

## **Impact of water on the BrO + HO<sub>2</sub> gas-phase reaction: mechanism, kinetics and products**

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### **Electronic Supplementary Information**

### S1. Eckart tunneling factor

By the Eckart function definition, the tunneling factor ( $\kappa$ ) is calculated by integrating the probability of transmission through the energy barrier. It takes into account the forward and reverse energy barriers  $\Delta E_f^\ddagger$  and  $E_r^\ddagger$ , respectively, and the imaginary frequency ( $\nu^\ddagger$ ) associated with the reaction coordinate of the transition state:

$$\kappa = \frac{1}{k_B T} \exp(\Delta E_f^\ddagger) \int_0^\infty p(E) \exp\left(-\frac{E}{k_B T}\right) dE$$

where

$$p(E) = 1 - \frac{\cosh[2\pi(\alpha - \beta)] + \cosh[2\pi\delta]}{\cosh[2\pi(\alpha + \beta)] + \cosh[2\pi\delta]}$$

$$\alpha = \frac{1}{2\sqrt{C}} \sqrt{E}$$

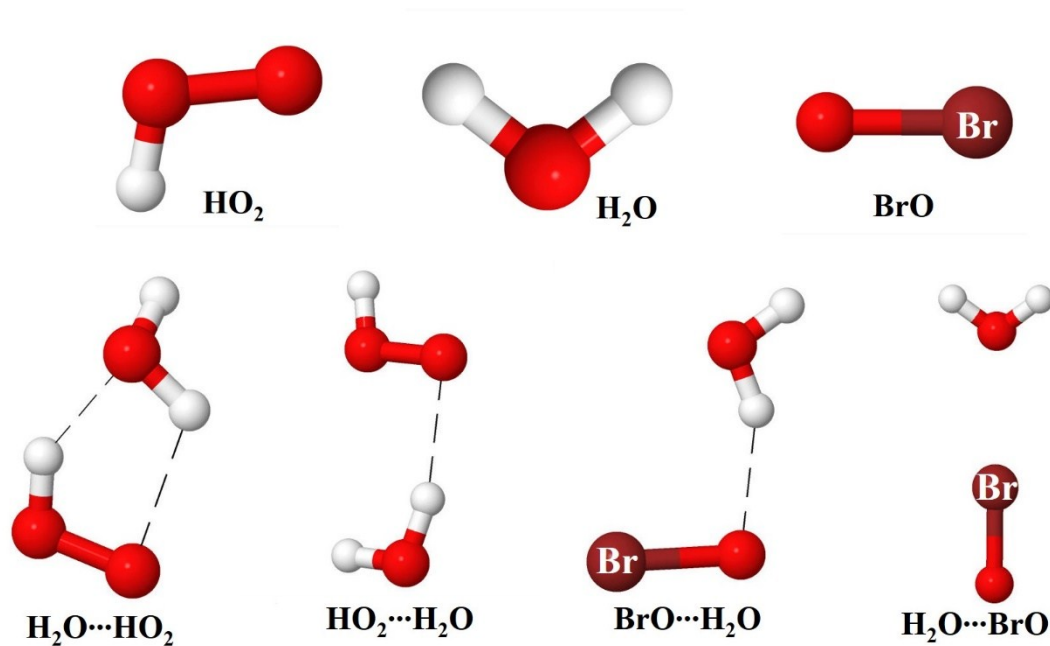
$$\beta = \frac{1}{2\sqrt{C}} \sqrt{E - A}$$

