

## *Supplementary Information*

### **Interaction of $\text{TiO}^+$ with water : Infrared photodissociation spectroscopy and density functional calculations**

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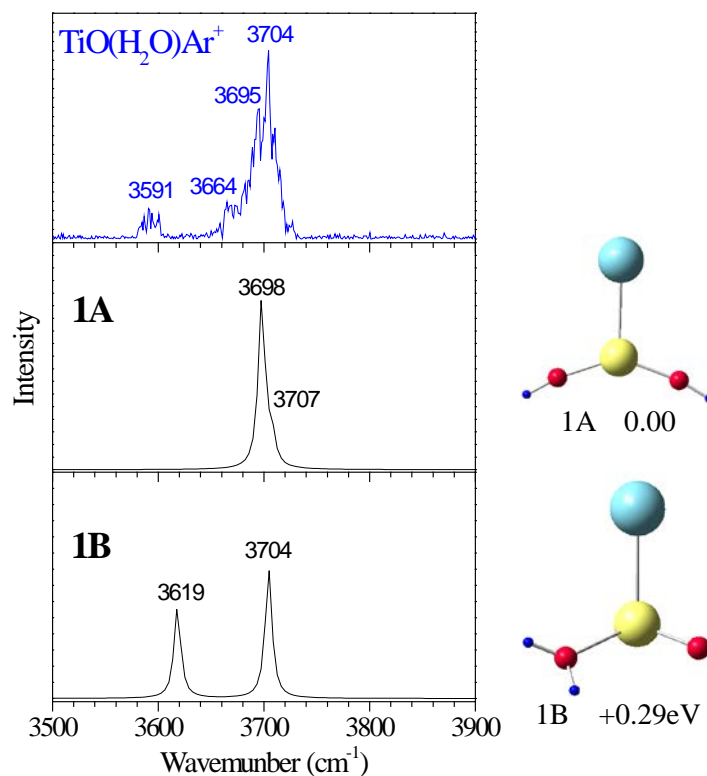
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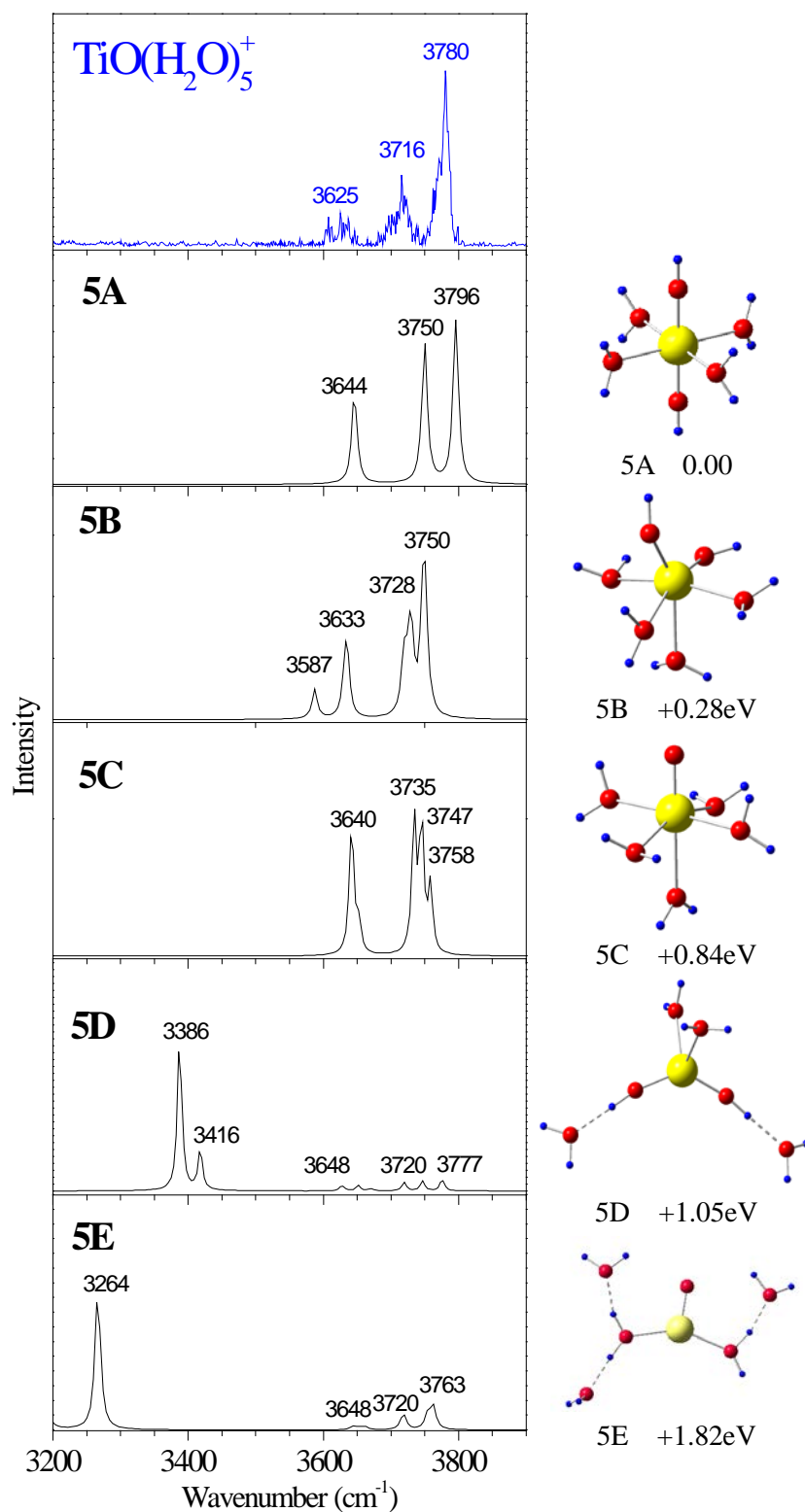
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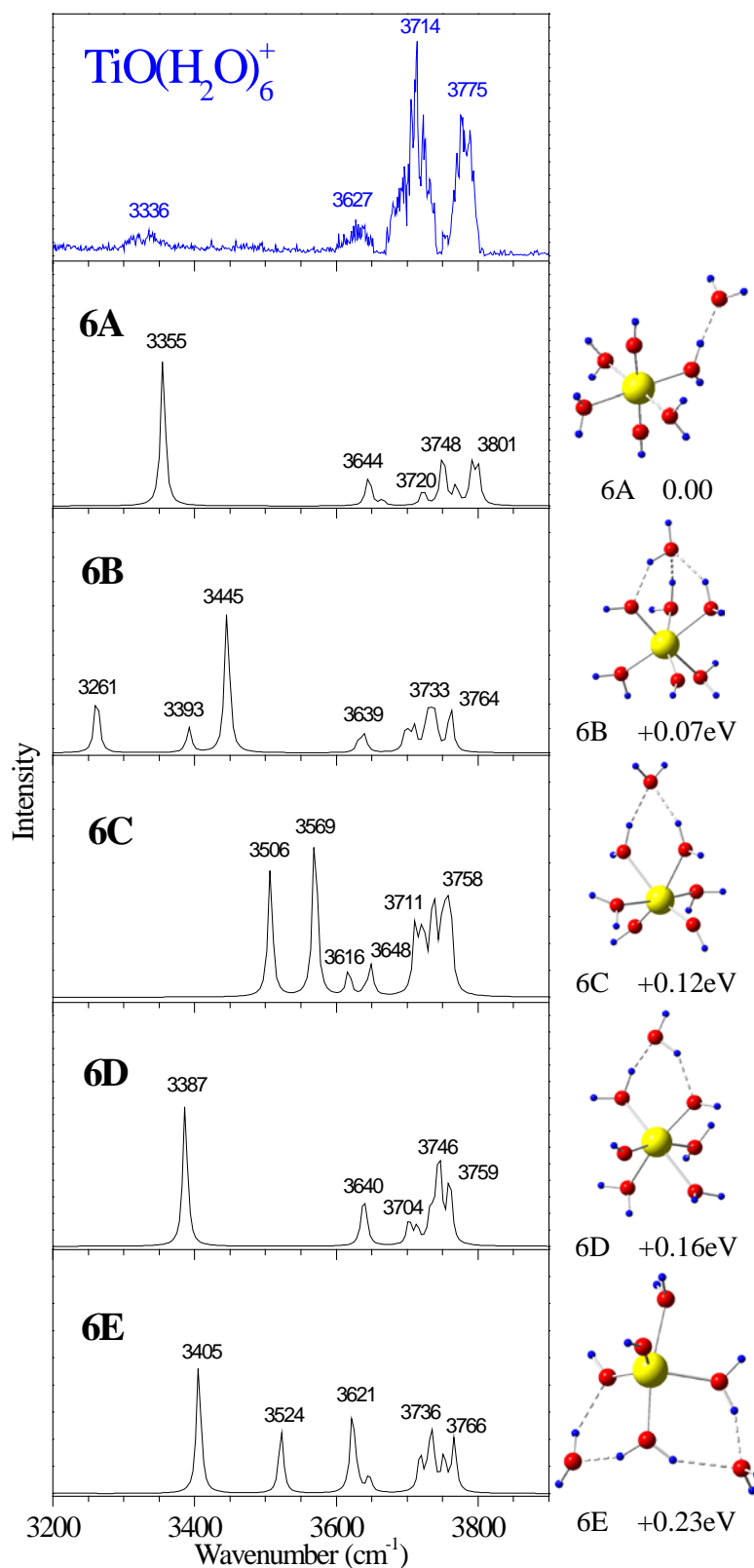
**Figure S1** Optimized geometries of the typical low-lying isomers of  $\text{TiO}(\text{H}_2\text{O})^+$  cluster obtained at B3LPY/6-311G+(d, p) level. The relative energy to the most stable isomer is shown. The yellow, red and blue spheres stand for Ti, O and H atoms, respectively.



