

SUPPORTING INFORMATION-DFT CALCULATIONS

Friedel-Crafts Alkylation of Indoles with p-Quinols. The role of hydrogen bonding of water for the desymmetrization of the cyclohexadienone system.

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DFT calculations with the hybrid ωB97XD (with dispersion correction)¹ have been carried out using Gaussian09² to locate and characterize the stationary points on the potential energy surface at the 6-31G* level. The optimized geometries have been characterized by harmonic analysis, and the nature of the stationary points determined according to the number of negative eigenvalues of the Hessian matrix. In several doubtful cases, internal reaction coordinates (IRCs) have been followed from the transition structures to verify the proper connections with reactants and products.³ Zero-point vibration energies (ZPVE) and thermal corrections (at 298 K, 1 atm) to the energy have been estimated using the computed frequencies applying the free particle, harmonic oscillator and rigid rotor approximations at the high temperature limit in a canonical ensemble. Solvation effects (to simulate the experimentally used CH₃CN) have been also included as single point corrections to the gas-phase free energy of the optimized structures computed with the ωB97XD functional with the self-consistent reaction field (SCRF) method using the polarizable continuum model (PCM)⁴ as implemented in Gaussian09.

Comprehensive DFT-based calculations were carried out using as model system the reaction of p-quinol **1a** and indole **2a** catalyzed by (*R*)-BINOL-3,3'-(9-anthracyl) phosphoric acid (*R*)-**12h** leading to the desymmetrization product. To address the stereoselectivity of the reaction, two descriptors will be used, which correspond to the face-selectivity and β-carbon selectivity, respectively. In all experimental

¹ Chai, J.-D.; Head-Gordon, M. *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615.

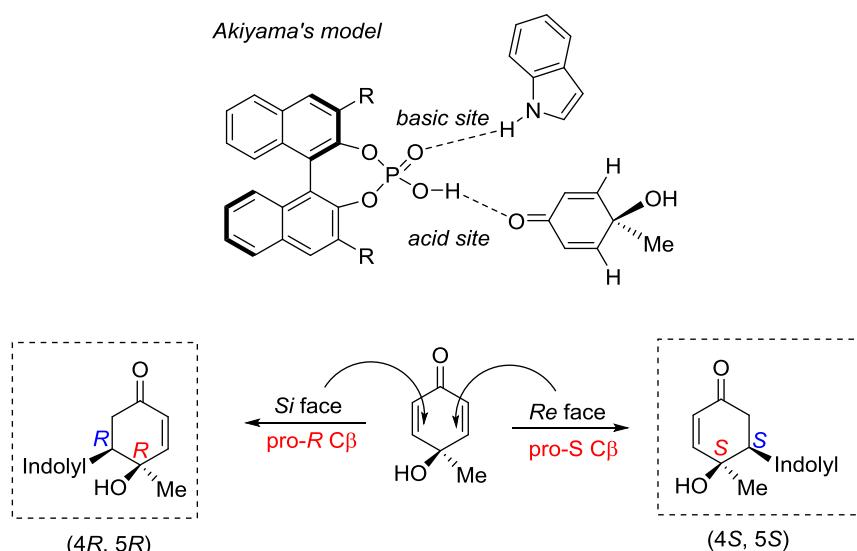
² Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian 09, Revision B.01, Wallingford CT, 2009.

³ (a) Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363. (b) Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523.

⁴ (a) Tomasi, J.; Persico, M. *Chem. Rev.* **1994**, *94*, 2027. (b) Cossi, M.; Scalmani, G.; Rega, N.; Barone, V. J. *Chem. Phys.* **2002**, *117*, 43. (c) Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999.

cases, compound **3a** was characterized as a single diastereoisomer resulting from a *Si* face-pro-*R* C β or *Re* face-pro-*S* C β selectivity in the (1,4)-addition of indole **2a** to the less hindered face of *p*-quinol **1a** (OH containing face), *anti* to the CH₃ group. In order to carry out conveniently the DFT study, we selected the reaction on the less hindered face as this is the experimentally obtained diastereoface-selective reaction. Therefore, enantiomers of the Friedel-Crafts-type reaction product **3a** would be formed by reaction of indole to the C β of **1a** with opposite topicities (i.e., *Si* face-pro-*R* C β or *Re* face-pro-*S* C β). In all cases, the two-point coordination Akiyama's model, which has been described for coordination of the BINOL phosphoric acid catalyst to the two reagents has been adopted. For this particular case, the coordination mode involves a double hydrogen bond established between the acidic position of catalyst **12h** and *p*-quinol **1a**, and between the basic position of catalyst **12h** and N-H of indole **2a** (Figure 1).^{5,6}

Figure 1. Representation of coordination modes of model reactants *p*-quinol **1a** and indole **2a** to the catalyst [(*R*)-BINOL-3,3'-(9-anthracenyl)-phosphoric acid **12h**] and structures of the four possible stereoisomers of the reaction product.



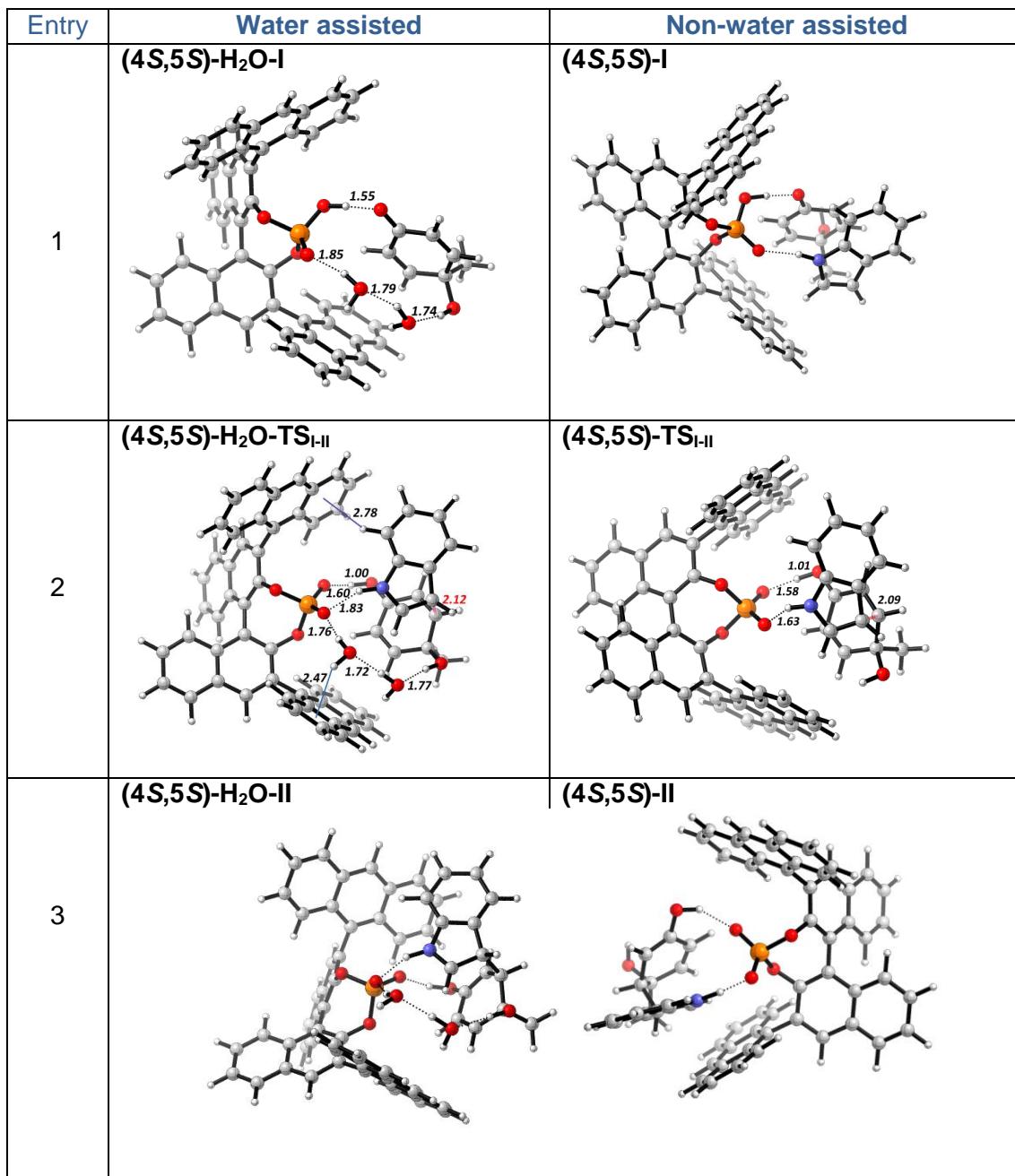
EFFECT OF THE WATER MOLECULES: WATER AND NON-WATER ASSISTED MODELS

In order to estimate the effect of the water molecules in the reaction, both the water and the non-water-assisted variants approaches have been computed of the *Re* face-pro-*S* C β (Figure 2). In Table 1 are shown the water and the non-water-assisted structures of: entry 1) *p*-quinol associated with (*R*)-**12h** (**I**), entry 2) the transitions state that incorporated the indole (**TS_{I-II}**), entry 3) the final adduct **3a** associated (*R*)-**12h** (**II**).