$$\delta = \frac{1}{2\sqrt{C}} \sqrt{B - C}$$

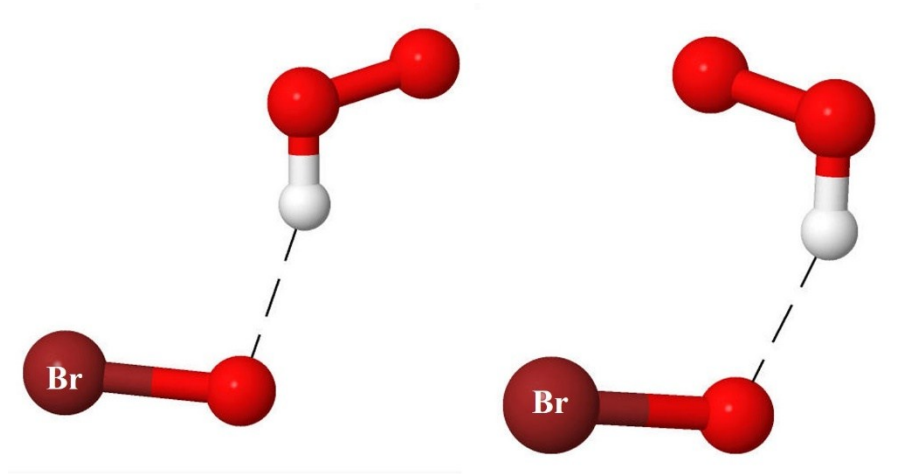
$$A = \Delta E_f^\ddagger - \Delta E_r^\ddagger$$

$$B = \sqrt{\Delta E_f^\ddagger} - \sqrt{\Delta E_r^\ddagger}$$

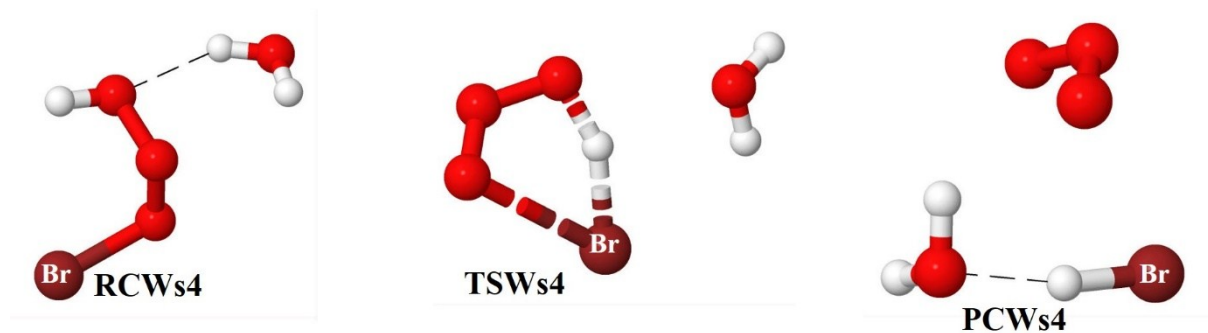
$$C = (\text{h.im}(\nu^\ddagger))^2 \left[ \frac{B^3}{A^2 - B^2} \right]^2$$



**Figure S1** Structures of all reactants optimized at the UM06-2X/AVDZ level of theory. The color coding is red for oxygen and white for hydrogen, while bromine is labelled as "Br".



**Figure S2** Structures of  $\text{BrO}\cdots\text{H}_2\text{O}$  optimized at the UM06-2X/AVDZ level of theory, for which transition states could not be located. The color coding is red for oxygen and white for hydrogen, while bromine is labelled as "Br".



**Figure S3** Structures of all intermediate species involved in the pathway of  $\text{BrH} + \text{O}_3$  from  $\text{HO}_2 + \text{BrO} \cdots \text{H}_2\text{O}$  interaction. The structures were optimized at the UM06-2X/AVDZ level of theory. The color coding is red for oxygen and white for hydrogen, while bromine is labelled as “Br”.

**Table S1** Polarizabilities and ionization energies of all reactants involved in the  $\text{BrO} + \text{HO}_2$  reaction, calculated with the UCCSD(T)/AVTZ//UM06-2X/AVDZ method. The structures of these reactants are given in **Fig. S1**.

Species	Polarizability ( $10^{-24} \text{ cm}^3$ )	Ionization energy ( $10^{-18} \text{ J}$ )
BrO	3.86	1.81
$\text{BrO} \cdots \text{H}_2\text{O}$	5.25	1.59
$\text{H}_2\text{O} \cdots \text{BrO}$	5.41	1.59
$\text{HO}_2$	1.82	1.85
$\text{H}_2\text{O} \cdots \text{HO}_2$	3.18	1.67
$\text{HO}_2 \cdots \text{H}_2\text{O}$	3.21	1.67

**Table S2** Calculated rate coefficients of the  $\text{BrO} + \text{HO}_2$  reaction in the absence and in the presence of one and two water molecules as a function of temperature in the range 250-350 K.

