

## Supplementary Information:

**The Non-Covalently Bound  $\text{SO}\cdots\text{H}_2\text{O}$  System, Including an  
Interpretation of the Differences Between  $\text{SO}\cdots\text{H}_2\text{O}$  and  
 $\text{O}_2\cdots\text{H}_2\text{O}$**

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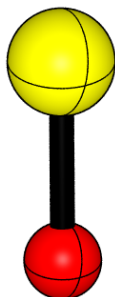
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# Contents

<b>1 Geometries and Frequencies</b>	<b>3</b>
1.1 Sulfur Monoxide . . . . .	3
1.2 Water . . . . .	4
1.3 Hydrogen Bonded Complex . . . . .	5
1.4 Transition State . . . . .	6
1.5 Chalcogen Bonded Complex . . . . .	7
1.6 Additional Transition State 1 . . . . .	8
1.7 Additional Transition State 2 . . . . .	9
<b>2 IRC Trajectory: Hydrogen Bonded to Chalcogen Bonded Complex</b>	<b>10</b>

# 1 Geometries and Frequencies

## 1.1 Sulfur Monoxide



### Level of Theory:

Method: UCCSD(T)

Basis: aug-cc-pV(Q+d)Z

Reference: ROHF

Program: MOLPRO 2010.1

### Convergence Thresholds (Program Specific):

energy =  $1.0 \times 10^{-12}$

orbital =  $1.0 \times 10^{-11}$

gradient =  $1.0 \times 10^{-8}$

oneint =  $1.0 \times 10^{-14}$

twoint =  $1.0 \times 10^{-14}$

### Wavefunction Diagnostics:

$\langle S^2 \rangle = 3.006$

$\mathcal{T}_1 = 0.024$

CASSCF(12,8)  $C_0^2 = 0.949$

CASSCF(12,8)  $C_1^2 = 0.020$

CASSCF(12,8)  $C_2^2 = 0.006$

Cartesian Coordinates of Optimized Geometry (Å):

S	0.0000000000	0.0000000000	0.5183229836
O	0.0000000000	0.0000000000	-0.9683229836

SCF Energy ( $E_h$ ): -472.4018524321

UCCSD(T) Energy ( $E_h$ ): -472.8603620067

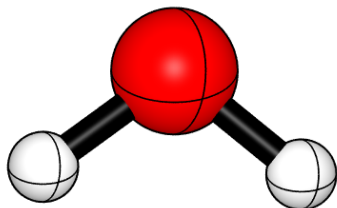
SCF Occupation:

	$a_1$	$b_1$	$b_2$	$a_2$
$\alpha$	7	3	3	0
$\beta$	7	2	2	0

Harmonic Frequencies ( $\text{cm}^{-1}$ ):

[ $\Sigma^+$ ] 1152

## 1.2 Water



### Level of Theory:

Method: CCSD(T)

Basis: aug-cc-pV(Q+d)Z

Reference: RHF

Program: MOLPRO 2010.1

### Convergence Thresholds (Program Specific):

energy =  $1.0 \times 10^{-12}$

orbital =  $1.0 \times 10^{-11}$

gradient =  $1.0 \times 10^{-8}$

oneint =  $1.0 \times 10^{-14}$

twoint =  $1.0 \times 10^{-14}$

### Wavefunction Diagnostics:

$\mathcal{T}_1 = 0.009$

CASSCF(8,6)  $C_0^2 = 0.978$

CASSCF(8,6)  $C_1^2 = 0.005$

CASSCF(8,6)  $C_2^2 = 0.005$

Cartesian Coordinates of Optimized Geometry (Å):

H	0.0000000000	-0.7575220311	0.5227227005
O	0.0000000000	0.0000000000	-0.0652457683
H	0.0000000000	0.7575220311	0.5227227005

SCF Energy ( $E_h$ ): -76.0658643993

CCSD(T) Energy ( $E_h$ ): -76.3635876011

SCF Occupation:

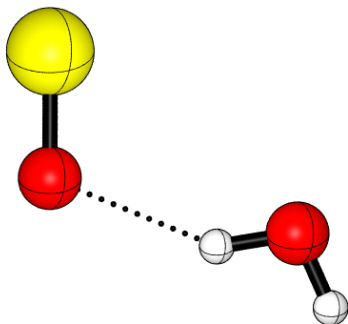
$a_1$	$b_1$	$b_2$	$a_2$
3	1	1	0

Harmonic Frequencies ( $\text{cm}^{-1}$ ):

$[a_1]$  3831     $[b_2]$  3940

$[a_1]$  1650

### 1.3 Hydrogen Bonded Complex



#### Level of Theory:

Method: UCCSD(T)  
 Basis: aug-cc-pV(Q+d)Z  
 Reference: ROHF  
 Program: MOLPRO 2010.1

#### Convergence Thresholds (Program Specific):

energy =  $1.0 \times 10^{-12}$   
 orbital =  $1.0 \times 10^{-11}$   
 gradient =  $1.0 \times 10^{-8}$   
 oneint =  $1.0 \times 10^{-14}$   
 twoint =  $1.0 \times 10^{-14}$

#### Wavefunction Diagnostics:

$\langle S^2 \rangle = 3.004$   
 $\mathcal{T}_1 = 0.021$   
 CASSCF(20,14)  $C_0^2 = 0.944$   
 CASSCF(20,14)  $C_1^2 = 0.012$   
 CASSCF(20,14)  $C_2^2 = 0.005$

Cartesian Coordinates of Optimized Geometry (Å):

