Supplementary Material to the Paper entitled

Unexpected Radical Mechanism in a [4 + 1] Cycloaddition Reaction

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General

Schlenk-type inert gas technics were used thorough and solvents were purified by standard methods.[1] UV-Vis spectra were recorded on an Agilent 8453 spectrophotometer. All infrared spectra were obtained using a ThermoNicolet Avatar 330 FT-IR. All EPR spectra were measured by a Bruker ElexSys E500 X-band spectrometer with 1 mW microwave power at 100 kHz modulation frequency. ^{1}H NMR and ^{31}P NMR spectra were recorded at 400 MHz on a Bruker Avance 400 MHz spectrometer. Chemical shifts (δ) are reported in ppm proton shifts downfield from tetramethylsilane (TMS), phosphorous shifts downfield from phosphorous acid (H_3PO_4). Cyclic voltammetry were carried out with a VoltaLab PST006 potentiostat. Melting points were obtained by using a calibrated melting point microscope.

Cyclic voltammetry

The cyclic voltammograms of 1 mM solutions of 9,10-phenanthrenequinone monoimines and 0.5 mM solutions of 2,7-disubstituted 1,3,2-oxazaphospholes

were recorded in dried and argon saturated acetonitrile solutions with 0.1 M tetrabutylammonium perchlorate as a supporting electrolyte. The reversible one electron Fc/Fc^+ (ferrocene/ferrocenium) couple has $E^0_{1/2}$= +428 mV *vs*. Ag/AgCl. A three-electrode configuration composed of Pt-wire counter electrode, glassy carbon working electrode and a Ag/AgCl reference electrode. The cyclic voltammograms displays reversible oxidation waves in the case of 1,3,2-oxazaphospholes and irreversible waves in the case of imines.

Materials

The starting materials, triphenylphosphine (A.R.) and phenanthrene (puriss) were purchased from Sigma-Aldrich and Merck respectively. Triphenylphosphine were further purified by two times recrystallization from 95% ethanol[1]. H-abstractor TEMPO ((2,2,6,6-tetramethyl-piperidin-1-yl)oxyl) (98%), hydroxylamine hydrochloride and methylamine 40 wt. % aqueous solution were provided by Aldrich. All solvents were purchased from Molar Chemicals. Ammonia cylinder was ordered from Messer Griesheim. All other reagents were used as received unless otherwise noted.

Preparation of starting compounds

9,10-Phenanthrenequinone and 2,7-*tert*-butyl-9,10-phenanthrenequinone[2] were prepared from phenanthrene and 2,7-di-*tert*-butylphenanthrene by CrO_3 oxidation. 2,7-Dinitro-9,10-phenanthrenequinone[3] was prepared by nitration of 9,10-phenanthrenequinone and 2,7-dibromo-9,10-phenanthrenequinone[4] by the reaction between NBS (*N*-bromosuccinimide) and 9,10-phenanthrenequinone. Amino[5]- methylamino[6]- and iodosubstituted[7] phenanthrenequinones were prepared *via* reduction and further methylation or diazotation of 2,7-dinitro-9,10-phenanthrenequinone. Hydroxylamine hydrochloride was used for the synthesis of 9,10-phenanthrenequinone-monoxime[8], methylamine for *N*-methylphenanthrenequinone and a Staudinger reagent, namely *N*-phenyliminophosphorane (prepared according to the literature), was applied to synthesize *N*-phenylphenanthrenequinone[9].

General procedure for the synthesis of 9,10-phenanthrenequinone monoimines (**1a-1d**).

2,7-disubstituted derivate of phenanthrenequinone (10 mmol) were dissolved in a mixture of 30 ml $CHCl_3$ and 60 ml ethanol. NH_3(g) was bubbled through the solution at reflux temperature for two hours. After cooling yellow, needle like crystals were separated and dried in vacuum.

R= -H Yield: 1.55 g (75%). m.p. 165-167 °C. – FTIR (KBr) v/cm^{-1}: 3199 (m, N-H stretch), 1674 (s, C=O stretch), 1589, 1451, 1282, 1251, 1227, 1122, 1011, 942, 923, 897, 758, 714, 696, 534, 433. UV-Vis (CH_3CN), λ_{max}/nm (log *ε*): 213 (*4.44*), 257 (*4.49),* 265 (*4.49*), 314 (*3.54*), 393 (*3.21*) (mol^{-1} dm^3 cm^{-1}).

