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Supporting Information

Mechanism for the Nonadiabatic Photooxidation of Benzene to Phenol: Orientation-Dependent Proton-Coupled Electron Transfer

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1 Computational Methods

1.1 CASSCF and CASPT2 Methods

Minima and minimum-energy crossing points in the $^1\pi\pi^*$, $^1n\pi^*$, $^3\pi\pi^*$, and $^3n\pi^*$ excited states of DDQ were determined from two-root state-averaged complete active space self-consistent field (SA2-CASSCF) calculations (equal state weights). All SA2-CASSCF geometry optimizations employed an active space of 10 electrons in 8 orbitals, including 4 lone-pair electrons (2 orbitals) and 6 π electrons (6 π and π^* orbitals). More accurate potential energy profiles were obtained by using complete active space second-order perturbation theory (CASPT2) [1, 2] to re-evaluate the energies at all SA2-CASSCF optimized geometries. In these single-point CASPT2 calculations, a level shift of 0.2 a.u. was adopted to avoid intruder-state problems. [3]

The 6-31G* [4, 5] and 6-31+G* [5, 6] basis sets were used in all SA2-CASSCF optimizations and single-point CASPT2 computations, respectively. All CASSCF and CASPT2 computations were performed with MOLPRO2010. [7, 8]

1.2 DFT Methods

All minima, transition states, and crossing points involving the T_1 and S_0 states were optimized using the unrestricted UB3LYP-D3/6-31G* approach [9–12] including the dispersion correction of Grimme et al. [13] The nature of all stationary points was confirmed by harmonic vibrational frequency analysis. Transition states were further verified by intrinsic reaction coordinate (IRC) calculations. [14, 15] The polarizable continuum model (PCM) [16–18] was employed to implicitly consider solvation effects of surrounding acetonitrile molecules. Gibbs free energies of all optimized structures were calculated at 298.15 K and 1 atm. Singly occupied molecular orbitals (SOMOs) associated with triplet structures were obtained through biorthogonalizing unrestricted molecular orbitals to ensure maximum alignment. All DFT computations were conducted using GAUSSIAN09. [19]

In order to examine the topology of potential energy surfaces, the nudged elastic band (NEB) method was employed to optimize the relevant reaction paths. [20–22]

The penalty function method was invoked to optimize T_1/S_0 crossing points. We adopted the penalty function method of Ciminelli et al. [23] implemented in the DL-FIND module of the ChemShell-3.5 package. [24] The objective function is defined as

$$f(R) = \frac{E_I + E_J}{2} + c_1 c_2^2 ln[1 + (\frac{E_J - E_I}{c_2})^2] \quad (1)$$

in which E_I and E_J are the QM/MM energies of electronic states I and J. For the parameters c_1 and c_2, we used the recommended values of 5.0 (kcal/mol)$^{-1}$ and 5.0 kcal/mol, respectively. [23] This optimization scheme

Table 1: Vertical Excitation Energies (in eV) and Oscillator Strengths (f) of DDQ in Acetonitrile Solution Computed by TD-DFT and CASPT2/6-31+G*//CASSCF(10,8)/6-31G* Methods

	B3LYP	CAM-B3LYP	ωB97XD	CASPT2	exp.[a]
S_1	2.58 (0.01)	3.09 (0.00)	3.07 (0.00)	2.94	-
S_2	2.65 (0.00)	3.17 (0.01)	3.13 (0.01)	3.37	3.10

[a]Experimental value in dichloromethane solution.

for conical intersection structures has recently been shown to be practical for large systems, in particular in the condensed phase. [25]

2 Convergence Criteria

In optimizations of minima and transition states, the following convergence thresholds had to be satisfied: (1) energy converged to within 1.0×10^{-6} hartree; (2) maximum force component less than 4.5×10^{-4} hartree/bohr; (3) root-mean-square force less than 3.0×10^{-4} hartree/bohr; (4) maximum step size component less than 1.8×10^{-3} bohr; (5) root-mean-square step size less than 1.2×10^{-3} bohr.

For optimizations of crossing points, we loosened the thresholds: (1) energy converged to within 1.0×10^{-5} hartree; (2) maximum force component less than 6.0×10^{-3} hartree/bohr; (3) root-mean-square force less than 4.0×10^{-3} hartree/bohr; (4) maximum step size component less than 2.4×10^{-3} bohr; (5) root-mean-square step size less than 1.6×10^{-3} bohr.

3 Mechanistic Photophysics of DDQ

Table 1 lists vertical excitation energies (in eV) and oscillator strengths (f) of DDQ to the S_1 and S_2 states. The S_1 state is spectroscopically dark as a $n \rightarrow \pi^*$ electronic transition. The corresponding vertical excitation energy is computed to be 3.09 and 3.07 eV at the TD-CAM-B3LYP and TD-ωB97XD levels, respectively, close to the CASPT2 result of 2.94 eV. The S_2 state is a $^1\pi\pi^*$ state with a rather small oscillator strength ($f \simeq$0.01). Its vertical excitation energy is predicted to be 3.17 and 3.13 eV at the TD-CAM-B3LYP and TD-ωB97XD levels, respectively. CASPT2 gives a value of 3.37 eV, i.e. 0.27 eV higher than experimental value of 3.10 eV measured in dichloromethane solution. In both cases, TD-B3LYP significantly underestimates the transition energies by more than about 0.5 eV.

Experimentally, it is known from the triplet-triplet absorption spectrum of DDQ that the photocatalytic reaction is initialized by an intermolecular electron transfer from ground-state benzene to triplet DDQ. Our computations show that the $^3\pi\pi^*$ state of DDQ (see the SOMOs in Fig. 4 of the main text) is responsible for this initial intermolecular electron transfer, not the lowest $^3n\pi^*$ triplet state. At the CASPT2 level, the $^3n\pi^*$ state is energetically

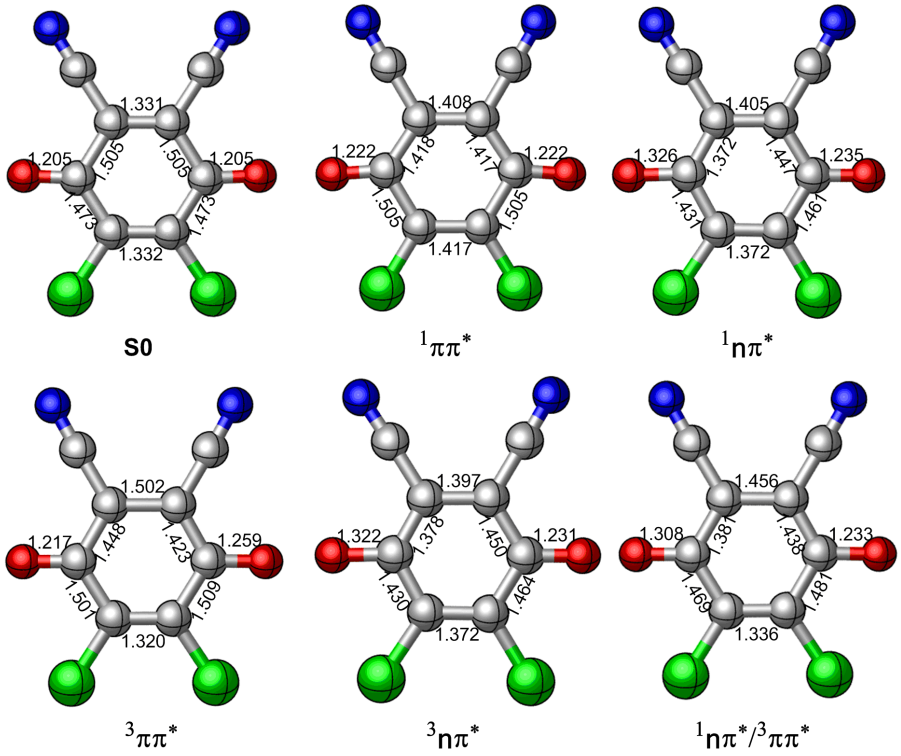


Figure 1: CASSCF(10,8)/6-31G* optimized minima and minimum-energy crossing point for the $^1\pi\pi^*$, $^1n\pi^*$, $^3\pi\pi^*$, and $^3n\pi^*$ excited states. Also shown are some selected geometric parameters (distances in Å).

Table 2: Relative Energies (in kcal/mol) of Excited-State Minima and Crossing Point of DDQ from CASPT2/6-31+G*//CASSCF(10,8)/6-31G* Calculations.

	CASPT2
$^1\pi\pi^*$	77.2
$^1n\pi^*$	53.6
$^3\pi\pi^*$	58.8
$^3n\pi^*$	52.0
$^1n\pi^*$ /$^3\pi\pi^*$	59.8/59.3

below the $^3\pi\pi^*$ state at the Franck-Condon point (69.8 vs. 54.1 kcal/mol) and at the respective minima (58.8 vs. 52.0 kcal/mol, see Table 2).

Furthermore, we found an efficient relaxation pathway from the initially populated singlet state $^1\pi\pi^*$ to the $^3\pi\pi^*$ state (see panel (a) of Fig. 2 of the main text). On this route, the $^1\pi\pi^*$ state first relaxes via internal conversion to the dark $^1n\pi^*$ doorway state, which then decays to the reactive $^3\pi\pi^*$ state via the $^1n\pi^*$ /$^3\pi\pi^*$ minimum-energy crossing point.

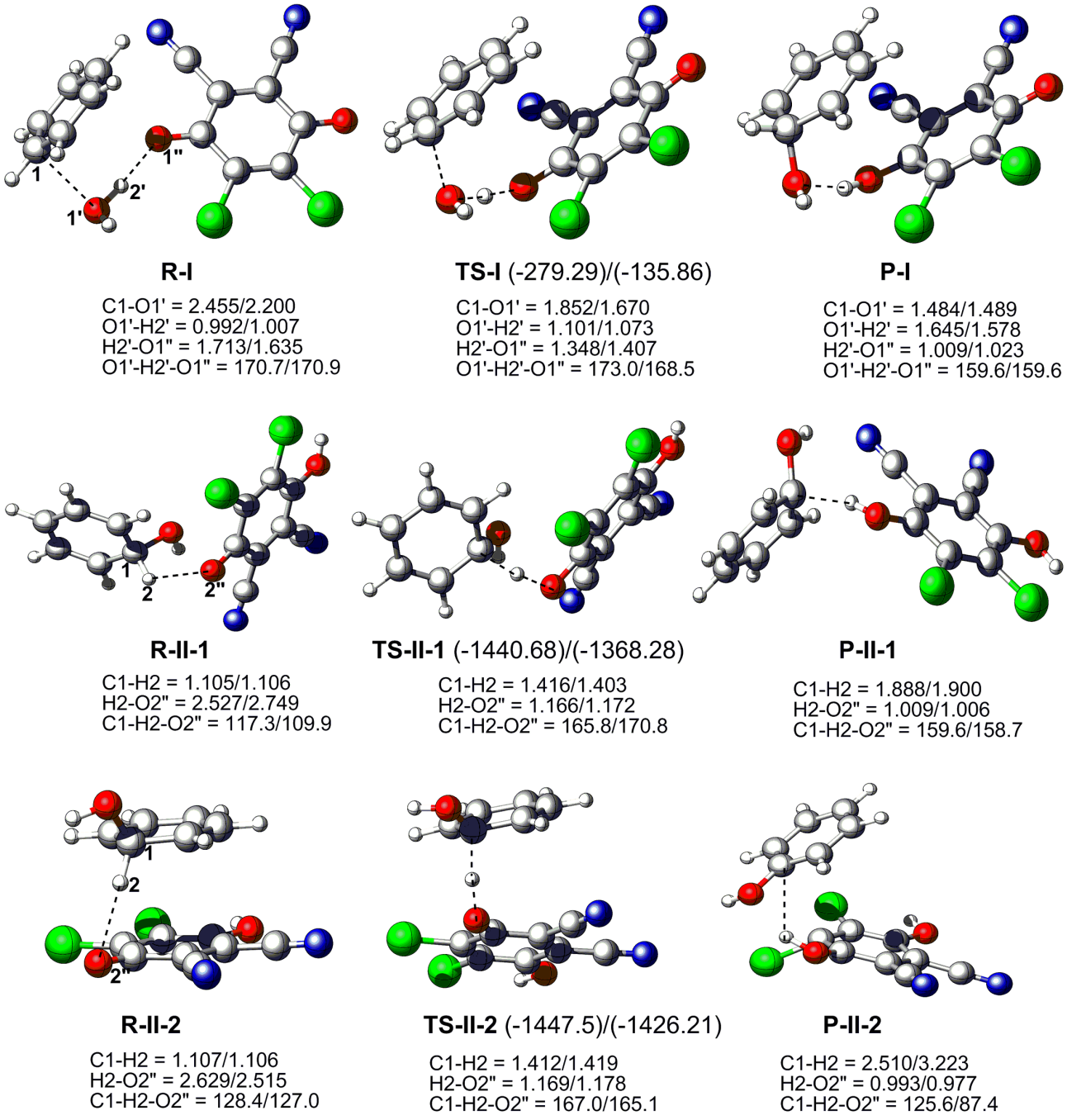
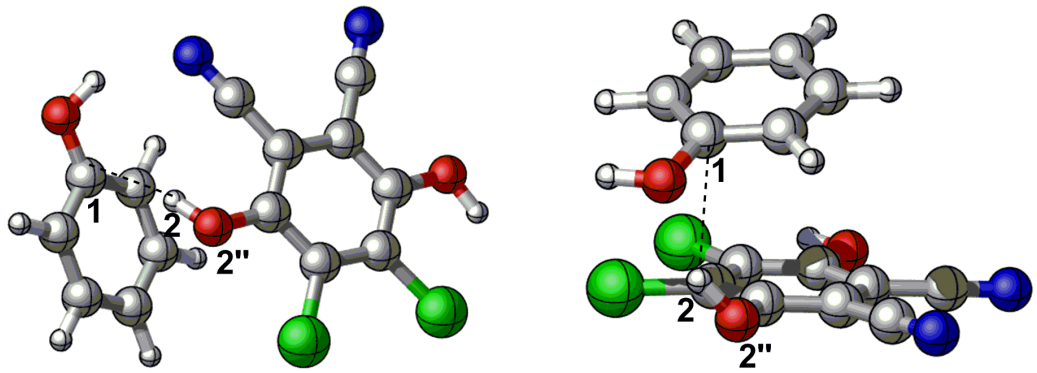


