

## Electronic Supplementary Information

### **DFT characterization on the mechanism of sulfoxidation with H<sub>2</sub>O<sub>2</sub> catalyzed by tetranuclear peroxotungstates [XO<sub>4</sub>{WO(O<sub>2</sub>)<sub>2</sub>}]<sub>4</sub><sup>n-</sup> (X = Si<sup>IV</sup>, P<sup>V</sup>, S<sup>VI</sup>, As<sup>V</sup>, and Se<sup>VI</sup>)**

Bo Zhu, Li-Kai Yan\*, Wei Guan\* and Zhong-Min Su\*

*Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun 130024, P. R. China; E-mail: [yanlk924@nenu.edu.cn](mailto:yanlk924@nenu.edu.cn); [guanw580@nenu.edu.cn](mailto:guanw580@nenu.edu.cn); [zmsu@nenu.edu.cn](mailto:zmsu@nenu.edu.cn)*

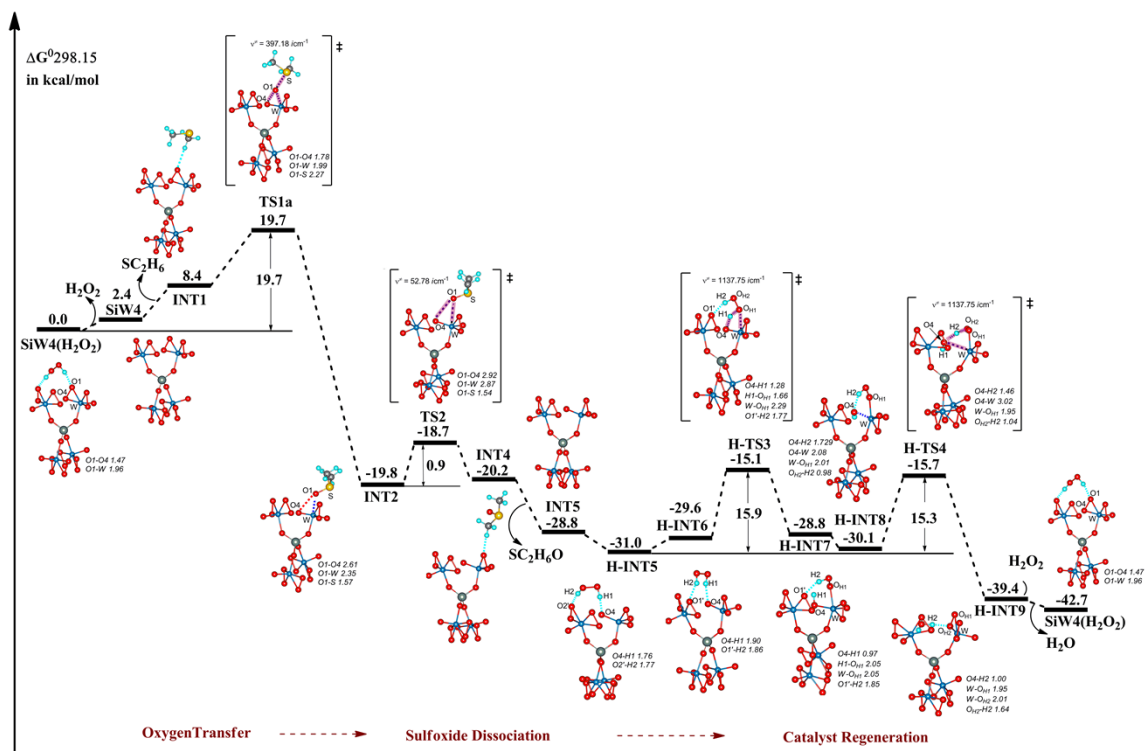
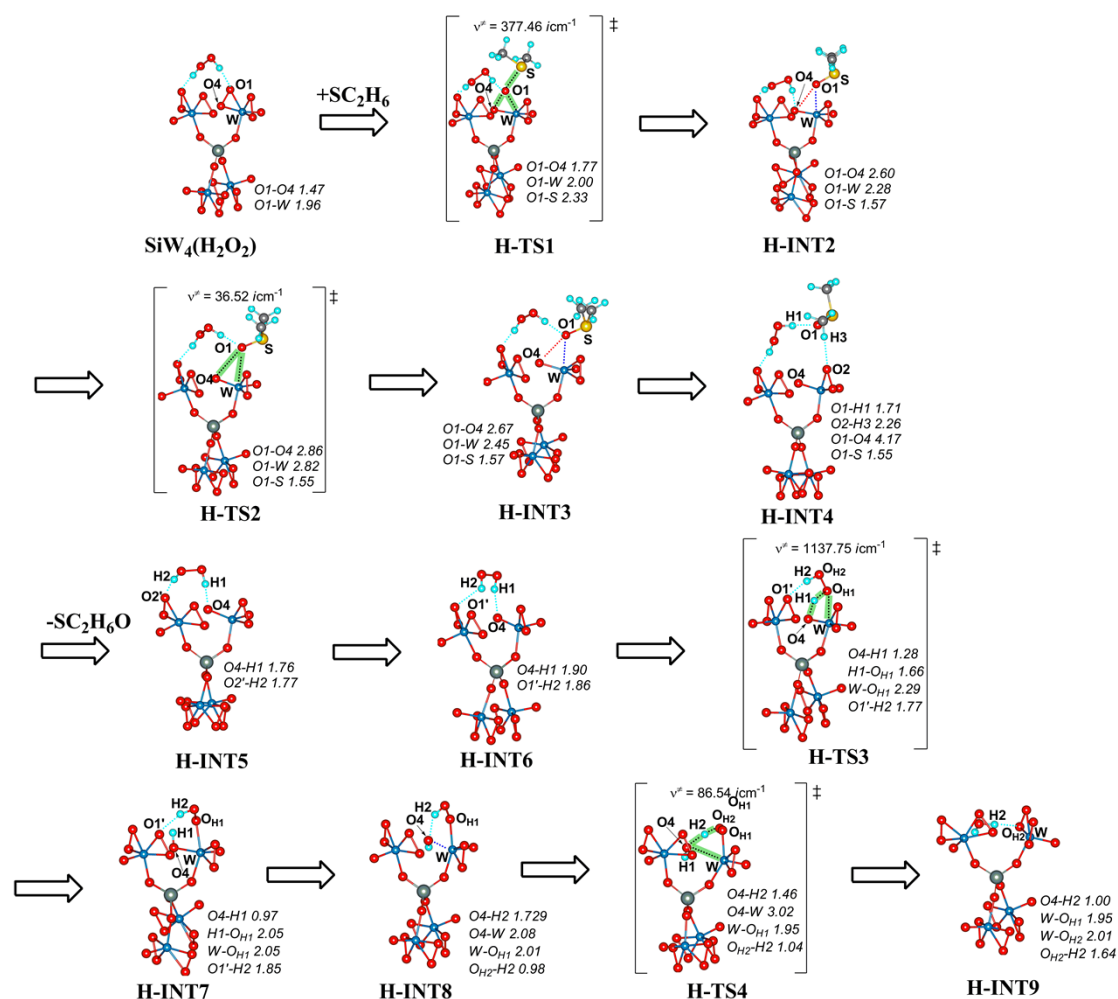
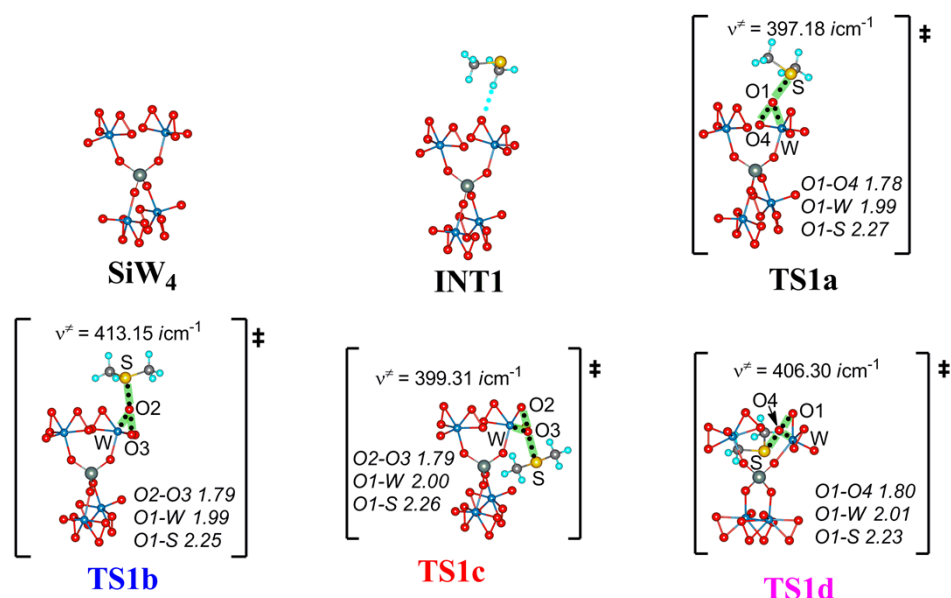