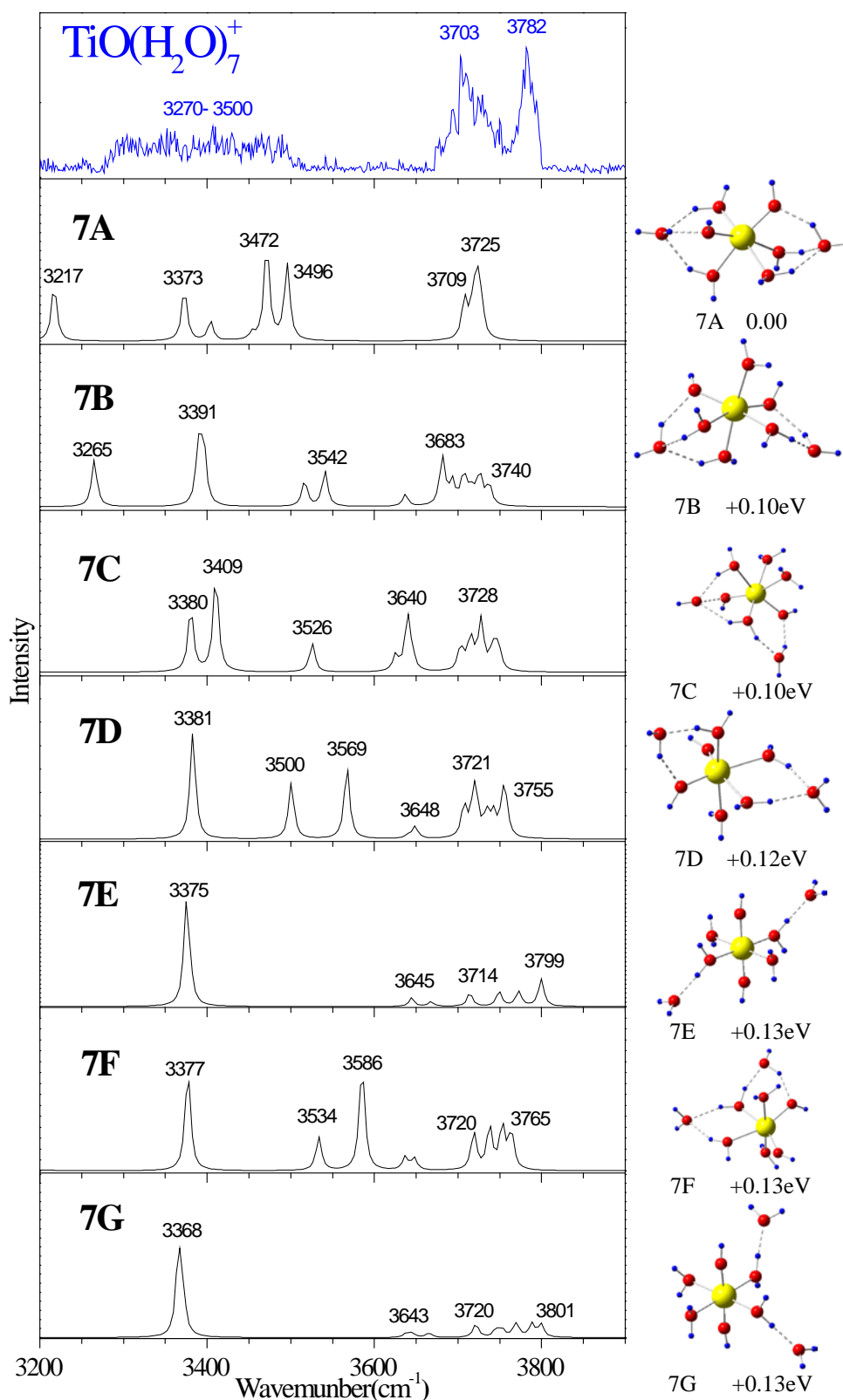
**Figure S2.** IRPD spectrum of  $\text{TiO}(\text{H}_2\text{O})\text{Ar}^+$  cluster and the simulated theoretical IR spectra of its low-lying isomers obtained at MP2/6-311G+ (d, p) level. The theoretical IR spectra were produced by using Lorentzian components with a full width at half-maximum of  $10 \text{ cm}^{-1}$ .