Figure 2: UB3LYP-D3/6-31G* and UB3LYP-D3/6-31G*/PCM(acetonitrile) optimized stationary points (reactants, transition states, and products) involved (a) in the triplet-state reaction between DDQ radical anion, water, and benzene radical cation that generates DDQH and phenol-OH radicals [top panel; step (2) in Fig. 1 in the main text]; and (b) in the subsequent proton-coupled electron transfer reaction that produces the products phenol and $DDQH_2$ [middle and bottom panels; step (3) in Fig. 1 of the main text]. Also shown are selected geometric parameters (distances in Å, angles in degree) and computed imaginary frequencies of transition states (in parentheses).



S0-II-1-P

C1-H2 = 2.441
H2-O2" = 0.977
C1-H2-O2" = 154.4

S0-II-2-P

C1-H2 = 2.583
H2-O2" = 0.988
C1-H2-O2" = 125.8

Figure 3: UB3LYP-D3/6-31G*/PCM(acetonitrile) optimized ground-state products. Selected geometric parameters are given in Å for distances and in degree for angles.

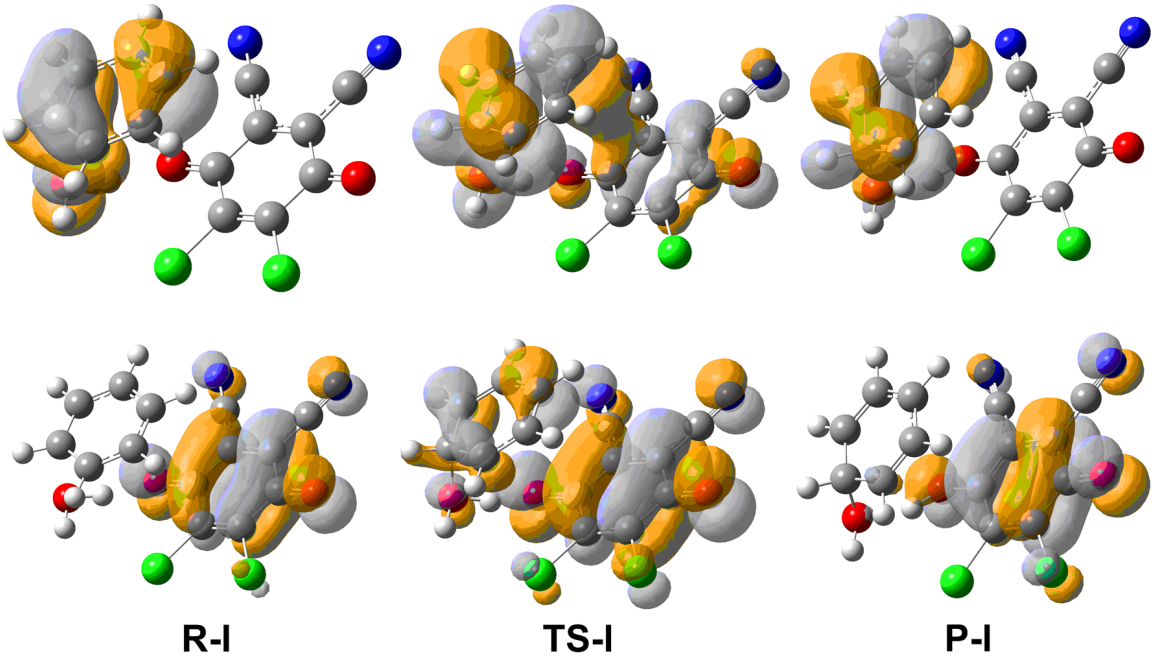


Figure 4: UB3LYP-D3/6-31G*/PCM(acetonitrile) calculations yield singly occupied molecular orbitals for reactant R-I, transition state TS-I, and product P-I, see step (2) in Fig. 1 of the main text.

Table 3: Energy Gaps (in kcal/mol) at T_1/S_0 Crossing Points from UB3LYP-D3/6-31G*/PCM Calculations.

	T1S0-II-1-R	T1S0-II-1-P	T1S0-II-2-R	T1S0-II-2-P
$\triangle E$	1.0	0.2	0.0	0.7

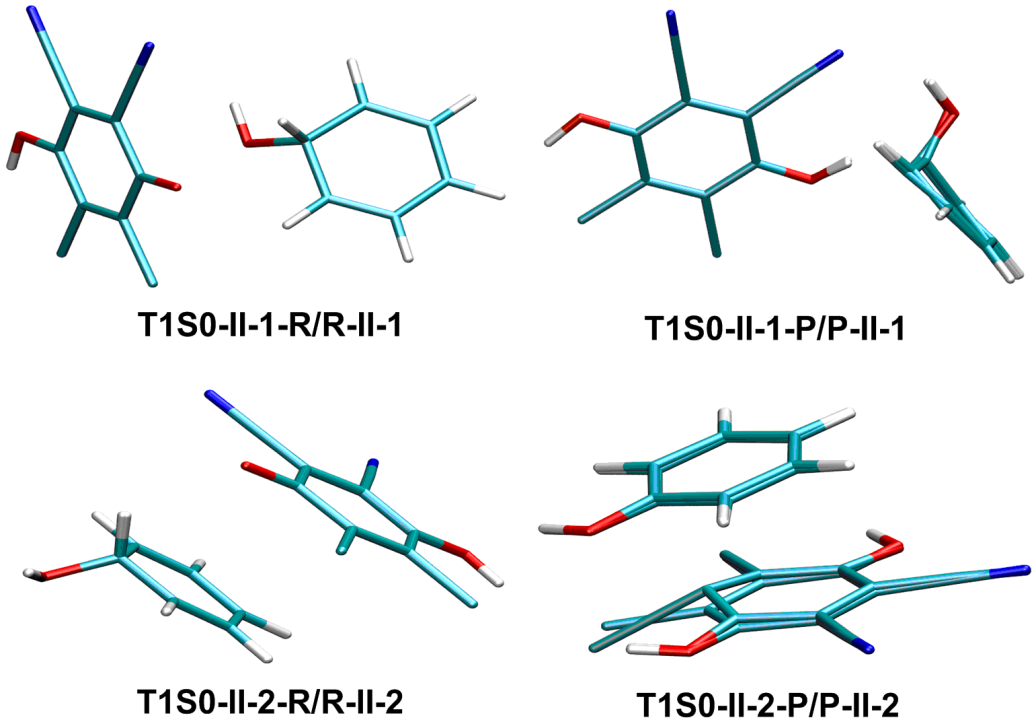


Figure 5: Spatial superposition of T_1/S_0 crossing points and their associated reactants and products in **II-1** and **II-2**.

4 T_1/S_0 Crossing Points

Table 3 lists the T_1-S_0 energy gaps computed at the optimized T_1/S_0 crossing points. Evidently, the two electronic states involved at a given crossing point are essentially degenerate (UB3LYP-D3/6-31G*/PCM results). Fig. 6 shows the corresponding structures with key geometric parameters. In all cases, the T_1/S_0 crossing points are structurally close to the associated reactants and products in **II-1** and **II-2** (see Fig. 5). Hence, these crossings are easily accessible both structurally and energetically.

5 Mulliken Population Analysis

It has been shown experimentally that the initial intermolecular triplet-state electron transfer generates DDQ anion and benzene cation radicals. [26] This is consistent with Mulliken population analysis for **R-I** which yields positive and negative charges of 0.68|**e**| for the benzene and DDQ moieties, respectively (Table 4), and with molecular orbital plots that show two SOMOs separately localized on the benzene and DDQ fragments (Fig. 4).

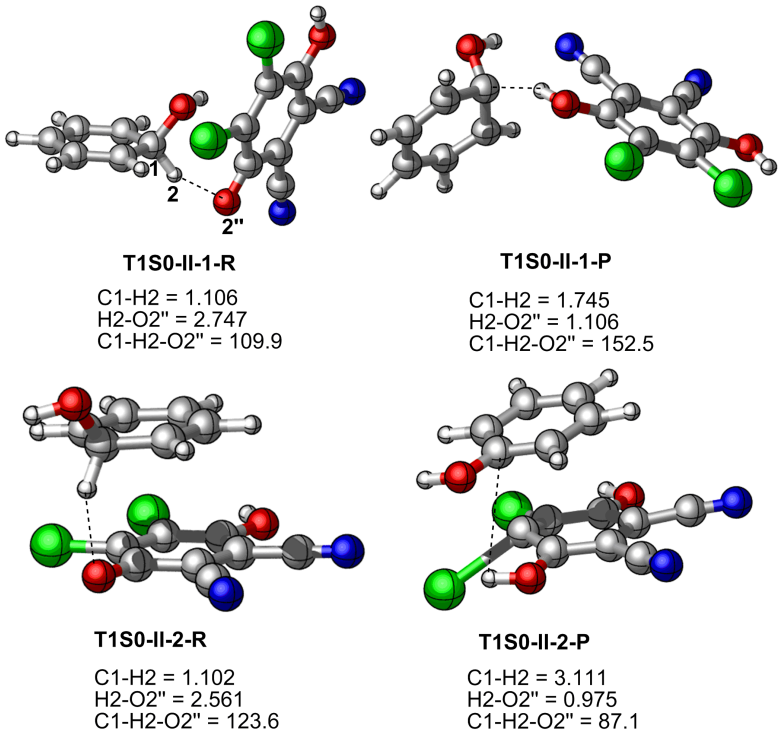


Figure 6: UB3LYP-D3/6-31G*/PCM(acetonitrile) optimized T_1/S_0 crossing points close to reactants and products in **II-1** and **II-2** (distances in Å, angles in degree).

Table 4: UB3LYP-D3/6-31G*/PCM Mulliken Charges (in |**e**|) of the Benzene-OH Moiety at the Optimized Stationary Points (Reactants, Transition States, and Products; see Fig. 2) and Crossing Points (see Fig. 4).

R-I	TS-I	P-1	R-II-1	TS-II-1
0.68	0.53	0.13	0.02	0.09
P-II-1	R-II-2	TS-II-2	P-II-2	S0-II-1-P
0.07	0.01	0.12	0.23	0.02
S0-II-2-P	T1S0-II-1-R	T1S0-II-1-P	T1S0-II-2-R	T1S0-II-2-P
0.06	0.70/0.02	0.26/0.07	0.66/0.01	0.16/0.46

The subsequent triplet-state reaction produces neutral DDQH and benzene-OH radicals [see step (2) in Fig. 1 of the main text]. This is reflected in the computed Mulliken charges for **P-I** (benzene-OH: 0.13|**e**|; Table 4).

6 Nudged Elastic Band Pathways

As discussed in the main text, we could not locate any transition states for the final proton-coupled electron transfer in the S_0 state [step (3) in Fig. 1 of the main text, orientations **II-3** and **II-4**], since all attempts converged either towards the initial triplet radical pairs or to the products $DDQH_2$ and phenol. This implies that the paths are barrierless. To verify this notion, the corresponding patways were subjected to optimization by the nudged elastic band (NEB) method.