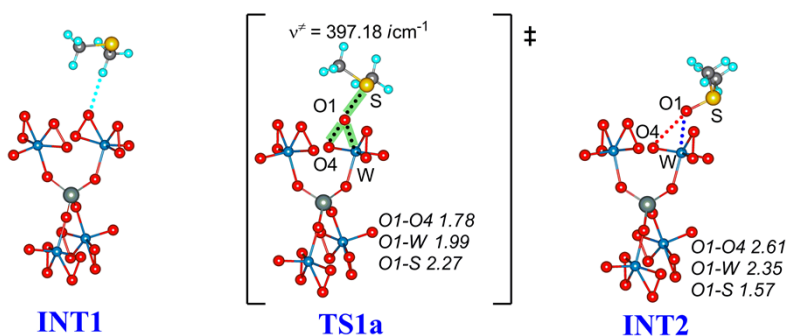
Fig. S1 Energy profiles ( $\Delta G^{\circ}_{298.15}$ ) of the catalytic cycle of  $\text{SiW}_4$  catalyzed reaction.



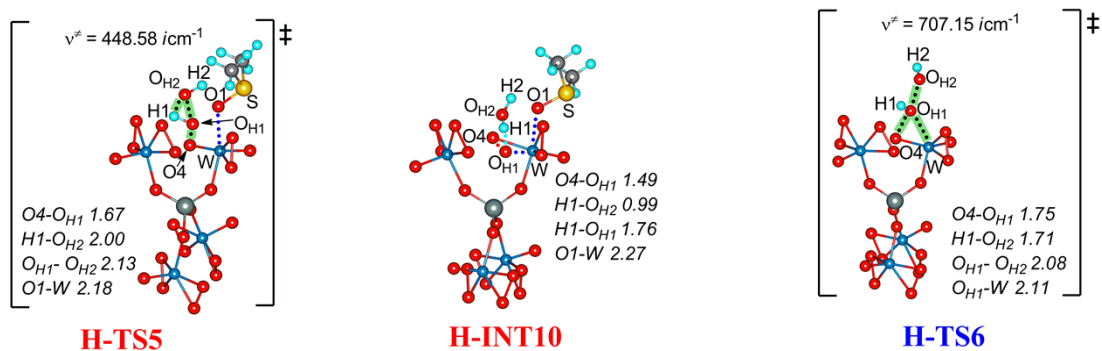
**Fig. S2** Optimized structures and selected geometrical parameters (bond lengths in angstroms) of stationary points in **Fig. 1**.



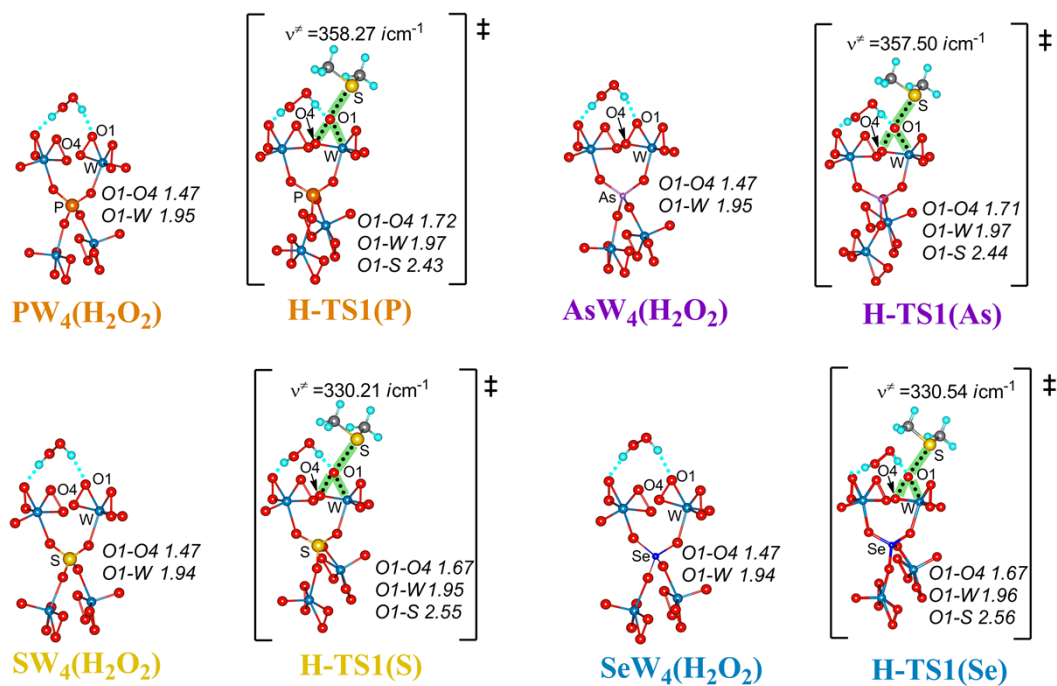
**Fig. S3** Optimized structures and selected geometrical parameters (bond lengths in angstroms) of stationary points in **Fig. 2**.



**Fig. S4** Optimized structures and selected geometrical parameters (bond lengths in angstroms) of stationary points in **Fig. 3**.



**Fig. S5** Optimized structures and selected geometrical parameters (bond lengths in angstroms) of stationary points in **Fig. 4**.



**Fig. S6** Optimized structures and selected geometrical parameters (bond lengths in angstroms) of stationary points in **Fig. 5**.

**Table S1** The natural charge of **WO<sub>5</sub>** group and the outer peroxy atoms (**O1-O4**) of tetranuclear peroxotungstates  $[\text{XO}_4\{\text{WO}(\text{O}_2)_2\}_4]^{n-}$  (X = Si<sup>IV</sup>, P<sup>V</sup>, As<sup>V</sup>, S<sup>VI</sup> and Se<sup>VI</sup>).

	<b>WO<sub>5</sub></b>	<b>O1</b>	<b>O2</b>	<b>O3</b>	<b>O4</b>
<b>SiW<sub>4</sub></b>	-0.567	-0.422	-0.464	-0.437	-0.419
<b>PW<sub>4</sub></b>	-0.422	-0.386	-0.420	-0.411	-0.416
<b>AsW<sub>4</sub></b>	-0.427	-0.384	-0.418	-0.412	-0.421
<b>SW<sub>4</sub></b>	-0.302	-0.350	-0.374	-0.388	-0.417
<b>SeW<sub>4</sub></b>	-0.305	-0.348	-0.372	-0.388	-0.422

**Table S2** The calculated condensed Fukui function ( $f^+$ ) of the outer peroxy atoms (**O1-O4**) of tetranuclear peroxotungstates  $[\text{XO}_4\{\text{WO}(\text{O}_2)_2\}_4]^{n-}$  (X = Si<sup>IV</sup>, P<sup>V</sup>, As<sup>V</sup>, S<sup>VI</sup> and Se<sup>VI</sup>).