⁵ Akiyama, T.; Itoh, J.; Yokota, K.; Fuchibe, K. *Angew. Chem. Int. Ed.* **2004**, *43*, 1566-1568.

⁶ Parmar, D.; Sugiono, E.; Raja, S.; Rueping, M. *Chem. Rev.* **2014**, *114*, 9047-9153.

Table 1. Representation of the structures corresponding to the water and the non-water assisted phosphoric acid-promoted [(*R*)-12h] FC reaction between *p*-quinol **1a** and indole **2a** (wB97XD/6-31G*, in gas phase). Relevant atom distances (in Å) are shown.



In Table 2 are shown all the calculated energies (ΔG , kcal/mol, gas phase) for the water assisted and the non-water assisted structures. A comparison of the energies of activation (in gas phase) and the structures of transition states of the Friedel-Crafts reaction indicates that the network of water molecules favors (by 9 kcal/mol) the (1,4)-addition of indole **2a** to **1a** (entry 2 and 5, Table 2). This effect might be due to the modulation of the acidity of phosphoric acid **12h**, which translates into an increase of the nucleophilicity of indole at its C₃ position.

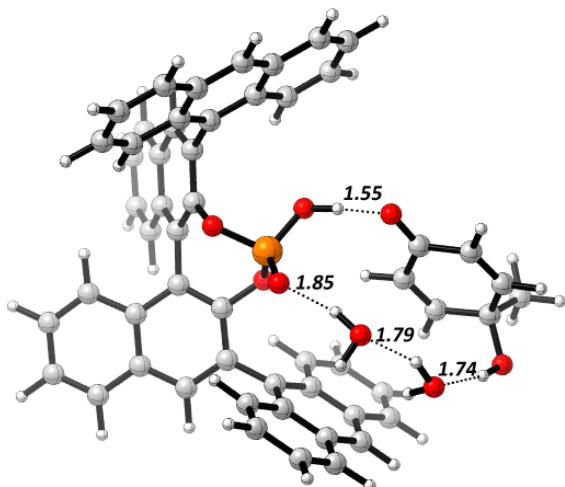
Table 2. Calculated energies (ΔG , kcal/mol, gas phase) for the non-assisted and for the water-assisted phosphoric acid-promoted [(*R*)-12h] FC reaction between *p*-quinol **1a** (*Re*-face-pro-S C β) and indole **2a**.^a

entry		Structures	ΔG (kcal/mol)
1		(4S,5S)-H ₂ O-I	0.0
2	H ₂ O-assisted	<i>Re face-pro-S Cβ</i>	<i>41.1</i>
3		(4S,5S)-H ₂ O-II	5.2
4		(4S,5S)-I	0.0
5	Non-water assisted	<i>Re face- pro-S Cβ</i>	<i>50.5</i>
6		(4S,5S)-II	16.6

^a Energies were computed at the wB97XD/6-31G* level in gas phase. ^b The activation energies are shown in italic blue.

As shown in Figure 2, the approach to the rear face of *p*-quinol **1a** is blocked by steric interference of the methyl group. In contrast, the coordination of water molecules opens a cavity in the front face that can be occupied by indole **2a**. Without disturbing the water-mediated H-bonding network, indole N-H group also binds the phosphoric acid basic site.

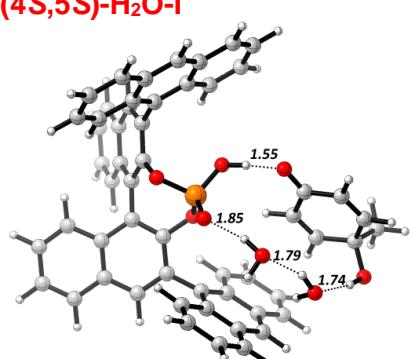
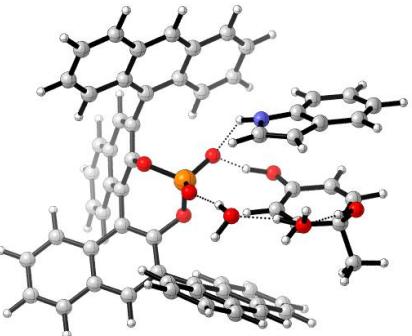
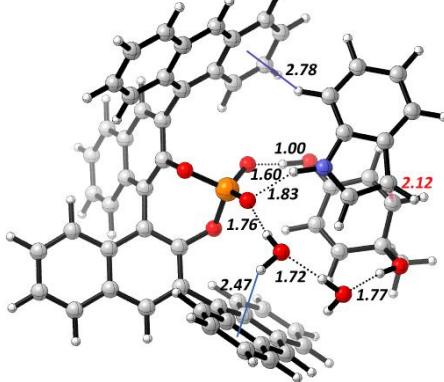
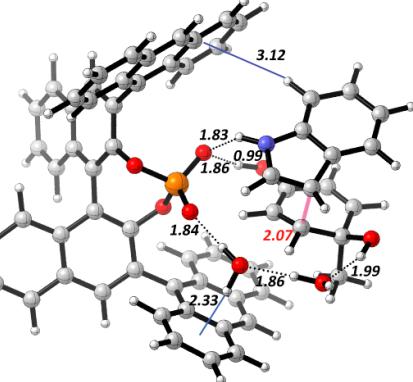
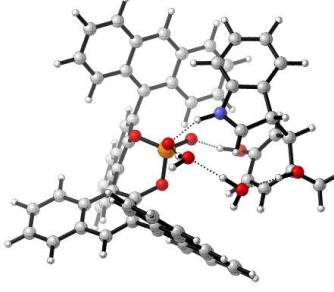
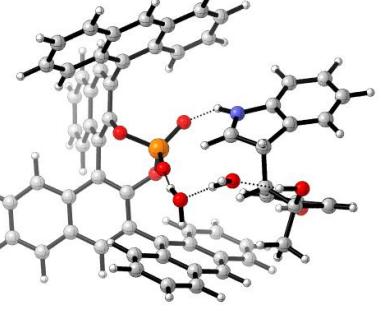
Figure 2. Representation of the (*R*)-12h phosphoric acid-complex with *p*-quinol **1a** and 2·H₂O (wB97XD/PCM(CH₃CN)/6-31G*/wB97XD/6-31G*). Relevant atom distances (in Å) are shown.



COMPUTATIONAL STUDIES: DESYMMETRIZATION OF THE *p*-QUINOL

In Table 3 are shown the water assisted diastereotopic approaches computed: entry 1) *p*-quinol associated with (*R*)-12h (**I**), entry 2) the transitions state that incorporated the indole (**TS_{I-II}**), entry 3) the final adduct **3a** associated (*R*)-12h (**II**). The named (4S,5S) correspond to the *Re* face-pro-S C β approach and (4*R*,5*R*) to the *Si* face-pro-R C β approach.

Table 3. Representation of the structures corresponding to the water-assisted, phosphoric acid-promoted (*R*)-**12h** Friedel-Crafts-type reaction between *p*-quinol **1a** and indole **2a** computed at the wB97XD/PCM(CH₃CN)/6-31G*/wB97XD/6-31G* level. Relevant atom distances (in Å) are shown.

Entry	Water assisted complex 4S,5S	Water assisted complex 4R,5R
1	(4S,5S)-H₂O-I 	(4R,5R)-H₂O-I 
2	(4S,5S)-H₂O-TS_{I-II} 	(4R,5R)-H₂O-TS_{I-II} 
3	(4S,5S)-H₂O-II 	(4R,5R)-H₂O-II 

In Table 4 are shown all the calculated energies (in CH₃CN) for the water assisted FC reaction promoted by (*R*)-**12h** between *p*-quinol **1a** and indole **2a** for both diastereomeric approaches (*4R,5R*)·(*R*)-**12h** and (*4S,5S*)·(*R*)-**12h**. As shown the *S*/face-pro-*R* C β approach of indole [(4*R*,5*R*)-H₂O-TS_{I-II}] (Table 3, entry 5) is less favored (by 3.9 kcal/mol in CH₃CN and 6.7 kcal/mol in gas phase) than the corresponding *Re* face-pro-*S* C β counterpart (Table 3, entry 2) [(4*S*,5*S*)-H₂O-TS_{I-II}]. Although the reactions are exergonic, transition state leading to the (4*S*,5*S*) enantiomer (ΔG -15.3 kcal/mol, (4*S*,5*S*)-H₂O-II, table 3, entry 3) is 3.5 kcal/mol more stable than the one giving the (4*R*,5*R*) enantiomer (ΔG -11.8 kcal/mol, (4*R*,5*R*)-H₂O-II, Table 3, entry 6).