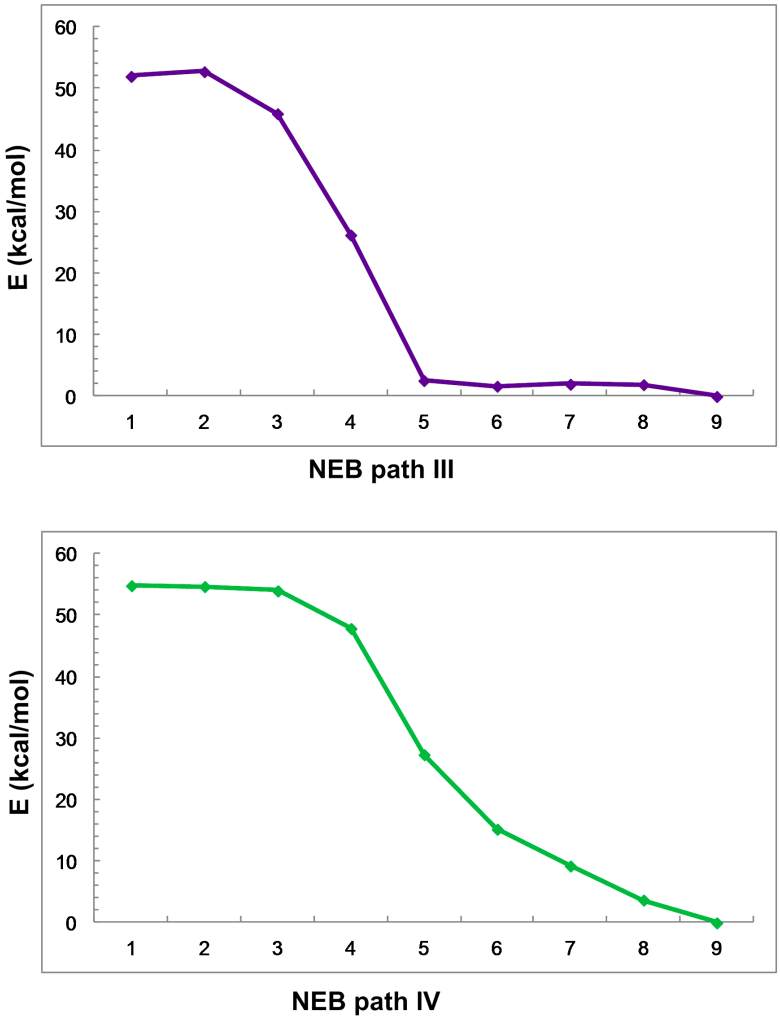


Figure 7: Ground-state nudged elastic band paths connecting **R-II-1** and **P-II-1** (top) as well as **R-II-2** and **P-II-2** (bottom). Both paths are essentially barrierless due to the zwitterionic ground-state electronic structure. See text.

Fig. 7 shows the computed NEB paths connecting **R-II-1** and **P-II-1** (top) as well as **R-II-2** and **P-II-2** (bottom), which indeed turn out to be essentially barrierless. The underlying reasons are explained in the main text. Briefly, the intersystem crossing via the T_1/S_0 crossing points in **II-3** and **II-4** causes a sudden electronic reorganization towards a zwitterionic structure, which triggers a barrierless ground-state proton transfer.

7 Solvent and Entropy Effects

As shown in Fig. 2, solvent effects on the optimized geometries are generally rather small. Exceptions are **R-I** and **TS-1**, which have much shorter C1-O1$^{'}$ distances in acetonitrile solution, and **P-II-2** with longer C1-H2 distance and a smaller C1-H2-O2$^{''}$ angle in acetonitrile solution (Fig. 2).

Solvent effects on reaction barriers, both on potential energy surfaces and on free-energy surfaces, are again small (on average below 1 kcal/mol, see Table 5). By contrast, solvents have a notable influence on reaction energies and reaction free energies. One example is the reaction free energy for step (2) in Fig. 1 of the main text, which amounts to -4.6 kcal/mol in vacuo and to 0.8 kcal/mol in acetonitrile solution. Entropy effects change the computed barriers and reaction energies by at most 2 kcal/mol and are thus less important.

Table 5: Activation (Free) Energies $\Delta H^{\ddagger}$ ($\Delta G^{\ddagger}$) and Reaction (Free) Energies ΔH_{rxn} (ΔG_{rxn}) (in kcal/mol) of the Three Elementary Reactions Considered in the Gas Phase (g; UB3LYP-D3/6-31G*) and in Acetonitrile Solution (w; UB3LYP-D3/6-31G*/PCM)

path	$\Delta G^{\ddagger}$(w)	$\Delta H^{\ddagger}$(w)	ΔG_{rxn}(w)	ΔH_{rxn}(w)		$\Delta G^{\ddagger}$(g)	$\Delta H^{\ddagger}$(g)	ΔG_{rxn}(g)	ΔH_{rxn}(g)
I	3.1	0.9	0.7	-1.1		2.2	0.1	-4.6	-6.9
II-1	18.3	16.2	17.0	16.2		18.3	15.6	14.3	12.9
II-2	18.0	15.8	-7.8	-9.3		18.2	16.4	-5.6	-6.8

8 Relative Energies, Enthalpies, and Gibbs Free Energies

In Tables 6-9 we document the computed relative energies (E), enthalpies (H) and Gibbs free energies (G) at 298 K for all species involved in steps 2 and 3 of the proposed mechanism (see Fig. 1 of the main paper).

Table 6: Relative Energies E, Enthalpies H, and Gibbs Free Energies G (in kcal/mol) at 298 K of the Stationary Points Computed at the UB3LYP-D3/6-31G* Level in the Gas Phase.

	R-I	TS-I	P-1
E	0.0	1.9	-7.1
H	0.0	0.1	-6.9
G	0.0	2.2	-4.6
	R-II-1	TS-II-1	P-II-1
E	0.0	19.4	13.3
H	0.0	15.6	12.9
G	0.0	18.3	14.3
	R-II-2	TS-II-2	P-II-2
E	-0.2	20.1	-8.2
H	-0.4	16.0	-7.2
G	-0.4	17.8	-6.0

Table 7: Relative Energies E, Enthalpies H, and Gibbs Free Energies G (in kcal/mol) of the Stationary Points Computed at the UB3LYP-D3/6-31G*/PCM Level in Acetonitrile Solution. In the Case of the Crossing Points, Two Values are Given for the Two States Involved.

	R-I	TS-I	P-1			
E	0.0	2.3	-0.8			
H	0.0	0.9	-1.1			
G	0.0	3.1	+0.7			
	R-II-1	TS-II-1	P-II-1	S0-II-1-P	T1S0-II-1-R	T1S0-II-1-P
E	0.0	20.1	16.9	-63.9	0.01/-1.0	34.5/34.3
H	0.0	16.2	16.2	-62.1		
G	0.0	18.3	17.0	-59.4		
	R-II-2	TS-II-2	P-II-2	S0-II-2-P	T1S0-II-2-R	T1S0-II-2-P
E	-1.3	19.9	-9.7	-67.3	-1.0/-1.0	5.7/5.0
H	-1.9	15.8	-9.3	-65.3		
G	+0.5	18.0	-7.8	-62.5		

Table 8: Relative Energies E, Enthalpies H, and Gibbs Free Energies G (in kcal/mol) of the R-I Complex Relative to the Separated Reactant Molecules before and after Intermolecular Electron Transfer. First Value: Gas phase (UB3LYP-D3/6-31G*); Second Value: Acetonitrile Solution (UB3LYP-D3/6-31G*/PCM).

	DDQ(neutral, T_1)+H_2O+Benzene	DDQ(radical)+H_2O+Benzene(radical)	R-I
E	0.0/0.0	69.6/2.5	-38.4/-26.6
H	0.0/0.0	69.0/1.8	-35.3/-23.5
G	0.0/0.0	68.7/1.4	-14.3/-2.0

Table 9: Relative Energies E, Enthalpies H, and Gibbs Free Energies G (in kcal/mol) of Three Binary Complexes Relative to the Separated Reactant Molecules in Acetonitrile Solution (UB3LYP-D3/6-31G*/PCM).

	DDQ(T_1)+H_2O+Benzene	DDQ(T_1)-H_2O+Benzene	DDQ(T_1)-Benzene+H_2O	DDQ(T_1)+Benzene-H_2O
E	0.0	-5.7	-15.2	-3.2
H	0.0	-4.1	-14.3	-1.8
G	0.0	3.6	-2.8	3.7

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10. Cartesian Coordinates for All Optimized Structures

In xyz format (unit: angström)

DDQ: CASSCF in vacuo

$^1\pi\pi^*$

C	1.487858400	0.169894460	0.000000000
C	0.704506340	1.350727610	0.000000000
C	-0.703825570	1.350676750	0.000000000
C	-1.487864680	0.168682160	0.000000000
C	-0.708204120	-1.118700020	0.000000000
C	0.708616580	-1.117981550	0.000000000
Cl	-1.575465190	-2.536007430	0.000000000
Cl	1.576229350	-2.534729940	0.000000000
O	-2.706665470	0.086546480	0.000000000
O	2.707208170	0.086323710	0.000000000
C	-1.430643500	2.585926940	0.000000000
C	1.430257240	2.586507480	0.000000000
N	-2.011609900	3.562414290	0.000000000
N	2.009602360	3.564001050	0.000000000

$^1n\pi^*$

C	1.459100306	0.124404792	0.000000000
C	0.712119121	1.363572226	0.000000000
C	-0.692991692	1.356832890	0.000000000
C	-1.362051332	0.158534465	0.000000000
C	-0.677273757	-1.097999361	0.000000000
C	0.694489657	-1.120017160	0.000000000
Cl	-1.641089451	-2.522656978	0.000000000
Cl	1.574840251	-2.588348139	0.000000000
O	-2.687675230	0.127268133	0.000000000
O	2.694490671	0.122865210	0.000000000
C	-1.455588509	2.578476701	0.000000000
C	1.445115074	2.596385517	0.000000000
N	-2.077981223	3.527032005	0.000000000
N	2.014496115	3.577931701	0.000000000

$^3n\pi^*$

C	1.461075575	0.124537638	0.000000000
C	0.708542624	1.364483345	0.000000000
C	-0.688509879	1.358072925	0.000000000
C	-1.361491226	0.155701396	0.000000000
C	-0.677725545	-1.100424978	0.000000000
C	0.693755563	-1.121768258	0.000000000
Cl	-1.643072443	-2.524079577	0.000000000
Cl	1.575198868	-2.588937877	0.000000000

O	-2.682872837	0.132517111	0.000000000
O	2.691858829	0.123428172	0.000000000
C	-1.453254354	2.579194150	0.000000000
C	1.442339683	2.597190305	0.000000000
N	-2.078167028	3.525945230	0.000000000
N	2.012322170	3.578422418	0.000000000

$^{3}\pi\pi^{*}$

C	1.447940910	0.137286980	0.000000000
C	0.754609850	1.379553460	0.000000000
C	-0.747334720	1.376818200	0.000000000
C	-1.468012410	0.120719450	0.000000000
C	-0.667724040	-1.149663500	0.000000000
C	0.651864740	-1.144212360	0.000000000
Cl	-1.604130840	-2.588683820	0.000000000
Cl	1.600268810	-2.572976280	0.000000000
O	-2.684560810	0.117063690	0.000000000
O	2.706731640	0.120256560	0.000000000
C	-1.471491180	2.602643250	0.000000000
C	1.477277910	2.609494260	0.000000000
N	-2.024850740	3.594527510	0.000000000
N	2.029410900	3.601454590	0.000000000

S0

C	1.442267260	0.104825440	0.000000000
C	0.665193490	1.393516720	0.000000000
C	-0.665430080	1.393295900	0.000000000
C	-1.442049160	0.104316410	0.000000000
C	-0.665481400	-1.147037390	0.000000000
C	0.666147960	-1.146809690	0.000000000
Cl	-1.604338250	-2.585338290	0.000000000
Cl	1.605484290	-2.584822980	0.000000000
O	-2.645582840	0.153748830	0.000000000
O	2.645784290	0.154709760	0.000000000
C	-1.434778580	2.609224880	0.000000000
C	1.434093180	2.609734650	0.000000000
N	-2.034140280	3.572008160	0.000000000
N	2.032830100	3.572909600	0.000000000

$^{1}n\pi^{*}/^{3}\pi\pi^{*}$

C	1.398350750	0.149913240	0.000000000
C	0.729686360	1.358542740	0.000000000
C	-0.726764720	1.364613040	0.000000000
C	-1.453694540	0.124067380	0.000000000
C	-0.675949140	-1.135824760	0.000000000
C	0.659949560	-1.119840800	0.000000000
Cl	-1.590774860	-2.582564070	0.000000000

Cl	1.608285490	-2.549529600	0.000000000
O	-2.686729430	0.122513980	0.000000000
O	2.706609230	0.129123160	0.000000000
C	-1.455726290	2.595509250	0.000000000
C	1.467461280	2.592318860	0.000000000
N	-2.017030240	3.581939220	0.000000000
N	2.036326570	3.573500360	0.000000000