**Figure S3.** IRPD spectrum of  $\text{TiO}(\text{H}_2\text{O})_5^+$  cluster and the simulated theoretical IR spectra of its low-lying isomers obtained at MP2/6-311G+(d, p) level.. The theoretical IR spectra were produced by using Lorentzian components with a full width at half-maximum of  $10 \text{ cm}^{-1}$ .



**Figure S4.** IRPD spectrum of  $\text{TiO}(\text{H}_2\text{O})_6^+$  cluster and the simulated theoretical IR spectra of its low-lying isomers obtained at MP2/6-311G+(d, p) level. The theoretical IR spectra were produced by using Lorentzian components with a full width at half-maximum of  $10 \text{ cm}^{-1}$ .



**Figure S5.** IRPD spectrum of  $\text{TiO}(\text{H}_2\text{O})_7^+$  cluster and the simulated theoretical IR spectra of its low-lying isomers obtained at MP2/6-311G+(d, p) level. The theoretical IR spectra were produced by using Lorentzian components with a full width at half-maximum of  $10 \text{ cm}^{-1}$ .

**Table S1.** Cartesian coordinates for stable isomers of  $\text{TiO}(\text{H}_2\text{O})_n^+$  clusters obtained at B3LPY/6-311G+(d, p) level

<b><math>\text{TiO}(\text{H}_2\text{O})^+</math></b>								
	<b>A</b>				<b>B</b>			
	X	Y	Z		X	Y	Z	
Ti	-0.00070600	-0.29867500	0.00000000	Ti	0.00000000	0.54056600	0.00000000	
O	-0.00070600	0.31085300	1.64935700	O	-1.18577600	-1.24070100	0.00000000	
O	-0.00070600	0.31085300	-1.64935700	O	1.54519000	0.19410200	0.00000000	
H	0.01341500	0.79859800	2.48281800	H	-0.73721400	-2.10143600	0.00000000	
H	0.01341500	0.79859800	-2.48281800	H	-2.13810300	-1.41822300	0.00000000	

<b><math>\text{TiO}(\text{H}_2\text{O})\text{Ar}^+</math></b>								
	<b>1A</b>				<b>1B</b>			
	X	Y	Z		X	Y	Z	
Ti	0.18898000	0.61751700	0.00000000	Ti	0.45272100	0.12711300	-0.16550400	
O	-0.10357800	1.21141500	1.63080000	O	2.26415100	-0.97141300	0.11815100	
O	-0.10357800	1.21141500	-1.63080000	O	0.72553700	1.65931100	0.14415600	
H	-0.31795600	1.68753700	2.44211400	H	3.05188800	-0.48931400	0.41540600	
H	-0.31795600	1.68753700	-2.44211400	H	2.53037300	-1.89098200	-0.02648800	
Ar	-0.10357800	-2.01906100	0.00000000	Ar	-2.19220200	-0.32885400	0.06409500	

<b><math>\text{TiO}(\text{H}_2\text{O})_5^+</math></b>								
	<b>5A</b>				<b>5B</b>			
	X	Y	Z		X	Y	Z	
Ti	-0.00002800	-0.00036800	0.00016600	Ti	-0.06926100	0.12982600	-0.22452400	
O	-1.61067500	-1.53397500	0.00521400	O	-0.08343800	-1.56675700	1.30684400	
H	-1.73002300	-2.08831700	-0.77545000	H	-0.94417300	-1.67480800	1.73333800	
H	-1.73235800	-2.09117600	0.78340700	H	0.21231800	-2.45099500	1.05541000	
O	-0.00871900	-0.00160500	-1.84151700	O	-1.31159100	-0.75516100	-1.30576700	
H	-0.00689600	-0.00198600	-2.79855000	H	-1.32589700	-1.30018500	-2.09625000	
O	1.53621700	-1.60847800	-0.00561300	O	1.65703500	-0.92390900	-1.04234500	
H	2.08808000	-1.73312200	0.77592900	H	2.52463100	-0.69398700	-0.68383700	
H	2.09572500	-1.72524100	-0.78289200	H	1.77151800	-1.14069800	-1.97612200	
O	-1.53506600	1.60919800	0.00482700	O	-2.00113900	0.51584900	0.80764800	
H	-2.09021000	1.72824100	0.78491900	H	-2.30210100	1.35714700	1.17182500	
H	-2.09225100	1.72679700	-0.77405900	H	-2.62868800	0.23381800	0.12058700	
O	1.60842700	1.53601200	-0.00684200	O	0.31500500	1.85250400	-0.69241500	
H	1.71895200	2.10204000	-0.78029700	H	0.10499600	2.49785900	-1.37235100	
O	0.01045400	0.00009600	1.84215000	O	1.52489700	0.66944700	1.35055600	
H	0.01101900	-0.00168700	2.79918800	H	1.57888800	0.36525200	2.26404700	
H	1.73347300	2.08256600	0.77840700	H	1.72610600	1.61465000	1.32672300	

	<b>5C</b>				<b>5D</b>			
	X	Y	Z		X	Y	Z	
Ti	-0.00001000	0.33854100	-0.10258100	Ti	-0.00003900	0.00034900	-0.25295800	
O	-1.62592000	-0.37997300	-0.09197100	O	-0.00029800	0.00148300	-1.89763300	
H	-2.42707600	-0.94490400	-0.06434600	O	-1.90602600	1.23498100	-0.20519900	
O	1.62607500	-0.37956400	-0.09033400	H	-2.21041200	1.97958000	0.32637200	
H	2.42716200	-0.94462500	-0.06341100	H	-2.07283400	1.44894500	-1.13408000	
O	-0.00030600	1.76945800	1.57516700	O	1.90607400	-1.23426500	-0.20767200	
H	0.77696200	1.80691400	2.14923800	H	2.21056500	-1.97980600	0.32251600	
H	-0.77729600	1.80654500	2.14963400	H	2.07252500	-1.44668400	-1.13697500	
O	3.86766800	-1.91769500	0.02319500	O	1.48820800	1.61611900	0.21847700	
H	3.89720900	-2.85346500	0.24854400	H	2.40441100	1.31642200	0.14263400	
H	4.70196200	-1.71472500	-0.41276000	H	1.43530500	2.44106100	-0.28014600	
O	-3.86728400	-1.91820400	0.02365500	O	-1.48805700	-1.61652500	0.21584200	
H	-3.89518000	-2.85640200	0.23898200	H	-2.40430900	-1.31673400	0.14095300	
H	-4.70498600	-1.71040500	-0.40344300	H	-1.43516900	-2.44005300	-0.28512300	
O	-0.00002100	2.15994100	-1.25219300	O	0.00014100	-0.00230500	2.13356000	
H	0.00001800	2.24358400	-2.21355300	H	0.47590100	0.61124100	2.70581700	
H	-0.00025900	3.04788600	-0.87225400	H	-0.47546900	-0.61755000	2.70411900	

	<b>5E</b>		
	X	Y	Z
Ti	0.43974700	-0.14507400	-0.05797100
O	1.14998600	1.31020000	-0.04914600
O	-1.60253400	-0.02203900	-0.01858700
H	-2.28391900	-0.74295300	0.00975100
H	-2.06476400	0.86362800	-0.00292200
O	-3.30376300	-2.05968000	0.05672700
H	-3.78740400	-2.33008300	0.84592300

