å. The parameters of the Ti-off unit cells are also reported: *a, b, c* in Å, α, β, γ in degrees.

57 Optimized geometry for the hydrated site in Tioff (system Ti-L)
Cell 13.229 13.229 7.338 90. 90. 120.
Ti .00000000 .00000000 .00000000 1
Si .41098438 -5.53744201 .13844160 2
Si 4.94968373 -2.81499944 .40309802 3
Si .48342391 -.41781168 -3.34108689 4
Si .49381186 -5.64663185 -2.95117828 5
Si 5.19925267 -2.90354374 -2.72431029 6
Si -1.23639200 -2.93535642 .05203110 7
Si 3.26249545 -.23734296 .14497927 8
Si 3.43701785 -5.61771518 .38523468 9
Si -1.18019078 -2.95435563 -3.06594683 10
Si 3.51809967 -.38388951 -3.05760816 11
Si 3.54081473 -5.58051129 -2.75435218 12
Si .49918555 2.14057081 2.14423916 13
Si -8.06626067 4.67695452 2.29208114 14
Si 6.94771451 -3.91435679 2.44563507 15
Si -3.09957641 -4.17194069 2.21694849 16
Si 3.59383700 1.93484347 2.22232497 17
Si -1.25236548 4.76210284 2.47585405 18
O .08246234 1.72498414 .62428678 19
O -7.31105497 5.00189406 .88672128 20
O 6.28496593 -2.93127246 1.32516913 21
O .08984787 .88534439 3.10722821 22
O -7.00787499 4.75102842 3.53351513 23
O 6.63762915 -3.30556715 -3.39886674 24
O -2.51865826 -3.63288856 .78743650 25
O 3.81055839 1.15848333 .80162254 26
O -2.28337159 4.73436848 1.19860709 27
O -2.55369187 -3.28744046 3.47131592 28
O 3.93776525 .99141143 3.51478109 29
O -2.08227821 4.79978995 -3.45942004 30
O 3.96048049 -4.09605159 .66356429 31
O 1.69761566 -.49475644 .50513313 32
O .06232970 -3.93611158 .18279877 33
O 4.05928861 -4.05073053 -2.99119408 34
O 2.03821525 -.88587214 -3.57208132 35
O -.06055283 -4.13326699 -3.19649353 36
O -.89498539 -1.46679561 .65312612 37
O -4.74080642 5.71773478 .84067047 38
O 4.14554020 -1.45901091 .78248282 39
O -.52501409 -1.63005057 3.59288151 40
O 2.05643354 -5.70467747 -3.41518233 41
O 4.63790958 -1.52646377 -3.39732502 42
O .20123858 -.04008299 -1.79356727 43
O -6.20733105 5.36977341 -1.39099708 44
O 5.47424202 -2.73944159 -1.13607977 45
O -1.63864725 -2.72423022 -1.52166236 46
O 3.50843781 -.11262132 -1.45764159 47

O -3.06543055 5.45385277 -1.18920745 48
O 6.35633353 -5.42242514 2.32405726 49
O 2.07278126 2.53309050 2.33185092 50
O -9.32942251 5.70911669 2.46893707 51
O 4.64807944 3.15456567 2.25360710 52
O 8.52988008 -3.99227257 2.16412641 53
O -.37761575 3.42113646 2.58398661 54
O -2.11264830 .70902131 -.35529498 55
H -2.64178995 .19010981 -.99221530 56
H -2.13573910 1.63690790 -.66355225 57