UB3LYP-D3/6-31G* level in vacuo

R-I

C	-4.123865000	-0.750879000	1.133637000
C	-3.304532000	0.198903000	1.704035000
C	-2.929354000	1.328925000	0.949300000
C	-3.434279000	1.529994000	-0.365354000
C	-4.265386000	0.588610000	-0.931698000
C	-4.584904000	-0.579812000	-0.205481000
H	-4.415439000	-1.639926000	1.684559000
H	-2.927751000	0.074850000	2.714012000
H	-2.273736000	2.079684000	1.374003000
H	-3.126486000	2.417869000	-0.906064000
H	-4.644419000	0.712348000	-1.940477000
H	-5.253615000	-1.315217000	-0.636840000
C	0.210590000	0.021249000	-0.166405000
C	0.840182000	1.317084000	-0.150368000
C	2.225199000	1.464787000	-0.043149000
C	3.117183000	0.313519000	0.050576000
C	2.453024000	-1.006412000	0.028710000
C	1.089136000	-1.134582000	-0.071525000
Cl	3.497739000	-2.375224000	0.161080000
Cl	0.319909000	-2.702583000	-0.070655000
O	-1.053741000	-0.106415000	-0.257387000
O	4.346457000	0.434318000	0.145482000
C	2.822052000	2.757386000	-0.028607000
C	-0.014979000	2.452551000	-0.259540000
N	3.287890000	3.824033000	-0.014714000
N	-0.743783000	3.357071000	-0.339568000
O	-2.789015000	-1.983706000	-1.116316000
H	-2.605492000	-2.717609000	-0.506433000
H	-2.091852000	-1.318507000	-0.879048000

TS-I

C	-2.164964000	-0.950279000	1.693264000
C	-1.221517000	-0.008848000	2.028848000
C	-1.392795000	1.341591000	1.646026000
C	-2.536130000	1.744991000	0.918625000
C	-3.496256000	0.826309000	0.572735000

C	-3.324924000	-0.577372000	0.903408000
H	-2.054044000	-1.984893000	2.003412000
H	-0.343073000	-0.296840000	2.597881000
H	-0.634779000	2.074046000	1.903642000
H	-2.639891000	2.782990000	0.622225000
H	-4.376403000	1.116960000	0.009378000
H	-4.232507000	-1.156444000	1.056326000
C	-0.108072000	0.014731000	-1.142540000
C	0.535899000	1.279995000	-0.905495000
C	1.748510000	1.374421000	-0.222238000
C	2.451410000	0.191620000	0.269859000
C	1.796761000	-1.099588000	-0.023270000
C	0.598453000	-1.169791000	-0.689611000
Cl	2.625718000	-2.508570000	0.539896000
Cl	-0.155039000	-2.716342000	-1.030070000
O	-1.256829000	-0.015357000	-1.697987000
O	3.513470000	0.267018000	0.902712000
C	2.322771000	2.642976000	0.077108000
C	-0.184689000	2.451082000	-1.292002000
N	2.764472000	3.688801000	0.333907000
N	-0.797149000	3.405019000	-1.553470000
O	-3.088927000	-1.339595000	-0.767872000
H	-2.735124000	-2.234156000	-0.598563000
H	-2.245440000	-0.802450000	-1.227529000

P-I

C	-2.070340000	-0.914875000	1.592549000
C	-1.287885000	0.109735000	2.048492000
C	-1.582599000	1.458581000	1.723169000
C	-2.705156000	1.759964000	0.910003000
C	-3.520740000	0.772702000	0.434076000
C	-3.269325000	-0.674106000	0.723293000
H	-1.840950000	-1.946259000	1.850202000
H	-0.420459000	-0.110122000	2.665965000
H	-0.941950000	2.257443000	2.081903000
H	-2.903781000	2.794702000	0.647342000
H	-4.365554000	0.998514000	-0.209085000
H	-4.166023000	-1.129466000	1.176505000
C	-0.067528000	0.030676000	-1.094415000
C	0.572037000	1.282583000	-0.865770000
C	1.789907000	1.350072000	-0.194165000
C	2.460668000	0.144140000	0.297418000
C	1.781806000	-1.131603000	0.004955000
C	0.579098000	-1.172325000	-0.668902000
Cl	2.577555000	-2.558677000	0.547865000
Cl	-0.186377000	-2.691850000	-1.061616000
O	-1.229628000	0.061518000	-1.717732000

O	3.528331000	0.197189000	0.921223000
C	2.408821000	2.601001000	0.084108000
C	-0.113203000	2.469656000	-1.273736000
N	2.900772000	3.629850000	0.315383000
N	-0.672677000	3.441460000	-1.579162000
O	-3.124776000	-1.344393000	-0.592693000
H	-2.972007000	-2.291747000	-0.434320000
H	-1.880738000	-0.644977000	-1.411135000

R-II-1

C	2.689580000	-1.071128000	-0.109689000
C	3.742872000	-1.738465000	-0.666434000
C	4.882195000	-1.045188000	-1.150573000
C	4.946380000	0.367227000	-1.042899000
C	3.921535000	1.078249000	-0.484784000
C	2.662659000	0.422946000	0.007200000
H	1.824568000	-1.604943000	0.269676000
H	3.714780000	-2.823354000	-0.737154000
H	5.705462000	-1.594732000	-1.596387000
H	5.830743000	0.887299000	-1.403751000
H	3.982718000	2.160672000	-0.388048000
H	2.484916000	0.697319000	1.062405000
C	-2.516694000	0.375430000	-0.638405000
C	-1.833815000	1.490200000	-0.088533000
C	-0.831081000	1.293387000	0.856822000
C	-0.464552000	-0.043984000	1.329224000
C	-1.196328000	-1.165102000	0.715397000
C	-2.179805000	-0.945129000	-0.226261000
Cl	-0.763854000	-2.745804000	1.233010000
Cl	-3.067151000	-2.256343000	-0.968120000
O	-3.463701000	0.633320000	-1.542396000
O	0.413295000	-0.218844000	2.182729000
C	-0.077365000	2.385932000	1.369517000
C	-2.173426000	2.799951000	-0.549212000
N	0.566700000	3.273620000	1.758071000
N	-2.440947000	3.868648000	-0.919335000
O	1.498948000	0.889236000	-0.752066000
H	1.539269000	1.861071000	-0.747598000
H	-3.856906000	-0.198354000	-1.867770000

TS-II-1

C	2.368462000	-0.761776000	-0.902070000
C	3.476990000	-1.406950000	-1.360895000
C	4.783679000	-0.905749000	-1.090138000
C	4.953701000	0.258795000	-0.287534000
C	3.881478000	0.939107000	0.215395000
C	2.495465000	0.544958000	-0.188612000

H	1.367507000	-1.140584000	-1.080945000
H	3.368609000	-2.333320000	-1.920043000
H	5.653543000	-1.436983000	-1.462632000
H	5.961366000	0.589515000	-0.046216000
H	4.002348000	1.798096000	0.870593000
H	1.708625000	0.391304000	0.978589000
C	-2.695151000	0.014278000	-0.443352000
C	-2.149200000	1.269741000	-0.120553000
C	-0.957329000	1.343092000	0.628722000
C	-0.297328000	0.176691000	1.083517000
C	-0.869940000	-1.081169000	0.756609000
C	-2.045656000	-1.154408000	0.007788000
Cl	-0.043288000	-2.509246000	1.281079000
Cl	-2.754661000	-2.691860000	-0.432904000
O	-3.819649000	-0.002760000	-1.182500000
O	0.844479000	0.255666000	1.750024000
C	-0.334866000	2.600020000	0.902617000
C	-2.801118000	2.453078000	-0.583653000
N	0.222517000	3.601138000	1.102119000
N	-3.325257000	3.421175000	-0.957176000
O	1.785889000	1.519684000	-0.894182000
H	1.967001000	2.398318000	-0.508516000
H	-4.085579000	-0.922680000	-1.358189000

P-II-1

C	4.021683000	-1.109363000	-0.634655000
C	4.885688000	-1.544811000	0.321617000
C	5.027629000	-0.846514000	1.563321000
C	4.212156000	0.288935000	1.845226000
C	3.313766000	0.759494000	0.932582000
C	3.296389000	0.181407000	-0.451242000
H	3.874640000	-1.650916000	-1.564418000
H	5.452604000	-2.459716000	0.165021000
H	5.719121000	-1.214845000	2.314045000
H	4.279639000	0.755602000	2.825854000
H	2.656250000	1.593037000	1.160697000
H	1.509254000	-0.314237000	-0.806348000
C	-2.990113000	0.682185000	0.291031000
C	-1.927303000	1.554198000	0.034157000
C	-0.670059000	1.044480000	-0.384268000
C	-0.451995000	-0.340966000	-0.525946000
C	-1.539927000	-1.211434000	-0.265839000
C	-2.778878000	-0.704006000	0.128636000
Cl	-1.283839000	-2.914550000	-0.447351000
Cl	-4.129149000	-1.763952000	0.452700000
O	-4.164712000	1.217803000	0.680594000
O	0.694887000	-0.898201000	-0.919911000

C	0.391540000	1.947803000	-0.679406000
C	-2.119369000	2.960153000	0.189404000
N	1.280645000	2.656527000	-0.925788000
N	-2.257421000	4.107919000	0.314314000
O	3.594251000	1.064310000	-1.466360000
H	3.162568000	1.922414000	-1.270791000
H	-4.818500000	0.511406000	0.823031000

R-II-2

C	-1.554528000	-1.812724000	-1.052460000
C	-0.742514000	-1.091708000	-1.883459000
C	-1.031009000	0.263134000	-2.194878000
C	-2.193743000	0.877826000	-1.660961000
C	-3.039365000	0.192878000	-0.833992000
C	-2.792487000	-1.229883000	-0.423703000
H	-1.328969000	-2.850042000	-0.817067000
H	0.134699000	-1.562064000	-2.323285000
H	-0.376336000	0.822270000	-2.857045000
H	-2.411448000	1.911598000	-1.917582000
H	-3.936764000	0.655424000	-0.435501000
H	-2.674520000	-1.256559000	0.676635000
C	1.619661000	1.343597000	-0.148271000
C	0.418456000	1.725696000	0.502344000
C	-0.278190000	0.803933000	1.278027000
C	0.182238000	-0.578811000	1.425454000
C	1.435378000	-0.921502000	0.730487000
C	2.115625000	0.017349000	-0.016339000
Cl	1.973093000	-2.545463000	0.866687000
Cl	3.586208000	-0.368550000	-0.879816000
O	2.225281000	2.274196000	-0.888244000
O	-0.456536000	-1.413259000	2.079698000
C	-1.489802000	1.157726000	1.932587000
C	-0.075825000	3.051309000	0.302662000
N	-2.480813000	1.443332000	2.471346000
N	-0.488380000	4.123906000	0.130534000
O	-3.971199000	-1.996592000	-0.764726000
H	-3.989152000	-2.771585000	-0.180948000
H	3.034976000	1.910834000	-1.293993000

TS-II-2

C	2.201029000	-1.402941000	1.044936000
C	1.719286000	-0.776743000	2.153939000
C	1.914852000	0.622844000	2.361072000
C	2.652901000	1.389319000	1.411630000
C	3.164700000	0.820391000	0.285088000
C	2.977300000	-0.639626000	0.015126000
H	2.004893000	-2.455340000	0.856112000

H	1.158382000	-1.346450000	2.891084000
H	1.497839000	1.102591000	3.239974000
H	2.783956000	2.454998000	1.577900000
H	3.690031000	1.400497000	-0.465102000
H	2.062281000	-0.620270000	-1.059608000
C	-2.370701000	0.585211000	0.205916000
C	-1.473447000	1.575112000	-0.229940000
C	-0.281545000	1.206673000	-0.889847000
C	0.039711000	-0.152620000	-1.126555000
C	-0.875398000	-1.137618000	-0.664616000
C	-2.056746000	-0.772125000	-0.020597000
Cl	-0.470953000	-2.803977000	-0.920744000
Cl	-3.199630000	-1.969290000	0.549750000
O	-3.493040000	0.992037000	0.829555000
O	1.144336000	-0.490184000	-1.771227000
C	0.641655000	2.201692000	-1.331231000
C	-1.780069000	2.948207000	0.016998000
N	1.410132000	3.003917000	-1.674776000
N	-2.019232000	4.067129000	0.222917000
O	4.169380000	-1.217894000	-0.396583000
H	4.094894000	-2.186189000	-0.325293000
H	-4.035217000	0.220043000	1.069366000

P-II-2

C	-3.107920000	0.134685000	0.408413000
C	-3.022318000	0.794137000	1.635028000
C	-2.388296000	0.189023000	2.721208000
C	-1.838916000	-1.088242000	2.577455000
C	-1.918045000	-1.760792000	1.359493000
C	-2.552070000	-1.139042000	0.281957000
H	-3.578839000	0.613820000	-0.446302000
H	-3.444028000	1.790018000	1.732021000
H	-2.319147000	0.709264000	3.671614000
H	-1.340547000	-1.565399000	3.416240000
H	-1.484558000	-2.746614000	1.226366000
H	-0.866359000	-2.133204000	-1.289992000
C	1.551257000	1.450496000	0.162340000
C	2.420705000	0.266048000	0.209375000
C	1.890413000	-0.991627000	-0.209813000
C	0.628998000	-1.042060000	-0.799661000
C	-0.123961000	0.197688000	-1.072958000
C	0.319801000	1.390193000	-0.443044000
Cl	-0.862462000	0.291536000	-2.714690000
Cl	-0.714903000	2.821446000	-0.410642000
O	2.046377000	2.526208000	0.780809000
O	0.107836000	-2.216110000	-1.115228000
C	2.590347000	-2.206524000	0.055531000