S	-0.3387469593	0.0000000000	-1.1908558477
O	0.8847472382	0.0000000000	-0.3445279161
H	0.4210342108	0.0000000000	1.7275935987
O	-0.2480570158	0.0000000000	2.4179317954
H	0.2472257748	0.0000000000	3.2385953098

SCF Energy ( $E_h$ ): -548.4712571063

UCCSD(T) Energy ( $E_h$ ): -549.228570555

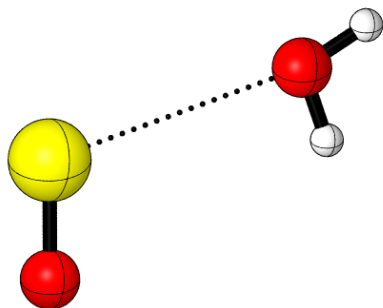
SCF Occupation:

	$a'$	$a''$
$\alpha$	14	4
$\beta$	13	3

Harmonic Frequencies ( $\text{cm}^{-1}$ ):

[ $a'$ ] 3925 H <sub>2</sub> O anti. stretch	[ $a''$ ] 327 H-bonded H
[ $a'$ ] 3809 H <sub>2</sub> O symm. stretch	out-of-plane bend
[ $a'$ ] 1653 H <sub>2</sub> O bend	[ $a''$ ] 59 Not H-bonded H
[ $a'$ ] 1153 SO stretch	out-of-plane bend
[ $a'$ ] 238 H <sub>2</sub> O rock	
[ $a'$ ] 138 Monomers slide into each other	
[ $a'$ ] 22 Monomers rotate into each other	

## 1.4 Transition State



### Level of Theory:

Method: UCCSD(T)

Basis: aug-cc-pV(Q+d)Z

Reference: ROHF

Program: MOLPRO 2010.1

### Convergence Thresholds (Program Specific):

energy =  $1.0 \times 10^{-12}$

orbital =  $1.0 \times 10^{-11}$

gradient =  $1.0 \times 10^{-8}$

oneint =  $1.0 \times 10^{-14}$

twoint =  $1.0 \times 10^{-14}$

### Wavefunction Diagnostics:

$\langle S^2 \rangle = 3.004$

$\mathcal{T}_1 = 0.020$

CASSCF(20,14)  $C_0^2 = 0.935$

CASSCF(20,14)  $C_1^2 = 0.013$

CASSCF(20,14)  $C_2^2 = 0.009$

Cartesian Coordinates of Optimized Geometry (Å):

S	0.7165773104	0.5084165444	0.0000000000
O	-2.5601893246	-0.1774984079	0.0000000000
O	1.4974546058	-0.7590810826	0.0000000000
H	-3.5191152209	-0.1516743100	0.0000000000
H	-2.3470783155	-1.1130778864	0.0000000000

SCF Energy ( $E_h$ ): -548.4687550165

UCCSD(T) Energy ( $E_h$ ): -549.2260200436

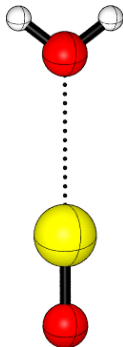
SCF Occupation:

	$a'$	$a''$
$\alpha$	14	4
$\beta$	13	3

Harmonic Frequencies ( $\text{cm}^{-1}$ ):

[ $a'$ ] 49i	[ $a''$ ] 105
Monomers bend	H <sub>2</sub> O out-of-plane bend
into each other	[ $a''$ ] 58
[ $a'$ ] 3934	H <sub>2</sub> O out-of-plane twist
H <sub>2</sub> O anti. stretch	
[ $a'$ ] 3825	
H <sub>2</sub> O aymm. stretc	
[ $a'$ ] 1652	
H <sub>2</sub> O bend	
[ $a'$ ] 1148	
SO stretch	
[ $a'$ ] 103	
H <sub>2</sub> O rock	
[ $a'$ ] 66	
Monomer	
approach	

## 1.5 Chalcogen Bonded Complex



### Level of Theory:

Method: UCCSD(T)  
 Basis: aug-cc-pV(Q+d)Z  
 Reference: ROHF  
 Program: MOLPRO 2010.1

### Convergence Thresholds (Program Specific):

energy =  $1.0 \times 10^{-12}$   
 orbital =  $1.0 \times 10^{-11}$   
 gradient =  $1.0 \times 10^{-8}$   
 oneint =  $1.0 \times 10^{-14}$   
 twoint =  $1.0 \times 10^{-14}$

### Wavefunction Diagnostics:

$\langle S^2 \rangle = 3.004$   
 $\mathcal{T}_1 = 0.020$   
 CASSCF(20,14)  $C_0^2 = 0.929$   
 CASSCF(20,14)  $C_1^2 = 0.019$   
 CASSCF(20,14)  $C_2^2 = 0.006$

Cartesian Coordinates of Optimized Geometry (Å):

H	-0.7589216703	0.0000000000	3.1082565820
H	0.7589216703	0.0000000000	3.1082565820
O	0.0000000000	0.0000000000	2.5216012101
S	0.0000000000	0.0000000000	-0.4748174225
O	0.0000000000	0.0000000000	-1.9641940526

SCF Energy ( $E_h$ ): -548.4702192342

UCCSD(T) Energy ( $E_h$ ): -549.2282563211

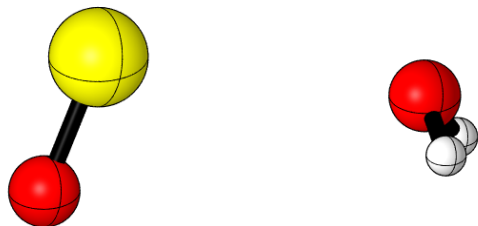
SCF Occupation:

	$a_1$	$b_1$	$b_2$	$a_2$
$\alpha$	10	4	4	0
$\beta$	10	3	3	0

Harmonic Frequencies ( $\text{cm}^{-1}$ ):

[ $a_1$ ] 3829 H <sub>2</sub> O symm. stretch	[ $b_1$ ] 84 H <sub>2</sub> O out-of-plane bend	[ $b_2$ ] 3937 H <sub>2</sub> O anti. stretch
[ $a_1$ ] 1651 H <sub>2</sub> O bend	[ $b_1$ ] 70 Both monomers bend to-	[ $b_2$ ] 146 H <sub>2</sub> O water rock
[ $a_1$ ] 1144 SO stretch	wards each other	[ $b_2$ ] 61 Monomers bend
[ $a_1$ ] 98 Monomer approach		into each other

## 1.6 Additional Transition State 1



### Level of Theory:

Method: CCSD(T)

Basis: aug-cc-pV(D+d)Z

Reference: UHF

Program: CFOUR 2.0, ECC

### Convergence Thresholds (Program Specific):

SCF\_CONV =  $1.0 \times 10^{-10}$

CC\_CONV =  $1.0 \times 10^{-10}$

LINEQ\_CONV =  $1.0 \times 10^{-10}$

CONVERGENCE =  $1.0 \times 10^{-8}$

INTEGRAL THRESHOLD =  $1.0 \times 10^{-14}$

### Wavefunction Diagnostics:

$\langle S^2 \rangle = 3.004$

$\mathcal{T}_1 = 0.022$

CASSCF(20,14)  $C_0^2 = 0.922$

CASSCF(20,14)  $C_1^2 = 0.021$

CASSCF(20,14)  $C_2^2 = 0.006$

Cartesian Coordinates of Optimized Geometry (Å):

O	-1.4294684395	0.8570715330	0.0000000000
S	-0.7639174244	-0.5107487413	0.0000000000
O	2.5978875666	0.0848079938	0.0000000000
H	2.8453637895	0.6272975168	0.7611379315
H	2.8453637895	0.6272975168	-0.7611379315

SCF Energy ( $E_h$ ): -548.4117632054

CCSD(T) Energy ( $E_h$ ): -548.9892433998

SCF Occupation:

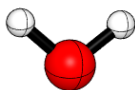
	$a'$	$a''$
$\alpha$	14	4
$\beta$	13	3

Harmonic Frequencies ( $\text{cm}^{-1}$ ):

$[a']$ 42i	$[a'']$ 53i
$[a']$ 3782	$[a'']$ 3899
$[a']$ 1640	$[a'']$ 94
$[a']$ 1084	
$[a']$ 101	
$[a']$ 61	



## 1.7 Additional Transition State 2



### Level of Theory:

Method: CCSD(T)

Basis: aug-cc-pV(D+d)Z

Reference: UHF

Program: CFOUR 2.0, ECC

### Convergence Thresholds (Program Specific):

SCF\_CONV =  $1.0 \times 10^{-10}$

CC\_CONV =  $1.0 \times 10^{-10}$

LINEQ\_CONV =  $1.0 \times 10^{-10}$

CONVERGENCE =  $1.0 \times 10^{-8}$

INTEGRAL THRESHOLD =  $1.0 \times 10^{-14}$

### Wavefunction Diagnostics:

$\langle S^2 \rangle = 3.004$

$\mathcal{T}_1 = 0.022$

CASSCF(20,14)  $C_0^2 = 0.938$

CASSCF(20,14)  $C_1^2 = 0.014$

CASSCF(20,14)  $C_2^2 = 0.005$

Cartesian Coordinates of Optimized Geometry (Å):

O	0.0000000000	0.0000000000	3.0247617033
H	0.0000000000	-0.7540004840	2.4196902343
O	0.0000000000	0.0000000000	-0.0974788044
H	0.0000000000	0.7540004840	2.4196902343
S	0.0000000000	0.0000000000	-1.6170015804

SCF Energy ( $E_h$ ): -548.4130693442

CCSD(T) Energy ( $E_h$ ): -548.9905833148

SCF Occupation:

	$a_1$	$b_1$	$b_2$	$a_2$
$\alpha$	10	4	4	0
$\beta$	10	3	3	0

Harmonic Frequencies ( $\text{cm}^{-1}$ ):

$[a_1]$ 3794	$[b_1]$ 260	$[b_2]$ 134i
$[a_1]$ 1644	$[b_1]$ 2	$[b_2]$ 3898
$[a_1]$ 1086		$[b_2]$ 29
$[a_1]$ 84		