T(K)	Singlet surface				Triplet surface		
	$k_{\text{HBr}+\text{O}_3}$	$k_{\text{BrOH}+\text{O}_2}$	$k_{\text{BrOH}+\text{O}_2+\text{H}_2\text{O}}$	$k_{\text{BrOH}+\text{O}_2+2\text{H}_2\text{O}}$	$k_{\text{BrOH}+\text{O}_2}$	$k_{\text{BrOH}+\text{O}_2+\text{H}_2\text{O}}$	$k_{\text{BrOH}+\text{O}_2+2\text{H}_2\text{O}}$
250	$1.34 \times 10^{-21}$	$2.15 \times 10^{-11}$	$2.18 \times 10^{-11}$	$1.41 \times 10^{-10}$	$2.15 \times 10^{-11}$	$2.19 \times 10^{-11}$	$4.75 \times 10^{-10}$
260	$2.54 \times 10^{-21}$	$2.16 \times 10^{-11}$	$2.19 \times 10^{-11}$	$6.29 \times 10^{-11}$	$2.16 \times 10^{-11}$	$2.20 \times 10^{-11}$	$3.17 \times 10^{-10}$
270	$4.60 \times 10^{-21}$	$2.17 \times 10^{-11}$	$2.21 \times 10^{-11}$	$2.99 \times 10^{-11}$	$2.17 \times 10^{-11}$	$2.22 \times 10^{-11}$	$2.18 \times 10^{-10}$
280	$8.02 \times 10^{-21}$	$2.19 \times 10^{-11}$	$2.22 \times 10^{-11}$	$1.51 \times 10^{-11}$	$2.19 \times 10^{-11}$	$2.23 \times 10^{-11}$	$1.54 \times 10^{-10}$
290	$1.35 \times 10^{-20}$	$2.20 \times 10^{-11}$	$2.23 \times 10^{-11}$	$7.98 \times 10^{-12}$	$2.20 \times 10^{-11}$	$2.24 \times 10^{-11}$	$1.12 \times 10^{-10}$
300	$2.20 \times 10^{-20}$	$2.21 \times 10^{-11}$	$2.24 \times 10^{-11}$	$4.42 \times 10^{-12}$	$2.21 \times 10^{-11}$	$2.25 \times 10^{-11}$	$8.31 \times 10^{-11}$

310	$3.47 \times 10^{-20}$	$2.22 \times 10^{-11}$	$2.26 \times 10^{-11}$	$2.54 \times 10^{-12}$	$2.22 \times 10^{-11}$	$2.27 \times 10^{-11}$	$6.29 \times 10^{-11}$
320	$5.35 \times 10^{-20}$	$2.24 \times 10^{-11}$	$2.27 \times 10^{-11}$	$1.52 \times 10^{-12}$	$2.24 \times 10^{-11}$	$2.28 \times 10^{-11}$	$4.85 \times 10^{-11}$
330	$8.04 \times 10^{-20}$	$2.25 \times 10^{-11}$	$2.28 \times 10^{-11}$	$9.39 \times 10^{-13}$	$2.25 \times 10^{-11}$	$2.29 \times 10^{-11}$	$3.80 \times 10^{-11}$
340	$1.18 \times 10^{-19}$	$2.26 \times 10^{-11}$	$2.29 \times 10^{-11}$	$5.98 \times 10^{-13}$	$2.26 \times 10^{-11}$	$2.30 \times 10^{-11}$	$3.03 \times 10^{-11}$
350	$1.70 \times 10^{-19}$	$2.27 \times 10^{-11}$	$2.30 \times 10^{-11}$	$3.92 \times 10^{-13}$	$2.27 \times 10^{-11}$	$2.31 \times 10^{-11}$	$2.45 \times 10^{-11}$

**Cartesian coordinates of structures shown in Figs. 1, 2, and 3 in the main manuscript, and Figs. S1 and S3 in this Supplementary Information.**