Table 4. Calculated energies (in CH₃CN) for the water assisted FC reaction promoted by (*R*)-**12h** between *p*-quinol **1a** and indole **2a**.

Entry		Structures ^a	ΔG (kcal/mol) ^b
1		(4S,5S)-H ₂ O-I	2.4
2	<i>Re face-pro-S Cβ</i> ^c	(4S,5S)-H ₂ O-TS _{I-II}	5.3 (2.9) ^d
3		(4S,5S)-H ₂ O-II	-15.3
4		(4R,5R)-H ₂ O-I	0.0
5	<i>Si face-pro-S Cβ</i> ^c	(4R,5R)-TS _{I-II}	9.2 (9.2) ^d
6		(4R,5R)-H ₂ O-II	-11.8

^a (4S,5S) and (4R,5R) descriptors refer to the configuration of the final product **3a** obtained. ^b Energies (in kcal/mol) were computed at the wb97XD/PCM(CH₃CN)/6-31G*//wb97XD/6-31G* level and refers to (4R,5R)-H₂O-I. ^c Both approaches are obtained from (*R*)-phosphoric acid and are diastereomeric. ^d Activation energies are shown in brackets.

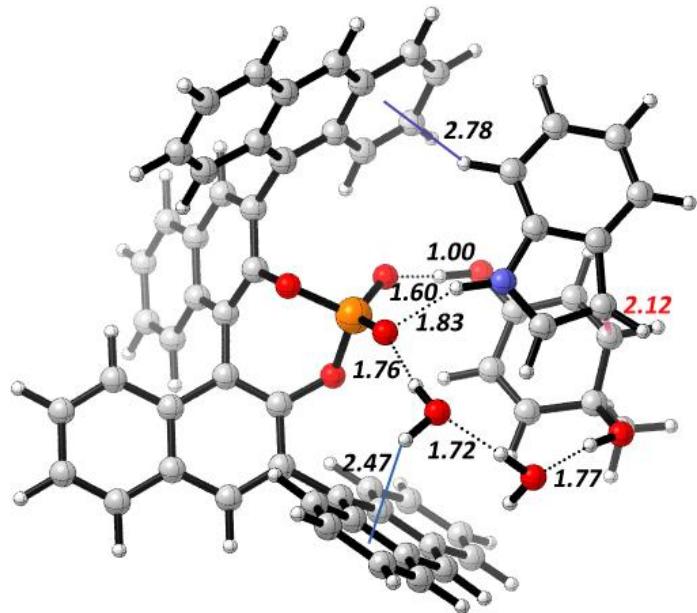
Interestingly, it was found that the presence of water molecules, not only forms a more compact cavity in the transition state (4S,5S)-H₂O-TS_{I-II} (H--O distances 1.76, 1.72 and 1.77 Å) than in (4R,5R)-H₂O-TS_{I-II} (H--O distances 1.84, 1.86 and 1.99 Å), but also these molecules interact with the aryl ring of the phosphoric acid catalyst through OH--π interactions (2.47 Å for (4S,5S)-H₂O-TS_{I-II} and 2.33 Å for (4R,5R)-H₂O-TS_{I-II}) (Figure 4, A and B).⁷ Moreover, a comprehensive analysis of both transition structures reveals that the lowest-energy transition state exhibits another important noncovalent interaction, namely *edge-to-face* π-π interaction (2.78 Å) between the indole and an aryl ring of the catalyst (Figure 4 A). These types of interactions have been recognized to play important roles in chemical and biological recognition processes⁸ and also in the enantioselectivity, as shown by the desymmetrization of *p*-quinol **1a**.

⁷ Takahashi, O.; Kohno, Y.; Nishio, M. *Chem. Rev.* **2010**, *110*, 6049-6079.

⁸ Review about non-covalent interactions: (a) Salonen, L. M.; Ellermann, M.; Diederich, F. *Angew. Chem. Int. Ed.* **2011**, *50*, 4808-4842. (b) Krenske, E. K.; Houk, K. N. *Acc. Chem. Res.* **2013**, *46*, 979-989. For examples in Stereoselective Organic reactions: (a) Calleja, J.; González Pérez, A. B.; de Lera, A. R.; Álvarez, R.; Fañanas, F.; Rodríguez, F. *Chem. Sci.*, **2014**, *5*, 996-1007. (b) Liu, C.; Besora, M.; Maseras, F. *Chem Asian J.* **2016**, *2016*, *11*, 411-416.

Figure 4. Representation of the transition structures corresponding to the water-assisted, phosphoric acid-promoted (*R*)-**12h** Friedel-Crafts-type reaction between *p*-quinol **1a** and indole **2a**: (4*S*,5*S*)-H₂O-**TS_{I-II}** and (4*R*,5*R*)-H₂O-**TS_{I-II}**. Relevant atom distances (in Å) are shown.

A. (4*S*,5*S*)-H₂O-**TS_{I-II}**



B. (4*R*,5*R*)-H₂O-**TS_{I-II}**

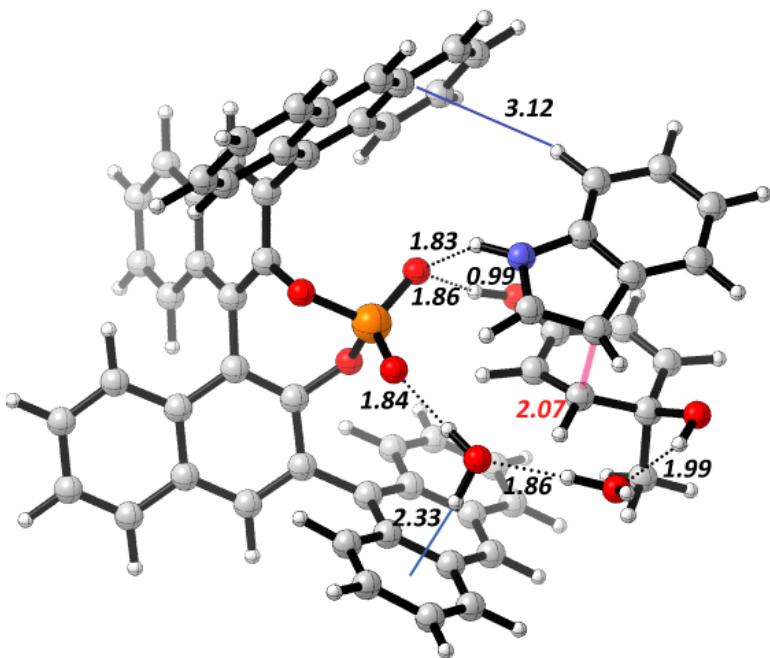


Table 3. Calculated energies (kcal/mol, yellow in gas phase and blue in CH₃CN) for the water-assisted (*R*)-**12h** catalyzed FC reaction of indole **2a** to both enantiotopic double bonds of *p*-quinol **1a**.

	E _{SCF}	E _{SCF+ZVE}	H	S	G		G (CH ₃ CN)	
(4S,5S)-H₂O-I	-2150268,8	-2149662,7	-2149624,5	98,3	-2149722,8	ref	-2150308,6	2,4
(4S,5S)-H₂O-TS_{I-II}	-2150232,5	-2149623,9	-2149586,7	94,7	-2149681,4	41,4	-2150300,5	5,3
(4S,5S)-H₂O-II	-2150269,6	-2149660,0	-2149622,7	94,9	-2149717,6	5,2	-2150320,3	-15,4
(4R,5R)-H₂O-I	-2150269,4	-2149662,7	-2149624,5	97,8	-2149722,3	0,5	-2150309,7	ref
(4R,5R)-H₂O-TS_{I-II}	-2150226,5	-2149617,5	-2149580,1	94,9	-2149675,0	47,8	-2150296,1	9,2
(4R,5R)-H₂O-II	-2150265,6	-2149656,3	-2149618,7	96,8	-2149715,5	7,4	-2150318,6	-11,8

Table 4. Calculated energies (kcal/mol, in gas phase) for the FC reaction promoted by (*R*)-**12h** phosphoric acid between *p*-quinol **1a** and indole **2a**, water assisted or non-water assisted.