H	-3.82009200	-2.36520000	-0.69816000
O	2.06349600	-1.43263600	-0.03652600
H	2.26050500	-2.37333300	0.02769200
H	2.91880400	-0.88313600	0.01045600
O	3.86998000	0.34842800	0.16049400
H	3.32069100	1.14570400	0.08739500
H	4.72691300	0.52942300	-0.23962900
O	-2.82919200	2.30436100	0.03601600
H	-2.76726200	2.90462600	0.78797500
H	-2.96167800	2.85388400	-0.74492700

**TiO(H<sub>2</sub>O)<sub>6</sub><sup>+</sup>**

<b>6A</b>				<b>6B</b>			
Ti	-0.48129200	0.00454600	0.03779500	Ti	0.63026100	-0.01357300	0.16200400
O	-0.87410300	2.18564600	-0.19335600	O	2.59036000	-0.77354800	-0.66329800
H	-0.92698100	2.72160000	0.60706900	H	3.22023200	-0.97934900	0.04057300
H	-0.34736600	2.67285100	-0.83820700	H	3.09336200	-0.43140600	-1.41239000
O	-1.21335100	0.06272000	1.73369000	O	0.75950700	1.54909800	-0.89542500
H	-1.58730100	0.08901200	2.61375500	H	1.53525700	1.95869700	-1.28976300
O	1.49350900	0.45146000	0.86249100	O	-1.44969700	2.96633200	-0.07954500
H	2.35043000	0.24840300	0.42339400	H	-1.98835000	3.63421300	-0.51360900
H	1.61027000	0.32331300	1.80986600	H	-0.63635400	2.82100300	-0.60038600
O	-2.51248900	-0.43778800	-0.79352100	O	-1.37861600	0.47772200	0.55365600
H	-2.65272100	-0.23731400	-1.72687400	H	-2.12961700	-0.12534800	0.45536400
H	-3.29396300	-0.14745700	-0.30833000	H	-1.65367400	1.42542200	0.39101600
O	-0.15070900	-2.18670000	0.25473800	O	1.28880200	-0.34272100	1.80840600
H	-0.68312500	-2.65446900	0.90935900	H	1.47002800	-0.13206400	2.72653500
O	0.16089300	-0.06180900	-1.68844100	O	-2.82635600	-1.96088200	-0.15353000
H	0.63303500	-0.08755100	-2.51998400	H	-3.51469100	-1.96558800	-0.83158400
H	-0.14154000	-2.71931300	-0.54950400	H	-3.14396800	-2.54447500	0.54826800
O	3.92873300	-0.02477100	-0.23999500	O	-0.15627200	-1.77034600	-0.73564100
H	4.60290800	0.65320400	-0.35860800	H	0.35797900	-2.49478000	-1.10958300
H	4.36491000	-0.87234300	-0.37826500	H	-1.09778600	-2.03295700	-0.64550100
<b>6C</b>				<b>6D</b>			
Ti	-0.41047900	0.10120300	-0.27662000	Ti	-0.69620200	0.01527300	0.04776500
O	-1.63026500	0.44878100	1.61143800	O	-1.68957000	-0.33620000	-1.50086600
H	-1.15061000	0.48338400	2.44908100	H	-2.18239800	0.19220400	-2.13351500
H	-2.19456700	1.23123900	1.56154800	O	-0.59836000	2.21386300	-0.22882200
O	-1.55212300	1.29407000	-1.02581200	H	-0.17727000	2.65083000	-0.97743700
H	-2.02548400	1.65111900	-1.78010700	H	-1.27677100	2.80041400	0.12539400
O	-1.66814300	-1.69800600	-0.33235900	O	-0.68595700	-2.19250300	0.00911500
H	-2.48001200	-1.71069800	0.19083400	H	-0.76452600	-2.75419500	0.78876800
H	-1.79889100	-2.27616700	-1.09431700	H	-1.38817900	-2.42988400	-0.61564600
O	1.04298300	1.67536900	0.22377900	O	-1.57615600	0.21818600	1.64313300
H	1.96985200	1.35489300	0.21263000	H	-2.43546800	0.19520500	2.06893800
H	0.99870900	2.48939400	-0.29185800	O	3.54788400	-0.11836200	-0.02768800
O	0.89989600	-0.68723800	-1.42978900	H	4.03950000	-0.94878800	0.01680600
H	0.79196700	-1.22980600	-2.21560100	H	4.21441500	0.57594200	-0.10951700
O	2.97903300	-0.18773100	0.12470500	O	1.11038000	0.01355700	1.41406900
H	3.92749100	-0.33452900	0.04622900	H	2.06185500	0.05957200	1.22822700
H	2.52219200	-0.50861600	-0.69032600	H	0.93351000	0.28688600	2.32117900
O	0.70850600	-0.93021900	1.43212400	O	1.06598100	0.12246000	-1.36440600
H	0.55908600	-1.86920100	1.59612000	H	1.99644000	-0.02088100	-1.11012600
H	1.67172600	-0.82768700	1.26871700	H	0.90170000	-0.31132500	-2.21017700
<b>6E</b>							
Ti	0.28222400	0.05639700	-0.21579600				
O	0.55301600	-0.89797600	1.81793900				
H	0.91300000	-0.45333000	2.59489300				
H	-0.18289400	-1.45915500	2.09383300				
O	-1.02241100	-1.34747200	-0.38768600				
H	-0.84978100	-2.19985700	-0.80046600				
O	2.07222100	-1.24457700	-0.61625500				
H	2.28916800	-2.04924800	-0.13005000				
H	2.35727100	-1.36058900	-1.53125600				
O	-1.30383300	1.29153100	0.53762200				
H	-2.21844300	0.88893500	0.39255300				
H	-1.36639400	2.23230800	0.34017000				
O	0.60899300	0.92003600	-1.77241500				
H	0.31022200	1.11800600	-2.66290200				



O	-3.36614300	-0.08233900	-0.09794800
H	-2.76537400	-0.83557500	-0.28874600
H	-4.15433800	-0.40874900	0.34657300
O	1.83734200	1.33077300	0.87292300
H	2.72443200	1.25955000	0.49649300
H	1.70072000	2.26716300	1.06296500