R= -*t*Bu Yield: 2.31 g (72%). m.p. 174-175 °C. FTIR (KBr) v/cm^{-1}: 3199 (m, N-H stretch), 3077 (w, C-H stretch), 2958 (s, C-H stretch), 1669 (s, C=O stretch). UV-Vis (CH_3CN), λ_{max}/nm (log *ε*): 213 (*4.67*), 265 (*4.86*), 274 (*4.83*), 315 (*3.74*), 420 (*3.53*) (mol^{-1} dm^3 cm^{-1}).

R= -NO_2 Yield: 1.95 g (66%). m.p. 291-293 °C. FTIR (KBr) v/cm^{-1}: 3211 (m, N-H stretch), 3166, 1674 (s, C=O stretch), 1516, 1348. UV-Vis (CH_3CN), λ_{max}/nm (log *ε*): 204 (*4.36*), 224 (*4.36*), 296 (*4.41*), 369 (*3.80*) (mol^{-1} dm^3 cm^{-1}).

R= -Br Yield: 2.88 g (79%). m.p. 235-237 °C. FTIR (KBr) v/cm^{-1}: 3199 (m, N-H stretch), 1677 (s, C=O stretch), 1077 (m, C_{arom}-Br stretch), 1033 (w, C_{arom}-Br stretch). UV-Vis(CH_3CN), λ_{max}/nm (log *ε*): 191 (*4.42*), 213 (*4.41*), 276 (*4.65*), 411 (*3.39*) (mol^{-1} dm^3 cm^{-1}).

General procedure for the synthesis of 2,7-disubstituted 2,3-dihydro-2,2,2-*triphenylphenanthro[9,10-]-1,3,2*λ^5*-oxazaphospholes.* (**4a-d**).

In an argon flushed Schlenk-tube 2 mmol of 2,7-substituted 9,10-phenanthrenequinone monoimine and 0.53 g (2 mmol) triphenylphosphine were dissolved in 10 ml argon saturated CH_3CN and refluxed for two hours. After cooling the precipitate was filtered off under argon and dried in vacuum.

R= -H Yield: 0.58 g (62%). m.p.153-155°C (benzene/hexane). FTIR (KBr) v/cm^{-1}: 3383 (m, N-H stretch), 3050, 1583, 1434, 1396, 1363, 1350, 1286, 1203, 1136, 1103, 763, 717, 694.MS (70eV): *m*/*z*(%) 469 (M^+, 30), 392 (8), 277 (22), 262 (100), 183 (35), 108 (20). ^{1}H NMR ($CDCl_3$): δ = 7.3 (br). ^{31}P NMR (C_6D_6): δ = -31.4; (CD_2Cl_2) -28.0.[10] UV-Vis (CH_3CN), λ_{max}/nm (log *ε*): 260 (*4.92*), 339 (*4.37*), 339 (*3.73*) (mol^{-1} dm^3 cm^{-1}).

R= -*t*Bu Yield: 0.64 g (55%). m.p. 258-261°C (mother liquor). FTIR (KBr) v/cm^{-1}: 3452 (m, N-H stretch), 3051, 2954 (s, C-H stretch), 2905 (m, C-H stretch), 2858 (m, C-H stretch), 1612, 1586, 1435, 1365, 1306, 1187, 1110. UV-Vis (CH_3CN), λ_{max}/nm (log *ε*): 262 (*4.64*), 274 (*4.61*), 335 (*3.95*), 413 (*3.48*), 526 (*3.13*) (mol^{-1} dm^3 cm^{-1}).

R= -NO_2 Yield: 0.61 g (55%). m.p. 134-135°C (CH_3CN). FTIR (KBr) v/cm^{-1}: 3419 (m, N-H stretch), 3314 (m, stretch) 1602 (m, stretch), 1508 (s, stretch), 1434 (s, stretch), 1341 (s, stretch). UV-Vis (CH_3CN), λ_{max}/nm (log *ε*): 322 (*4.53*), 540 (*3.30*) (mol^{-1} dm^3 cm^{-1}).

R= -Br Yield: 0.72 g (57%). m.p. 214-216 °C (mother liquor). FTIR (KBr) v/cm^{-1}: 3407 (m, N-H stretch), 3052, 1618, 1588, 1414, 1366, 1311, 1086, 1073 (m, C_{arom}-Br stretch), 1057, 1025, 993. UV-Vis($CH_3CN_{(Ar)}$), λ_{max}/nm (log *ε*): 268 (*4.54*), 282 (*4.46*), 346 (*3.88*), 414 (*3.30*), 500 (*2.89*), 536 (*2.87*) (mol^{-1} dm^3 cm^{-1}).