	E _{SCF}	E _{SCF+ZVE}	H	S	G	
(4S,5S)-H₂O-I	-2150268,8	-2149662,7	-2149624,5	98,3	-2149722,8	ref
(4S,5S)-H₂O-TS_{I-II}	-2150232,5	-2149623,9	-2149586,7	94,7	-2149681,4	41,4
(4S,5S)-H₂O-II	-2150269,6	-2149660,0	-2149622,7	94,9	-2149717,6	5,2
(4S,5S)-I	-2054375,4	-2053801,4	-2053766,0	94,8	-2053860,8	ref
(4S,5S)-TS_{I-II}	-2054331,2	-2053755,6	-2053721,5	88,8	-2053810,3	50,5
(4S,5S)-II	-2054363,9	-2053788,4	-2053754,0	90,3	-2053844,2	16,6

(S,S)-H₂O-I

Num.	Imaginary Frequencies:	0	H	-1.880303	2.869247	-2.348695	
C	3.039020	-4.426697	-2.334537	H	4.375713	2.796115	-1.860917
C	2.344990	-4.335450	-1.086186	H	6.350127	1.327709	-1.458525
C	0.994095	-3.851454	-1.067767	H	3.700743	-2.103533	-1.093898
C	0.392611	-3.501906	-2.319687	H	1.761309	-0.644518	-1.403835
C	1.092939	-3.583424	-3.486391	H	5.648070	-1.289920	0.323228
C	2.439074	-4.048258	-3.497218	H	1.737268	-0.983985	2.039604
C	0.304908	-3.755695	0.158421	H	1.975915	-2.042291	3.144717
C	0.956979	-4.083179	1.364466	H	3.877688	-1.951306	1.864418
C	2.303848	-4.578440	1.333792	H	4.590035	-3.065632	1.074746
C	2.959191	-4.706765	0.110310	H	5.620680	-2.210174	-2.840772
C	2.952875	-4.919621	2.562832	H	5.116876	-0.705973	-3.662642
C	2.317692	-4.769915	3.757435	H	6.764012	-0.861303	-2.985216
C	0.987238	-4.258640	3.797533	H	4.150147	0.183152	2.256550
C	0.332273	-3.927192	2.646683	H	6.294733	1.776733	1.852541
C	-1.142407	-3.395362	0.196097	H	2.118181	1.346279	1.422919
C	-1.616024	-2.100553	-0.151133	H	6.398780	4.547977	0.640129
C	-2.959119	-1.774221	-0.136404	H	4.949269	6.271243	-0.392167
C	-3.891349	-2.731315	0.384396	H	1.450187	3.833741	0.217102
C	-3.434493	-4.035323	0.716735	H	2.507942	5.915917	-0.595491
C	-2.059280	-4.339233	0.587184				
C	-4.355385	-5.000916	1.201385				
C	-5.674508	-4.682523	1.381899				
C	-6.124838	-3.373589	1.094320				
C	-5.261250	-2.425782	0.610061				
O	-0.684954	-1.200348	-0.599265				
P	-0.379159	0.233671	0.143544				
O	-1.817300	0.567358	0.817138				
C	-2.857872	0.697571	-0.080881				
C	-3.418524	-0.440714	-0.612339				
C	-4.416758	-0.292584	-1.631621				
C	-4.876315	1.013463	-1.958260				
C	-4.312918	2.139313	-1.305444				
C	-3.294885	2.009897	-0.397085				
C	-4.943390	-1.392259	-2.360387				
C	-5.897584	-1.205563	-3.327313				
C	-6.381986	0.088896	-3.621162				
C	-5.875979	1.172286	-2.953054				
C	-2.656281	3.194800	0.243377				
C	-2.914844	3.475678	1.598319				
C	-2.303678	4.617866	2.212570				
C	-1.474446	5.442355	1.453594				
C	-1.217052	5.177652	0.110449				
C	-1.807136	4.025875	-0.510588				
C	-2.563199	4.889274	3.592490				
C	-3.382456	4.083721	4.323555				
C	-4.000068	2.954187	3.714076				
C	-3.776898	2.662396	2.401659				
C	-1.480771	3.760844	-1.880839				
C	-0.653223	4.586492	-2.579787				
C	-0.091382	5.744159	-1.967871				
C	-0.364881	6.027246	-0.664554				
O	-0.122782	1.176956	-1.005557				
O	0.626439	0.088525	1.235249				
O	1.986200	1.955644	-1.902643				
C	2.963373	1.164338	-1.715771				
C	4.291370	1.718969	-1.766008				
C	5.346630	0.919448	-1.536032				
C	5.249629	-0.578501	-1.461833				
C	3.835500	-1.044501	-1.286051				
C	2.768754	-0.248778	-1.448257				
O	6.132056	-1.115810	-0.517031				
C	5.711204	-1.120417	-2.843996				
C	5.265618	1.993730	1.603599				
C	4.747862	3.199858	1.026480				
C	3.347537	3.022401	0.898181				
N	3.044271	1.766878	1.372657				
C	4.196873	1.161583	1.804271				
C	5.327077	4.388024	0.555262				
C	4.513109	5.348031	-0.020962				
C	3.122517	5.149910	-0.133545				
C	2.519036	3.992418	0.326073				
O	2.436000	-1.414308	2.575045				
O	4.756706	-2.218230	1.501464				
H	1.034189	1.573850	-1.559741				
H	-4.575176	-2.390806	-2.153456				
H	-6.281959	-2.060738	-3.874993				
H	-7.143066	0.221427	-4.384017				
H	-6.224821	2.175945	-3.181696				
H	-4.657571	3.132265	-1.558032				
H	-1.715347	-5.339201	0.839123				
H	-5.622501	-1.424679	0.404844				
H	-7.156577	-3.115399	1.264117				
H	-6.372592	-5.424677	1.756621				
H	-3.987697	-5.996342	1.436630				
H	-1.014501	6.310031	1.921531				
H	3.967632	-5.118395	0.083482				
H	-0.671581	-3.521040	2.695430				
H	0.495307	-4.124661	4.756134				
H	2.822859	-5.024806	4.683575				
H	3.972964	-5.292551	2.522604				
H	-0.635261	-3.158636	-2.333509				
H	0.619213	-3.299002	-4.420707				
H	2.976890	-4.111854	-4.438232				
H	4.060722	-4.798818	-2.330852				
H	-4.257441	1.800547	1.950622				
H	-4.654002	2.320530	4.305762				
H	-3.569974	4.296816	5.371616				
H	-2.088328	5.755862	4.045122				
H	0.068369	6.899542	-0.181857				
H	0.562518	6.391170	-2.545041				
H	-0.409626	4.359167	-3.613088				