**TiO(H<sub>2</sub>O)<sub>7</sub><sup>+</sup>**

<b>7A</b>				<b>7B</b>			
Ti	0.02169600	0.03490600	-0.17559500	Ti	0.01034600	-0.54440700	0.00162100
O	-1.20238200	0.53104000	1.59201800	O	-1.61990400	0.56204800	-0.96000900
H	-1.03656800	0.31307900	2.51543400	H	-2.25387400	1.14987300	-0.49285700
H	-2.16561700	0.52193400	1.41503500	H	-1.38265300	0.98948000	-1.78992700
O	-1.26013600	1.04611200	-1.18497600	O	-0.88144600	-0.64367100	1.62033700
H	-1.08256000	1.81794300	-1.73184400	H	-1.44968200	-0.58675400	2.38727800
O	-3.36460200	0.08450700	0.01965400	O	0.98395200	1.31107200	0.63835400
H	-4.30871500	0.21889800	-0.11308500	H	1.85269200	1.61914300	0.29723400
H	-2.85696800	0.62846800	-0.63658000	H	0.96808600	1.47755300	1.58678100
O	1.32695500	1.66025500	0.33089100	O	-0.96430900	-2.46777800	-0.61594500
H	2.28001000	1.44585700	0.26257200	H	-1.00606600	-2.62088100	-1.56773300
H	1.19014800	2.61332400	0.31381600	H	-1.83386800	-2.66594700	-0.24856000
O	1.16397100	-0.66348400	-1.49245700	O	1.64307500	-1.75083800	0.95122600
H	0.99717000	-0.76172900	-2.43513100	H	1.36426900	-2.22293000	1.74551900
O	3.36932900	-0.06013700	-0.04756100	O	0.91751400	-0.58067400	-1.60915400
H	4.31796300	-0.14709400	-0.19113500	H	1.47999700	-0.46902000	-2.37431000
H	2.89485100	-0.40281000	-0.83700100	H	2.12434000	-2.37455500	0.39477900
O	1.24943600	-0.97839500	1.39441200	O	3.37947500	2.29601700	-0.20921200
H	1.09952000	-1.88962600	1.67127800	H	4.25300300	1.90221200	-0.11291300
H	2.20384000	-0.87247300	1.20490600	H	3.51591900	3.19153300	-0.53668000
O	-1.34229500	-1.68010100	-0.18365700	O	-3.47089000	2.20453100	0.18042000
H	-1.25460200	-2.39615300	-0.82286200	H	-4.41941900	2.11944100	0.03559700
H	-2.27799300	-1.37593600	-0.17891500	H	-3.34007900	3.02214900	0.67199400
<b>7C</b>				<b>7D</b>			
Ti	-0.24769700	0.42995200	0.10033800	Ti	0.10169200	-0.38411100	-0.20130700
O	-3.41074200	-1.34774500	-0.09860700	O	-3.25637000	1.09191600	0.01431400
H	-3.03988600	-0.72342100	-0.76115900	H	-3.94929400	1.51563200	-0.50070700
H	-3.98549300	-1.97368000	-0.54907100	H	-3.01045800	0.24711400	-0.41681800
O	-1.61140200	0.28581000	-1.24381500	O	-1.65212300	-0.98588400	-0.66052300
H	-1.72597500	0.89783100	-1.97774100	H	-1.86687200	-1.83335700	-1.06398600
O	0.76529900	2.17816400	-0.89555500	O	1.09586600	-2.34565800	-0.65279800
H	1.02210700	2.27815300	-1.81880100	H	0.92843800	-3.16943500	-0.17954700
H	0.51755100	3.04524700	-0.55227500	H	1.45309800	-2.56479300	-1.52163900
O	-1.03808500	-1.38340000	0.87809300	O	-0.76487200	1.36241100	0.61875900
H	-0.83975200	-1.71755500	1.75858000	H	-0.24779900	2.18220600	0.60420700
H	-1.99556400	-1.57160100	0.64183300	H	-1.72949400	1.53049300	0.41988800
O	-0.62814900	1.59561300	1.45869400	O	0.95990900	0.43726400	-1.63686300
H	-1.38658300	1.99664000	1.89013400	H	0.66573200	0.53300700	-2.54840800
O	3.53338500	-1.40653400	-0.18310500	O	1.72868600	2.58118100	0.00992600
H	3.74684500	-2.30617200	0.09708200	H	2.22119700	3.40462000	-0.07899700
H	4.35296900	-1.04401000	-0.54362600	H	1.67466000	2.15697400	-0.86738800
O	1.58393000	-0.03313600	1.36654800	O	1.88022200	0.11838200	1.08376500
H	2.44806500	-0.36577900	1.07356500	H	2.70953700	-0.36082800	0.96902400
H	1.70985000	0.60937500	2.07487300	H	2.08047600	1.07233300	0.95530200
O	1.06751300	-0.67247600	-1.33912400	O	-0.26185100	-1.45594700	1.74379600
H	1.92694200	-1.07691800	-1.11718300	H	0.19116000	-1.11350200	2.52556700
H	0.60426600	-1.23742600	-1.96866700	H	-1.19334600	-1.57934400	1.96924600
<b>7E</b>				<b>7F</b>			
Ti	-0.49904600	-0.57990800	-0.02480700	Ti	-0.03149600	0.30877000	-0.27306800
O	-1.06381200	3.02525100	0.08097400	O	3.17450900	-1.33915300	0.26846300
H	-1.41495800	3.82662200	0.48068900	H	4.12600800	-1.46775200	0.20684500
H	-1.72955500	2.30996900	0.17290700	H	2.83245200	-1.06397600	-0.60481500
O	-2.05946200	0.50246600	0.31723800	O	1.42742900	-0.07969000	-1.43364700
H	-2.66211800	0.37166100	1.05593700	H	1.85315500	0.54703100	-2.02799300
O	-0.06083600	-1.04942800	2.10829700	O	0.45658900	2.45320100	0.04347300
H	0.09796500	-0.35159600	2.75432200	H	1.23994900	2.66524100	0.56687100
H	-0.45506400	-1.80475400	2.55947800	H	0.27133200	3.19426600	-0.54513000
O	-0.84370700	0.20627300	-2.00888100	O	-0.38892800	-1.81918500	-0.19734100
H	-0.49570000	-0.08541300	-2.85835200	H	-1.32733200	-2.06776200	-0.08865300
H	-1.73348100	0.56459900	-2.13076400	H	0.01628600	-2.37947300	-0.87124000

O	-0.89327000	-2.33503000	-0.32993200	O	-1.60322900	0.66109200	-1.23234300
H	-1.58973200	-2.96965400	-0.50974200	H	-1.71096100	0.83568700	-2.17283300
O	3.49079600	0.77173300	-0.09773700	O	-3.02973500	-1.20497200	0.20485800
H	3.92388700	1.20351300	-0.84529500	H	-3.92883200	-1.55187400	0.20660300
H	4.14132900	0.77171800	0.61586500	H	-2.95010400	-0.53562700	-0.50504700
O	1.58058900	-1.21724400	-0.66896500	O	-1.33440700	0.43360600	1.58868000
H	2.42420700	-0.77113100	-0.48048200	H	-1.66281800	1.29065400	1.88615000
H	1.71305400	-2.17210500	-0.67926300	H	-2.11725200	-0.14099800	1.46379500
O	0.70969300	1.16534700	0.55182700	O	1.39753700	0.18728100	1.39156200
H	1.65088400	1.27982700	0.34230600	H	1.05369800	-0.08848700	2.24962400
H	0.22838200	2.02978300	0.44558200	H	2.19922300	-0.36730900	1.17367100