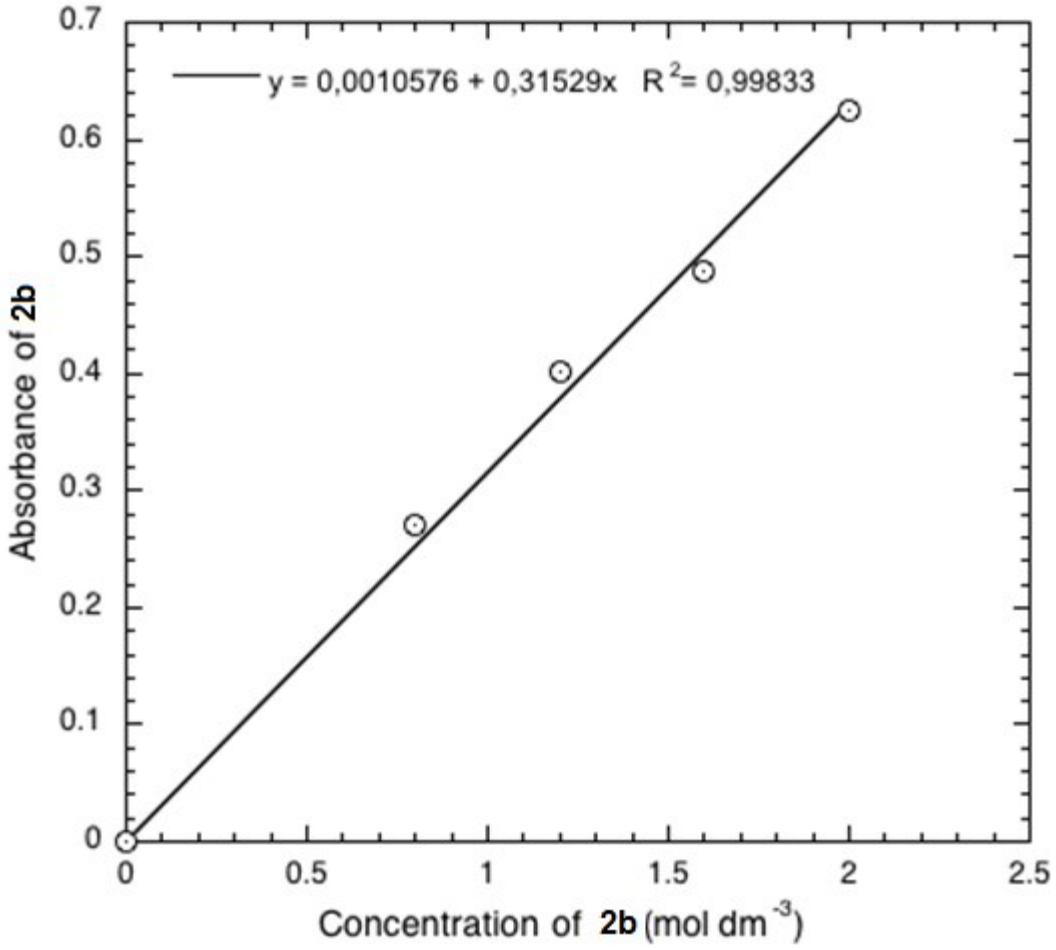
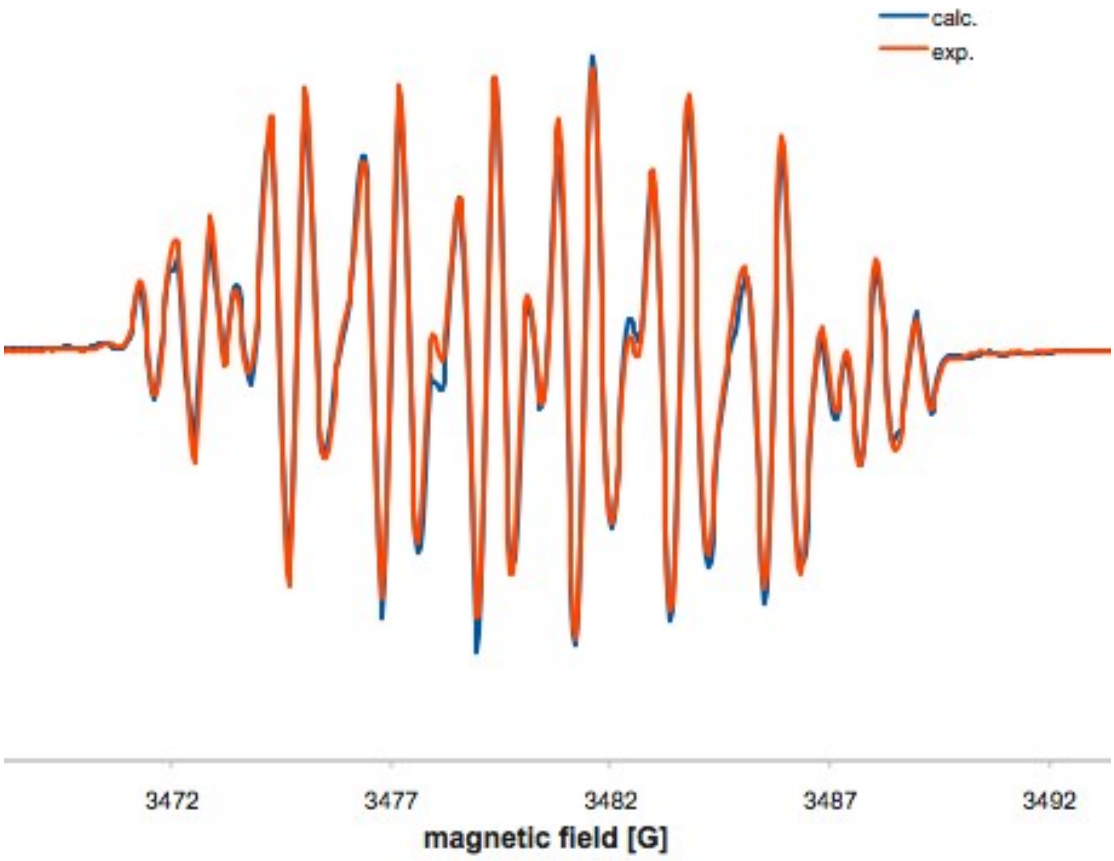