	<b>O1</b>	<b>O2</b>	<b>O3</b>	<b>O4</b>
<b>SiW<sub>4</sub></b>	0.063	0.054	0.053	0.032
<b>PW<sub>4</sub></b>	0.069	0.047	0.060	0.025
<b>AsW<sub>4</sub></b>	0.066	0.048	0.058	0.027
<b>SW<sub>4</sub></b>	0.072	0.043	0.066	0.020
<b>SeW<sub>4</sub></b>	0.070	0.0433	0.064	0.021

## Optimized Cartesian Coordinates

### SiW<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>

O	-1.11359900	-0.98358400	-0.93667000
O	-2.64753200	-3.30681000	-0.72892000
O	-2.86422800	-1.42734900	-2.92668600
O	-4.25256500	-1.64325500	-2.44818100
O	-4.46520700	-1.38823000	0.23604200
O	-3.23667100	-0.89831400	0.88362800
O	-1.21552000	0.96397700	0.89293900
O	-2.78702400	3.24758100	0.54533800
O	-3.13249400	1.36557000	2.72616000
O	-4.48172400	1.54696300	2.13548300
O	-4.46892600	1.27803100	-0.55499200
O	-3.17938500	0.82274100	-1.10053900
O	0.80257600	0.88329400	-0.90879700
W	-2.96008600	-1.63402200	-0.98585100
W	-3.07407500	1.56755600	0.78322400
O	0.70016400	-0.89995100	1.07129800
O	2.35665400	-3.13742600	1.18732000
O	2.34242200	-1.03640300	3.18304000
O	3.76460300	-1.21999800	2.80400000
O	4.12679100	-1.23177900	0.11746900
O	2.91575900	-0.87266200	-0.64032100
O	2.24115000	3.26708800	-0.73601300
O	2.76800500	1.20097000	-2.70619300
O	4.08333900	1.53542400	-2.10789500
O	3.96182400	1.48612000	0.60769800
O	2.67165800	1.03380300	1.15193700
W	2.56125900	-1.43382500	1.28537500
W	2.61123200	1.59061800	-0.79447300
Si	-0.21338300	-0.01056600	0.03149100
O	6.39594700	-0.69744000	-1.38619200
O	5.70816500	-0.60535600	-2.66787200
H	5.13196700	0.18617400	-2.52339200
H	5.66554400	-0.98638700	-0.79450100

### H-TS1

O	-1.28657100	0.94607600	0.72628800
O	-2.43687600	3.48122500	0.53986400
O	-2.79094800	1.71289100	2.81344900
O	-4.15674400	2.14265400	2.42265600
O	-4.60508300	1.85985100	-0.22663700
O	-3.52257200	1.16735900	-0.94587100
O	-1.82552100	-0.98512900	-1.03433000
O	-3.70505400	-2.98449600	-0.51140200
O	-3.90694700	-1.11865300	-2.72348800
O	-5.22149600	-1.06701200	-2.03659700
O	-4.97474900	-0.75239500	0.63699700
O	-3.59438200	-0.49796200	1.08298200
O	0.18387100	-1.30359900	0.73240600
W	-2.99123500	1.88637200	0.87635200
W	-3.74070000	-1.28449300	-0.78237300
O	0.43959700	0.41120500	-1.29629500
O	2.21233400	2.52926400	-1.45865700
O	2.21059600	0.16776600	-3.18103100
O	3.61067500	0.39033700	-2.77213200

O	3.96011800	0.76837600	-0.12465400
O	2.38016700	0.40623500	0.58415400
O	1.65640500	-3.60027300	1.12709400
O	1.82030400	-1.32158000	2.86726100
O	3.23063200	-1.66252200	2.54741100
O	3.56832200	-2.03528800	-0.16437500
O	2.38668800	-1.68533600	-0.97088800
W	2.36539800	0.81595600	-1.32894900
W	2.01255200	-1.91870600	1.00861200
Si	-0.61543900	-0.22424300	-0.21769700
C	7.00586300	0.11216500	-0.19346000
H	6.68620000	0.08086600	0.85040900
H	8.06235100	0.38291600	-0.26327700
H	6.84849800	-0.86305200	-0.65764500
S	5.99897300	1.31151800	-1.12124600
C	6.37677800	2.84478400	-0.21387800
H	5.78071300	3.63945200	-0.66662400
H	6.11284100	2.74191800	0.84095600
H	7.43847600	3.08365000	-0.31622100
O	5.00171800	1.13995000	2.39081100
O	4.03645100	0.81790200	3.43192400
H	3.77430000	-0.09866900	3.17308600
H	4.46080000	1.09603000	1.56594300