**7G**

Ti	0.00374800	0.00397600	0.00059800
O	-0.40338400	2.18266300	-0.25784700
H	-0.33399400	2.73351100	0.53028900
H	0.11529700	2.60737900	-0.95335300
O	-0.69857100	0.05332100	1.71228100
H	-1.20727600	0.09435900	2.52215400
O	1.95044700	0.53445700	0.87338900
H	2.82035500	0.30868200	0.47270800
H	2.01606000	0.39114100	1.82310000
O	-1.94593800	-0.52333000	-0.86926500
H	-2.00778800	-0.38191400	-1.82072300
H	-2.81860900	-0.30355200	-0.47482800
O	0.41389900	-2.17495500	0.26327700
H	-0.10228000	-2.59936400	0.95845600
O	0.70123700	-0.04734500	-1.69874100
H	1.23607100	-0.08798000	-2.51677700
H	0.34265000	-2.72636100	-0.52638900
O	4.40389400	-0.03248800	-0.14362100
H	4.79387400	-0.90979700	-0.21665200
H	5.13407400	0.59568400	-0.16881100
O	-4.43300500	0.00417100	0.11160100
H	-4.83647600	0.86394700	0.27139600
H	-5.14304200	-0.64516800	0.15768200

**Table S2.** Cartesian coordinates for stable isomers of  $\text{TiO}(\text{H}_2\text{O})_n^+$  clusters obtained at MP2/6-311G+(d, p) level

<b><math>\text{TiO}(\text{H}_2\text{O})\text{Ar}^+</math></b>									
<b>1A</b>				<b>1B</b>					
O	-0.00029700	1.22309900	1.66276600	O	-1.67657700	1.40733300	0.17870800		
H	-0.00081500	1.70589900	2.49656600	H	-2.42249500	1.28900100	0.78259900		
O	-0.00029700	1.22309900	-1.66276600	H	-1.49739200	2.35562600	0.16821000		
H	-0.00081500	1.70589900	-2.49656600	Ti	-0.52980300	-0.34797900	-0.40237600		
Ti	0.00053300	0.62998200	0.00000000	O	-0.88775200	-1.55568300	0.56698900		
Ar	-0.00029700	-2.04672200	0.00000000	Ar	2.00501000	0.28876200	0.10754900		

<b><math>\text{TiO}(\text{H}_2\text{O})_5^+</math></b>									
<b>5A</b>				<b>5B</b>					
Ti	0.00015000	-0.00007200	-0.00000700	Ti	-0.06196600	0.05692600	-0.25710200		
O	-1.62331600	-1.50647200	0.00458700	O	-0.06092800	-1.13775000	1.68540800		
H	-1.75834700	-2.06490000	-0.76869200	H	-0.93943100	-1.26895100	2.06296400		
H	-1.75501000	-2.06803900	0.77613800	H	0.35212500	-2.00903900	1.69956400		
O	-0.00663200	-0.00139400	-1.84359400	O	-1.23176300	-1.17198600	-1.05476800		
H	-0.00406500	-0.00161100	-2.79965000	H	-1.19993000	-1.93327000	-1.63647600		
O	1.50689600	-1.62311300	-0.00282700	O	1.72526700	-1.13536800	-0.66962200		
H	2.06798400	-1.75579200	0.76892600	H	2.59214100	-0.75011400	-0.49372500		
H	2.06582800	-1.75711400	-0.77590000	H	1.81872200	-1.64764400	-1.48109300		
O	-1.50659800	1.62302400	0.00229400	O	-2.00882900	0.68385700	0.57208600		
H	-2.06452600	1.75831100	0.77586800	H	-2.32616400	1.58594400	0.68953400		
H	-2.06886400	1.75367100	-0.76895300	H	-2.64621000	0.22985300	0.00041700		
O	1.62288500	1.50694900	-0.00433500	O	0.32195700	1.55585200	-1.22866000		
H	1.75308700	2.06983500	-0.77518400	O	0.13276500	1.96107100	-2.07748800		
O	0.00641600	0.00134000	1.84366000	O	1.33953500	1.13506900	1.17608600		
H	0.00480600	0.00029200	2.79971700	H	1.35815600	1.10162300	2.13803000		
H	1.75860100	2.06427300	0.76961900	H	1.53916000	2.04076300	0.91028100		

<b>5C</b>									
Ti	0.00001700	0.29593500	-0.11367200	Ti	0.00000800	0.00003600	0.30107600		
O	-1.65308100	-0.37405200	-0.11123500	O	0.00009300	0.00010500	1.94694800		
H	-2.47061300	-0.90813000	-0.08961600	O	1.90295900	1.22096200	0.11000100		
O	1.65313100	-0.37400500	-0.10959300	H	2.16412100	1.91204700	-0.50682900		
H	2.47061200	-0.90817900	-0.08841200	H	2.19212000	1.51653800	0.98162800		
O	-0.00067100	1.63460700	1.62931700	O	-1.90297300	-1.22088100	0.11030500		
H	0.76969200	1.65420700	2.21053500	H	-2.16418000	-1.91199400	-0.50647400		
H	-0.77150500	1.65441500	2.20990100	H	-2.19206200	-1.51641800	0.98196900		
O	3.96599000	-1.80552200	0.02730600	O	-1.39284000	1.70654700	-0.18972200		
H	4.01489300	-2.75664900	0.15872200	H	-2.33123800	1.49178300	-0.13577200		
H	4.75750300	-1.58727400	-0.47282100	H	-1.30063300	2.51763500	0.32267500		
O	-3.96584200	-1.80557200	0.02744400	O	1.39283700	-1.70656000	-0.18954600		
H	-4.01439700	-2.75661400	0.15960900	H	2.33123800	-1.49175500	-0.13582100		
H	-4.75727300	-1.58808100	-0.47314700	H	1.30073100	-2.51744500	0.32319200		
O	0.00043600	2.14813800	-1.22627800	O	-0.00009200	-0.00024500	-2.10932400		
H	0.00063800	2.27181300	-2.18151000	H	-0.45287800	0.62096300	-2.68885000		
H	0.00036300	3.02516900	-0.82816500	H	0.45273400	-0.62157400	-2.68868900		

<b>5E</b>			
Ti	0.33257200	-0.26407700	-0.15436800
O	0.99226200	1.21993600	-0.08620200
O	-1.71667500	-0.02005600	-0.13437400
H	-2.50644100	-0.59496000	-0.01074000
H	-1.97933600	0.93152300	-0.06468100
O	-3.75516100	-1.69061500	0.18818100
H	-4.23838900	-1.81895800	1.01029700
H	-4.37438400	-1.93478800	-0.50664200
O	1.97944700	-1.56262500	-0.05436300
H	2.16147400	-2.49564900	0.09159300
H	2.82878300	-1.04565400	0.05633900
O	3.88718900	0.13240900	0.29075400
H	3.50491300	1.01405800	0.20942600
H	4.79708100	0.20596500	-0.01183800
O	-1.89221000	2.58540400	0.13412200
H	-0.99929900	2.94576100	0.09736500
H	-2.46979500	3.28679000	-0.17998100