C	3.717846000	0.392155000	0.731698000
N	3.162735000	-3.197441000	0.263805000
N	4.796603000	0.494815000	1.173087000
O	-2.571200000	-1.833192000	-0.920595000
H	-2.945952000	-1.264478000	-1.614037000
H	1.408112000	3.262218000	0.714475000

UB3LYP-D3/6-31G*/PCM level in acetonitrile solution

R-I

C	-2.711576000	-0.804193000	1.548934000
C	-1.521496000	-0.259713000	1.977508000
C	-1.263722000	1.114991000	1.767893000
C	-2.202470000	1.945549000	1.111278000
C	-3.396979000	1.417242000	0.678999000
C	-3.675833000	0.026858000	0.888956000
H	-2.940459000	-1.851560000	1.712620000
H	-0.782507000	-0.873486000	2.480634000
H	-0.323573000	1.537417000	2.107424000
H	-1.971480000	2.993094000	0.953139000
H	-4.136253000	2.031017000	0.176912000
H	-4.692852000	-0.328723000	0.777212000
C	-0.009449000	0.192831000	-1.108725000
C	0.883146000	1.283449000	-0.786746000
C	2.089154000	1.082191000	-0.112278000
C	2.531432000	-0.240995000	0.304282000
C	1.616278000	-1.347124000	-0.039575000
C	0.436607000	-1.141751000	-0.702360000
Cl	2.131885000	-2.927828000	0.457127000
Cl	-0.629063000	-2.460976000	-1.105487000
O	-1.108538000	0.408194000	-1.682885000
O	3.601883000	-0.423760000	0.909320000
C	2.939427000	2.175960000	0.214314000
C	0.448652000	2.592509000	-1.144363000
N	3.628758000	3.076146000	0.480304000
N	0.090062000	3.666134000	-1.417031000
O	-3.467721000	-0.655198000	-1.191741000
H	-3.376217000	-1.618945000	-1.076180000
H	-2.540367000	-0.335834000	-1.418815000

TS-I

C	-2.400251000	-0.950232000	1.477981000
C	-1.435694000	-0.126845000	1.999151000
C	-1.488082000	1.273348000	1.792331000
C	-2.554998000	1.847724000	1.058432000
C	-3.539704000	1.062858000	0.519279000
C	-3.487302000	-0.403201000	0.647759000

H	-2.382632000	-2.020371000	1.656802000
H	-0.628163000	-0.548661000	2.589415000
H	-0.709580000	1.908409000	2.201183000
H	-2.592981000	2.924821000	0.930715000
H	-4.365687000	1.490501000	-0.038424000
H	-4.458131000	-0.875898000	0.802540000
C	-0.058641000	0.106050000	-1.066274000
C	0.709365000	1.294429000	-0.800178000
C	1.941483000	1.245165000	-0.150058000
C	2.532964000	-0.012825000	0.288493000
C	1.742422000	-1.220155000	-0.013450000
C	0.531582000	-1.159305000	-0.652954000
Cl	2.442953000	-2.722484000	0.490876000
Cl	-0.377853000	-2.598670000	-1.026022000
O	-1.192865000	0.200311000	-1.631396000
O	3.627497000	-0.059552000	0.874887000
C	2.672134000	2.433649000	0.132589000
C	0.127277000	2.540047000	-1.179430000
N	3.263803000	3.409574000	0.362953000
N	-0.342802000	3.563116000	-1.473420000
O	-3.264895000	-0.934533000	-0.919805000
H	-3.204893000	-1.911183000	-0.916667000
H	-2.324875000	-0.550884000	-1.266304000

P-I

C	-2.201315000	-0.919755000	1.473111000
C	-1.429945000	0.095791000	1.969182000
C	-1.743927000	1.453212000	1.701270000
C	-2.882466000	1.773704000	0.917227000
C	-3.683655000	0.796062000	0.396724000
C	-3.391367000	-0.657838000	0.598099000
H	-1.961307000	-1.957668000	1.685715000
H	-0.558213000	-0.137487000	2.574877000
H	-1.113023000	2.244088000	2.093021000
H	-3.114624000	2.817602000	0.725498000
H	-4.546978000	1.039175000	-0.214975000
H	-4.279737000	-1.175803000	0.989508000
C	-0.033589000	0.065664000	-1.011418000
C	0.655297000	1.293030000	-0.785947000
C	1.894601000	1.313098000	-0.154519000
C	2.539991000	0.083852000	0.302826000
C	1.809023000	-1.162874000	0.023520000
C	0.586807000	-1.164544000	-0.612794000
Cl	2.578280000	-2.620748000	0.526437000
Cl	-0.233960000	-2.647869000	-0.996612000
O	-1.198416000	0.147722000	-1.610404000
O	3.636129000	0.100096000	0.883280000

C	2.576083000	2.536605000	0.097661000
C	0.012359000	2.506321000	-1.181660000
N	3.130481000	3.538736000	0.303770000
N	-0.495397000	3.504749000	-1.492069000
O	-3.182763000	-1.231547000	-0.760204000
H	-3.128883000	-2.200374000	-0.679214000
H	-1.883256000	-0.571552000	-1.364418000

R-II-1

C	2.928779000	-0.647520000	0.310597000
C	4.155262000	-1.139152000	-0.038163000
C	5.008858000	-0.432793000	-0.925961000
C	4.594627000	0.815922000	-1.457997000
C	3.380463000	1.353728000	-1.132280000
C	2.406088000	0.650271000	-0.230248000
H	2.279314000	-1.183432000	0.994792000
H	4.490043000	-2.088609000	0.373035000
H	5.976138000	-0.845228000	-1.195084000
H	5.259462000	1.351835000	-2.131309000
H	3.070883000	2.315456000	-1.535663000
H	2.140901000	1.308996000	0.617350000
C	-2.444184000	0.074505000	-0.690530000
C	-2.011259000	1.290317000	-0.100854000
C	-1.052031000	1.276591000	0.908737000
C	-0.467612000	0.027052000	1.396250000
C	-0.953275000	-1.204628000	0.751333000
C	-1.898374000	-1.168663000	-0.249264000
Cl	-0.271416000	-2.681151000	1.306078000
Cl	-2.471173000	-2.610590000	-1.038017000
O	-3.360082000	0.171936000	-1.646099000
O	0.386588000	0.017307000	2.293133000
C	-0.578941000	2.481199000	1.497079000
C	-2.567933000	2.518652000	-0.572914000
N	-0.180851000	3.466000000	1.972755000
N	-3.009493000	3.526492000	-0.947200000
O	1.161321000	0.348251000	-0.939643000
H	0.839925000	1.186449000	-1.314459000
H	-3.605653000	-0.706145000	-1.998399000

TS-II-1

C	2.646614000	-0.866034000	-0.955315000
C	3.843734000	-1.452057000	-1.245539000
C	5.073266000	-0.875437000	-0.808805000
C	5.069881000	0.311453000	-0.017435000
C	3.904268000	0.939904000	0.316351000
C	2.608914000	0.456148000	-0.257254000
H	1.700618000	-1.305139000	-1.257480000

H	3.865213000	-2.389190000	-1.797002000
H	6.013137000	-1.363754000	-1.045197000
H	6.015426000	0.702174000	0.351782000
H	3.886030000	1.816111000	0.959543000
H	1.728543000	0.262406000	0.817271000
C	-2.825414000	0.131602000	-0.378758000
C	-2.155908000	1.332345000	-0.090186000
C	-0.906315000	1.307286000	0.566183000
C	-0.302592000	0.090169000	0.951420000
C	-0.982726000	-1.115182000	0.628027000
C	-2.222929000	-1.092731000	-0.009427000
Cl	-0.213546000	-2.610249000	1.047112000
Cl	-3.079102000	-2.561269000	-0.395168000
O	-4.011825000	0.221333000	-1.000194000
O	0.862125000	0.073140000	1.583178000
C	-0.205143000	2.518546000	0.846149000
C	-2.752906000	2.570775000	-0.471161000
N	0.384445000	3.498009000	1.062619000
N	-3.227303000	3.587755000	-0.776164000
O	1.924531000	1.384536000	-1.044792000
H	2.095552000	2.284691000	-0.705972000
H	-4.384600000	-0.664638000	-1.162215000

P-II-1

C	4.035817000	-1.061563000	-0.670655000
C	4.886791000	-1.532047000	0.282349000
C	4.991017000	-0.894375000	1.560629000
C	4.147194000	0.209687000	1.883673000
C	3.262095000	0.713251000	0.974339000
C	3.297605000	0.214020000	-0.438871000
H	3.913564000	-1.562449000	-1.626716000
H	5.468898000	-2.431288000	0.094740000
H	5.669822000	-1.292003000	2.307658000
H	4.179196000	0.620140000	2.890556000
H	2.576074000	1.514324000	1.232903000
H	1.509503000	-0.286344000	-0.840820000
C	-2.986512000	0.667340000	0.295611000
C	-1.928729000	1.544166000	0.036123000
C	-0.668440000	1.049541000	-0.393107000
C	-0.445430000	-0.331059000	-0.544446000
C	-1.526930000	-1.208196000	-0.281635000
C	-2.768235000	-0.718484000	0.124725000
Cl	-1.257797000	-2.910390000	-0.477102000
Cl	-4.102535000	-1.789599000	0.449417000
O	-4.156634000	1.199713000	0.692659000
O	0.704355000	-0.880203000	-0.950762000
C	0.379933000	1.968368000	-0.683636000

C	-2.132534000	2.946486000	0.198795000
N	1.246385000	2.707675000	-0.922620000
N	-2.284818000	4.092311000	0.328645000
O	3.632006000	1.159172000	-1.389775000
H	3.196217000	2.004477000	-1.154582000
H	-4.818272000	0.500798000	0.844379000

R-II-2

C	-2.048559000	-1.731755000	-0.851428000
C	-1.063967000	-1.314962000	-1.704605000
C	-0.971056000	0.042982000	-2.107767000
C	-1.924324000	0.984659000	-1.636445000
C	-2.931052000	0.612571000	-0.789596000
C	-3.090578000	-0.796624000	-0.298431000
H	-2.111217000	-2.771664000	-0.540395000
H	-0.335105000	-2.029301000	-2.080021000
H	-0.179416000	0.359916000	-2.779328000
H	-1.844258000	2.021158000	-1.955503000
H	-3.662477000	1.333450000	-0.436085000
H	-3.009444000	-0.791662000	0.804261000
C	2.021536000	0.866214000	-0.297881000
C	1.029548000	1.726233000	0.242403000
C	0.040400000	1.217186000	1.078092000
C	-0.011629000	-0.200436000	1.428008000
C	1.038989000	-1.048662000	0.843840000
C	2.011118000	-0.525168000	0.018976000
Cl	0.974582000	-2.720759000	1.228551000
Cl	3.246881000	-1.514286000	-0.701005000
O	2.917244000	1.426502000	-1.099294000
O	-0.899489000	-0.655330000	2.165834000
C	-0.975063000	2.054491000	1.618024000
C	1.050127000	3.108587000	-0.116389000
N	-1.803150000	2.740242000	2.062317000
N	1.047647000	4.234452000	-0.404608000
O	-4.433009000	-1.231381000	-0.643837000
H	-4.627429000	-2.010182000	-0.096183000
H	3.562087000	0.770973000	-1.431419000

TS-II-2

C	2.113217000	-1.318549000	1.149638000
C	1.455057000	-0.586135000	2.087457000
C	1.613455000	0.835410000	2.172082000
C	2.547307000	1.498460000	1.319330000
C	3.229042000	0.821608000	0.354978000
C	2.996684000	-0.643678000	0.146025000
H	1.978255000	-2.392823000	1.065600000
H	0.791980000	-1.084558000	2.789454000

H	1.048358000	1.400179000	2.904841000
H	2.699212000	2.567973000	1.433791000
H	3.920863000	1.313768000	-0.319956000
H	2.126251000	-0.621991000	-0.974577000
C	-2.350074000	0.499620000	0.197669000
C	-1.491337000	1.524064000	-0.226981000
C	-0.270638000	1.211841000	-0.869630000
C	0.110320000	-0.128730000	-1.109290000
C	-0.779221000	-1.152876000	-0.674817000
C	-1.979180000	-0.845653000	-0.039528000
Cl	-0.309069000	-2.796427000	-0.957818000
Cl	-3.074666000	-2.090829000	0.501936000
O	-3.489849000	0.860237000	0.810965000
O	1.244836000	-0.412976000	-1.727975000
C	0.591457000	2.253500000	-1.322419000
C	-1.860336000	2.881564000	0.010053000
N	1.285417000	3.110652000	-1.692493000
N	-2.147804000	3.992670000	0.199455000
O	4.169999000	-1.290384000	-0.186160000
H	4.050581000	-2.254207000	-0.099511000
H	-4.009694000	0.074066000	1.059584000