## 2 IRC Trajectory: Hydrogen Bonded to Chalcogen Bonded Complex

```
5
IRC point -35: -548.9921064975300
S 0.3611186196 1.0430485656 0.0000000000
O 0.3611194184 -2.2684524304 0.0000000000
O -1.0583644698 0.4953284826 0.0000000000
H 0.0719295742 -3.1901588489 0.0000000000
H -0.4622202706 -1.7586001993 0.0000000000
5
IRC point -34: -548.9920152871130
S 0.3637141815 1.0357856280 0.0000000000
O 0.3637151805 -2.2743918285 0.0000000000
O -1.0667816603 0.5174081906 0.0000000000
H 0.0857114115 -3.1995750577 0.0000000000
H -0.4659552043 -1.7749418090 0.0000000000
5
IRC point -33: -548.9919145079730
S 0.3661356191 1.0288455677 0.0000000000
O 0.3661352605 -2.2811393122 0.0000000000
O -1.0746610108 0.5397438466 0.0000000000
H 0.0992623187 -3.2096340398 0.0000000000
H -0.4696648318 -1.7920667852 0.0000000000
5
IRC point -32: -548.9918060823400
S 0.3683874087 1.0221273128 0.0000000000
O 0.3683876262 -2.2884499082 0.0000000000
O -1.0820292492 0.5622694826 0.0000000000
H 0.1127994033 -3.2201518667 0.0000000000
H -0.4734514098 -1.8099137105 0.0000000000
5
IRC point -31: -548.9916919192580
S 0.3704754201 1.0155626556 0.0000000000
O 0.3704764492 -2.2961583761 0.0000000000
O -1.0889063033 0.5849494219 0.0000000000
H 0.1264729448 -3.2309967658 0.0000000000
H -0.4773811271 -1.8284506969 0.0000000000
5
IRC point -30: -548.9915738533240
S 0.3724042873 1.0091026666 0.0000000000
O 0.3724050499 -2.3041496330 0.0000000000
O -1.0953077087 0.6077613667 0.0000000000
H 0.1403786596 -3.2420662933 0.0000000000
H -0.4814880409 -1.8476511849 0.0000000000
5
IRC point -29: -548.9914536082960
S 0.3741765403 1.0027091269 0.0000000000
O 0.3741775756 -2.3123424382 0.0000000000
O -1.1012464353 0.6306890506 0.0000000000
H 0.1545625961 -3.2532745014 0.0000000000
H -0.4857767447 -1.8674783568 0.0000000000
5
IRC point -28: -548.9913327698760
S 0.3757955248 0.9963527083 0.0000000000
O 0.3757963701 -2.3206761961 0.0000000000
O -1.1067318270 0.6537243822 0.0000000000
H 0.1690242565 -3.2645439303 0.0000000000
```

H	-0.4902307291	-1.8878766184	0.0000000000
5			
IRC point -27: -548.9912127615841			
S	0.3772640939	0.9900085242	0.0000000000
O	0.3772636391	-2.3291059644	0.0000000000
O	-1.1117709351	0.6768641105	0.0000000000
H	0.1837200584	-3.2758034235	0.0000000000
H	-0.4948139716	-1.9087657384	0.0000000000
5			
IRC point -26: -548.9910948233340			
S	0.3785834997	0.9836533060	0.0000000000
O	0.3785830405	-2.3375991341	0.0000000000
O	-1.1163699052	0.7001063127	0.0000000000
H	0.1985741035	-3.2869903491	0.0000000000
H	-0.4994755478	-1.9300439045	0.0000000000
5			
IRC point -25: -548.9909799947480			
S	0.3797563660	0.9772673731	0.0000000000
O	0.3797559387	-2.3461295460	0.0000000000
O	-1.1205312616	0.7234556519	0.0000000000
H	0.2134791542	-3.2980476694	0.0000000000
H	-0.5041599610	-1.9515890218	0.0000000000
5			
IRC point -24: -548.9908691064049			
S	0.3807844570	0.9708320256	0.0000000000
O	0.3807839292	-2.3546769491	0.0000000000
O	-1.1242558521	0.7469180312	0.0000000000
H	0.2283105090	-3.3089279553	0.0000000000
H	-0.5088085652	-1.9732629232	0.0000000000
5			
IRC point -23: -548.9907627787441			
S	0.3816688423	0.9643297590	0.0000000000
O	0.3816682585	-2.3632249979	0.0000000000
O	-1.1275420750	0.7705002916	0.0000000000
H	0.2429334444	-3.3195934248	0.0000000000
H	-0.5133674953	-1.9949220926	0.0000000000
5			
IRC point -22: -548.9906614343211			
S	0.3824100322	0.9577446567	0.0000000000
O	0.3824095066	-2.3717592741	0.0000000000
O	-1.1303861587	0.7942088929	0.0000000000
H	0.2572163532	-3.3300167527	0.0000000000
H	-0.5177909549	-2.0164231591	0.0000000000
5			
IRC point -21: -548.9905653179610			
S	0.3830078889	0.9510627002	0.0000000000
O	0.3830073544	-2.3802663484	0.0000000000
O	-1.1327817442	0.8180493032	0.0000000000
H	0.2710362175	-3.3401798369	0.0000000000
H	-0.5220459290	-2.0376336966	0.0000000000
5			
IRC point -20: -548.9904745269240			
S	0.3834614359	0.9442718625	0.0000000000
O	0.3834609424	-2.3887329783	0.0000000000
O	-1.1347209035	0.8420240836	0.0000000000
H	0.2842905373	-3.3500734456	0.0000000000
H	-0.5261118983	-2.0584366390	0.0000000000
5			
IRC point -19: -548.9903890432990			