**In Fig. S1**

**H<sub>2</sub>O**

O	0.00000000	0.00000000	0.11748300
H	0.00000000	0.76197900	-0.46993200
H	0.00000000	-0.76197900	-0.46993200

**HO<sub>2</sub>**

H	-0.88299800	-0.86566000	0.00000000
O	0.05518700	-0.59956200	0.00000000
O	0.05518700	0.70776900	0.00000000

**BrO**

Br	0.00000000	0.00000000	0.32336000
O	0.00000000	0.00000000	-1.41470100

**BrO...H<sub>2</sub>O**

Br	0.79292800	-0.20432400	-0.00000200
O	-0.17354400	1.23675200	0.00023100
O	-2.60708700	-0.38760900	0.00016000
H	-3.49377000	-0.01660100	0.00166700
H	-2.01367100	0.37479000	-0.00473100

**H<sub>2</sub>O...BrO**

Br	0.28095100	0.00011100	0.00019800
O	2.02319600	-0.00028900	0.00358200
O	-2.49078900	-0.00005300	-0.03787000
H	-3.04691500	0.76616800	0.13378700
H	-3.04562900	-0.76731700	0.13359800

**H<sub>2</sub>O...HO<sub>2</sub>**

H	0.00210300	-0.80994200	-0.00058400
O	-0.97312000	-0.64078400	0.00807100
O	-1.06725900	0.66088800	0.01177600
O	1.61355700	-0.02088600	-0.09200300
H	1.14693200	0.82564500	-0.03744800
H	2.26553700	-0.00944700	0.61527900

**HO<sub>2</sub>...H<sub>2</sub>O**

H	-2.18514200	-0.60102800	0.00028300
O	-1.21004300	-0.55713200	-0.00007000
O	-0.91025200	0.71408900	0.00001900
O	2.01887600	-0.00977800	-0.00004100
H	1.86027000	-0.95808500	0.00031900
H	1.13622700	0.38168100	0.00012800

**In Fig. 1**

**RCs1**

Br	-0.56474800	-0.31383500	-0.07942600
O	-0.96792700	1.29772900	0.16933700
H	1.87771500	1.24343600	0.07724600
O	1.99201200	0.36658900	-0.32649800
O	1.21197200	-0.44671800	0.49499500

**TSs1**

Br	-0.73476400	-0.19846000	-0.02668600
O	-0.08634900	1.39856200	0.09656000
H	1.18720500	1.02912500	0.08760600
O	1.91733800	0.21109600	-0.14933000
O	1.23520500	-0.87003400	0.15857200

**PCs1**

Br	1.27875800	-0.19827400	-0.00026500
O	0.13531100	1.23821800	0.00075900
H	-0.74044800	0.82016300	0.00161100
O	-2.31207000	-0.54894100	0.00216000
O	-3.32525400	0.07565300	-0.00196100

**RCs2**

Br	-1.01144000	-0.11701800	-0.01943300
O	0.52639900	0.90185400	0.32621800
H	1.66100600	-1.40365200	-0.19667400
O	2.12328700	-0.65686200	0.22089300
O	1.56773600	0.44241800	-0.43750700

**TSs2**

Br	1.10556700	-0.00450500	0.01721500
O	-1.34107200	1.05092600	-0.22099400
H	-0.31979600	-0.84425400	-0.22923100
O	-1.55295800	-1.04041800	-0.16309200
O	-1.90285100	0.11473200	0.33742600

**PCs2**

Br	1.38546400	0.00242400	-0.02405100
O	-1.91241100	-1.05463300	0.16207500
H	0.23574400	-0.18160200	0.81073900
O	-1.89573700	1.05642000	0.18279100
O	-2.28272400	0.01031000	-0.34098400

**PCt1**

Br	1.03739500	-0.30172500	0.03483600
O	0.46669600	1.42579200	-0.21357000
H	-0.43843800	1.42303200	0.13080500
O	-2.39069700	0.33094700	0.37520600
O	-2.55979600	-0.61457200	-0.33039300