#### H-INT2

O	-1.21796400	0.76582200	0.81086700
O	-2.14161200	3.39736700	0.86641800
O	-2.75219300	1.43550500	2.91344300
O	-4.05752700	2.02083200	2.51713500
O	-4.39259200	2.06470500	-0.16701300
O	-3.33668400	1.35515500	-0.90960400
O	-1.83093900	-0.92932700	-1.15383900
O	-3.89894000	-2.78919300	-0.93192600
O	-3.82597700	-0.69579800	-2.93687400
O	-5.16420000	-0.59421700	-2.30247000
O	-5.02545900	-0.58156900	0.39712600
O	-3.65274100	-0.49993200	0.92458700
O	0.12225400	-1.55885900	0.57826600
W	-2.84056500	1.82897700	0.99975900
W	-3.77048700	-1.07397300	-1.01866200
O	0.50263500	0.35945700	-1.25670000
O	2.34058300	2.37065000	-1.26471600
O	2.29851100	-0.06682900	-2.98857300
O	3.68166700	0.11377500	-2.56084200
O	4.57799600	1.06838100	-0.39179900
O	2.37357400	0.16158500	0.64699800
O	1.63271100	-3.76418400	1.18169500
O	1.52014100	-1.48316900	2.89990500
O	2.96757000	-1.78273700	2.74612300
O	3.62593900	-2.17741900	0.06569100
O	2.51047100	-1.91296400	-0.86318100
W	2.45408300	0.64531400	-1.13076400
W	1.94509200	-2.06885000	1.07273700
Si	-0.58689900	-0.32941000	-0.25098900
C	6.86970900	0.93636900	-1.76537400
H	7.27621000	0.41725600	-0.89498500
H	7.63136300	1.55214800	-2.24982400

H	6.44623500	0.22840900	-2.47878300
S	5.50657800	2.01303900	-1.23782900
C	6.36834700	2.98527000	0.02790900
H	5.62666600	3.64272500	0.48312800
H	6.79648100	2.31133100	0.77219100
H	7.14345800	3.57766400	-0.46422200
O	4.22060000	1.17312900	2.43405100
O	3.48467800	0.78553000	3.63331600
H	3.34285400	-0.17379700	3.45767600
H	3.59856200	0.90334600	1.70693000

### H-INT3

O	1.43678300	-0.72636200	1.15857100
O	2.56738900	-3.26016700	1.47734000
O	3.24492100	-0.97077400	3.12643600
O	4.54045200	-1.52768100	2.66299900
O	4.57799500	-1.96692000	-0.00373900
O	3.39200500	-1.45757100	-0.71216300
O	1.68050000	0.63287900	-1.12366200
O	3.58166600	2.65426400	-1.42659700
O	3.48551600	0.26803700	-3.07308200
O	4.88768600	0.36702900	-2.59559700
O	5.04248600	0.77206400	0.07011500
O	3.74882200	0.68161900	0.76737400
O	-0.14044900	1.38690700	0.71840100
W	3.15053200	-1.64997500	1.29471000
W	3.60207000	0.94233800	-1.24127300
O	-0.48353100	-0.88272800	-0.72231600
O	-2.43283200	-2.65122500	0.03665900
O	-2.02978300	-1.21306400	-2.72532500
O	-3.46951000	-1.22820700	-2.41457000
O	-4.79761300	-1.26923600	-0.22112500
O	-2.68952400	0.28652700	0.30231100
O	-1.11762600	3.95714400	1.00734200
O	-2.14039800	1.80521500	2.56484200
O	-3.31919400	2.49121500	1.98761300
O	-3.05889600	2.87839400	-0.73158200
O	-1.77896500	2.37771200	-1.27923900
W	-2.41961600	-1.11195900	-0.77708600
W	-1.81758300	2.40819900	0.70043100
Si	0.60060800	0.11071500	0.00886400
C	-6.82203100	-2.05359400	-1.80181900
H	-7.42308500	-1.26188000	-1.35029600
H	-7.43813100	-2.91932900	-2.05660800
H	-6.30193100	-1.68927400	-2.68875100
S	-5.53546800	-2.59151500	-0.63816700
C	-6.56985200	-2.99834100	0.79711100
H	-5.89238500	-3.27449700	1.60644300
H	-7.17318700	-2.13180000	1.07426900
H	-7.20153600	-3.84917000	0.53109300
O	-6.05380900	0.80645600	1.03910500
O	-5.42337400	0.83023800	2.35230600
H	-4.62887500	1.40102700	2.17951100
H	-5.57616200	0.06003500	0.59804700