S	0.3837689770	0.9373625101	0.0000000000
O	0.3837684737	-2.3971456247	0.0000000000
O	-1.1361936694	0.8661332717	0.0000000000
H	0.2968981371	-3.3596946646	0.0000000000
H	-0.5299828859	-2.0787385083	0.0000000000
5			
IRC point -18: -548.9903087691190			
S	0.3839281445	0.9303272436	0.0000000000
O	0.3839276719	-2.4054904044	0.0000000000
O	-1.1371894149	0.8903731214	0.0000000000
H	0.3088063272	-3.3690457631	0.0000000000
H	-0.5336642641	-2.0984691053	0.0000000000
5			
IRC point -17: -548.9902335567120			
S	0.3839359833	0.9231611188	0.0000000000
O	0.3839354750	-2.4137531878	0.0000000000
O	-1.1376962323	0.9147372611	0.0000000000
H	0.3199857142	-3.3781316156	0.0000000000
H	-0.5371725738	-2.1175851782	0.0000000000
5			
IRC point -16: -548.9901632362240			
S	0.3837891072	0.9158613270	0.0000000000
O	0.3837886501	-2.4219199114	0.0000000000
O	-1.1377025439	0.9392159400	0.0000000000
H	0.3304335547	-3.3869587771	0.0000000000
H	-0.5405310307	-2.1360656954	0.0000000000
5			
IRC point -15: -548.9900976352380			
S	0.3834838076	0.9084271704	0.0000000000
O	0.3834833518	-2.4299767663	0.0000000000
O	-1.1371961019	0.9637976735	0.0000000000
H	0.3401643269	-3.3955335861	0.0000000000
H	-0.5437689749	-2.1539119972	0.0000000000
5			
IRC point -14: -548.9900365943170			
S	0.3830162429	0.9008595655	0.0000000000
O	0.3830158200	-2.4379106540	0.0000000000
O	-1.1361656248	0.9884685860	0.0000000000
H	0.3492110020	-3.4038619177	0.0000000000
H	-0.5469174029	-2.1711403424	0.0000000000
5			
IRC point -13: -548.9899799752141			
S	0.3823824152	0.8931609703	0.0000000000
O	0.3823819969	-2.4457093375	0.0000000000
O	-1.1345995786	1.0132139053	0.0000000000
H	0.3576148550	-3.4119482836	0.0000000000
H	-0.5500090230	-2.1877813755	0.0000000000
5			
IRC point -12: -548.9899276665360			
S	0.3815784443	0.8853349518	0.0000000000
O	0.3815781184	-2.4533614963	0.0000000000
O	-1.1324877327	1.0380174820	0.0000000000
H	0.3654266291	-3.4197957634	0.0000000000
H	-0.5530746872	-2.2038718962	0.0000000000
5			
IRC point -11: -548.9898795843520			
S	0.3806004704	0.8773860685	0.0000000000
O	0.3806001751	-2.4608567728	0.0000000000
O	-1.1298196151	1.0628630748	0.0000000000