57 Optimized geometry for the hydrolysed Ti site in Ti-off (system Ti-H)
Cell 13.229 13.229 7.338 90. 90. 120.
Ti .00000000 .00000000 .00000000 1
Si .01403035 -5.32259831 -.03277760 2
Si 4.84370061 -2.76783521 .30314955 3
Si .15021942 -.39975564 -3.25564471 4
Si .36085291 -5.69146746 -3.14755045 5
Si 4.85463873 -2.96219120 -2.82069030 6
Si -2.23204406 -3.42546933 -.69677567 7
Si 3.16542387 -.23568663 .05366269 8
Si 3.09861297 -5.44606365 .39064338 9
Si -1.33514612 -3.24172138 -3.59351375 10
Si 3.26269155 -.40240213 -3.07679040 11
Si 3.34476188 -5.65061841 -2.71827180 12
Si .30495874 2.17466705 2.12913632 13
Si -8.25952833 4.60539264 2.16590532 14
Si 6.72745042 -4.01615651 2.32623679 15
Si -3.39902224 -4.43438247 1.81704839 16
Si 3.30557566 1.97545810 2.19699292 17
Si -1.53614221 4.77425494 2.41407281 18
O .17482423 1.72093417 .56049001 19
O -7.50745567 5.04203209 .78138332 20
O 6.21363807 -2.98236847 1.16520699 21
O -.04337089 .84436630 3.03870928 22
O -7.22524880 4.70571729 3.42662946 23
O 6.21578673 -3.48507036 -3.55160559 24
O -3.31715695 -4.33367039 .17115020 25
O 3.35639033 1.21735770 .75642918 26
O -2.81072084 4.89752088 1.37736099 27
O -2.31528103 -3.36277068 2.44270508 28
O 3.60926958 .93636856 3.41255867 29
O -2.07032619 4.91905075 -3.38273658 30
O 3.80005919 -3.98719801 .61919041 31
O 1.63027680 -.75083260 .24358513 32
O -.72035853 -3.83993564 -.09852000 33
O 3.63382336 -4.05096658 -2.94549991 34
O 1.71063471 -.90333151 -3.30899483 35
O .02267323 -4.16378394 3.66331730 36
O -2.74942833 -1.87872448 -.82495950 37
O -1.03230729 -1.11907044 .98473820 38
O 1.49440540 -5.23986959 .67937999 39
O 4.15512879 -1.34958089 .72269759 40
O -.81969827 -1.67051866 3.64019177 41
O -4.68320855 5.44094318 -3.45895260 42
O 4.30132866 -1.58695866 -3.51377726 43
O -.35165661 .03887996 -1.78281672 44
O -6.46325558 5.56563475 -1.54851980 45
O 5.26568581 -2.71818700 -1.26812522 46
O -2.19201842 -3.77348354 -2.30660086 47
O 3.50687157 -.02897526 -1.51749059 48
O -3.31220177 5.45158551 -1.13025270 49
O 6.18379422 -5.53503010 2.03945278 50
O 1.83508204 2.69250258 2.45163851 51
O -9.61209530 5.52457892 2.35639673 52
O 4.50729923 3.05621378 2.13611521 53

O 8.34960265 -4.04253114 2.35190015 54
O -.81435900 3.32070139 2.37272347 55
H -.91125098 -1.38592968 1.93695293 56
H -2.72121423 -1.30965388 -.03455842 57

73 Optimized geometry of W6 system
Cell 13.229 13.229 7.338 90. 90. 120.
Ti .0000 .0000 .0000
Si .3067 -5.7051 .1940
Si 4.8511 -2.9304 .3975
Si .3423 -.4506 -3.2945
Si .4002 -5.6886 -2.9151
Si 4.9708 -3.0248 -2.7482
Si -1.4217 -3.1574 .0331
Si 3.2348 -.3189 .1811
Si 3.3360 -5.7030 .3883
Si -1.1882 -3.0491 -3.0659
Si 3.3889 -.4716 -2.9799
Si 3.3967 -5.6653 -2.7670
Si .4308 2.1079 2.1225
Si -8.2264 4.5940 2.3091
Si 6.8296 -4.0617 2.4219
Si -3.2452 -4.2924 2.1975
Si 3.4627 1.8871 2.2741
Si -1.3353 4.6714 2.4486
H -4.3750 .2150 2.2945
H -5.3923 1.3824 -1.7196
H -6.8225 -.4716 2.2444
H -6.2144 .6557 3.1606
H -2.8379 .0110 2.1310
H -4.4622 1.9871 .4500
H -5.8525 1.4168 .7136
H -4.4624 1.0115 -2.9487
H 1.2997 6.8321 -1.3180
H 1.2956 5.3254 -.9396
H .9496 3.0056 -.8561
H 2.3910 3.3114 -1.3022
O 1.2443 6.2355 -.5502
O 1.4665 3.5705 -1.4740
O -5.3500 1.9452 .0456
O -1.7004 -.5480 .5732
O -5.3957 1.1502 -2.6843
O -6.2857 .3415 2.2118
O -3.5001 .5613 2.5970
O .1166 1.7441 .5418
O -7.3852 4.8016 .9339
O 6.2059 -3.0600 1.2920
O .1374 .7345 2.9522
O -7.2987 4.8847 3.6117
O 6.3614 -3.5261 -3.4323
O -2.7816 -3.6384 .7589
O 3.6725 1.1033 .8585
O -2.3798 4.6482 1.1854
O -2.4547 -3.5696 3.4230
O 3.6771 .9019 3.5493
O -2.1204 4.8386 -3.4764
O 3.8255 -4.1707 .7037
O 1.6607 -.6401 .4576
O -.1498 -4.1196 .3322
O 3.7458 -4.0816 -3.0018