**TiO(H<sub>2</sub>O)<sub>6</sub><sup>+</sup>**

<b>6A</b>				<b>6B</b>			
Ti	0.47331300	-0.00480200	0.05476400	Ti	0.63774300	0.03123000	0.14172700
O	0.98137100	-2.14932100	-0.19969300	O	2.64556100	-0.65342000	-0.60696700
H	1.09761500	-2.70582700	0.57770200	H	3.25185200	-0.77303400	0.13525600
H	0.47610900	-2.66644500	-0.83616800	H	3.17032700	-0.29515800	-1.33074900
O	1.27919600	-0.01281300	1.71818900	O	0.62973000	1.53316800	-1.00213600
H	1.68229700	-0.02803600	2.58464700	H	1.32730200	1.97349600	-1.49343900
O	-1.44835800	-0.53784000	0.92740800	O	-1.59888400	2.87274900	-0.04549500
H	-2.30209800	-0.34277200	0.48700100	H	-2.18285700	3.53017900	-0.43092400
H	-1.58143400	-0.39828700	1.86953400	H	-0.83432200	2.77485300	-0.63680900
O	2.40223100	0.53945400	-0.90853200	O	-1.38915200	0.40200900	0.62446100
H	2.46381700	0.34889000	-1.85135100	H	-2.11015000	-0.22136700	0.46889200
H	3.24011200	0.27209200	-0.51624200	H	-1.71069900	1.32568900	0.45081500
O	0.03783600	2.15865700	0.28181400	O	1.34415600	-0.24263500	1.78843100
H	0.53676700	2.65119900	0.94261200	H	1.31133600	-0.13285600	2.73989200
O	-0.23794800	0.01288400	-1.65600100	O	-2.72703000	-2.07140400	-0.16884300
H	-0.90450800	0.02374500	-2.34150000	H	-3.40325800	-2.11273500	-0.85539900
H	0.02456700	2.70526400	-0.51122700	H	-3.05132600	-2.66357900	0.52017000
O	-3.81100700	-0.00548600	-0.28237400	O	-0.06516000	-1.77972000	-0.71249700
H	-4.52166800	-0.64806700	-0.36871600	H	0.47586800	-2.48927800	-1.07261100
H	-4.25102300	0.84961400	-0.28758600	H	-0.98819300	-2.08923700	-0.62873200
<b>6C</b>				<b>6D</b>			
Ti	0.41623900	-0.07416000	-0.27669500	Ti	-0.69491300	0.02588700	0.03559300
O	1.67106900	-0.60895900	1.52087900	O	-1.71714100	-0.37585600	-1.48837800
H	1.24240000	-0.77019300	2.36934300	H	-2.19711500	0.12818600	-2.14775900
H	2.28097100	-1.34244000	1.37710600	O	-0.48026600	2.20419600	-0.32974600
O	1.56026500	-1.14645000	-1.18636500	H	-0.29144700	2.60506700	-1.18423700
H	1.88211100	-1.48050500	-2.02527600	H	-1.08140100	2.79945700	0.13147000
O	1.59148800	1.76757700	-0.14279700	O	-0.73811400	-2.16321200	0.15041200
H	2.47587400	1.75476200	0.24158200	H	-0.75558100	-2.68931700	0.95633000
H	1.59204700	2.45854300	-0.81422100	H	-1.45666000	-2.47479600	-0.41613600
O	-1.02020800	-1.68011000	0.12984800	O	-1.56801800	0.39594300	1.61024500
H	-1.95084100	-1.38371800	0.10133000	H	-2.43358500	0.37714000	2.02154900
H	-0.96444600	-2.49179100	-0.38518300	O	3.53718100	-0.10243400	-0.03020000
O	-0.91819200	0.78688100	-1.37210400	H	4.08462300	-0.88647900	0.09420900
H	-0.80128600	1.38950700	-2.11053100	H	4.17240400	0.60529700	-0.18928400
O	-2.96666900	0.15987500	0.13985200	O	1.09098500	-0.00649700	1.41022600
H	-3.90945500	0.32574800	0.05003400	H	2.03185600	0.10924500	1.21438400
H	-2.50874600	0.54885000	-0.64121300	H	0.91246400	0.35202200	2.28596400
O	-0.70104100	0.75547800	1.51202300	O	1.05374000	-0.04991100	-1.35604900
H	-0.56632200	1.67592300	1.76328900	H	1.98527900	-0.17638200	-1.11081800
H	-1.66327000	0.67249800	1.35035000	H	0.89032400	-0.53677600	-2.17080100
<b>6E</b>							
Ti	0.30277000	0.03737300	-0.22736100				
O	0.42170700	-0.84526400	1.83663300				
H	0.72540700	-0.41705500	2.64408800				
H	-0.31299900	-1.42560900	2.06777700				
O	-1.01033400	-1.36544500	-0.42371300				
H	-0.83841800	-2.20410500	-0.86085100				
O	2.09171300	-1.27035500	-0.48377800				
H	2.25862300	-2.08660500	-0.00027500				
H	2.44928100	-1.39194600	-1.37068100				
O	-1.27829100	1.34425800	0.42385100				
H	-2.18298600	0.92122700	0.33562900				
H	-1.36622800	2.22153900	0.03694200				
O	0.71739700	0.86580300	-1.78380500				
H	0.48091900	1.05563300	-2.69330300				
O	-3.32791100	-0.08049100	-0.09921100				
H	-2.73427500	-0.83373600	-0.29558700				
H	-4.11008100	-0.42546900	0.33824200				
O	1.73994900	1.36115500	0.91602100				
H	2.62947400	1.42373800	0.54810000				
H	1.50650700	2.26289600	1.16387600				