H	-5.282351	-2.241176	0.076470	C	2.822439	-0.529526	-1.990669
H	-6.620538	-4.162156	0.780124	C	4.852996	1.234586	0.440390
H	-5.539557	-6.356681	1.257339	C	4.399634	2.631862	0.773018
H	-3.082177	-6.575771	1.087245	C	3.083896	2.560191	1.232087
H	-2.370472	6.083034	2.225643	N	2.733194	1.192274	1.316703
H	4.738432	-4.492714	0.403996	C	3.701808	0.435101	0.927603
H	-0.268049	-3.614684	2.654892	C	4.994554	3.873969	0.626576
H	0.821337	-4.045539	4.802281	C	4.249223	5.007263	0.958921
H	3.257332	-4.583092	4.906879	C	2.931269	4.902280	1.406990
H	4.592501	-4.661925	2.837225	C	2.313078	3.662054	1.547496
H	0.080443	-3.224077	-2.352533	O	6.050327	-1.108985	-0.447320
H	1.490787	-3.159976	-4.344268	C	6.049269	-0.607159	-2.765057
H	3.938902	-3.608983	-4.186501	O	2.388379	-1.784065	2.904781
H	4.959147	-4.140721	-2.003542	O	4.326572	-2.639061	1.207521
H	-4.504254	0.967542	1.831331	H	1.028457	1.337282	-2.204485
H	-5.263460	1.300587	4.128950	H	-4.606698	-1.927081	-2.305295
H	-4.772773	3.428556	5.335314	H	-6.109063	-1.376416	-4.154547
H	-3.509737	5.222514	4.208697	H	-6.579065	0.999791	-4.741735
H	-1.231464	6.979243	0.256844	H	-5.471549	2.816520	-3.483939
H	-0.367109	6.668054	-2.033160	H	-3.918902	3.557014	-1.755864
H	-0.688465	4.489290	-3.203680	H	-2.295267	-5.209099	0.832575
H	-1.935784	2.674221	-2.134767	H	-5.675924	-0.856597	0.174325
H	3.763693	3.407997	-2.127870	H	-7.459547	-2.345991	0.941444
H	5.894354	2.443246	-1.252968	H	-6.975704	-4.731254	1.479217
H	3.953890	-1.444204	-0.922604	H	-4.664294	-5.585312	1.298870
H	1.849186	-0.421572	-1.632738	H	-0.372055	6.477087	1.831136
H	5.640080	-0.490474	0.544937	H	3.483089	-5.503762	0.319153
H	1.817718	-0.686343	2.394686	H	-1.102351	-3.524114	2.750352
H	2.179197	-1.791871	3.408369	H	-0.077042	-4.237069	4.852849
H	4.073117	-1.349065	2.270201	H	2.156417	-5.354770	4.863564
H	4.545116	-2.304433	1.177724	H	3.364435	-5.712139	2.743140
H	6.068756	-1.069483	-2.590073	H	-0.856996	-3.189532	-2.270372
H	5.323455	0.339061	-3.396483	H	0.469078	-3.408640	-4.306157
H	6.898496	0.498025	-2.567367	H	2.762315	-4.384878	-4.233339
H	3.830101	0.484668	1.447979	H	3.704253	-5.167513	-2.091769
H	5.819049	2.256861	1.092139	H	-3.917587	2.200002	1.837802
H	1.689476	1.592318	1.160020	H	-4.449459	2.869978	4.127768
H	5.626619	5.225136	0.323496	H	-3.294988	4.817958	5.178827
H	3.941848	6.998506	-0.096563	H	-1.617535	6.096725	3.902728
H	0.716700	4.189454	0.447979	H	0.929010	6.850904	-0.209674
H	1.525389	6.484250	-0.051461	H	1.639337	6.102989	-2.447251
H	0.657099			H	0.657099	4.033869	-3.442950
(S,S)-H₂O-II							
Num. Imaginary Frequencies: 0							
C	-2.118132	5.240760	3.456987	H	3.914565	2.712966	-2.030803
C	-1.777331	4.877811	2.115851	H	6.001567	1.535351	-1.337119
C	-2.426510	3.750014	1.512108	H	3.927861	-2.266654	-1.527066
C	-3.407738	3.047559	2.282954	H	1.884729	-1.052482	-2.158484
C	-3.703033	3.422681	3.559320	H	5.481324	-1.629281	0.153874
C	-3.047381	4.535470	4.159917	H	1.624996	-1.404262	2.420188
C	-2.093163	3.379544	0.195625	H	2.010100	-2.489050	3.445163
C	-1.109057	4.088841	-0.518882	H	3.717738	-2.383836	1.941224
C	-0.490895	5.236703	0.081370	H	3.746637	-3.145789	0.622591
C	-0.840906	5.604293	1.379710	H	6.150355	-1.659984	-3.042775
C	0.489818	5.965658	-0.663168	H	5.541462	-0.068420	-3.570717
C	0.879355	5.552739	-1.900336	H	7.052884	-0.190169	-2.628243
C	0.301593	4.387556	-2.481268	H	3.620568	-0.643352	0.951666
C	-0.667419	3.693239	-1.822773	H	5.776606	0.906740	0.926498
C	-2.827614	2.265015	-0.470009	H	1.807539	0.790319	1.590880
C	-2.619591	0.909551	-0.104096	H	6.011856	3.968397	0.258668
C	-3.294709	-0.140325	-0.687528	H	4.700829	5.989254	0.858412
C	-4.177005	0.133877	-1.782909	H	1.280391	3.570318	1.866879
C	-4.410252	1.487285	-2.152258	H	2.370947	5.800080	1.644557
C	-3.735257	2.526105	-1.464568				
C	-4.804347	-0.888388	-2.544854				
C	-5.643976	-0.578383	-3.583559				
C	-5.905780	0.768568	-3.921970				
C	-5.295569	1.776151	-3.223421				
C	-3.047619	-1.521534	-0.193588				
C	-1.755877	-2.006636	-0.133834				
C	-1.460190	-3.347492	0.229975				
C	-2.501722	-4.175292	0.567378				
C	-3.836725	-3.707784	0.617815				
C	-4.116529	-2.360148	0.261666				
C	-4.893994	-4.553798	1.044557				
C	-6.174150	-4.078853	1.146658				
C	-6.448836	-2.727949	0.833393				
C	-5.451531	-1.892379	0.402181				
O	-0.703142	-1.216236	-0.512942				
P	-0.255699	0.102257	0.358639				
O	-1.708291	0.635184	0.890539				
C	-0.060376	-3.858952	0.251794				
C	0.513068	-4.241809	1.481829				
C	1.809815	-4.854868	1.499548				
C	2.503534	-5.029751	0.301616				
C	1.973944	-4.595303	-0.914008				
C	0.663765	-4.010532	-0.946656				
C	2.380012	-5.252730	2.749212				
C	1.713437	-5.049862	3.920483				
C	0.435409	-4.416837	3.912675				
C	-0.141099	-4.024759	2.739103				
C	0.140292	-3.610835	-2.218795				
C	0.880020	-3.736178	-3.356464				
C	2.189755	-4.295383	-3.315445				
C	2.712450	-4.724356	-2.133646				
O	0.367243	1.057438	-0.596058				
O	0.505192	-0.295530	1.599778				
O	1.772539	1.480919	-2.831403				
C	2.852564	0.923026	-2.228414				
C	3.929274	1.644345	-1.886980				
C	5.060460	1.016229	-1.121190				
C	5.265657	-0.490148	-1.452576				
C	3.929472	-1.183863	-1.624760				