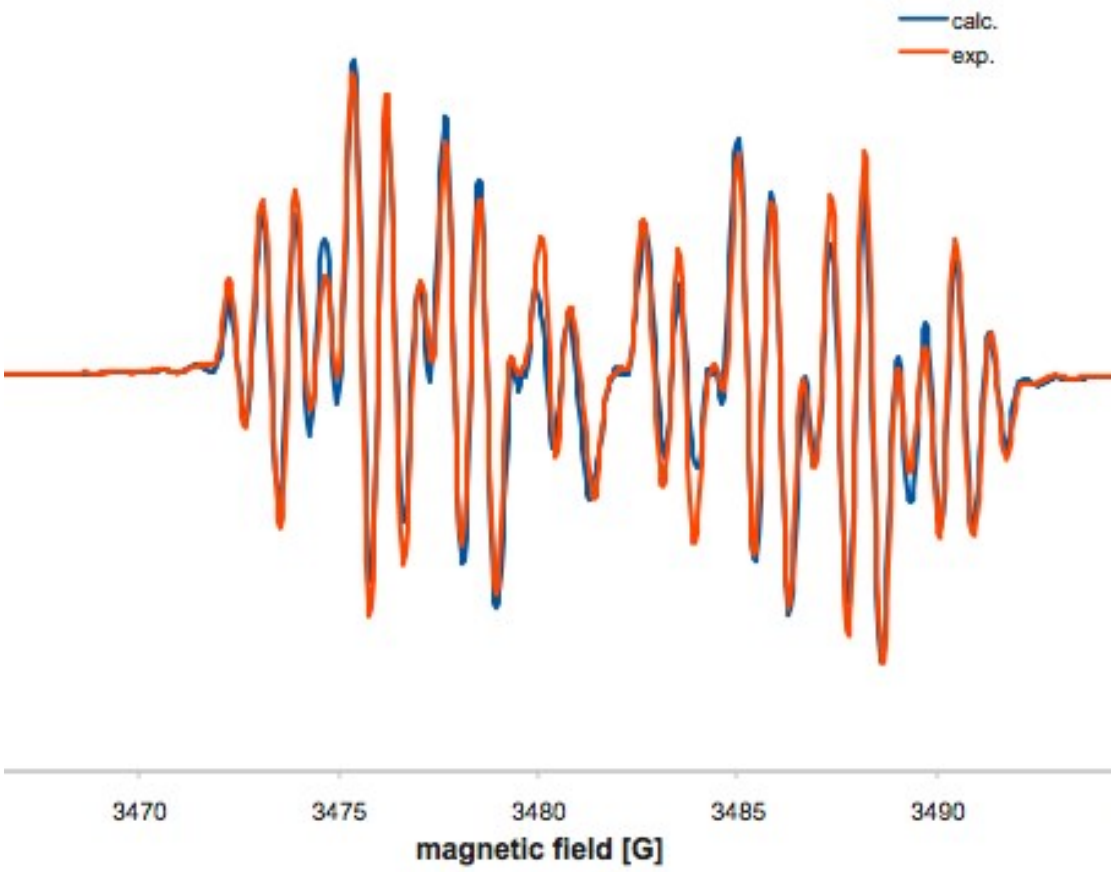