O 1.8788 -1.0218 -3.3116
O .0671 -4.0924 -3.0958
O -.8132 -1.7375 .7712
O -4.8356 5.6206 .8692
O 4.1336 -1.5263 .8188
O -.6897 -1.6422 3.6318
O -4.6883 5.5116 -3.4201
O 4.4962 -1.5994 -3.4043
O -.0576 .0606 -1.8033
O -6.3268 5.3201 -1.3614
O 5.2815 -2.8689 -1.1659
O -1.7128 -2.8512 -1.5228
O 3.5475 -.1373 -1.4015
O -3.1729 5.4156 -1.1918
O 6.3765 -5.6069 2.2113
O 1.9784 2.5843 2.3119
O -9.5560 5.5589 2.2740
O 4.5704 3.0478 2.3997
O 8.4336 -3.9521 2.4108
O -.5786 3.2569 2.6070

67 Optimized geometry for W4 eta2 system
Cell 13.229 13.229 7.338 90. 90. 120.
Ti .00000000 .00000000 .00000000 1
Si -6.28432049 5.70170613 .23801718 2
Si 4.83632199 -2.96638002 .44706695 3
Si .36200135 -.49908852 -3.27504483 4
Si -6.18961087 5.69476741 -2.87939561 5
Si 4.98093291 -3.06454555 -2.70836903 6
Si -1.34263499 -3.18676295 .09795453 7
Si 3.26247290 -.32628878 .18587913 8
Si -3.26152173 5.70549983 .45475357 9
Si -1.16669590 -3.09568283 -3.01264282 10
Si 3.41876915 -.50428653 -2.95686915 11
Si 3.42264961 -5.69558853 -2.70866407 12
Si .42169963 2.05918299 2.14145010 13
Si -8.20143480 4.55368978 2.35467314 14
Si 6.84064046 -4.09688475 2.46805805 15
Si -3.20741615 -4.29608358 2.27204796 16
Si 3.46314939 1.85365674 2.29042161 17
Si -1.30121941 4.62972507 2.51530077 18
O .06639140 1.72605954 .57387343 19
O -7.39008711 4.77223109 .96232796 20
O 6.20485670 -3.11462574 1.32463439 21
O .15268479 .66662361 2.95227373 22
O -7.23653482 4.77192442 3.64395175 23
O 6.37590890 -3.57889348 -3.38624941 24
O -2.70132600 -3.67288424 .83039694 25
O 3.71253692 1.08079833 .87896093 26
O -2.35319595 4.60933569 1.25885467 27
O -2.50309662 -3.55191631 3.53379670 28
O 3.69255839 .85957849 3.55660342 29
O -2.05264829 4.83888679 -3.39618539 30
O 3.82402297 -4.21315873 .78534358 31
O 1.67938980 -.61975307 .41635746 32
O -.07242145 -4.15511675 .38763452 33
O 3.74554657 -4.10986941 -2.96566507 34
O 1.90450050 -1.05979889 -3.26420564 35
O .05148624 -4.17920448 -3.09287592 36
O -.75529917 -1.75883763 .81530660 37
O -4.81767547 5.53695291 .91793592 38
O 4.12655642 -1.55594927 .84877073 39
O -.63567402 -1.72019557 3.65411979 40
O -4.65330452 5.45447417 -3.36996471 41
O 4.52310368 -1.64202349 -3.37813046 42
O -.08443558 .02879783 -1.80531301 43
O -6.31023052 5.27682373 -1.31886018 44
O 5.27282471 -2.93824238 -1.11858395 45
O -1.63126714 -2.88476387 -1.45703475 46
O 3.62222135 -.16199553 -1.38696222 47
O -3.14132796 5.38845313 -1.13136161 48
O 6.41583641 -5.65293858 2.22951342 49
O 1.97170573 2.53568422 2.33430493 50
O -9.50030170 5.56145650 2.36102262 51
O 4.55347108 3.02550548 2.42993523 52
O 8.44485645 -4.00149712 2.34987173 53