C	0.958423	-3.807745	1.220510	C	-4.086897	-2.642747	0.301170
C	2.346219	-4.169047	1.148701	C	-3.620746	-3.967464	0.532228
C	2.970072	-4.254417	-0.094434	C	-2.250367	-4.271219	0.335954
C	2.278756	-3.983472	-1.273911	C	-4.531436	-4.957083	0.987664
C	0.889655	-3.631376	-1.214680	C	-5.843299	-4.647160	1.231601
C	3.060943	-4.443322	2.357756	C	-6.300035	-3.322868	1.038673
C	2.442663	-4.370343	3.569706	C	-5.447395	-2.348311	0.587705
C	1.071931	-3.981153	3.648689	O	-0.931366	-1.057997	-0.705162
C	0.360843	-3.698099	2.518649	P	-0.469282	0.111897	0.349587
C	0.211366	-3.367205	-2.448121	O	-1.919598	0.541748	0.971030
C	0.868053	-3.423635	-3.640718	C	-2.924177	0.791183	0.065844
C	2.247288	-3.775725	-3.695387	C	-3.578630	-0.269265	-0.526323
C	2.924392	-4.058563	-2.548111	C	-4.580010	0.011145	-1.512976
O	0.047602	1.234282	-0.476835	C	-4.934449	1.365447	-1.769893
O	0.270612	-0.336296	1.597038	C	-4.261214	2.407761	-1.084675
N	2.296100	2.630599	0.684862	C	-3.248408	2.147787	-0.197392
C	3.348442	3.078004	-0.077578	C	-5.210130	-1.004845	-2.282057
C	4.545146	2.710720	0.583800	C	-6.163965	-0.693381	-3.216925
C	4.158392	2.013138	1.775060	C	-6.541576	0.650087	-3.442041
C	2.791937	1.980381	1.788111	C	-5.933788	1.654399	-2.735999
C	3.349458	3.754713	-1.301748	C	-2.493860	3.249676	0.465542
C	4.577964	4.066112	-1.858910	C	-1.592737	4.028371	-0.285630
C	5.781539	3.709765	-1.217931	C	-0.906394	5.119434	0.346517
C	5.775075	3.036366	-0.008482	C	-1.119280	5.373415	1.700536
C	3.957072	-0.946650	-0.100553	C	-1.993727	4.595480	2.458547
C	2.810001	-0.478056	-0.612779	C	-2.701388	3.516987	1.831655
C	2.848047	0.407870	-1.745565	C	-0.020103	5.929669	-0.432725
C	4.103683	0.717498	-2.384550	C	0.184813	5.672050	-1.754779
C	5.249286	0.292853	-1.827757	C	-0.461891	4.563023	-2.375824
C	5.308264	-0.682721	-0.689803	C	-1.312925	3.768419	-1.667222
O	1.796801	0.968628	-2.208826	C	-3.607109	2.750838	2.633858
O	6.233218	-0.209707	0.257407	C	-3.784093	3.027720	3.956565
C	5.803233	-2.033838	-1.274860	C	-3.075207	4.096435	4.577434
O	2.603248	-1.081218	2.836403	C	-2.210474	4.855831	3.848650
O	5.309326	-1.109402	2.691276	O	0.086545	1.189379	-0.548274
H	0.986833	0.956613	-1.533084	O	0.339989	-0.441396	1.476417
H	-4.754074	-2.236501	-2.187316	O	1.967478	0.682355	-2.568883
H	-6.418906	-1.806441	-3.927354	C	3.013240	0.323954	-1.835874
H	-7.177932	0.518223	-4.407766	C	2.897251	-0.276987	-0.612930
H	-6.198825	2.411778	-3.157101	C	4.022791	-0.365244	0.245926
H	-4.622332	3.276690	-1.508325	C	5.384462	-0.490127	-0.414555
H	-1.732519	-5.268406	0.721633	C	5.437583	0.289510	-1.703982
H	-5.772077	-1.475148	0.341462	C	4.334168	0.614699	-2.391483
H	-7.262524	-3.237026	1.159541	O	6.450645	-0.112965	0.425851
H	-6.388939	-5.524239	1.615048	C	5.545223	-1.989677	-0.777526
H	-3.985986	-6.008068	1.294542	C	4.198692	1.343008	1.392594
H	-0.757917	6.156642	2.081219	C	4.547579	2.384267	0.430726
H	4.019014	-4.539052	-0.145504	C	3.336195	2.866016	-0.082856
H	-0.668574	-3.368492	2.595004	N	2.299174	2.276714	0.646671
H	0.597393	-3.890904	4.620999	C	2.799478	1.465190	1.568848
H	2.992417	-4.585669	4.480793	C	3.265469	3.783253	-1.127582
H	4.112485	-4.707698	2.286862	C	4.471974	4.261448	-1.616463
H	-0.842665	-3.113660	-2.424057	C	5.698810	3.842553	-1.070896
H	0.336024	-3.208080	-4.562159	C	5.751712	2.898157	-0.058054
H	2.748851	-3.831853	-4.656743	O	2.562768	-1.462890	2.870675
H	3.969604	-4.355720	-2.579446	O	5.402495	-1.370816	2.859823
H	-4.394634	1.959147	1.984696	H	1.167807	0.716952	-1.986085
H	-4.820432	2.508258	4.328994	H	-4.925055	-2.039554	-2.128919
H	-3.606429	4.384468	5.435437	H	-6.629318	-1.486769	-3.794222
H	-1.959974	5.709458	4.164328	H	-7.300953	0.882369	-4.182424
H	0.451443	6.639169	0.017398	H	-6.197739	2.693871	-2.912931
H	0.927256	6.129846	-2.345403	H	-4.531099	3.439504	-1.295130
H	-0.214160	4.211584	-3.464438	H	-1.904291	-5.285269	0.519987
H	-1.831970	2.843118	-2.243911	H	-5.809095	-1.335240	0.450360
H	4.081977	1.423055	-3.205832	H	-7.335271	-3.075411	1.253570
H	6.208618	0.631374	-2.207910	H	-6.531084	-5.410039	1.583438
H	3.914530	-1.606671	0.759630	H	-4.161914	-5.966557	1.149292
H	1.867734	-0.735100	-0.149768	H	-0.594585	6.199945	2.175454
H	5.948253	-0.507682	1.151874	H	3.900969	-4.502926	-0.448097
H	1.847966	-0.720517	2.326776	H	-0.775473	-3.685974	2.432682
H	2.264635	-1.905035	3.208621	H	0.506429	-4.418545	4.377709
H	4.331336	-0.995843	2.754838	H	2.899530	-5.102343	4.142897
H	5.668306	-0.656111	3.461567	H	4.000959	-4.978686	1.936674
H	5.866524	-2.765232	-0.463528	H	-0.998968	-2.957184	-2.555060
H	5.130179	-2.408661	-2.051679	H	0.176563	-2.776731	-4.686286
H	6.804303	-1.891458	-1.690924	H	2.614092	-3.279979	-4.841683
H	2.113239	1.528371	2.496309	H	3.855178	-3.997332	-2.836470
H	4.814860	1.575380	2.511549	H	-4.155553	1.935850	2.173873
H	1.332259	2.559944	0.374295	H	-4.470257	2.428679	4.547693
H	6.704683	2.743502	0.469109	H	-3.230931	4.301025	5.632486
H	6.728158	3.968378	-1.684474	H	-1.667966	5.677101	4.310162
H	2.416525	4.011749	-1.792511	H	0.482246	6.761034	0.055228
H	4.615213	4.594052	-2.808009	H	0.851681	6.300305	-2.338715
				H	-0.263841	4.346064	-3.421215
				H	-1.776961	2.911543	-2.140635
				H	4.378327	1.147327	-3.334990
				H	6.428077	0.533533	-2.076716
				H	3.881378	-1.022675	1.094535
				H	1.931375	-0.535550	-0.208709
				H	6.300649	-0.575356	1.273572
				H	1.796240	-1.160069	2.338238
				H	2.339049	-2.373942	3.103483
				H	4.423230	-1.366815	2.913753
				H	5.709364	-1.162877	3.748848
				H	5.502790	-2.588922	0.138902
				H	4.757183	-2.316768	-1.458759
				H	6.523620	-2.132405	-1.244926
				H	2.138559	0.890815	2.200252
				H	4.859894	0.953303	2.152982
				H	1.320419	2.221212	0.329050
				H	6.696841	2.531650	0.325933
				H	6.621642	4.257461	-1.465483
				H	2.310407	4.109064	-1.524806