P-II-2

C	-1.813406000	-0.420466000	1.897491000
C	-1.041662000	0.564220000	2.500388000
C	0.335984000	0.371466000	2.697593000
C	0.930861000	-0.834246000	2.309021000
C	0.175816000	-1.824678000	1.691861000
C	-1.197407000	-1.609733000	1.467929000
H	-2.874017000	-0.265042000	1.721561000
H	-1.508855000	1.494915000	2.806462000
H	0.934029000	1.153012000	3.154829000
H	1.994447000	-0.989610000	2.459928000
H	0.622594000	-2.753051000	1.352984000
H	-1.091050000	-2.343264000	-1.669022000
C	0.720038000	1.690475000	-0.380534000
C	1.800485000	0.720131000	-0.519887000
C	1.477960000	-0.604562000	-0.987903000
C	0.123433000	-0.924071000	-1.266488000
C	-0.908097000	0.053171000	-1.155607000
C	-0.590457000	1.366634000	-0.711080000
Cl	-2.522750000	-0.387036000	-1.621527000
Cl	-1.836203000	2.567744000	-0.490037000
O	1.099270000	2.883830000	0.068091000
O	-0.129122000	-2.174197000	-1.629873000
C	2.452024000	-1.617408000	-1.060123000
C	3.098249000	1.082546000	-0.152786000

N	3.278230000	-2.444366000	-1.115059000
N	4.196877000	1.364450000	0.152129000
O	-1.870909000	-2.587957000	0.807019000
H	-2.809789000	-2.348352000	0.721266000
H	0.332252000	3.484493000	0.147965000

T1S0-II-1-R

C	2.934275000	-0.644236000	0.313217000
C	4.164055000	-1.130196000	-0.029811000
C	5.016494000	-0.424251000	-0.919693000
C	4.594660000	0.818467000	-1.460386000
C	3.376733000	1.350985000	-1.141355000
C	2.404992000	0.647265000	-0.236378000
H	2.285720000	-1.180091000	0.998426000
H	4.503879000	-2.075436000	0.387976000
H	5.986432000	-0.831960000	-1.183593000
H	5.257967000	1.354340000	-2.135932000
H	3.061578000	2.307830000	-1.551858000
H	2.135026000	1.309877000	0.606995000
C	-2.449845000	0.072830000	-0.687558000
C	-2.014030000	1.290273000	-0.098701000
C	-1.053272000	1.277439000	0.906914000
C	-0.466426000	0.027917000	1.394814000
C	-0.952188000	-1.204554000	0.750557000
C	-1.899710000	-1.169937000	-0.247551000
Cl	-0.266500000	-2.679213000	1.302850000
Cl	-2.471561000	-2.611449000	-1.035695000
O	-3.368264000	0.169560000	-1.637310000
O	0.387984000	0.019871000	2.289980000
C	-0.578555000	2.482562000	1.494078000
C	-2.573527000	2.517686000	-0.570327000
N	-0.180134000	3.467061000	1.968652000
N	-3.016787000	3.524807000	-0.943142000
O	1.161959000	0.334040000	-0.944919000
H	0.835097000	1.168308000	-1.322993000
H	-3.616574000	-0.709037000	-1.988746000

T1S0-II-1-P

C	3.986126000	-1.131482000	-0.690957000
C	4.929464000	-1.471352000	0.207008000
C	5.004140000	-0.866644000	1.572928000
C	4.198617000	0.270920000	1.828066000
C	3.122952000	0.670151000	1.014158000
C	3.147551000	0.183588000	-0.529931000
H	3.881877000	-1.670204000	-1.622078000
H	5.510069000	-2.415448000	0.062324000
H	5.674640000	-1.289667000	2.309500000

H	4.204379000	0.660002000	2.875985000
H	2.518386000	1.520350000	1.304367000
H	1.497192000	-0.240049000	-0.904969000
C	-2.986175000	0.666289000	0.295485000
C	-1.931021000	1.543777000	0.034413000
C	-0.667570000	1.048827000	-0.395629000
C	-0.441483000	-0.328876000	-0.536635000
C	-1.521540000	-1.205703000	-0.285978000
C	-2.764050000	-0.718319000	0.122655000
Cl	-1.255372000	-2.911099000	-0.478787000
Cl	-4.100337000	-1.791074000	0.450041000
O	-4.155717000	1.199311000	0.694664000
O	0.713034000	-0.886229000	-0.917894000
C	0.374081000	1.978386000	-0.686851000
C	-2.132837000	2.945897000	0.198263000
N	1.250563000	2.697272000	-0.923222000
N	-2.285723000	4.091093000	0.329017000
O	3.785531000	1.153811000	-1.230838000
H	3.274768000	2.007614000	-1.113459000
H	-4.817436000	0.500573000	0.847438000

T1S0-II-2-R

C	-2.055813000	-1.728825000	-0.839494000
C	-1.074263000	-1.317857000	-1.701126000
C	-0.969202000	0.036547000	-2.112078000
C	-1.925960000	0.976408000	-1.640710000
C	-2.931080000	0.611499000	-0.788297000
C	-3.104107000	-0.795510000	-0.289207000
H	-2.111984000	-2.768457000	-0.528606000
H	-0.349874000	-2.038641000	-2.075944000
H	-0.166789000	0.352559000	-2.771357000
H	-1.846738000	2.012957000	-1.963012000
H	-3.653085000	1.342470000	-0.438298000
H	-3.064024000	-0.798423000	0.812207000
C	2.037384000	0.866218000	-0.284708000
C	1.045996000	1.736528000	0.253196000
C	0.050989000	1.228204000	1.071806000
C	0.002790000	-0.194997000	1.419168000
C	1.053315000	-1.053454000	0.842877000
C	2.030146000	-0.530394000	0.025758000
Cl	0.966665000	-2.720631000	1.222696000
Cl	3.253644000	-1.521218000	-0.706935000
O	2.918615000	1.424819000	-1.093258000
O	-0.886783000	-0.643485000	2.152153000
C	-0.974207000	2.057921000	1.608604000
C	1.066828000	3.116464000	-0.115397000
N	-1.801975000	2.740631000	2.056584000

N	1.052066000	4.240427000	-0.411053000
O	-4.449402000	-1.232420000	-0.655598000
H	-4.640157000	-2.009780000	-0.104255000
H	3.559869000	0.769056000	-1.432474000

T1S0-II-2-P

C	-1.797583400	-0.358024000	1.802117200
C	-1.037055600	0.606407800	2.449206200
C	0.335827200	0.405986700	2.632752500
C	0.950898000	-0.798276800	2.230027500
C	0.216781700	-1.779591400	1.600115900
C	-1.176089700	-1.563153200	1.384954700
H	-2.860654100	-0.234585600	1.658258200
H	-1.516681400	1.517432800	2.802152600
H	0.929077900	1.163719500	3.125681400
H	1.999841400	-0.969356200	2.456797500
H	0.639677500	-2.744179800	1.326773900
H	-1.133974900	-2.230313200	-1.653664800
C	0.722207200	1.649017000	-0.309768800
C	1.766729700	0.678614800	-0.411141800
C	1.474558300	-0.628931700	-0.874379200
C	0.104758600	-0.954402800	-1.055429700
C	-0.891972200	-0.061451000	-0.695290000
C	-0.605499800	1.271195000	-0.527365700
Cl	-2.772232300	-0.477689100	-2.178770300
Cl	-1.850677700	2.535204400	-0.445810400
O	1.123456200	2.872486400	0.010872800
O	-0.165328300	-2.126943100	-1.612480900
C	2.494696100	-1.630573100	-1.046042800
C	3.094572400	1.070441800	-0.094307600
N	3.297092100	-2.478603900	-1.108725500
N	4.193457400	1.381131800	0.127900000
O	-1.845482300	-2.565724900	0.818289400
H	-2.783054300	-2.337894300	0.695209400
H	0.374471500	3.492548600	0.109223600

S0-II-1-P

C	3.969754000	-1.005442000	-0.100942000
C	3.356262000	-2.101497000	0.507713000
C	2.365021000	-1.916842000	1.476081000
C	1.999518000	-0.619867000	1.843573000
C	2.614212000	0.486994000	1.253976000
C	3.600151000	0.296148000	0.271869000
H	4.730234000	-1.134915000	-0.864679000
H	3.645580000	-3.105140000	0.209358000
H	1.879292000	-2.773153000	1.933412000
H	1.228710000	-0.460289000	2.592151000

H	2.338090000	1.494480000	1.551027000
H	1.750602000	-0.357694000	-1.179930000
C	-2.526030000	0.867826000	0.253049000
C	-1.431996000	1.686822000	-0.050824000
C	-0.255884000	1.132815000	-0.616976000
C	-0.152803000	-0.246957000	-0.855432000
C	-1.261084000	-1.066208000	-0.548294000
C	-2.426657000	-0.516332000	-0.010371000
Cl	-1.123379000	-2.769069000	-0.840200000
Cl	-3.802078000	-1.510926000	0.375565000
O	-3.614767000	1.454058000	0.781100000
O	0.927867000	-0.837466000	-1.395558000
C	0.843703000	1.979713000	-0.939999000
C	-1.515580000	3.086796000	0.208666000
N	1.757070000	2.653215000	-1.198673000
N	-1.569596000	4.229881000	0.416544000
O	4.237673000	1.334212000	-0.345645000
H	3.678554000	2.131184000	-0.299699000
H	-4.308321000	0.793531000	0.960351000

S0-II-2-P

C	-2.676207000	-0.408507000	1.304295000
C	-2.082919000	0.179728000	2.423665000
C	-0.907492000	-0.346859000	2.963739000
C	-0.331203000	-1.482022000	2.385452000
C	-0.916327000	-2.083578000	1.271611000
C	-2.079186000	-1.531918000	0.729765000
H	-3.577871000	0.013975000	0.869595000
H	-2.540957000	1.060210000	2.864901000
H	-0.444756000	0.121792000	3.826856000
H	0.583223000	-1.900121000	2.796274000
H	-0.470235000	-2.952554000	0.798015000
H	-1.244841000	-1.824746000	-1.697590000
C	1.460619000	1.477348000	0.092706000
C	2.135832000	0.264329000	-0.107610000
C	1.515337000	-0.788689000	-0.819086000
C	0.230560000	-0.636488000	-1.356042000
C	-0.420177000	0.605091000	-1.197785000
C	0.172536000	1.633429000	-0.460002000
Cl	-1.981670000	0.814893000	-1.929510000
Cl	-0.648278000	3.145383000	-0.191636000
O	2.090314000	2.426445000	0.807598000
O	-0.319963000	-1.679558000	-2.012633000
C	2.163077000	-2.054681000	-0.943417000
C	3.438604000	0.094288000	0.448245000
N	2.695470000	-3.085085000	-1.027280000
N	4.500208000	-0.055314000	0.899150000

O	-2.560793000	-2.112372000	-0.432903000
H	-3.399897000	-1.692761000	-0.688483000
H	1.539922000	3.227355000	0.877110000

NEB path connecting R-II-1 and P-II-1

1

C	2.933981800	-0.644169200	0.313110100
C	4.164346200	-1.130347300	-0.029566000
C	5.015836400	-0.423988100	-0.919476300
C	4.594920300	0.818630200	-1.460565400
C	3.376521900	1.350821400	-1.141342300
C	2.404731700	0.647354200	-0.236438100
H	2.285616600	-1.180111300	0.998325300
H	4.503867300	-2.075363600	0.387935100
H	5.986363700	-0.831972200	-1.183631300
H	5.257930500	1.354280400	-2.135884600
H	3.061602900	2.307749600	-1.551880400
H	2.135287600	1.309839400	0.606907200
C	-2.449197700	0.073161000	-0.686759200
C	-2.014702600	1.289621400	-0.099389000
C	-1.052542300	1.277099400	0.907322300
C	-0.466716100	0.028185000	1.394529400
C	-0.952167300	-1.203908300	0.750541200
C	-1.899853500	-1.169321300	-0.247606100
Cl	-0.266367100	-2.679571700	1.303024400
Cl	-2.471648700	-2.611651700	-1.035812300
O	-3.369069900	0.169441000	-1.638181500
O	0.388553100	0.019590000	2.290601600
C	-0.578645200	2.482261700	1.493973400
C	-2.573466700	2.517431700	-0.570264200
N	-0.180081100	3.467297000	1.968769600
N	-3.016847800	3.524969000	-0.943199300
O	1.162675300	0.333979100	-0.944947300
H	0.835051200	1.168348300	-1.322927400
H	-3.616506000	-0.708901200	-1.988658600

2

C	2.807727200	-0.802445100	0.074453900
C	4.087533600	-1.291646700	-0.228707200
C	5.028003200	-0.426139100	-0.867119400
C	4.770730800	0.947369700	-1.194676500
C	3.524051200	1.475455000	-0.895523500
C	2.425030900	0.646477700	-0.229662900
H	2.046743100	-1.420263100	0.562598300
H	4.338130100	-2.340901900	-0.000875600