O -.56012359 3.20915268 2.70414566 54
O -5.34875906 1.08846513 -2.66389783 55
O -6.25105947 .34916207 2.22270035 56
O -3.46396028 .43333317 2.63245287 57
O -5.27643868 1.89866356 .04925768 58
O -1.68030517 -.60486162 .59150482 59
H -4.34628976 .12412264 2.31270254 60
H -5.35420147 1.33261132 -1.70097046 61
H 6.38726674 -.42544443 2.26539768 62
H -6.16211397 .66784529 3.17044274 63
H -2.81173579 -.09013247 2.12108882 64
H -4.37825995 1.91019008 .43209292 65
H -5.78455464 1.39091649 .73074716 66
H -4.41559220 .91422802 -2.90811162 67

67 Optimized geometry for W4-eta1 system
Cell 13.229 13.229 7.338 90. 90. 120.
Ti .00000000 .00000000 .00000000 1
Si -6.14139870 5.32246507 .27704093 2
Si 4.91831834 -3.30508929 .59884436 3
Si .55012746 -.75202111 -3.25329914 4
Si -6.03062567 5.33745139 -2.81519944 5
Si 5.15034944 -3.40451764 -2.49761479 6
Si -1.22393218 -3.57061450 .14558057 7
Si 3.20890810 -.70214800 .34370439 8
Si -3.10506671 5.27108296 .53527871 9
Si -.99521761 -3.42314688 -2.95278427 10
Si 3.62220697 -.80386592 -2.81261073 11
Si -3.03309896 5.41520618 -2.57387237 12
Si .64615292 1.78254969 2.30676180 13
Si -8.06121989 4.21217009 2.40927322 14
Si 6.96998364 -4.38260431 2.59728148 15
Si -3.07052244 -4.63982524 2.31446533 16
Si 3.67843797 1.45512559 2.51059766 17
Si -1.10770102 4.33203991 2.59807259 18
O -3.80476115 -.02927262 -1.70992379 19
O -1.40632988 -1.04018475 .62752097 20
O -5.04460514 1.54562502 -3.45204821 21
O -1.89734723 1.09886195 -.38593262 22
O -4.32500654 .84404837 1.34274707 23
O .42183122 1.65309877 .70037955 24
O -7.25893683 4.40704631 1.00774266 25
O 6.25062963 -3.34712905 1.55306356 26
O .15623612 .36757917 2.96343149 27
O -7.05684948 4.41590086 -3.66235865 28
O 6.50714585 -3.98873406 -3.21485349 29
O -2.59653889 -4.15724772 .81435017 30
O 3.79778652 .61788789 1.12055164 31
O -2.19028383 4.19060312 1.36574449 32
O -2.29258470 -3.82758436 3.49234342 33
O 4.14716729 .55746954 -3.54342771 34
O -1.86964455 4.58872794 -3.33064488 35
O 4.02101460 -4.66154776 .82767690 36
O 1.60242991 -.80225434 .50747454 37
O .06202511 -4.55172317 .37428777 38
O 3.87848667 -4.43406733 -2.64904237 39
O 2.12849161 -1.20858493 -3.36467746 40
O .19054888 -4.54481381 -3.00721598 41
O -.63839811 -2.24022326 .95553817 42
O -4.67565000 5.12818413 .97065306 43
O 3.97219862 -2.03006781 .95222275 44
O -.40971610 -2.03671696 -3.53679802 45
O -4.47907340 5.13530832 -3.27682757 46
O 4.68979232 -1.99456461 -3.17702856 47
O .21537013 -.14655790 -1.79803419 48
O -6.14537473 4.84842493 -1.27146779 49
O 5.50236394 -3.20932571 -.92199581 50
O -1.53956788 -3.25254687 -1.41527571 51
O 3.64710492 -.53320086 -1.21716171 52
O -2.97932607 4.86835656 -1.03843736 53