**In Fig. 2****RCWs1**

H	-2.10856000	-0.67405400	-0.61371900
O	-1.31889200	-1.25079900	-0.52290600
O	-0.85132800	-0.86933500	0.73003000
O	-3.06687700	0.81254300	-0.13861400
H	-2.34652700	1.33923600	0.22982200
H	-3.53125900	1.39627700	-0.74623400
Br	1.47893300	0.15741900	-0.12001800
O	-0.23494200	0.36119900	0.59783500

**TSWs1**

H	-1.89937100	0.45293700	-0.61214200
O	-1.58931900	-0.84255500	-0.78598300
O	-1.41064500	-1.10624300	0.43633200
O	-1.75378000	1.39872100	-0.03455800
H	-0.95892000	0.95679100	0.59672100
H	-1.37986300	2.08125000	-0.60518800
Br	1.23545000	0.02500700	-0.13749800
O	-0.12158100	0.00429800	1.06333600

**PCWs1=PCWs2**

H	-2.25282400	0.97416000	-0.48505000
O	-2.44328900	-1.08339200	-0.21349600
O	-1.57033100	-1.10108300	0.59915500
O	-1.60774900	1.68737300	-0.40195700
H	-2.09325300	2.51142400	-0.49572600
H	-0.14701700	1.32798300	0.57958600
Br	1.25700600	-0.25347300	-0.21050600
O	0.68360500	1.00435200	0.98741100

**RCWs2**

H	1.84759400	0.70738600	-0.25376400
O	1.23403100	1.48341500	-0.35132000
O	0.26426200	1.19330400	0.60475700
O	2.37548200	-0.90523300	-0.08354300
H	2.84771600	-1.16342000	0.71389300
H	1.51470600	-1.36536700	-0.04021400
Br	-0.98577700	0.00244200	-0.07376100
O	-0.33725100	-1.55449500	0.10032100

**TSWs2**

H	-1.95252900	-0.12255300	0.01055100
O	-1.44642900	-1.07718900	-0.55863700
O	-0.55076900	-1.47631800	0.24406000
O	-2.01783500	0.94854000	0.54911200
H	-2.76018600	1.48282500	0.24756900
H	-1.09370600	1.23489000	0.01872500
Br	1.08360700	0.04076800	0.11074200
O	0.00005800	1.10221300	-0.75363800

**RCWs3**

Br	-0.07425500	-1.11861200	-0.02919700
O	-0.04696300	0.66002900	0.56127000
O	2.86521700	0.98199700	-0.14545500
H	3.38934300	1.71990500	0.17909700
H	1.97733800	1.13949500	0.19509200
H	-2.42265300	0.65146300	-0.54426700
O	-2.10288900	1.35776700	0.04289400
O	-0.75850300	1.45527700	-0.30971200

**TSWs3**

Br	1.29676600	0.00750400	0.00526900
O	-1.12263900	-0.87873900	1.07086700
O	-1.36189100	1.99209300	0.03080000



H	-1.51258200	2.59391700	-0.70465500
H	-0.40188200	1.96270800	0.13493200
H	-0.07159600	-0.73913500	-0.79216300
O	-1.17764500	-1.01750300	-1.02852300
O	-1.76292000	-0.60586800	0.07404000

**PCWs3**

Br	-1.79744900	-0.32178400	-0.04615400
O	1.33844800	0.31662200	0.97924500
O	3.35839900	-1.27820500	-0.31582900
H	3.88314100	-2.07333700	-0.44550300
H	2.86049700	-1.43122100	0.49425500
H	-1.19434400	0.90992600	0.36731700
O	0.88082000	1.82287100	-0.42046100
O	1.59251200	0.87084800	-0.09304200

**RCWs4**

H	0.61214700	1.88174500	-0.11926600
O	1.30620200	1.20351000	-0.18048800
O	0.90277500	0.26244800	0.77079500
O	3.74073500	-0.56510600	-0.28334100
H	3.19504900	0.15675600	-0.61334100
H	3.26302100	-0.87847500	0.49092900
Br	-1.59789900	-0.08089500	-0.09079000
O	0.15731900	-0.69193900	0.12045100