H	6.011439900	-0.846351300	-1.140640200
H	5.545796600	1.568205200	-1.671718700
H	3.285981300	2.520748100	-1.110486500
H	2.131652300	1.105074200	0.703471900
C	-2.583576700	0.009373500	-0.604883300
C	-2.104295100	1.244998100	-0.132950000
C	-1.028669000	1.307850300	0.787139900
C	-0.369475800	0.106732500	1.329848100
C	-0.940835600	-1.162317900	0.805008900
C	-1.971157500	-1.192469900	-0.118050800
Cl	-0.185519000	-2.616254700	1.385885100
Cl	-2.607893800	-2.712340400	-0.746884900
O	-3.595547400	0.016173500	-1.490348400
O	0.583050000	0.128224200	2.120803300
C	-0.518428100	2.577914500	1.253652200
C	-2.696800700	2.443277700	-0.640703600
N	-0.088497200	3.578025100	1.569457300
N	-3.169096400	3.430680200	-1.049798900
O	1.289788200	0.587872800	-1.161664600
H	1.009661600	1.500278600	-1.310189900
H	-3.826052900	-0.902846900	-1.718923900

3

C	2.760691200	-0.817324800	-0.231047700
C	4.023793900	-1.327257200	-0.486822400
C	5.067920600	-0.448689400	-0.839303700
C	4.875408400	0.944556800	-0.854223500
C	3.628344700	1.475681400	-0.589546500
C	2.474379700	0.619385700	-0.328132100
H	1.919519100	-1.450428400	0.032592900
H	4.216782700	-2.394153800	-0.462756100
H	6.042677700	-0.870897900	-1.088462000
H	5.719655300	1.569130900	-1.116160400
H	3.441901800	2.538068900	-0.602069800
H	1.993495700	0.872279700	0.753708400
C	-2.662784500	-0.062330300	-0.494990000
C	-2.159660900	1.205921900	-0.167883900
C	-1.050236500	1.318703800	0.685320300
C	-0.353103200	0.176883700	1.201176300
C	-0.907441000	-1.109104600	0.840770700
C	-2.025372900	-1.212471300	0.020784800
Cl	-0.103989800	-2.530345100	1.448488500
Cl	-2.690551900	-2.768026200	-0.427147300
O	-3.751776100	-0.104381500	-1.287629100
O	0.724404800	0.312690200	1.873191900
C	-0.489616500	2.596550400	0.969666200
C	-2.797039700	2.370401000	-0.706953100

N	-0.027357600	3.635992300	1.180422600
N	-3.307952500	3.320947900	-1.136961500
O	1.389326200	0.845183100	-1.191756200
H	1.248754800	1.805062500	-1.280412000
H	-4.000699200	-1.031276000	-1.435355000

4

C	2.702941200	-0.795008600	-0.535157100
C	3.987614500	-1.334195700	-0.747649200
C	5.087933600	-0.478672000	-0.808174600
C	4.983654900	0.884131600	-0.506019300
C	3.700871100	1.446077200	-0.278344400
C	2.546000300	0.621532200	-0.435133500
H	1.820025200	-1.409236400	-0.524441700
H	4.112773100	-2.394026000	-0.951253400
H	6.078989300	-0.901889800	-1.036024600
H	5.866096200	1.510987700	-0.529280100
H	3.577547000	2.504133300	-0.062407000
H	1.782904500	0.679693100	0.833198300
C	-2.756895700	-0.114905700	-0.395111200
C	-2.223675100	1.167260500	-0.200800900
C	-1.037707300	1.323826000	0.539643500
C	-0.314779300	0.226645100	1.065275000
C	-0.880443900	-1.065555800	0.862174800
C	-2.075228200	-1.225927900	0.146983000
Cl	-0.028931700	-2.449692700	1.488283300
Cl	-2.771532000	-2.811383300	-0.129968700
O	-3.906645500	-0.204438400	-1.091429500
O	0.877513500	0.421258300	1.639717400
C	-0.458729200	2.624773700	0.697514900
C	-2.902086400	2.297845200	-0.761564000
N	0.021233800	3.668302000	0.808442000
N	-3.442955300	3.220763700	-1.209109600
O	1.491021100	1.116197900	-1.235184300
H	1.527238400	2.091222700	-1.210947500
H	-4.165273500	-1.138964400	-1.154721400

5

C	2.707783400	-0.694076800	-0.850094500
C	3.964823300	-1.265215300	-1.007262000
C	5.110445000	-0.504734900	-0.772433700
C	5.013103400	0.742773200	-0.167903700
C	3.762785600	1.342506600	0.005625100
C	2.706581500	0.693676800	-0.645579100
H	1.808667000	-1.264659800	-1.073173700
H	4.040550200	-2.262428700	-1.433675500
H	6.081798800	-0.928869000	-0.969033300

H	5.904684500	1.321275900	0.058255500
H	3.682397900	2.328132000	0.462317000
H	1.592262900	0.554192500	0.868349000
C	-2.841291000	-0.167444100	-0.284031400
C	-2.288960500	1.124791400	-0.235642400
C	-1.035394000	1.331895800	0.380649200
C	-0.298523600	0.264619100	0.919899900
C	-0.863610600	-1.025952000	0.877349300
C	-2.119178700	-1.234948500	0.279414400
Cl	0.040544900	-2.355633000	1.524512800
Cl	-2.835805200	-2.828141600	0.189858000
O	-4.043906000	-0.301423900	-0.873635300
O	0.907723300	0.481514200	1.492574300
C	-0.445402600	2.635409400	0.407034700
C	-3.007791600	2.215264900	-0.815450400
N	0.058837100	3.683118200	0.421865500
N	-3.581541800	3.110229100	-1.281889300
O	1.667953300	1.381037200	-1.216154500
H	1.831630800	2.337620900	-1.127709300
H	-4.321692800	-1.233776100	-0.855526200

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C	2.893458600	-0.733849800	-0.985618900
C	4.186557200	-1.226870100	-0.844373400
C	5.223445800	-0.396496800	-0.422918700
C	4.923544200	0.870170000	0.105732500
C	3.634953200	1.378705200	-0.008881600
C	2.755228300	0.662531400	-0.838151800
H	2.077679400	-1.374924000	-1.319437900
H	4.389669700	-2.242612700	-1.197637200
H	6.240299400	-0.741533700	-0.452093800
H	5.708301400	1.527297700	0.476486900
H	3.379340200	2.379409000	0.402188400
H	1.575401800	0.388559300	0.470111400
C	-2.984790000	-0.068326100	-0.123080200
C	-2.299190700	1.150089500	-0.230961200
C	-0.957447300	1.227857600	0.179988100
C	-0.284271600	0.096907100	0.689417400
C	-0.971811200	-1.129178900	0.771913600
C	-2.304129200	-1.207661200	0.379539200
Cl	-0.117610100	-2.517227300	1.353749600
Cl	-3.175824900	-2.717666400	0.482403300
O	-4.267817900	-0.104352900	-0.511804400
O	0.955510300	0.157615200	1.177197900
C	-0.277492100	2.484788600	0.057867800
C	-2.977090300	2.308862400	-0.746915300
N	0.225303700	3.512359600	-0.087233400

N	-3.480785700	3.262029500	-1.156335400
O	1.780325100	1.301910500	-1.546944700
H	1.926150100	2.252109400	-1.403819900
H	-4.577432700	-1.019748400	-0.391877800

7

C	3.143273600	-0.751446700	-1.112342800
C	4.395431400	-1.161553100	-0.686320800
C	5.260700700	-0.260892200	-0.066346800
C	4.786857500	0.979157000	0.350468300
C	3.530381800	1.405942300	-0.043663700
C	2.857888900	0.616077000	-0.976538600
H	2.428449100	-1.449770700	-1.540592300
H	4.715723200	-2.161386900	-0.948461400
H	6.294440200	-0.526540000	0.064426300
H	5.420651500	1.685901200	0.865128200
H	3.104213400	2.342980500	0.316115700
H	1.537695700	0.220524400	0.083412900
C	-3.080853200	0.034746100	0.050043300
C	-2.310583400	1.169158500	-0.221798200
C	-0.912918000	1.110983100	-0.029891900
C	-0.326225700	-0.070952500	0.446539600
C	-1.099962500	-1.222120900	0.662425500
C	-2.466771500	-1.156461500	0.482825900
Cl	-0.300698300	-2.666325900	1.174747700
Cl	-3.450750000	-2.555432000	0.787698300
O	-4.407171600	0.110102700	-0.123854300
O	0.961724200	-0.187050300	0.754607200
C	-0.169628700	2.291338400	-0.307624500
C	-2.923661600	2.387180100	-0.665716900
N	0.364167200	3.298941400	-0.591233500
N	-3.371587600	3.392534600	-1.023934100
O	1.979343600	1.200628900	-1.833921900
H	2.024756300	2.164354900	-1.680861800
H	-4.785412100	-0.759865000	0.093175100

8

C	3.384215300	-0.768110900	-1.164135000
C	4.570353700	-1.084493600	-0.526759000
C	5.241871600	-0.127117900	0.234087000
C	4.603416500	1.062805900	0.564722700
C	3.401324300	1.394491000	-0.039168300
C	2.973739300	0.572405700	-1.081730900
H	2.809929100	-1.514088100	-1.708047400
H	5.007797500	-2.053362200	-0.727174900
H	6.255700100	-0.312208000	0.540207800
H	5.080698200	1.811133200	1.179852400

H	2.856328200	2.297724500	0.235253000
H	1.470243000	0.067486800	-0.286269400
C	-3.132436900	0.153339100	0.227760100
C	-2.304646100	1.194045700	-0.194971100
C	-0.903496500	0.991719100	-0.234207700
C	-0.374130100	-0.246402200	0.162124700
C	-1.217413800	-1.294808600	0.566901700
C	-2.578117300	-1.088080100	0.601956700
Cl	-0.489355400	-2.798068100	1.006508500
Cl	-3.631821300	-2.373521300	1.104738700
O	-4.456422500	0.360003700	0.262341200
O	0.911713000	-0.551394200	0.210991700
C	-0.116967800	2.089908300	-0.673320600
C	-2.857164900	2.460631200	-0.580299200
N	0.449526800	3.045750300	-1.060430700
N	-3.256690000	3.499360900	-0.899733700
O	2.225947800	1.096768500	-2.086977200
H	2.151574400	2.057851400	-1.923624500
H	-4.876241700	-0.463016200	0.567913900

9

C	3.607978200	-0.784483000	-1.155446400
C	4.722840700	-0.991082200	-0.379657700
C	5.201437200	0.020849600	0.476911700
C	4.382081200	1.125272800	0.736806900
C	3.234512500	1.350386700	-0.010616200
C	3.094950400	0.530384400	-1.157301400
H	3.237958100	-1.570098000	-1.834088400
H	5.316223900	-1.900394400	-0.519521200
H	6.149317600	-0.095277600	0.976393300
H	4.696955400	1.899670400	1.432588900
H	2.596797700	2.212900200	0.162694400
H	1.364387600	-0.160245000	-0.674659300
C	-3.144889700	0.281767900	0.409355400
C	-2.285511600	1.225287600	-0.161851300
C	-0.944197300	0.878616500	-0.431545200
C	-0.454746000	-0.416672300	-0.118980100
C	-1.335229300	-1.358916100	0.453877100
C	-2.647611900	-1.017514700	0.709229700
Cl	-0.707061000	-2.927020600	0.813240900
Cl	-3.736009000	-2.183529600	1.411921800
O	-4.414908700	0.642485300	0.651675800
O	0.782841300	-0.856860800	-0.320822500
C	-0.118751100	1.877006500	-1.041587800
C	-2.771430000	2.537316400	-0.471609500
N	0.495805100	2.723910100	-1.537876300
N	-3.115789000	3.609227700	-0.736465200

O	2.534960500	1.006930600	-2.316214200
H	2.310876900	1.949411300	-2.140405700
H	-4.854315100	-0.128576500	1.052462900

NEB path connecting R-II-2 and P-II-2

1

C	-1.554528400	-1.812724500	-1.052460300
C	-0.742514200	-1.091708300	-1.883459500
C	-1.031009300	0.263134100	-2.194878600
C	-2.193743600	0.877826200	-1.660961500
C	-3.039365900	0.192878100	-0.833992200
C	-2.792487800	-1.229883300	-0.423703100
H	-1.328969400	-2.850042800	-0.817067200
H	0.134699000	-1.562064400	-2.323285700
H	-0.376336100	0.822270200	-2.857045800
H	-2.411448700	1.911598500	-1.917582500
H	-3.936765100	0.655424200	-0.435501100
H	-2.674520700	-1.256559400	0.676635200
C	1.619661500	1.343597400	-0.148271000
C	0.418456100	1.725696500	0.502344100
C	-0.278190100	0.803933200	1.278027400
C	0.182238100	-0.578811200	1.425454400
C	1.435378400	-0.921502300	0.730487200
C	2.115625600	0.017349000	-0.016339000
Cl	1.973093600	-2.545463700	0.866687200
Cl	3.586209000	-0.368550100	-0.879816200
O	2.225281600	2.274196600	-0.888244200
O	-0.456536100	-1.413259400	2.079698600
C	-1.489802400	1.157726300	1.932587500
C	-0.075825000	3.051309900	0.302662100
N	-2.480813700	1.443332400	2.471346700
N	-0.488380100	4.123907200	0.130534000
O	-3.971200100	-1.996592600	-0.764726200
H	-3.989153100	-2.771585800	-0.180948100
H	3.034976800	1.910834500	-1.293993400