H	0.3726968313	-3.4274058146	0.0000000000
H	-0.5561443241	-2.2194547518	0.0000000000
5			
IRC point -10: -548.9898356716780			
S	0.3794448736	0.8693194004	0.0000000000
O	0.3794446719	-2.4681859567	0.0000000000
O	-1.1265862340	1.0877334256	0.0000000000
H	0.3794788020	-3.4347786769	0.0000000000
H	-0.5592442196	-2.2345724190	0.0000000000
5			
IRC point -9: -548.9897958951700			
S	0.3781081200	0.8611407188	0.0000000000
O	0.3781079557	-2.4753404828	0.0000000000
O	-1.1227783204	1.1126116822	0.0000000000
H	0.3858202125	-3.4419130619	0.0000000000
H	-0.5623985945	-2.2492674524	0.0000000000
5			
IRC point -8: -548.9897602418890			
S	0.3765866819	0.8528553967	0.0000000000
O	0.3765876176	-2.4823132938	0.0000000000
O	-1.1183884640	1.1374791891	0.0000000000
H	0.3917692747	-3.4488072928	0.0000000000
H	-0.5656271250	-2.2635792388	0.0000000000
5			
IRC point -7: -548.9897287146100			
S	0.3748781268	0.8444707933	0.0000000000
O	0.3748790670	-2.4890961842	0.0000000000
O	-1.1134077810	1.1623207757	0.0000000000
H	0.3973623437	-3.4554570944	0.0000000000
H	-0.5689491539	-2.2775417750	0.0000000000
5			
IRC point -6: -548.9897013277000			
S	0.3729794696	0.8359927306	0.0000000000
O	0.3729800827	-2.4956828764	0.0000000000
O	-1.1078297330	1.1871179287	0.0000000000
H	0.4026362965	-3.4618587328	0.0000000000
H	-0.5723785551	-2.2911842882	0.0000000000
5			
IRC point -5: -548.9896781023000			
S	0.3708878936	0.8274273249	0.0000000000
O	0.3708884089	-2.5020673233	0.0000000000
O	-1.1016476196	1.2118525307	0.0000000000
H	0.4076203170	-3.4680078493	0.0000000000
H	-0.5759276334	-2.3045335876	0.0000000000
5			
IRC point -4: -548.9896590627581			
S	0.3686012212	0.8187811329	0.0000000000
O	0.3686015404	-2.5082431400	0.0000000000
O	-1.0948555481	1.2365067760	0.0000000000
H	0.4123410959	-3.4738988212	0.0000000000
H	-0.5796065700	-2.3176101833	0.0000000000
5			
IRC point -3: -548.9896442323800			
S	0.3661169705	0.8100612899	0.0000000000
O	0.3661175066	-2.5142034826	0.0000000000
O	-1.0874488867	1.2610605068	0.0000000000
H	0.4168473650	-3.4795236066	0.0000000000
H	-0.5834289658	-2.3304585013	0.0000000000
5			

```

IRC point -2: -548.9896336292870
S 0.3634355719 0.8012631901 0.0000000000
O 0.3634353803 -2.5199547718 0.0000000000
O -1.0794107183 1.2855149734 0.0000000000
H 0.4208176194 -3.4849080929 0.0000000000
H -0.5873375242 -2.3427698011 0.0000000000
5
IRC point -1: -548.9896272723130
S 0.3605407999 0.7923054986 0.0000000000
O 0.3605410510 -2.5251737053 0.0000000000
O -1.0707585678 1.3097374138 0.0000000000
H 0.4255091601 -3.4896513236 0.0000000000
H -0.5915774804 -2.3554700864 0.0000000000
5
IRC point 0: -548.9896251542040
S 0.3574435331 0.7833151476 0.0000000000
O 0.3574435331 -2.5301829488 0.0000000000
O -1.0614856951 1.3337974494 0.0000000000
H 0.4301726622 -3.4941078342 0.0000000000
H -0.5959908790 -2.3681434601 0.0000000000
5
IRC point 1: -548.9896272673579
S 0.3541669489 0.7744639720 0.0000000000
O 0.3541669730 -2.5355347909 0.0000000000
O -1.0515650917 1.3578622047 0.0000000000
H 0.4329266775 -3.4989925351 0.0000000000
H -0.6002450675 -2.3794527320 0.0000000000
5
IRC point 2: -548.9896335909020
S 0.3506836888 0.7655722392 0.0000000000
O 0.3506834223 -2.5406043801 0.0000000000
O -1.0410215720 1.3817100763 0.0000000000
H 0.4358682538 -3.5035182942 0.0000000000
H -0.6047299750 -2.3908749546 0.0000000000
5
IRC point 3: -548.9896440984980
S 0.3469849722 0.7565586859 0.0000000000
O 0.3469850519 -2.5451594364 0.0000000000
O -1.0298516735 1.4052653865 0.0000000000
H 0.4394042995 -3.5074085298 0.0000000000
H -0.6095082571 -2.4025886216 0.0000000000
5
IRC point 4: -548.9896587354590
S 0.3430820053 0.7475110206 0.0000000000
O 0.3430818498 -2.5494683870 0.0000000000
O -1.0180368251 1.4285994047 0.0000000000
H 0.4425645599 -3.5110149085 0.0000000000
H -0.6144145651 -2.4138933500 0.0000000000
5
IRC point 5: -548.9896774395989
S 0.3389736983 0.7384458198 0.0000000000
O 0.3389736767 -2.5535159551 0.0000000000
O -1.0055892300 1.4516762009 0.0000000000
H 0.4456169905 -3.5142960578 0.0000000000
H -0.6194886074 -2.4250402078 0.0000000000
5
IRC point 6: -548.9897001334330
S 0.3346606892 0.7293712616 0.0000000000
O 0.3346606544 -2.5572985962 0.0000000000

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O	-0.9925105498	1.4744760635	0.0000000000
H	0.4485648685	-3.5172458605	0.0000000000
H	-0.6247286065	-2.4360295945	0.0000000000
5			
IRC point 7: -548.9897267256340			
S	0.3301434786	0.7202959921	0.0000000000
O	0.3301433983	-2.5608115430	0.0000000000
O	-0.9788037673	1.4969774778	0.0000000000
H	0.4514292456	-3.5198544038	0.0000000000
H	-0.6301341644	-2.4468783526	0.0000000000
5			
IRC point 8: -548.9897571114240			
S	0.3254232535	0.7112287079	0.0000000000
O	0.3254230433	-2.5640502750	0.0000000000