H	4.468150	4.985931	-2.425291	H	0.796231	6.137480	-2.301786					
(R,R)-H₂O-II												
Num.	Imaginary Frequencies:	0		H	-0.394521	4.259955	-3.445200					
C	5.657414	2.854122	-0.911487	H	-2.009098	2.886983	-2.224985					
C	4.426267	2.401767	-0.465105	H	6.807704	-0.527844	-2.466519					
C	3.269709	2.794529	-1.141122	H	7.747324	-0.021730	-0.218241					
C	3.271335	3.596725	-2.268116	H	3.76920	-0.476511	1.381686					
C	4.518074	4.026832	-2.716790	H	2.834857	-0.819703	-0.858352					
C	5.689664	3.667349	-2.044396	H	5.854724	0.596261	2.600877					
N	2.159498	2.254102	-0.446753	H	1.390485	-0.581330	2.615698					
C	2.544374	1.599647	0.598206	H	2.360734	-1.693223	3.051079					
C	4.017007	1.525548	0.685524	H	3.568512	0.184260	3.543923					
C	4.352971	-0.016528	0.576376	H	4.447048	0.769028	4.683368					
C	3.894460	-0.607609	-0.731999	H	5.417367	-1.752480	2.437359					
C	4.766638	-0.812913	-1.731160	H	5.507212	-2.457964	0.804218					
C	6.193304	-0.516216	-1.571734	H	7.000787	-1.979340	1.655601					
C	6.694323	-0.245186	-0.366302	H	1.816969	1.067126	1.205685					
C	5.851390	-0.305547	0.884904	H	4.388044	1.863876	1.657916					
O	4.460372	-1.299690	-2.959002	H	1.149727	2.177198	-0.734022					
O	6.394673	0.635841	1.784751	H	6.565220	2.571982	-0.389602					
C	5.952459	-1.721244	1.480601	H	6.644089	4.030028	-2.413326					
O	-0.209408	1.270875	-0.753564	H	2.348001	3.879465	-2.761699					
P	-0.624363	0.186386	0.190378	H	4.578339	4.658520	-3.597383					
O	0.274223	-0.263092	1.297147	(S,S)-I								
O	-1.057540	-1.068804	-0.778116	Num.	Imaginary Frequencies:	0						
C	-1.927077	-2.011771	-0.302813	C	-4.829787	0.836871	1.272351					
C	-1.392642	-3.288995	0.014649	C	-5.816660	-0.016501	0.987501					
C	-2.257469	-4.267421	0.433166	C	-5.647293	-1.512323	0.947765					
C	-3.639158	-4.007903	0.611801	C	-4.207179	-1.927936	1.101550					
C	-4.153232	-2.711968	0.325423	C	-3.211730	-1.086723	1.393985					
C	-3.270815	-1.713568	-0.199824	C	-3.464196	0.356478	1.524403					
C	-4.512744	-5.011187	1.107151	O	-6.185244	-2.033195	-0.255797					
C	-5.835092	-4.741024	1.338614	C	-6.466546	-2.148063	2.081230					
C	-6.339374	-3.443184	1.094464	O	-2.573997	1.163498	1.814511					
C	-5.523227	-2.456812	0.604326	C	-5.258742	-0.098096	-2.664423					
C	0.076561	-3.523195	-0.079085	C	-4.969796	1.228970	-2.199299					
C	0.832664	-3.680463	1.098293	C	-3.625217	1.216551	-1.756177					
C	2.247403	-3.908556	1.006901	N	-3.131509	-0.051573	-1.943833					
C	2.858715	-3.955320	-0.243489	C	-4.113319	-0.834773	-2.480856					
C	2.120367	-3.796717	-1.415037	C	-5.715235	2.412208	-2.080354					
C	0.705688	-3.578930	-1.337007	C	-5.111968	3.527662	-1.528095					
C	0.249273	-3.604882	2.405741	C	-3.768790	3.492865	-1.101113					
C	0.999644	-3.795672	3.527471	C	-3.004586	2.346525	-1.212698					
C	2.400320	-4.050831	3.431574	O	-0.056931	0.571608	1.708595					
C	3.004482	-4.088331	2.209310	P	0.319050	-0.065805	0.335969					
C	2.748739	-3.844719	-2.699772	O	-0.767806	-0.595463	-0.506743					
C	2.022136	-3.673929	-3.841642	O	1.437126	-1.120500	0.825588					
C	0.614528	-3.464672	-3.768104	C	2.233722	-1.653575	-0.172629					
C	-0.019310	-3.425774	-2.562683	C	3.261816	-0.893544	-0.682983					
C	-3.733153	-0.349637	-0.578194	C	4.028555	-1.441716	-1.763252					
C	-3.107240	0.740587	-0.011232	C	3.767694	-2.776425	-2.184700					
C	-3.481676	2.082556	-0.289403	C	2.728939	-3.521156	-1.569469					
C	-4.509136	2.294613	-1.171187	C	1.939014	-2.975551	-0.591824					
C	-5.152792	1.218857	-1.834375	C	5.016518	-0.696485	-2.460787					
C	-4.753199	-0.118664	-1.557663	C	5.728365	-1.259775	-3.488341					
C	-6.169866	1.457513	-2.795018	C	5.495575	-2.597947	-3.878160					
C	-6.752487	0.421837	-3.476345	C	4.532687	-3.334760	-3.241555					
C	-6.330618	-0.904389	-3.231043	C	3.492123	0.470022	-0.129169					
C	-5.358588	-1.167777	-2.300576	C	2.441887	1.359864	-0.064677					
O	-2.076822	0.533010	0.872918	C	2.559701	2.684686	0.426153					
C	-2.762486	3.210696	0.371003	C	3.790843	3.094012	0.867790					
C	-1.832846	3.978589	-0.355289	C	4.901538	2.212736	0.889935					
C	-1.138086	5.050239	0.299912	C	4.754577	0.879933	0.412619					
C	-1.398041	5.319752	1.642153	C	6.151677	2.630746	1.416445					
C	-2.318171	4.567095	2.370238	C	7.207067	1.761562	1.496282					
C	-3.013333	3.490551	1.727112	C	7.051716	0.426713	1.059719					
C	-0.181696	5.816614	-0.439929	C	5.860817	-0.003426	0.534076					
C	0.073247	5.543503	-1.749456	C	1.357924	3.566527	0.470468					
C	-0.609216	4.474832	-2.401986	C	0.853734	4.118869	-0.721481					
C	-1.523456	3.719252	-1.730328	C	-0.315143	4.947996	-0.676770					
C	-3.949084	2.735069	2.504355	C	-0.926811	5.201164	0.550549					
C	-4.171432	3.025078	3.817082	C	-0.442664	4.651140	1.735251					
C	-3.479331	4.095867	4.452440	C	0.721080	3.811914	1.701183					
C	-2.583423	4.842036	3.748736	C	1.462961	3.884452	-1.995745					
O	2.164848	-0.757545	3.193082	C	0.938580	4.416821	-3.135334					
O	4.414193	0.655851	3.728456	C	-0.230082	5.229469	-3.088565					
H	3.525459	-1.554180	-2.982808	C	-0.832072	5.489326	-1.895390					
H	-5.038129	-2.189563	-2.130374	C	-1.089213	4.896229	2.987482					
H	-6.776907	-1.722690	-3.788225	C	-0.622228	4.338073	4.137539					
H	-7.526050	0.616406	-4.212973	C	0.522302	3.490243	4.105561					
H	-6.469776	2.484459	-2.987386	C	1.168942	3.235156	2.934166					
H	-4.819552	3.312793	-1.392043	O	1.196558	0.978987	-0.527255					
H	-1.871311	-5.256116	0.668469	C	0.793635	-3.707858	0.026861					
H	-5.922166	-1.463634	0.431129	C	-0.402283	-3.875895	-0.690236					
H	-7.382670	-3.224784	1.301854	C	-1.501684	-4.562070	-0.072363					
H	-6.494796	-5.514348	1.720221	C	-1.373340	-5.031705	1.233432					
H	-4.105791	-5.998846	1.308513	C	-0.190574	-4.867430	1.953529					
H	-0.870210	6.134911	2.133147	C	0.920101	-4.200625	1.339634					
H	3.931663	-4.120296	-0.309977	C	2.215196	-4.545435	3.371122					
H	-0.806567	-3.378640	2.495356	C	1.711255	-4.750520	-0.813885					
H	0.536199	-3.726024	4.506249	C	-2.832571	-4.282445	-2.086472					
H	2.981578	-4.199145	4.336766	C	-1.752563	-3.577412	-2.694153					
H	4.073374	-4.265268	2.122942	C	-0.586248	-3.373762	-2.019744					
H	-1.091681	-3.270302	-2.520767	C	2.125911	-4.064582	2.099128					
H	0.046410	-3.337131	-4.684280	C	2.215196	-4.545435	3.371122					
H	2.511116	-3.709779	-4.810661	C	1.107042	-5.200218	3.980626					
H	3.821568	-4.010569	-2.745483	C	-0.056780	-5.356750	3.290901					
H	-4.483989	1.917976	2.032180	H	-1.037923	0.811215	1.793733					
H	-4.881132	2.435039	4.389149	H	5.754577	-1.034309	0.216029					
H	-3.670528	4.311059	5.499523	H	7.881218	-0.268401	1.147827					
H	-2.051051	5.662993	4.222487	H	8.156902	2.089826	1.906959					
H	0.334573	6.626855	0.068809	H	6.250720	3.654244	1.768308					
H				H	3.911476	4.106175	1.244802					
H				H	2.536780	-4.536754	-1.905410					