**TSWs4**

H	-0.04420400	0.56306200	-0.01558500
O	-0.90740600	1.41627300	-0.16588700
O	-1.96320900	0.66854300	-0.31139000
O	1.73676200	2.05331200	0.19980300
H	2.27542000	2.75881900	-0.17058500
H	2.26185500	1.25011700	0.10699400
Br	0.58916200	-1.01735300	-0.04531700
O	-2.00536300	-0.25870700	0.48563300

**PCWs4**

H	0.63386300	0.93490300	-0.15163400
O	-1.83151200	-0.35507000	-1.05016300
O	-1.93631100	-1.01077600	-0.01231200
O	-0.56749400	2.26070600	-0.08956300
H	-1.34905800	1.71086600	0.05219200
H	-0.45448700	2.75932200	0.72723600
Br	1.44847400	-0.26755200	0.00388300

O	-1.85554600	-0.39995400	1.05657700
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### RCWWs1

Br	-1.29851400	-0.50637900	-0.07955800
O	-0.68089800	1.11043700	0.64833800
O	1.80974300	-0.94688400	1.42933000
H	2.49065500	-0.96192300	2.10851400
H	1.51718800	-0.02466000	1.37515900
H	1.49271600	0.71049700	-0.79851500
O	1.37306200	1.45500800	-0.15330800
O	0.03441000	1.81731700	-0.29005400
O	2.02771700	-0.85965400	-1.34081000
H	2.04360400	-1.20956900	-0.43056200
H	1.39156300	-1.40087600	-1.81803000

### TSWWs1

Br	-1.80866200	0.04536400	-0.07318400
O	-0.18797900	-0.17245500	0.70869900
O	1.16182600	1.76914100	0.07585700
H	0.82274900	2.12330700	-0.75503900
H	2.17729100	1.20007000	-0.08800200
H	0.50268400	0.97203900	0.38711700
O	1.79537500	-1.58888200	0.17587700
O	0.77282400	-1.17333600	-0.43000100
O	3.12096500	0.42453300	-0.20597300
H	2.66715700	-0.53730400	-0.00551600
H	3.82918600	0.58215500	0.42721900

### PCWWs1

Br	1.81954500	-0.21852500	-0.01262900
O	0.09841800	-0.45441900	-0.60731000
O	-1.18795100	0.50821700	1.60165900
H	-1.22516600	1.32881400	1.07504100
H	-0.60217700	0.69676400	2.34130500
H	-0.42948300	-0.36125300	0.22196900
O	-2.61166100	-1.52604100	-0.00148600
O	-2.75401600	-0.49380000	-0.57526000
O	-0.94508000	2.22102700	-0.55372800
H	-0.57646000	1.42488100	-0.96946900
H	-1.64846700	2.51930700	-1.13781600

### TSWWs3

Br	-0.01296100	-1.13797100	-0.28171500
O	-2.20703700	0.03335800	0.93310700

O	3.07776800	0.04648500	0.71210500
H	2.34120600	-0.57203600	0.60429100
H	3.26691900	0.05408700	1.65558600
H	-0.36156600	0.54098800	-0.16837100
O	-1.12089400	1.49405200	-0.13083800
O	-2.26460000	0.91319300	0.08652900
O	1.43102200	2.02388400	-0.45446100
H	2.13264500	1.47396400	-0.06686500
H	1.74434800	2.24419900	-1.33614700

### PCWWs3

Br	1.35870100	-0.51008600	0.06760500
O	-1.58218300	-1.16105600	0.77574500
O	-0.99493000	1.73491000	1.22047300
H	-0.42605000	1.92912100	1.97578800
H	-1.01307800	0.76042100	1.17001900
H	0.85508000	1.07526400	-0.65984000
O	-1.71151400	-0.14078200	-1.06358300
O	-1.85055400	-1.19722300	-0.42803200
O	0.33103300	2.03490700	-0.89321500
H	-0.29284700	2.05004000	-0.06528700
H	-0.21248000	1.87212900	-1.67796600