O	-0.9644740001	1.5191590694	0.0000000000
H	0.4542345115	-3.5221112241	0.0000000000
H	-0.6357040196	-2.4576061932	0.0000000000
5			
IRC point 9: -548.9897911733530			
S	0.3205011905	0.7021784542	0.0000000000
O	0.3205009885	-2.5670105837	0.0000000000
O	-0.9495268110	1.5409988670	0.0000000000
H	0.4570070015	-3.5240047734	0.0000000000
H	-0.6414359599	-2.4682355047	0.0000000000
5			
IRC point 10: -548.9898287820760			
S	0.3153792731	0.6931544452	0.0000000000
O	0.3153790642	-2.5696886030	0.0000000000
O	-0.9339700191	1.5624756106	0.0000000000
H	0.4597756967	-3.5255229473	0.0000000000
H	-0.6473266913	-2.4787910389	0.0000000000
5			
IRC point 11: -548.9898697972990			
S	0.3100595102	0.6841663943	0.0000000000
O	0.3100592697	-2.5720811069	0.0000000000
O	-0.9178118573	1.5835677020	0.0000000000
H	0.4625712420	-3.5266525531	0.0000000000
H	-0.6533717543	-2.4893004355	0.0000000000
5			
IRC point 12: -548.9899140687420			
S	0.3045446749	0.6752239344	0.0000000000
O	0.3045443062	-2.5741855614	0.0000000000
O	-0.9010630290	1.6042542570	0.0000000000
H	0.4654268384	-3.5273800357	0.0000000000
H	-0.6595650390	-2.4997937020	0.0000000000
5			
IRC point 13: -548.9899614371510			
S	0.2988375299	0.6663372362	0.0000000000
O	0.2988372254	-2.5760002599	0.0000000000
O	-0.8837347769	1.6245142656	0.0000000000
H	0.4683764650	-3.5276907279	0.0000000000
H	-0.6658986812	-2.5103029902	0.0000000000
5			
IRC point 14: -548.9900117352540			
S	0.2929417176	0.6575163676	0.0000000000
O	0.2929412835	-2.5775243505	0.0000000000
O	-0.8658403936	1.6443280232	0.0000000000
H	0.4714550048	-3.5275697208	0.0000000000
H	-0.6723632880	-2.5208617599	0.0000000000

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5
IRC point 15: -548.9900647886950
S 0.2868608424 0.6487719186 0.0000000000
O 0.2868603594 -2.5787581436 0.0000000000
O -0.8473939835 1.6636758381 0.0000000000
H 0.4746983782 -3.5270009751 0.0000000000
H -0.6789471371 -2.5315060381 0.0000000000
5
IRC point 16: -548.9901204168530
S 0.2805992607 0.6401144486 0.0000000000
O 0.2805986745 -2.5797031197 0.0000000000
O -0.8284116233 1.6825396102 0.0000000000
H 0.4781428045 -3.5259683867 0.0000000000
H -0.6856364954 -2.5422728138 0.0000000000
5
IRC point 17: -548.9901784335860
S 0.2741613906 0.6315548298 0.0000000000
O 0.2741607913 -2.5803622490 0.0000000000
O -0.8089099530 1.7009016090 0.0000000000
H 0.4818237133 -3.5244549941 0.0000000000
H -0.6924151797 -2.5532003889 0.0000000000
5
IRC point 18: -548.9902386478300
S 0.2675523023 0.6231038754 0.0000000000
O 0.2675515618 -2.5807396462 0.0000000000
O -0.7889073088 1.7187459701 0.0000000000
H 0.4857758317 -3.5224437017 0.0000000000
H -0.6992647541 -2.5643271220 0.0000000000
5
IRC point 19: -548.9903008640410
S 0.2607770805 0.6147727601 0.0000000000
O 0.2607763079 -2.5808412841 0.0000000000
O -0.7684226434 1.7360575498 0.0000000000
H 0.4900326947 -3.5199167134 0.0000000000
H -0.7061639072 -2.5756925263 0.0000000000
5
IRC point 20: -548.9903648824310
S 0.2538413612 0.6065724578 0.0000000000
O 0.2538405020 -2.5806745902 0.0000000000
O -0.7474761611 1.7528231912 0.0000000000
H 0.4946258554 -3.5168564813 0.0000000000
H -0.7130889833 -2.5873353790 0.0000000000
5
IRC point 21: -548.9904304990800
S 0.2467508075 0.5985142214 0.0000000000
O 0.2467498927 -2.5802487583 0.0000000000
O -0.7260884397 1.7690308286 0.0000000000
H 0.4995844341 -3.5132446599 0.0000000000
H -0.7200134111 -2.5992944695 0.0000000000
5
IRC point 22: -548.9904975058580
S 0.2395114640 0.5906091496 0.0000000000
O 0.2395104147 -2.5795746041 0.0000000000
O -0.7042810224 1.7846704891 0.0000000000
H 0.5049351931 -3.5090632829 0.0000000000
H -0.7269081156 -2.6116076650 0.0000000000
5
IRC point 23: -548.9905656901500
S 0.2321293495 0.5828685206 0.0000000000

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O	0.2321282060	-2.5786649206	0.0000000000
O	-0.6820755360	1.7997335430	0.0000000000
H	0.5107009750	-3.5042940504	0.0000000000
H	-0.7337410968	-2.6243115028	0.0000000000
5			
IRC point 24: -548.9906348345251			
S	0.2246107523	0.5753032830	0.0000000000
O	0.2246094778	-2.5775339942	0.0000000000
O	-0.6594941439	1.8142133475	0.0000000000
H	0.5169013252	-3.4989191270	0.0000000000
H	-0.7404779832	-2.6374407737	0.0000000000
5			
IRC point 25: -548.9907047160571			
S	0.2169618741	0.5679245124	0.0000000000
O	0.2169605047	-2.5761979006	0.0000000000
O	-0.6365587772	1.8281047565	0.0000000000
H	0.5235507390	-3.4929205052	0.0000000000
H	-0.7470817318	-2.6510275825	0.0000000000
5			
IRC point 26: -548.9907751059040			
S	0.2091890555	0.5607429102	0.0000000000
O	0.2091875153	-2.5746740367	0.0000000000
O	-0.6132913931	1.8414045735	0.0000000000
H	0.5306588609	-3.4862811128	0.0000000000
H	-0.7535133440	-2.6651006663	0.0000000000
5			
IRC point 27: -548.9908457684630			