O -.05606819 5.53229674 2.24665665 54
O 2.18947855 2.09478616 2.75069025 55
O -9.37024582 5.20897206 2.47922004 56
O 4.74228430 2.66560183 2.45473503 57
O 8.58496143 -4.28057682 2.46886757 58
O -.29854599 2.96785529 2.88106068 59
H -3.40958843 .95812867 1.00323393 60
H -6.01810371 1.59236454 -3.41552501 61
H -2.59781755 .69106762 -1.03546768 62
H -1.76819183 2.04117473 -.60773807 63
H -4.70731590 .17266744 .74804134 64
H -4.30947955 .53348630 -2.39693023 65
H -3.55293588 -.84884870 -2.17283334 66
H -4.82933234 1.28971851 -4.39603230 67

58 Optimized geometry of W1 system
Cell 13.229 13.229 7.338 90. 90. 120.
Ti .0000 .0000 .0000
Si -6.1040 5.5392 .2547
Si 4.9789 -3.1507 .5368
Si .5808 -.6730 -3.2882
Si -6.0031 5.5107 -2.8446
Si 5.1883 -3.2627 -2.5620
Si -1.1938 -3.3579 .1052
Si 3.2650 -.5530 .2812
Si -3.0708 5.4376 .4865
Si -.9712 -3.2789 -2.9917
Si 3.6443 -.6774 -2.8846
Si -3.0085 5.5572 -2.6278
Si .6670 1.8946 2.2566
Si -8.0313 4.3717 2.3656
Si 7.0044 -4.2495 2.5411
Si -3.0395 -4.4932 2.2746
Si 3.7214 1.6069 2.4208
Si -1.0854 4.4638 2.5432
O -1.5587 -.8249 .5918
O -1.7576 1.3070 -.6786
O .3638 1.6854 .6710
O -7.2131 4.6114 .9783
O 6.3034 -3.2082 1.4950
O .1967 .5222 3.0098
O -7.0518 4.6135 3.6472
O 6.5412 -3.8558 -3.2733
O -2.5513 -3.9330 .8021
O 3.8624 .7854 1.0223
O -2.1665 4.3320 1.3038
O -2.2696 -3.7481 3.4979
O 4.1180 .6940 -3.6231
O -1.8568 4.7069 -3.3839
O 4.0849 -4.5093 .7733
O 1.6682 -.6769 .4981
O .0964 -4.3276 .3602
O 3.9167 -4.2977 -2.7137
O 2.1527 -1.1213 -3.4164
O .2558 -4.3606 -3.0116
O -.6346 -1.9570 .8646
O -4.6381 5.3499 .9530
O 4.0421 -1.8730 .8923
O -.4027 -1.9187 -3.6518
O -4.4588 5.2629 -3.3243
O 4.7210 -1.8594 -3.2485
O .2204 -.1914 -1.7930
O -6.1005 5.0479 -1.2894
O 5.5473 -3.0669 -.9893
O -1.5006 -3.0673 -1.4568
O 3.6696 -.4042 -1.2900
O -2.9730 5.0243 -1.0867
O -.0322 5.6627 2.1981
O 2.2210 2.2498 2.6077
O -9.3547 5.3511 2.3977