2

C	-1.548707800	-1.832905000	-1.126726300
C	-0.842776300	-1.071598000	-2.008744200
C	-1.228597500	0.256481700	-2.267942300
C	-2.353471100	0.819358600	-1.646544300
C	-3.091615900	0.082299100	-0.765197800
C	-2.735150800	-1.307581600	-0.408110300
H	-1.244011900	-2.851933700	-0.921418600
H	0.009489900	-1.495836800	-2.511191100
H	-0.655540100	0.852073200	-2.964930000

H	-2.640134300	1.835025900	-1.861378800
H	-3.959998300	0.510665600	-0.288108900
H	-2.464793700	-1.281506700	0.695783600
C	1.712407500	1.350584800	-0.065423800
C	0.514703500	1.785504400	0.516043800
C	-0.274743400	0.885379400	1.223982200
C	0.097994900	-0.502960900	1.361060500
C	1.349656400	-0.898987600	0.730700200
C	2.125651100	0.010806500	0.054062100
Cl	1.800258900	-2.552838900	0.853960400
Cl	3.616256500	-0.452449500	-0.722017500
O	2.421415800	2.267874600	-0.738126100
O	-0.625034200	-1.316625500	1.966516300
C	-1.494348700	1.300650100	1.812615500
C	0.103410400	3.135324600	0.344117700
N	-2.499581400	1.632725800	2.292113700
N	-0.244288200	4.231870600	0.191817600
O	-3.884320500	-2.105187000	-0.635453600
H	-3.772798900	-2.962823000	-0.194586300
H	3.222697700	1.852875800	-1.092685300

3

C	2.760691200	-0.817324800	-0.231047700
C	4.023793900	-1.327257200	-0.486822400
C	5.067920600	-0.448689400	-0.839303700
C	4.875408400	0.944556800	-0.854223500
C	3.628344700	1.475681400	-0.589546500
C	2.474379700	0.619385700	-0.328132100
H	1.919519100	-1.450428400	0.032592900
H	4.216782700	-2.394153800	-0.462756100
H	6.042677700	-0.870897900	-1.088462000
H	5.719655300	1.569130900	-1.116160400
H	3.441901800	2.538068900	-0.602069800
H	1.993495700	0.872279700	0.753708400
C	-2.662784500	-0.062330300	-0.494990000
C	-2.159660900	1.205921900	-0.167883900
C	-1.050236500	1.318703800	0.685320300
C	-0.353103200	0.176883700	1.201176300
C	-0.907441000	-1.109104600	0.840770700
C	-2.025372900	-1.212471300	0.020784800
Cl	-0.103989800	-2.530345100	1.448488500
Cl	-2.690551900	-2.768026200	-0.427147300
O	-3.751776100	-0.104381500	-1.287629100
O	0.724404800	0.312690200	1.873191900
C	-0.489616500	2.596550400	0.969666200
C	-2.797039700	2.370401000	-0.706953100
N	-0.027357600	3.635992300	1.180422600

N	-3.307952500	3.320947900	-1.136961500
O	1.389326200	0.845183100	-1.191756200
H	1.248754800	1.805062500	-1.280412000
H	-4.000699200	-1.031276000	-1.435355000

4

C	2.702941200	-0.795008600	-0.535157100
C	3.987614500	-1.334195700	-0.747649200
C	5.087933600	-0.478672000	-0.808174600
C	4.983654900	0.884131600	-0.506019300
C	3.700871100	1.446077200	-0.278344400
C	2.546000300	0.621532200	-0.435133500
H	1.820025200	-1.409236400	-0.524441700
H	4.112773100	-2.394026000	-0.951253400
H	6.078989300	-0.901889800	-1.036024600
H	5.866096200	1.510987700	-0.529280100
H	3.577547000	2.504133300	-0.062407000
H	1.782904500	0.679693100	0.833198300
C	-2.756895700	-0.114905700	-0.395111200
C	-2.223675100	1.167260500	-0.200800900
C	-1.037707300	1.323826000	0.539643500
C	-0.314779300	0.226645100	1.065275000
C	-0.880443900	-1.065555800	0.862174800
C	-2.075228200	-1.225927900	0.146983000
Cl	-0.028931700	-2.449692700	1.488283300
Cl	-2.771532000	-2.811383300	-0.129968700
O	-3.906645500	-0.204438400	-1.091429500
O	0.877513500	0.421258300	1.639717400
C	-0.458729200	2.624773700	0.697514900
C	-2.902086400	2.297845200	-0.761564000
N	0.021233800	3.668302000	0.808442000
N	-3.442955300	3.220763700	-1.209109600
O	1.491021100	1.116197900	-1.235184300
H	1.527238400	2.091222700	-1.210947500
H	-4.165273500	-1.138964400	-1.154721400

5

C	2.707783400	-0.694076800	-0.850094500
C	3.964823300	-1.265215300	-1.007262000
C	5.110445000	-0.504734900	-0.772433700
C	5.013103400	0.742773200	-0.167903700
C	3.762785600	1.342506600	0.005625100
C	2.706581500	0.693676800	-0.645579100
H	1.808667000	-1.264659800	-1.073173700
H	4.040550200	-2.262428700	-1.433675500
H	6.081798800	-0.928869000	-0.969033300
H	5.904684500	1.321275900	0.058255500

H	3.682397900	2.328132000	0.462317000
H	1.592262900	0.554192500	0.868349000
C	-2.841291000	-0.167444100	-0.284031400
C	-2.288960500	1.124791400	-0.235642400
C	-1.035394000	1.331895800	0.380649200
C	-0.298523600	0.264619100	0.919899900
C	-0.863610600	-1.025952000	0.877349300
C	-2.119178700	-1.234948500	0.279414400
Cl	0.040544900	-2.355633000	1.524512800
Cl	-2.835805200	-2.828141600	0.189858000
O	-4.043906000	-0.301423900	-0.873635300
O	0.907723300	0.481514200	1.492574300
C	-0.445402600	2.635409400	0.407034700
C	-3.007791600	2.215264900	-0.815450400
N	0.058837100	3.683118200	0.421865500
N	-3.581541800	3.110229100	-1.281889300
O	1.667953300	1.381037200	-1.216154500
H	1.831630800	2.337620900	-1.127709300
H	-4.321692800	-1.233776100	-0.855526200

6

C	2.893458600	-0.733849800	-0.985618900
C	4.186557200	-1.226870100	-0.844373400
C	5.223445800	-0.396496800	-0.422918700
C	4.923544200	0.870170000	0.105732500
C	3.634953200	1.378705200	-0.008881600
C	2.755228300	0.662531400	-0.838151800
H	2.077679400	-1.374924000	-1.319437900
H	4.389669700	-2.242612700	-1.197637200
H	6.240299400	-0.741533700	-0.452093800
H	5.708301400	1.527297700	0.476486900
H	3.379340200	2.379409000	0.402188400
H	1.575401800	0.388559300	0.470111400
C	-2.984790000	-0.068326100	-0.123080200
C	-2.299190700	1.150089500	-0.230961200
C	-0.957447300	1.227857600	0.179988100
C	-0.284271600	0.096907100	0.689417400
C	-0.971811200	-1.129178900	0.771913600
C	-2.304129200	-1.207661200	0.379539200
Cl	-0.117610100	-2.517227300	1.353749600
Cl	-3.175824900	-2.717666400	0.482403300
O	-4.267817900	-0.104352900	-0.511804400
O	0.955510300	0.157615200	1.177197900
C	-0.277492100	2.484788600	0.057867800
C	-2.977090300	2.308862400	-0.746915300
N	0.225303700	3.512359600	-0.087233400
N	-3.480785700	3.262029500	-1.156335400

O	1.780325100	1.301910500	-1.546944700
H	1.926150100	2.252109400	-1.403819900
H	-4.577432700	-1.019748400	-0.391877800

7

C	3.143273600	-0.751446700	-1.112342800
C	4.395431400	-1.161553100	-0.686320800
C	5.260700700	-0.260892200	-0.066346800
C	4.786857500	0.979157000	0.350468300
C	3.530381800	1.405942300	-0.043663700
C	2.857888900	0.616077000	-0.976538600
H	2.428449100	-1.449770700	-1.540592300
H	4.715723200	-2.161386900	-0.948461400
H	6.294440200	-0.526540000	0.064426300
H	5.420651500	1.685901200	0.865128200
H	3.104213400	2.342980500	0.316115700
H	1.537695700	0.220524400	0.083412900
C	-3.080853200	0.034746100	0.050043300
C	-2.310583400	1.169158500	-0.221798200
C	-0.912918000	1.110983100	-0.029891900
C	-0.326225700	-0.070952500	0.446539600
C	-1.099962500	-1.222120900	0.662425500
C	-2.466771500	-1.156461500	0.482825900
Cl	-0.300698300	-2.666325900	1.174747700
Cl	-3.450750000	-2.555432000	0.787698300
O	-4.407171600	0.110102700	-0.123854300
O	0.961724200	-0.187050300	0.754607200
C	-0.169628700	2.291338400	-0.307624500
C	-2.923661600	2.387180100	-0.665716900
N	0.364167200	3.298941400	-0.591233500
N	-3.371587600	3.392534600	-1.023934100
O	1.979343600	1.200628900	-1.833921900
H	2.024756300	2.164354900	-1.680861800
H	-4.785412100	-0.759865000	0.093175100

8

C	3.384215300	-0.768110900	-1.164135000
C	4.570353700	-1.084493600	-0.526759000
C	5.241871600	-0.127117900	0.234087000
C	4.603416500	1.062805900	0.564722700
C	3.401324300	1.394491000	-0.039168300
C	2.973739300	0.572405700	-1.081730900
H	2.809929100	-1.514088100	-1.708047400
H	5.007797500	-2.053362200	-0.727174900
H	6.255700100	-0.312208000	0.540207800
H	5.080698200	1.811133200	1.179852400
H	2.856328200	2.297724500	0.235253000

H	1.470243000	0.067486800	-0.286269400
C	-3.132436900	0.153339100	0.227760100
C	-2.304646100	1.194045700	-0.194971100
C	-0.903496500	0.991719100	-0.234207700
C	-0.374130100	-0.246402200	0.162124700
C	-1.217413800	-1.294808600	0.566901700
C	-2.578117300	-1.088080100	0.601956700
Cl	-0.489355400	-2.798068100	1.006508500
Cl	-3.631821300	-2.373521300	1.104738700
O	-4.456422500	0.360003700	0.262341200
O	0.911713000	-0.551394200	0.210991700
C	-0.116967800	2.089908300	-0.673320600
C	-2.857164900	2.460631200	-0.580299200
N	0.449526800	3.045750300	-1.060430700
N	-3.256690000	3.499360900	-0.899733700
O	2.225947800	1.096768500	-2.086977200
H	2.151574400	2.057851400	-1.923624500
H	-4.876241700	-0.463016200	0.567913900

9

C	3.607978200	-0.784483000	-1.155446400
C	4.722840700	-0.991082200	-0.379657700
C	5.201437200	0.020849600	0.476911700
C	4.382081200	1.125272800	0.736806900
C	3.234512500	1.350386700	-0.010616200
C	3.094950400	0.530384400	-1.157301400
H	3.237958100	-1.570098000	-1.834088400
H	5.316223900	-1.900394400	-0.519521200
H	6.149317600	-0.095277600	0.976393300
H	4.696955400	1.899670400	1.432588900
H	2.596797700	2.212900200	0.162694400
H	1.364387600	-0.160245000	-0.674659300
C	-3.144889700	0.281767900	0.409355400
C	-2.285511600	1.225287600	-0.161851300
C	-0.944197300	0.878616500	-0.431545200
C	-0.454746000	-0.416672300	-0.118980100
C	-1.335229300	-1.358916100	0.453877100
C	-2.647611900	-1.017514700	0.709229700
Cl	-0.707061000	-2.927020600	0.813240900
Cl	-3.736009000	-2.183529600	1.411921800
O	-4.414908700	0.642485300	0.651675800
O	0.782841300	-0.856860800	-0.320822500
C	-0.118751100	1.877006500	-1.041587800
C	-2.771430000	2.537316400	-0.471609500
N	0.495805100	2.723910100	-1.537876300
N	-3.115789000	3.609227700	-0.736465200
O	2.534960500	1.006930600	-2.316214200

H	2.310876900	1.949411300	-2.140405700
H	-4.854315100	-0.128576500	1.052462900