S	0.2012984980	0.5537691770	0.0000000000
O	0.2012967858	-2.5729813806	0.0000000000
O	-0.5897135668	1.8541109845	0.0000000000
H	0.5382301440	-3.4789838487	0.0000000000
H	-0.7597315022	-2.6796856691	0.0000000000
5			
IRC point 28: -548.9909164605980			
S	0.1932959755	0.5470133223	0.0000000000
O	0.1932962241	-2.5711401204	0.0000000000
O	-0.5658476840	1.8662231768	0.0000000000
H	0.5462646837	-3.4710132959	0.0000000000
H	-0.7656918140	-2.6948033079	0.0000000000
5			
IRC point 29: -548.9909869315620			
S	0.1851883138	0.5404856521	0.0000000000
O	0.1851885972	-2.5691710926	0.0000000000
O	-0.5417115903	1.8777436480	0.0000000000
H	0.5547492568	-3.4623548661	0.0000000000
H	-0.7713537666	-2.7104671392	0.0000000000
5			
IRC point 30: -548.9910569214881			
S	0.1769810835	0.5341954420	0.0000000000
O	0.1769814460	-2.5670957627	0.0000000000
O	-0.5173262166	1.8886739521	0.0000000000
H	0.5636714324	-3.4529951280	0.0000000000
H	-0.7766712623	-2.7266875961	0.0000000000
5			
IRC point 31: -548.9911261616400			
S	0.1686800224	0.5281518085	0.0000000000
O	0.1686804303	-2.5649364216	0.0000000000
O	-0.4927100405	1.8990177193	0.0000000000
H	0.5730080812	-3.4429230305	0.0000000000

H	-0.7815998918	-2.7434663997	0.0000000000
5			
IRC point 32: -548.9911943740100			
S	0.1602906541	0.5223631181	0.0000000000
O	0.1602911818	-2.5627150080	0.0000000000
O	-0.4678805308	1.9087791382	0.0000000000
H	0.5827285269	-3.4321304126	0.0000000000
H	-0.7860962829	-2.7607977357	0.0000000000
5			
IRC point 33: -548.9912612715760			
S	0.1518182840	0.5168373426	0.0000000000
O	0.1518189266	-2.5604536357	0.0000000000
O	-0.4428537466	1.9179633377	0.0000000000
H	0.5927944341	-3.4206118765	0.0000000000
H	-0.7901186246	-2.7786677024	0.0000000000
5			
IRC point 34: -548.9913265587720			
S	0.1432680007	0.5115816513	0.0000000000
O	0.1432687611	-2.5581735140	0.0000000000
O	-0.4176445613	1.9265756323	0.0000000000
H	0.6031605360	-3.4083657773	0.0000000000
H	-0.7936277518	-2.7970546213	0.0000000000
5			
IRC point 35: -548.9913899327810			
S	0.1346446227	0.5066026849	0.0000000000
O	0.1346455380	-2.5558954590	0.0000000000
O	-0.3922664526	1.9346217802	0.0000000000
H	0.6137747752	-3.3953942738	0.0000000000
H	-0.7965875668	-2.8159286863	0.0000000000
5			
IRC point 36: -548.9914510850870			
S	0.1259527585	0.5019064461	0.0000000000
O	0.1259538889	-2.5536389498	0.0000000000
O	-0.3667316626	1.9421074728	0.0000000000
H	0.6245796641	-3.3817040202	0.0000000000
H	-0.7989661409	-2.8352531070	0.0000000000
5			
IRC point 37: -548.9915097039740			
S	0.1171968092	0.4974984032	0.0000000000
O	0.1171982239	-2.5514229558	0.0000000000
O	-0.3410512400	1.9490384039	0.0000000000
H	0.6355136066	-3.3673059228	0.0000000000
H	-0.8007357104	-2.8549854070	0.0000000000
5			
IRC point 38: -548.9915654774420			
S	0.1083810403	0.4933837095	0.0000000000
O	0.1083827921	-2.5492647167	0.0000000000
O	-0.3152354348	1.9554200647	0.0000000000
H	0.6465128278	-3.3522148810	0.0000000000
H	-0.8018732179	-2.8750787974	0.0000000000
5			
IRC point 39: -548.9916180968420			
S	0.0995095993	0.4895671223	0.0000000000
O	0.0995118200	-2.5471812151	0.0000000000
O	-0.2892938840	1.9612576095	0.0000000000
H	0.6575130791	-3.3364497343	0.0000000000
H	-0.8023596845	-2.8954846925	0.0000000000
5			
IRC point 40: -548.9916672608870			

S 0.0905873201 0.4860537505 0.0000000000  
O 0.0905864079 -2.5451876567 0.0000000000  
O -0.2632340031 1.9665567380 0.0000000000  
H 0.6684489133 -3.3200316526 0.0000000000  
H -0.8021831586 -2.9161541859 0.0000000000

5

IRC point 41: -548.9917126796710

S 0.0816173623 0.4828475253 0.0000000000  
O 0.0816161761 -2.5433004163 0.0000000000  
O -0.2370694923 1.9713205973 0.0000000000  
H 0.6792671409 -3.3029847359 0.0000000000  
H -0.8013257371 -2.9370427520 0.0000000000

5

IRC point 42: -548.9917540793020

S 0.0726045492 0.4799536289 0.0000000000  
O 0.0726025563 -2.5415344445 0.0000000000  
O -0.2108079477 1.9755546961 0.0000000000  
H 0.6899073078 -3.2853365354 0.0000000000  
H -0.7997822387 -2.9581040144 0.0000000000

5

IRC point 43: -548.9917912055350

S 0.0635534010 0.4773773258 0.0000000000  
O 0.0635502621 -2.5399056625 0.0000000000  
O -0.1844604457 1.9792636764 0.0000000000  
H 0.7003189824 -3.2671147709 0.0000000000  
H -0.7975446862 -2.9793001461 0.0000000000

5

IRC point 44: -548.9918238276540

S 0.0544682692 0.4751238836 0.0000000000  
O 0.0544657827 -2.5384307220 0.0000000000  
O -0.1580397811 1.9824521702 0.0000000000  
H 0.7104574603 -3.2483495726 0.0000000000  
H -0.7946057308 -3.0005965246 0.0000000000

5

IRC point 45: -548.9918517414070

S 0.0453546076 0.4731999413 0.0000000000  
O 0.0453511645 -2.5371271192 0.0000000000  
O -0.1315560958 1.9851264568 0.0000000000  
H 0.7202762715 -3.2290735939 0.0000000000  
H -0.7909643452 -3.0219622533 0.0000000000