### RCWWs2

Br	-0.20723100	-0.82724600	-0.01084700
O	1.39973800	-1.35978100	0.05242500
O	-2.62841500	0.53982900	-0.54569800
H	-3.29036300	0.65533000	0.14374200
H	-2.09240200	1.34475700	-0.51100300
H	0.84451300	1.82612200	-0.09242700
O	-0.11546800	1.85210500	0.16797300
O	-0.20984100	0.73624300	1.00426500
O	2.35110400	1.16699100	-0.52070800
H	3.15262400	1.44094400	-0.06558900
H	2.26176200	0.20337300	-0.36111200

### TSWWs2

Br	-0.14504300	-0.87997200	0.00599400
O	1.59742800	-1.05297000	0.03080800
O	-2.56072400	0.42217000	-0.57488600
H	-3.29232700	0.54065100	0.03882700
H	-2.01260000	1.21782000	-0.46623300
H	1.02603900	1.68206600	-0.22765300
O	-0.19655100	1.83228300	0.21069700

O	-0.25870200	0.76054000	1.02461400
O	2.00399700	1.24093600	-0.58053500
H	2.74287300	1.66712000	-0.13381100
H	1.92894500	0.06768600	-0.30649200

**PCWwS2**

Br	-0.71343700	-0.74326100	-0.04293200
O	0.52076000	-2.03821700	-0.45337900
O	-2.30556100	1.47802300	0.42920500
H	-1.74006100	2.09548300	-0.04853900
H	-3.14859300	1.49230000	-0.03556000
H	3.00244800	0.10138900	0.10638000
O	1.50146100	2.07916600	-0.77439400
O	0.72421300	1.89781100	0.11287300
O	2.51264500	-0.43865500	0.73636700
H	1.88606500	0.17509400	1.14112300
H	1.34229600	-1.67517300	-0.06616400

**In Fig. 3**

**RCWt1**

Br	1.31055300	-0.19514900	-0.19765200
O	0.65944600	0.93391600	0.94667300
O	-1.76017300	1.59562600	-0.39898900
H	-2.34059500	2.21385200	0.05553900
H	-0.98705000	1.48335800	0.18244800
H	-2.28840000	-0.00329900	-0.52257400
O	-2.32737800	-0.98616300	-0.36117300
O	-1.60355900	-1.15134300	0.71379000

**TSWt1**

Br	1.40410700	-0.03673200	-0.15150700
O	0.03711200	0.28339100	0.95978600
O	-1.75190100	1.51605000	-0.23299900
H	-2.28309200	2.08855900	0.33170300
H	-0.92742800	1.20398300	0.30050200
H	-2.22064400	0.30320600	-0.37696600
O	-2.35543500	-0.81140800	-0.39326000
O	-1.39385000	-1.27679800	0.29741100

**PCWt1**

Br	1.21475200	-0.26273800	-0.20102300
O	0.23008500	0.24736900	1.25594800
O	-1.03809500	2.31814500	-0.08503700

H	-1.79111800	1.94010500	-0.55266600
H	-0.26669600	1.02145100	0.91436500
H	-0.41159200	2.56281600	-0.77544700
O	-2.17788200	-0.57569900	-0.46683100
O	-2.01997300	-1.53088300	0.22711300

**RCWt2**

H	1.40862200	-0.25600200	0.43673600
O	1.98521300	-1.03128900	0.22536000
O	2.99322000	-0.55758700	-0.45092500
O	1.40977500	1.63528400	-0.03774100
H	1.59832700	2.31725200	0.61416300
H	2.26841500	1.37802300	-0.40728500
Br	-1.48481500	-0.08316900	-0.23812900
O	-0.55156300	-0.11245000	1.22466700

**TSWt2**

H	0.98553100	-1.13199600	0.70623700
O	1.87904700	-1.26660300	0.22812600
O	1.81764400	-0.57731400	-0.85819400
O	1.21010400	2.05771300	0.29652300
H	1.89313500	2.68530800	0.55057900
H	1.65778600	1.40571100	-0.25581000
Br	-1.15443000	0.02970100	-0.21766900
O	-0.42322200	-0.71361400	1.16072000