### H-TS2



O	1.51995800	-0.75727800	1.17573500
O	2.71270300	-3.26834600	1.44635700
O	3.38322300	-0.97589400	3.09393000
O	4.67791000	-1.50300900	2.59552000
O	4.65760000	-1.92182700	-0.07601300
O	3.44366200	-1.42924700	-0.74787700
O	1.68115400	0.64444100	-1.09126200
O	3.54488700	2.69249100	-1.43555600
O	3.44033700	0.31353200	-3.09196500
O	4.85359600	0.43447200	-2.65444300
O	5.07461500	0.82313700	0.01021100
O	3.80099300	0.70479300	0.73947400
O	-0.13806600	1.30637000	0.80023100
W	3.25872300	-1.64615400	1.26141700
W	3.59840200	0.98068400	-1.26140600
O	-0.43226400	-0.94138600	-0.66751800
O	-2.52418400	-2.73001300	-0.12028700
O	-2.10552900	-0.95602300	-2.69111500
O	-3.52483000	-0.91355000	-2.25486500
O	-5.08995400	-1.28469400	-0.08579000
O	-2.67448800	0.11371200	0.52377100
O	-1.15679300	3.88724300	0.86111400
O	-2.10504800	1.84738400	2.63647700
O	-3.30891200	2.46374400	2.03272600
O	-3.11211200	2.59184600	-0.71427900
O	-1.84528300	2.03399000	-1.23185000
W	-2.35335400	-1.11103900	-0.72469800
W	-1.83035900	2.30433300	0.73063000
Si	0.64880100	0.07759000	0.05749800
C	-6.91454000	-1.66461200	-2.03153600
H	-7.51792100	-0.87454400	-1.57902800
H	-7.54719000	-2.43240200	-2.48372300
H	-6.23141900	-1.25271300	-2.77573400
S	-5.87346300	-2.44558600	-0.75904200
C	-7.17600000	-2.90178700	0.42746100
H	-6.67746600	-3.33359500	1.29681400
H	-7.74132900	-2.01104600	0.71007100
H	-7.82403000	-3.64719800	-0.03989300
O	-6.14746500	0.82724300	1.23440600
O	-5.43453600	0.81247800	2.50538300
H	-4.63702600	1.36136300	2.29308200
H	-5.75016700	0.04791400	0.76266000

#### H-INT4

O	1.71815100	-0.98373600	1.03936900
O	3.15565800	-3.37299600	1.01149100
O	3.61826700	-1.24187600	2.92365300
O	4.95281300	-1.57668100	2.36821800
O	4.94589900	-1.66852800	-0.33454000
O	3.68320100	-1.21160300	-0.93887100
O	1.72972500	0.74021000	-1.00734100
O	3.41736200	2.96278800	-1.10879300
O	3.48744900	0.80159100	-3.04122700
O	4.89108700	0.98756100	-2.59608600
O	5.10887100	1.06583100	0.09911800
O	3.85628500	0.74756600	0.80437600
O	-0.09429700	0.98166300	0.99387700

W	3.54200000	-1.69610700	1.02448300
W	3.61380900	1.25351700	-1.14436600
O	-0.27409700	-1.02311900	-0.78186100
O	-2.39152600	-2.91364200	-0.36061800
O	-2.29229500	-0.97109700	-2.71099100
O	-3.60462800	-0.86080400	-1.99691900
O	-6.60266800	-1.43062500	0.40582600
O	-2.59535600	-0.31535700	0.73368400
O	-1.18530300	3.53760400	0.86997200
O	-2.07188100	1.57232300	2.78696000
O	-3.29669900	2.11784600	2.15445100
O	-3.09361800	2.06850000	-0.59558100
O	-1.83918900	1.45540700	-1.06747400
W	-2.18267000	-1.23469100	-0.73603500
W	-1.81028000	1.93252900	0.87075000
Si	0.77816400	-0.05499800	0.06748700
C	-6.87851300	-0.32942500	-2.04786900
H	-7.14892300	0.61319200	-1.56603600
H	-7.42213500	-0.45775200	-2.98737600
H	-5.80222400	-0.38459700	-2.22408600
S	-7.29732200	-1.71850800	-0.94754100
C	-9.06416000	-1.34482100	-0.70006400
H	-9.44804500	-2.07481800	0.01458700
H	-9.17230900	-0.33032900	-0.30933700
H	-9.58099600	-1.45367800	-1.65698900
O	-6.41781600	0.85508600	1.83805400
O	-5.41142800	0.48633100	2.82735800
H	-4.62867700	1.00297600	2.51401900
H	-6.48107400	0.02624400	1.29230100

#### H-INT5

O	-1.14750400	-1.18403500	-0.86937600
O	-2.87908100	-3.33263900	-0.45720900
O	-2.99139900	-1.59383300	-2.77754900
O	-4.37845000	-1.65651300	-2.25436100
O	-4.49039300	-1.19293900	0.40744400
O	-3.20545200	-0.77421700	0.99142100
O	-1.02628400	0.89800000	0.80920700
O	-2.40680100	3.28298100	0.35215700
O	-2.83919400	1.59007600	2.66647900
O	-4.18773500	1.84651000	2.10253000
O	-4.28617300	1.39727400	-0.56390400
O	-3.05809700	0.79467600	-1.10873800
O	0.89791400	0.52661900	-1.07854900
W	-3.04915400	-1.66052400	-0.82590200
W	-2.83051200	1.65509300	0.71379800
O	0.75571100	-1.09302200	1.04024100
O	2.78915300	-3.07035200	1.39322400
O	2.46554700	-0.65275600	3.17095700
O	3.87448200	-0.75908100	2.67954400
O	3.31510800	-0.83840600	-0.26865500
O	2.12597600	3.02095800	-1.30218400
O	3.01260600	0.68322600	-2.74398500
O	4.22885300	1.27821700	-2.13618700
O	3.80359200	1.73779100	0.57168300
O	2.47494100	1.28726500	1.02162000
W	2.63451800	-1.34985200	1.31794800

W	2.64035300	1.41568400	-0.96411500
Si	-0.14317400	-0.19641100	-0.03343800
O	5.91079200	-1.29141100	-1.01042400
O	5.79961200	-0.95170000	-2.42519800
H	5.33274400	-0.08147200	-2.37794800
H	4.96471700	-1.26004100	-0.72332800