**TiO(H<sub>2</sub>O)<sub>7</sub><sup>+</sup>**

<b>7A</b>				<b>7B</b>			
Ti	0.02424000	0.02145600	-0.18034000	Ti	-0.02480000	0.39777900	-0.22679700
O	-1.18787000	0.64441600	1.54895500	O	2.74311000	-1.56535300	0.06159600
H	-1.03009300	0.48071800	2.48366800	H	3.60227400	-1.97934000	-0.06036800
H	-2.14955100	0.63197800	1.38744100	H	2.60995900	-0.93666200	-0.68482500
O	-1.26277000	0.97047600	-1.25060300	O	1.56509300	0.31980000	-1.30888500
H	-1.07931600	1.68999100	-1.86070600	H	1.94135300	1.03969800	-1.82237200
O	-3.35332600	0.07310500	0.00818400	O	0.08539800	2.56678300	0.18428600
H	-4.29150400	0.20192300	-0.15822600	H	0.90646700	2.97428500	0.48387900
H	-2.85134600	0.57519400	-0.67874600	H	-0.35713300	3.21551100	-0.37466600
O	1.31311400	1.68454900	0.22661400	O	0.02103200	-1.73565600	-0.02033500
H	2.26564800	1.49231700	0.15095400	H	-0.75189200	-2.30771300	-0.10546700
H	1.16529500	2.62522900	0.09156000	H	0.84988900	-2.23074600	-0.11743900
O	1.15934300	-0.77908300	-1.44237500	O	-1.47099100	0.48746400	-1.39527500
H	0.97899700	-0.93713000	-2.37353900	H	-1.43852200	0.54505000	-2.35523200
O	3.36168500	-0.06486000	-0.04478700	O	-2.79335200	-1.52478000	0.01459900
H	4.30825100	-0.17164500	-0.18024000	H	-3.64304400	-1.97293800	-0.04143000
H	2.91164000	-0.46738100	-0.81403100	H	-2.75213700	-0.91157300	-0.73904600
O	1.23231500	-0.86812600	1.45438100	O	-1.45297700	0.30633900	1.47966200
H	1.08675500	-1.76170700	1.78269200	H	-1.93892200	1.07865100	1.78758600
H	2.18525200	-0.79001700	1.26068000	H	-2.12508400	-0.37544100	1.27465700
O	-1.32768700	-1.68808400	-0.04956100	O	1.36771500	0.31674700	1.49792300
H	-1.25014300	-2.43013100	-0.65827700	H	1.02422700	0.03915700	2.35482900
H	-2.26159700	-1.39052000	-0.07221600	H	2.09794500	-0.29981600	1.28086500
<b>7C</b>				<b>7D</b>			
Ti	0.09006000	-0.38623500	-0.20273600	Ti	-0.24887900	0.45089900	0.09615500
O	-3.16761400	1.26081100	0.00535900	O	-3.35741800	-1.40043100	-0.07382900
H	-3.84420600	1.72024800	-0.49815400	H	-3.00672100	-0.77787700	-0.74339000
H	-2.95641100	0.43614300	-0.47538700	H	-3.92987700	-2.02040700	-0.53208000
O	-1.68553800	-0.83946500	-0.78153500	O	-1.60958000	0.24994600	-1.25611000
H	-1.93557400	-1.65360200	-1.22740900	H	-1.76221800	0.87569200	-1.96931100
O	0.97025400	-2.40892300	-0.53004800	O	0.76520600	2.16942300	-0.91347200
H	0.63562600	-3.23001600	-0.15357700	H	0.98973000	2.24754000	-1.84589700
H	1.40255400	-2.63644600	-1.36053300	H	0.52964400	3.05105100	-0.60395500
O	-0.67030000	1.42416500	0.57740100	O	-0.98687000	-1.38322000	0.88825400
H	-0.12842300	2.22347100	0.54158900	H	-0.84229400	-1.64646200	1.80164300
H	-1.62237100	1.63729400	0.38597200	H	-1.93288400	-1.59089500	0.64677200
O	1.07066600	0.31629900	-1.62038400	O	-0.67128700	1.61103400	1.44479200
H	0.82353200	0.40463900	-2.54562700	H	-1.42982200	1.99484700	1.88883100
O	1.93975200	2.43325100	0.01422600	O	3.48946100	-1.45320800	-0.15582800
H	2.50815900	3.20452800	-0.07447600	H	3.68252900	-2.33994100	0.17047200
H	1.89983300	2.01267200	-0.86113300	H	4.32153400	-1.15937600	-0.54456000
O	1.81121100	0.00646400	1.15166100	O	1.58517500	0.03848300	1.33845100
H	2.60455600	-0.53863400	1.11739600	H	2.44406500	-0.30701100	1.05475000
H	2.11008800	0.92769500	1.00436800	H	1.73499100	0.68172400	2.03946100
O	-0.50443000	-1.37964000	1.71104400	O	1.06126300	-0.65783300	-1.32574200
H	-0.13172200	-1.07139300	2.54559900	H	1.88994100	-1.11245600	-1.09909300
H	-1.45897600	-1.44314100	1.83978400	H	0.57911700	-1.20974300	-1.95116500
<b>7E</b>				<b>7F</b>			
Ti	-0.00086700	0.00557500	0.00830800	Ti	-0.49235300	-0.58067100	-0.03590300
O	0.53235700	-2.13455300	-0.26083900	O	-1.09145900	2.97071100	0.12132600
H	0.51961500	-2.70096600	0.51810300	H	-1.45697500	3.77213300	0.50465400
H	0.04551800	-2.60573200	-0.94595300	H	-1.74900500	2.25849700	0.26077500
O	0.72975300	-0.00300200	1.71390500	O	-2.05448900	0.47857000	0.39539100
H	1.35829900	-0.01842800	2.43365600	H	-2.67146700	0.27636800	1.10369500
O	-1.89578300	-0.61388000	0.90679600	O	-0.02955800	-1.20072600	2.04263200
H	-2.76651600	-0.37663700	0.52692300	H	0.00053200	-0.57038700	2.77001400
H	-1.95659000	-0.47458600	1.85703100	H	-0.3829400	-2.02479800	2.39442300
O	1.88998900	0.62580800	-0.89641200	O	-0.79205100	0.37110400	-1.95223600
H	1.94466800	0.49194700	-1.84780000	H	-0.47869600	0.09866200	-2.81998100
H	2.76378500	0.38734400	-0.52471100	H	-1.65876500	0.78094800	-2.06275400
O	-0.53203400	2.14591800	0.27798500	O	-0.90795400	-2.30633100	-0.46621700
H	-0.04463600	2.61635600	0.96322700	H	-1.61846900	-2.90246900	-0.70745200
O	-0.73155600	0.01382200	-1.69799900	O	3.47069400	0.78734100	-0.04096900
H	-1.37452500	0.02291700	-2.40503100	H	3.93595200	1.24482200	-0.75078000
H	-0.51842900	2.71252900	-0.50080100	H	4.10698200	0.76907700	0.68298000
O	-4.31992000	-0.02719400	-0.16879600	O	1.56448100	-1.15820500	-0.73763100
H	-4.74841600	0.83344500	-0.17984900	H	2.40729700	-0.73585400	-0.50946500
H	-5.04171100	-0.66194000	-0.20192300	H	1.71259100	-2.10562200	-0.82419600

O	4.33128800	-0.01442500	0.10984800	O	0.69644500	1.13730700	0.61784300
H	4.73392900	-0.88738100	0.10038000	H	1.62741400	1.28259900	0.39498300
H	5.07133200	0.59854600	0.14806800	H	0.20842600	1.99263100	0.51185300

**7G**

Ti	-0.00653900	-0.51192800	-0.01545500
O	-1.47746900	0.65607900	-1.12586300
H	-2.12310000	1.22810600	-0.66189200
H	-1.17929300	1.14037300	-1.90136400
O	-1.11632300	-0.57059600	1.48160000
H	-1.85828900	-0.26076900	1.99941300
O	0.97631300	1.29004600	0.72210200
H	1.85694100	1.56576700	0.39301100
H	0.98690500	1.41501800	1.67568100
O	-0.92595500	-2.39922600	-0.76076300
H	-0.81634200	-2.58127200	-1.70055500
H	-1.84219600	-2.59987700	-0.54277600
O	1.36107400	-1.76115500	1.21832600
H	0.91315100	-2.14395600	1.98193800
O	1.11594800	-0.61153100	-1.48576500
H	1.78726300	-0.41557600	-2.13714600
H	1.85779900	-2.47541300	0.80553900
O	3.39050700	2.08205700	-0.22881600
H	4.22356900	1.62543500	-0.07988100
H	3.63617400	2.99882200	-0.38444900
O	-3.31043300	2.14228400	0.21655200
H	-4.24600800	2.13073800	-0.00731400
H	-3.16202100	3.01135200	0.60081200