**PCWt2**

H	2.60656900	-1.16390200	0.71566800
O	-2.27117400	-1.58425100	0.07680000
O	-2.76301100	-0.51142700	-0.08397600
O	-1.03141200	2.07813600	0.11200700
H	-0.84409500	2.77270000	-0.52827400
H	-1.83550200	1.65120200	-0.20312800
Br	0.89283000	0.17405500	0.00977000
O	2.16859700	-1.15144900	-0.14560600

**RCWWt1**

Br	-1.34133800	-0.31621000	-0.02752700
O	-0.41657800	-1.78655500	-0.03164400
O	-2.66560000	2.02574700	-0.07894000
H	-3.49200900	2.27265000	0.34804500
H	-2.14713000	2.83560500	-0.13160200
H	1.24411500	-1.30396500	-0.31403700
O	2.08602000	-0.78124200	-0.27780400

O	1.93931300	-0.00826600	0.76510200
O	4.44943600	1.25997200	-0.17141700
H	4.53121200	0.63060200	-0.89395800
H	3.66990300	0.95521000	0.31263000

### TSWWt1

Br	-1.30268500	-0.34410200	-0.00716500
O	-0.34542300	-1.78959600	0.01220600
O	-2.72647300	1.96483100	-0.07562600
H	-2.98522300	2.42032200	0.73238700
H	-2.35731400	2.64604500	-0.64786200
H	1.12075100	-1.30435900	-0.14748400
O	1.99485100	-0.78402700	-0.09061100
O	1.67496000	0.41259600	0.28250800
O	4.57808200	1.07708300	-0.06450700
H	4.77553800	0.17373600	-0.32866600
H	3.63224600	1.06072100	0.13065300

### PCWWt1

Br	0.90429700	-0.35999100	-0.22777300
O	-0.54875000	-1.37192400	-0.76816500
O	3.01871500	1.03572900	0.64498400
H	2.80518800	1.40288300	1.50964300
H	3.78275400	0.46809800	0.79253500
H	-1.07737200	-0.76192100	-1.30368100
O	-2.16606700	1.18217100	-0.85637200
O	-1.98872500	1.83021900	0.12711500
O	-2.41357000	-0.88398700	1.37599400
H	-2.62741400	-1.58315200	1.99951800
H	-1.74638300	-1.26387800	0.78558900

### RCWWt2

Br	1.06957300	0.25644100	-0.00281400
O	1.68695000	-1.36962800	0.10242400
O	-0.36682600	2.53073100	-0.10361900
H	-1.24584400	2.12432000	-0.15852200
H	-0.43842400	3.22866900	0.55458000
H	-1.80704800	-1.10610300	0.45771500
O	-2.21820900	-0.21155200	0.65675700
O	-2.22344000	0.39819300	-0.49646600
O	-0.97411700	-2.40373400	-0.11417000
H	-1.16600000	-2.52342900	-1.05051400
H	-0.01259900	-2.25098700	-0.06419100

**TSWWt2**

Br	-0.51003200	0.81739000	0.04100900
O	0.95190400	1.69253600	-0.30219700
O	-2.60820700	-0.90978000	0.20280100
H	-2.16469300	-1.65610900	-0.22245300
H	-3.45667600	-0.83212900	-0.24639100
H	1.82796600	-1.20251500	0.12845900
O	1.19285100	-2.12302300	0.00886500
O	0.01393800	-1.74280200	-0.30229100
O	2.53328300	-0.12471400	0.13397500
H	3.05983700	0.01068400	0.92768900
H	1.91453700	0.73368300	0.04817700

**PCWWt2**

Br	-0.56344000	-0.81107100	-0.01988900
O	-2.31079000	-0.31939400	-0.30508200
O	2.08315900	-1.51459100	0.38351500
H	2.42828400	-1.68579100	-0.49966000
H	2.09304100	-2.37023100	0.82543100
H	-0.56526100	2.02825300	0.35411800
O	1.82468100	1.62802200	0.30031500
O	2.34521900	1.25034500	-0.70205000
O	-1.47175800	2.33196400	0.21693400
H	-1.72247600	2.75610900	1.04400700
H	-2.27729600	0.64836600	-0.17683700