**H-INT6**

O	1.20595100	-1.16191000	0.85270400
O	2.99919500	-3.27512600	0.54319000
O	3.05884400	-1.42472200	2.77855500
O	4.44757800	-1.47284800	2.25824600
O	4.55120300	-1.13153400	-0.41863200
O	3.25673600	-0.78537800	-1.02801500
O	1.02517700	0.80592000	-0.95219900
O	2.31448600	3.26160200	-0.60825700
O	2.82768600	1.46756700	-2.82859100
O	4.16108000	1.80366900	-2.27067000
O	4.25575700	1.49678400	0.41468000
O	3.04714800	0.88161200	0.98751300
O	-0.79857500	0.60055300	1.05415500
W	3.12003900	-1.58321400	0.83214400
W	2.80105600	1.63389300	-0.88225900
O	-0.79578200	-1.16578400	-0.95260000
O	-2.75947700	-3.24861400	-0.90616000
O	-2.76177700	-0.99366100	-2.90940900
O	-4.09752500	-1.08281800	-2.23729100
O	-3.22442200	-0.88783000	0.59291900
O	-2.10590500	3.06085600	1.20663200
O	-2.76665900	0.79933000	2.88762300
O	-4.04998600	1.27816600	2.32079000
O	-3.90191400	1.60162100	-0.41458800
O	-2.60761400	1.14262600	-0.94637100
W	-2.67760700	-1.52363100	-0.99816600
W	-2.58258200	1.41606000	1.03995500
Si	0.17075600	-0.21217900	0.00895600
O	-6.02449100	-1.00364800	0.48833700
O	-6.34251000	0.36341300	0.08720000
H	-5.50682100	0.66804000	-0.33701100
H	-5.10442200	-0.92631300	0.82961900

**H-TS3**

O	0.90528300	-0.80064000	0.85292700
O	2.19601600	-3.27703500	0.76296000
O	2.53317500	-1.35823900	2.91204100
O	3.90618500	-1.72866100	2.48778700
O	4.23288700	-1.58430600	-0.18912500
O	3.08345500	-1.00597700	-0.90464400
O	1.25383900	1.02156700	-1.06564700
O	3.01557400	3.16189800	-0.73522400
O	3.26082100	1.17566200	-2.83626200
O	4.59946400	1.25049500	-2.20016500
O	4.47236700	1.09227000	0.49335500
O	3.12983400	0.78500900	1.01349700
O	-0.78057100	1.29969700	0.66777300
W	2.66817600	-1.63595100	0.98135600
W	3.15421200	1.45405100	-0.90391100

O	-0.85098600	-0.61093500	-1.21185400
O	-2.32492500	-2.96632900	-1.07232400
O	-2.71758500	-0.73795800	-2.98679800
O	-4.02575600	-1.13473100	-2.46244300
O	-2.66716700	-0.74234500	0.77673500
O	-2.67298000	3.26123700	1.02134400
O	-2.30020300	1.12837600	2.92350000
O	-3.75496500	1.16647000	2.63681000
O	-4.32451200	1.27981200	-0.04189800
O	-3.14253500	1.13924400	-0.91202800
W	-2.67382300	-1.27837900	-1.08529700
W	-2.68266600	1.53666400	1.04924800
Si	0.12728400	0.21977200	-0.17605700
O	-4.58983500	-1.74832800	0.08615300
O	-5.80454200	-0.99829900	-0.16938500
H	-5.45409800	-0.07318700	-0.18900100
H	-3.86313400	-1.19980100	0.81377800

#### H-INT7

O	0.94565100	-0.60303600	1.05259100
O	2.14270400	-3.12212900	1.19923600
O	2.69869600	-0.96132000	3.05383700
O	4.02456000	-1.44047000	2.58947700
O	4.15426900	-1.65155400	-0.10515400
O	2.97496400	-1.11157300	-0.80221300
O	1.21392900	0.98126700	-1.07302800
O	3.07883500	3.05332100	-1.15545000
O	3.07905200	0.81079600	-2.99685700
O	4.46590600	0.90283000	-2.47566600
O	4.54383800	1.08239200	0.21773000
O	3.23373000	0.90179300	0.86648500
O	-0.79603800	1.41339000	0.65006400
W	2.68199900	-1.48715800	1.17092400
W	3.13344100	1.33271500	-1.11317000
O	-0.86094600	-0.70245400	-0.98328300
O	-2.32599600	-3.05446500	-0.89936800
O	-2.47730200	-0.96251800	-2.90318900
O	-3.86589200	-1.27900700	-2.58085800
O	-2.53470700	-0.76643400	0.95347100
O	-2.75728200	3.33904200	0.90090400
O	-2.29014500	1.33204700	2.91642100
O	-3.74373800	1.25471100	2.62808500
O	-4.31675600	1.20896500	-0.01783900
O	-3.13538500	1.00813400	-0.87799600
W	-2.72083600	-1.38259700	-1.00609100
W	-2.69077800	1.62380700	1.02604600
Si	0.11517300	0.25108500	-0.08629000
O	-4.55378200	-1.68355500	-0.13523000
O	-5.72307600	-1.04737800	-0.70747700
H	-5.54234600	-0.11571300	-0.45887400
H	-3.35387500	-1.04263900	1.39890900