H	5.200171	0.334245	-2.178978	C	-5.3151720	-1.282585	0.945220
H	6.474639	-0.669820	-4.011706	C	-3.912886	-1.607197	1.378497
H	6.070806	-3.032760	-4.689683	C	-2.994100	-0.668628	1.630843
H	4.330205	-4.359012	-3.543207	C	-3.312037	0.747680	1.435894
H	-1.807386	5.839808	0.583817	C	-4.539465	1.117540	0.915655
H	-2.212645	-5.544691	1.698932	O	-5.823823	-2.261680	0.051855
H	0.218027	-2.816072	-2.485465	C	-6.232824	-1.335628	2.184045
H	-1.867696	-3.188888	-3.701996	O	-2.451827	1.671091	1.786527
H	-3.753935	-4.439821	-2.640048	H	-1.52006	1.291428	1.896160
H	-3.532082	-5.282674	-0.339199	H	5.613270	-1.519086	-0.035760
H	2.980677	-3.573493	1.646208	H	7.866207	-0.954755	0.738167
H	3.140044	-4.430394	3.928181	H	8.410871	1.365914	1.465543
H	1.198775	-5.576681	4.994960	H	6.647766	3.098251	1.463448
H	-0.908138	-5.857960	3.744156	H	4.323354	3.758891	1.128667
H	2.356519	3.270905	-2.046522	H	1.871749	-4.643065	-2.020599
H	1.413445	4.221216	-4.092012	H	5.042763	-0.093426	-2.366920
H	-0.637304	5.638195	-4.008127	H	6.087714	-1.183201	-4.293462
H	-1.725236	6.106783	-1.848233	H	5.382882	-3.469602	-4.991480
H	-1.969146	5.534219	2.996099	H	3.575816	-4.625572	-3.764569
H	-1.123656	4.525610	5.082186	H	-1.264366	5.973935	1.006581
H	0.874075	3.033775	5.025784	H	-2.712418	-5.340673	1.792018
H	2.022423	2.566991	2.922017	H	-0.230317	-2.776837	-2.463461
H	-4.968405	1.912922	1.269168	H	-2.355097	-3.060841	-3.643420
H	-6.815826	0.343837	0.753955	H	-4.280399	-4.207871	-2.535774
H	-4.012593	-2.989190	0.966454	H	-4.061054	-5.018230	-0.214387
H	-2.191144	-1.434503	1.502823	H	2.585695	-3.679688	1.603179
H	-3.917691	-1.875211	-2.695853	H	2.747245	-4.529150	3.887433
H	-6.177923	-0.448001	-3.114935	H	0.765523	-5.546900	5.009107
H	-2.232890	-0.374873	-1.590033	H	-1.384376	-5.707197	3.809961
H	-6.749266	2.448124	-2.412773	H	2.376571	3.098326	-2.047769
H	-5.676177	4.450430	-1.426266	H	1.337342	4.179143	-3.981121
H	-1.971043	2.322717	-0.881624	H	-0.522920	5.813652	-3.675599
H	-3.321059	4.382918	-0.671603	H	-1.337986	6.344348	-1.406229
H	-5.762972	-1.547754	-0.987352	H	-1.234318	5.615375	3.416883
H	-6.375165	-3.237019	2.026763	H	-0.311719	4.463669	5.393366
H	-6.116336	-1.803971	3.058237	H	1.524438	2.796879	5.121686
H	-7.521150	-1.885098	1.958527	H	2.443043	2.303493	2.912539
H				H	-4.736768	2.171744	0.760203
H				H	-6.428158	0.446877	0.174285
H				H	-3.688466	-2.657552	1.548606
(S,S)-TS _{r-II}				H	-2.005418	-0.926793	1.990281
Num. Imaginary Frequencies:	1			H	-3.450075	-1.555565	-1.396131
C	-0.532956	5.628169	-1.553753	H	-5.945378	-0.582297	-1.919800
C	0.034164	5.000636	-0.399373	H	-1.885748	0.241619	-1.297448
C	1.112026	4.069573	-0.569233	H	-6.786181	2.335771	-2.364500
C	1.563487	3.801876	-1.902027	H	-5.805275	4.599459	-2.604444
C	0.984033	4.404749	-2.979432	H	-1.847962	3.072144	-1.841190
C	-0.079873	5.337248	-2.805590	H	-3.372829	4.964330	-2.343323
C	1.678224	3.447323	0.559276	H	-5.084391	-2.636228	-0.447270
C	1.170016	3.707760	1.845975	H	-6.159797	-2.324660	2.644118
C	0.091993	4.642584	2.004034	H	-5.948242	-0.572583	2.912611
C	-0.445349	5.268711	0.881713	H	-7.270728	-1.173904	1.876113
C	-0.421042	4.901546	3.314445				
C	0.089813	4.265107	4.404041				
C	1.143251	3.318121	4.248811				
C	1.662996	3.048183	3.018844				
C	2.795513	2.471745	0.397856				
C	2.519845	1.169524	-0.094981				
C	3.482500	0.188267	-0.226714				
C	4.810084	0.476916	0.228143				
C	5.112338	1.789320	0.690909				
C	4.086463	2.766933	0.752338				
C	5.837484	-0.504157	0.273428				
C	7.098591	-0.187285	0.709117				
C	7.406790	1.127157	1.128126				
C	6.431074	2.088793	1.123276				
C	3.083607	-1.142054	-0.768742				
C	2.014832	-1.796083	-0.191855				
C	1.544911	-3.063652	-0.631282				
C	2.201808	-3.667169	-1.672911				
C	3.279232	-3.028350	-2.338975				
C	3.712887	-1.742688	-1.907395				
C	4.730898	-1.091100	-2.654803				
C	5.313116	-1.701578	-3.736123				
C	4.909813	-2.995793	-4.136697				
C	3.910308	-3.638680	-3.454743				
O	1.363139	-1.207460	0.861712	P	0.268770	-0.037298	0.412135
P	0.286044	-0.043220	0.450479	O	-0.671832	-0.613647	-0.610314
O	1.233570	0.915026	-0.487248	O	1.373324	-1.172473	0.836158
C	0.364691	-3.692867	0.031916	C	2.080921	-1.716340	-0.204797
C	-0.862480	-3.795059	-0.651138	C	3.144597	-1.015233	-0.733097
C	-1.986294	-4.408108	-0.001350	C	3.828447	-1.571839	-1.863045
C	-1.857633	-4.874704	1.305002	C	3.448178	-2.860264	-2.334906
C	-0.649703	-4.772999	1.995745	C	2.374859	-3.549289	-1.713997
C	0.484650	-4.180550	1.348994	C	1.669840	-2.991268	-0.680074
C	-3.224861	-4.532586	-0.713134	C	4.849236	-0.874980	-2.564042
C	-3.345395	-4.082627	-1.995670	C	5.480225	-1.443207	-3.640849
C	-2.238260	-3.446406	-2.635103	C	5.127257	-2.738388	-4.082396
C	-1.051164	-3.294838	-1.982340	C	4.129094	-3.425677	-3.443992
C	1.714697	-4.116733	2.078670	C	3.477540	0.317077	-0.151508
C	1.804477	-4.592534	3.352771	C	2.477543	1.261419	-0.035896
C	0.672913	-5.172639	3.993954	C	2.687848	2.562475	0.491345
C	-0.515124	-5.261184	3.333477	C	3.950461	2.893060	0.908064
O	-0.744024	-0.588421	-0.488921	C	5.010456	1.950735	0.870739
O	-0.097776	0.616677	1.740225	C	4.774873	0.641505	0.362431
N	-2.869283	0.429787	-1.587697	C	6.296549	2.281352	1.371996
C	-3.485751	1.650322	-1.853697	C	7.303512	1.353100	1.397630
C	-4.863878	1.411981	-1.995637	C	7.061635	0.042544	0.927637
C	-5.072017	0.004148	-1.668887	C	5.833461	-0.304159	0.426316
C	-3.772929	-0.539324	-1.566957	C	1.522671	3.486927	0.612280
C	-2.914233	2.913181	-1.967001	C	0.998639	4.114411	-0.532965
C	-3.779482	3.963243	-2.239604	C	-0.147383	4.967889	-0.412438
C	-5.160397	3.753610	-2.385862	C	-0.735306	5.152974	0.837479
C	-5.715631	2.485571	-2.257553	C	-0.235874	4.523950	1.975184
C	-5.407310	0.136325	0.385816	C	0.914491	3.672454	1.867335

C	1.559213	3.924288	-1.836992
C	1.022626	4.531569	-2.933815
C	-0.108260	5.390130	-2.808387
C	-0.668622	5.602744	-1.583993
C	-0.858080	4.697001	3.251355
C	-0.378682	4.060961	4.354563
C	0.752473	3.201361	4.248749
C	1.373822	3.011066	3.052107
O	1.216281	0.969995	-0.477971
C	0.503326	-3.678721	-0.051373
C	-0.714522	-3.798266	-0.747080
C	-1.824675	-4.460092	-0.122768
C	-1.691020	-4.962884	1.168984
C	-0.491266	-4.847689	1.870679
C	0.628681	-4.202114	1.250906
C	-3.056644	-4.591222	-0.844180
C	-3.187589	-4.094590	-2.108284
C	-2.093036	-3.414389	-2.723161
C	-0.909083	-3.264153	-2.064095
C	1.850435	-4.121135	1.992258
C	1.945768	-4.632177	3.251755
C	0.828364	-5.265492	3.866280
C	-0.351358	-5.370651	3.194326
H	-1.732254	1.237946	2.151698
H	5.658542	-1.316644	0.079713
H	7.853299	-0.699442	0.970881
H	8.281066	1.615208	1.790809
H	6.462237	3.286684	1.750769
H	4.137535	3.883336	1.315466
H	2.091304	-4.529521	-2.089349
H	5.123923	0.123506	-2.242544
H	6.255913	-0.890472	-4.162517
H	5.638392	-3.178576	-4.933165
H	3.834445	-4.415118	-3.784557
H	-1.611336	5.792190	0.924638
H	-2.536615	-5.462842	1.637581
H	-0.095997	-2.717283	-2.526199
H	-2.213549	-3.002987	-3.720977
H	-4.119724	-4.220440	-2.652873
H	-3.880262	-5.118987	-0.367278
H	2.710778	-3.643395	1.536946
H	2.882258	-4.555888	3.795632
H	0.925070	-5.666434	4.870731
H	-1.210490	-5.854742	3.651401
H	2.426458	3.280960	-1.944452
H	1.463710	4.369011	-3.912663
H	-0.514080	5.875986	-3.691117
H	-1.526315	6.262072	-1.472088
H	-1.731521	5.340387	3.315366
H	-0.863619	4.192693	5.317111
H	1.109992	2.679742	5.131289
H	2.212820	2.328919	2.979558
H	-4.842409	2.021529	0.860884
H	-6.442425	0.254512	0.150769
H	-3.665942	-2.804690	1.466642
H	-2.100764	-1.032338	2.113666
H	-3.181834	-1.552941	-1.181169
H	-5.669598	-0.698956	-1.878735
H	-1.702081	0.209195	-1.403261
H	-6.739346	2.211948	-2.058304
H	-5.831152	4.446975	-2.641545
H	-1.790029	3.009015	-2.230200
H	-3.394073	4.848615	-2.708292
H	-4.921858	-2.895867	-0.464557
H	-6.231839	-2.528135	2.469994
H	-6.131976	-0.764061	2.709156
H	-7.337933	-1.453762	1.589199