O 4.7854 2.8215 2.3985
O 8.6161 -4.1499 2.4125
O -.2843 3.0899 2.8137
H -1.8674 1.3197 -1.6491
H -1.5441 2.2275 -.4176

58 Optimized geometry for W0-1 system
Cell 13.229 13.229 7.338 90. 90. 120.
Ti .0000 .0000 .0000
Si .3123 -5.6968 .1938
Si 4.8573 -2.9255 .4029
Si .3533 -.4495 -3.2944
Si .4076 -5.6891 -2.9158
Si 4.9738 -3.0219 -2.7442
Si -1.4191 -3.1503 .0367
Si 3.2378 -.3197 .1803
Si 3.3456 -5.7038 .3886
Si -1.1755 -3.0448 -3.0630
Si 3.3967 -.4723 -2.9812
Si 3.4073 -5.6663 -2.7682
Si .4385 2.1046 2.1197
Si -8.2202 4.5884 2.3069
Si 6.8316 -4.0562 2.4397
Si -3.2322 -4.2903 2.2078
Si 3.4651 1.8836 2.2734
Si -1.3197 4.6703 2.4461
O 1.4759 3.5638 -1.4870
O -1.6936 -.5483 .5693
O .1187 1.7420 .5440
O -7.3657 4.7891 .9341
O 6.2238 -3.0890 1.2734
O .1463 .7347 2.9537
O -7.2879 4.8774 3.6099
O 6.3652 -3.5288 -3.4230
O -2.7796 -3.6586 .7527
O 3.6880 1.1006 .8594
O -2.3693 4.6490 1.1858
O -2.4457 -3.5676 3.4284
O 3.6922 .9006 3.5473
O -2.1113 4.8388 -3.4817
O 3.8312 -4.1721 .7024
O 1.6653 -.6416 .4573
O -.1452 -4.1183 .3326
O 3.7496 -4.0832 -3.0033
O 1.8883 -1.0258 -3.3148
O .0776 -4.0948 -3.0958
O -.8128 -1.7414 .7755
O -4.8291 5.6121 .8660
O 4.1358 -1.5282 .8176
O -.6784 -1.6437 3.6303
O -4.6807 5.5005 -3.4185
O 4.5009 -1.6019 -3.4008
O -.0529 .0550 -1.8056
O -6.3179 5.3100 -1.3607
O 5.2911 -2.8800 -1.1617
O -1.7077 -2.8565 -1.5221
O 3.5584 -.1384 -1.4022
O -3.1668 5.4112 -1.1926
O 6.3932 -5.6073 2.1955
O 1.9861 2.5860 2.3097
O -9.5455 5.5573 2.2678

O 4.5864 3.0393 2.3969
O 8.4387 -3.9649 2.3849
O -.5772 3.2506 2.6074
H .9623 3.0095 -.8606
H 2.3981 3.3092 -1.3000

58 Optimized geometry for HP system
Cell 13.229 13.229 7.338 90. 90. 120.
Ti .0000 .0000 .0000
Si .0880 -5.4225 -.0311
Si 4.9137 -2.8595 .3108
Si .2411 -.4897 -3.2625
Si -6.1783 5.6659 -3.1440
Si 4.9243 -3.0597 -2.8164
Si -2.1646 -3.5336 -.6907
Si 3.1923 -.3441 .0656
Si 3.1744 -5.5409 .3933
Si -1.2677 -3.3484 -3.5881
Si 3.3419 -.4987 -3.0686
Si -3.1940 5.7081 -2.7131
Si .3905 2.0947 2.1206
Si -8.1878 4.5060 2.1703
Si 6.7991 -4.1127 2.3297
Si -3.3289 -4.5371 1.8227
Si 3.3783 1.8737 2.1953
Si -1.4660 4.6758 2.4195
O .3360 1.7050 .5289
O -7.4299 4.9449 .7884
O 6.2959 -3.0831 1.1581
O .0417 .7380 3.0079
O -7.1567 4.6152 3.4322
O 6.2854 -3.5817 -3.5487
O -3.2420 -4.4457 .1778
O 3.4321 1.1156 .7556
O -2.7376 4.7999 1.3780
O -2.2422 -3.4608 2.4452
O 3.6808 .8382 3.4156
O -1.9968 4.8184 -3.3754
O 3.8733 -4.0835 .6310
O 1.6401 -.8146 .2474
O -.6492 -3.9392 -.0926
O 3.7025 -4.1486 -2.9380
O 1.7903 -1.0104 -3.3175
O .0926 -4.2601 -3.6666
O -2.6729 -1.9974 -.8178
O -.8919 -1.4169 1.0333
O 1.5685 -5.3293 .6742
O 4.2091 -1.4483 .7347
O -.7429 -1.7641 3.6071
O -4.6085 5.3440 -3.4541
O 4.3720 -1.6878 -3.5141
O -.2718 -.0566 -1.7955
O -6.3921 5.4655 -1.5467
O 5.3287 -2.8158 -1.2631
O -2.1225 -3.8793 -2.3043
O 3.5719 -.1373 -1.5050
O -3.2310 5.3550 -1.1257
O 6.2528 -5.6315 2.0501
O 1.9154 2.5973 2.4734
O -9.5388 5.4269 2.3667
O 4.5776 2.9600 2.1434

O 8.4228 -4.1440 2.3601
O -.7436 3.2215 2.3853
O -1.6795 -.1863 .8456
H -.8095 -1.5066 2.0526
H -2.6824 -1.3429 -.0854