#### H-INT8

O	-1.14055800	-0.82094100	-1.16876300
O	-2.65657100	-3.16199700	-1.11285300
O	-3.11376500	-0.98898100	-2.98123900
O	-4.43745800	-1.28236300	-2.37760600

O	-4.33207900	-1.41301600	0.32054000
O	-3.03073200	-1.01738900	0.88566800
O	-0.99779000	0.84575500	0.91082600
O	-2.57952400	3.13643000	1.10580900
O	-2.66570300	0.95183500	3.01284100
O	-4.07673600	1.20194800	2.62540800
O	-4.39949900	1.33332500	-0.05460600
O	-3.19273800	0.97497600	-0.81888600
O	0.81921100	0.99442000	-1.08571800
W	-2.98072200	-1.47092400	-1.09071200
W	-2.84577200	1.43549700	1.12709500
O	0.87853400	-1.06863000	0.59914600
O	2.66180100	-3.09710200	0.94242800
O	2.08555500	-0.95555000	2.83408500
O	3.54106800	-1.08403400	2.85255600
O	3.00303800	-0.84682300	-0.93163600
O	2.39376800	3.26986300	-1.03418200
O	2.69972700	1.15746000	-3.00053500
O	4.06075500	1.43458200	-2.47598600
O	4.10816600	1.43487400	0.23727500
O	2.83743600	1.02375400	0.86079900
W	2.79004400	-1.38510800	1.06390100
W	2.68236400	1.57461500	-1.09399000
Si	-0.10461900	-0.01887300	-0.16983500
O	4.79136500	-1.31500000	0.84349000
O	5.32778200	-1.76318100	-0.43137700
H	4.63295400	-1.41541600	-1.04144200
H	2.35359400	-1.27600200	-1.50648300

#### H-TS4

O	-1.07731800	-0.27654400	-1.44968400
O	-2.36328800	-2.72395000	-1.86562200
O	-3.14729100	-0.24563300	-3.15730900
O	-4.39320800	-0.81004100	-2.58126800
O	-4.08465700	-1.52895800	0.01297200
O	-2.78855600	-1.13386200	0.58908600
O	-0.94426400	0.90492800	0.94641900
O	-2.72753900	2.89340400	1.74057900
O	-2.46790500	0.33711900	3.08782800
O	-3.91964600	0.51426200	2.83724600
O	-4.44320200	1.20681900	0.27856500
O	-3.26225400	1.15992800	-0.60090200
O	0.94415200	1.40061200	-0.92763500
W	-2.84172000	-1.12632100	-1.43930100
W	-2.82724100	1.21376700	1.37871000
O	0.83923900	-0.99013600	0.28675300
O	2.04231900	-3.40530300	0.68466800
O	1.97766200	-1.46128400	2.74993600
O	3.42335900	-1.76806900	2.63509600
O	2.99626300	-0.26026800	-1.64767900
O	2.68104900	3.22924800	0.15651900
O	2.89884900	2.42746300	-2.56994100
O	4.26355300	2.29562600	-2.00139900
O	4.27127000	0.95158300	0.40469700
O	2.96646400	0.51683100	0.91928600
W	2.47784800	-1.75698000	0.92006500
W	2.88134800	1.75122100	-0.72749900

Si	-0.05731800	0.27987300	-0.28689300
O	4.32563200	-1.90507900	0.30225000
O	4.19561400	-2.33883000	-1.07989700
H	3.80361900	-1.46371900	-1.48894900
H	2.27110600	-0.41829800	-2.26517000

**H-INT9**

O	0.95342500	0.57604300	-1.20333200
O	2.45473300	2.87605200	-1.70144700
O	2.79984600	0.38064100	-3.14070900
O	4.15893500	0.77877600	-2.69661500
O	4.23270300	1.42636900	-0.07306800
O	2.97598500	1.15352300	0.64473600
O	0.96918600	-0.65543800	1.16945100
O	2.57566400	-2.87765900	1.68864900
O	2.78198800	-0.36799700	3.13134400
O	4.16402800	-0.69972800	2.70312100
O	4.29809900	-1.34108800	0.08013200
O	3.03794500	-1.12877400	-0.65127000
O	-0.89130200	-1.27660400	-0.67467300
W	2.78947100	1.21899900	-1.37474900
W	2.83224300	-1.20604000	1.36598100
O	-0.94932700	1.11510700	0.62404300
O	-2.16124900	3.61263900	1.10249300
O	-2.75341700	1.28250200	2.65528200
O	-4.06558000	1.78130500	2.17939600
O	-3.02258700	-0.33273700	-2.35011600
O	-2.51827900	-3.16881100	0.63348900
O	-2.26363100	-2.98854100	-2.23870700
O	-3.71421300	-3.02793800	-1.93124300
O	-4.38583100	-1.10763200	-0.04860200
O	-3.19985400	-0.39265400	0.46372300
W	-2.67785400	1.99730500	0.82540500
W	-2.71268900	-1.99045800	-0.60759900
Si	-0.00041700	-0.05876000	-0.02060800
O	-4.11662200	2.26322700	-0.47150600
O	-2.84017200	2.01755700	-1.17462300
H	-2.96465900	0.58064400	-1.95191700
H	-2.29990700	-0.40887300	-2.98800300