Fig. S1 Determination of the molar absorptivity of **2b•** using TEMPO as H-abstractor. λ_{max} = 488 nm, ε = 3154 $Lmol^{-1}cm^{-1}$.



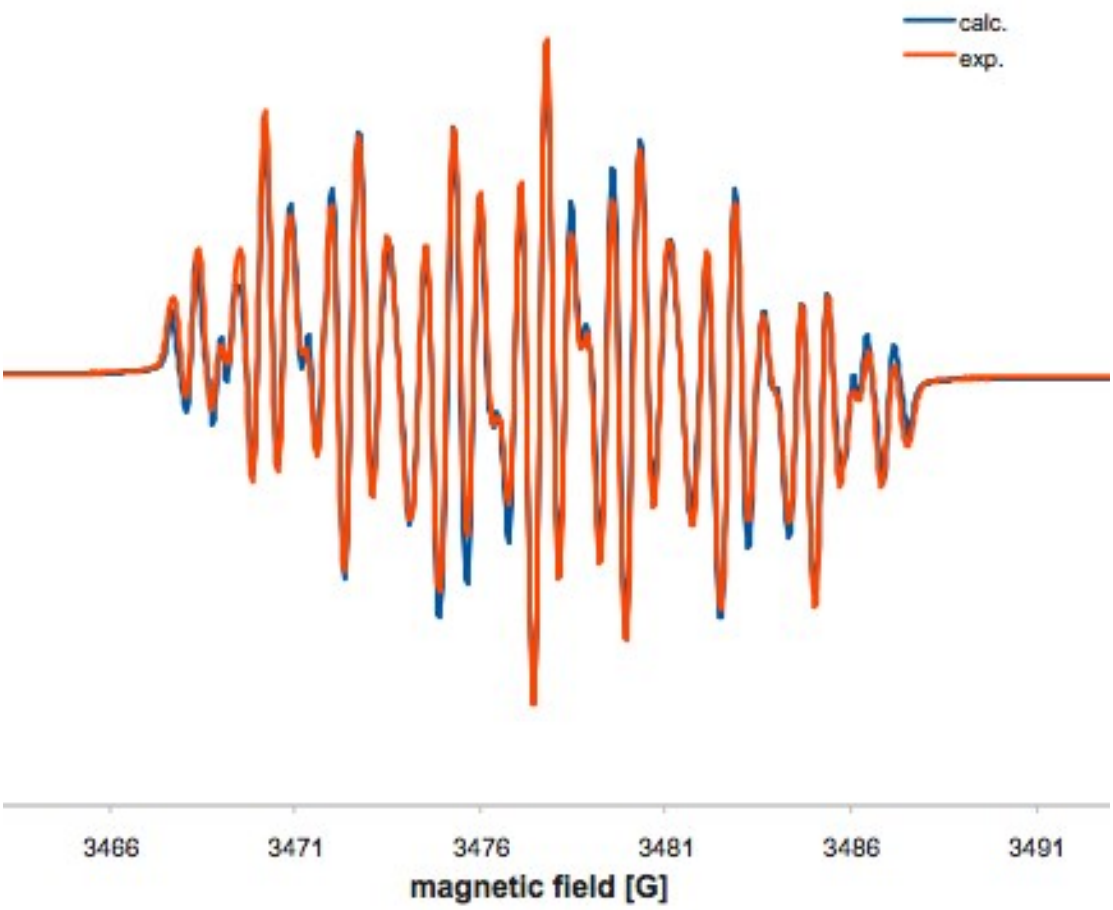
2.0039		2.0033
[MHz]	**[G]**	**[G]**
-18.0239	-6.44	6.59
9.9955	3.56	1.04
-6.8290	-2.44	2.31
-6.3920	-2.28	2.20
-3.1823	-1.14	2.13
-2.7653	-0.99	0.79
2.3713	0.84	0.79
		0.70
		0.15

Fig. S2. The EPR spectrum and calculated data of **2a**$^{\bullet}$ **(3a**$^{\bullet}$**)**. tBu; [**2a**] = [PPh_3] = 0.5 mM, 25°C.



g	2.0038		2.0033	2.0032
	[MHz]	[G]	[G]	
a_P	-21.8213	-7.79	7.35	7.22
a_N	17.5172	6.26	1.04	1.05
a_H	-6.0201	-2.15	2.52	2.59
a_H	5.5927	2.00	2.35	2.35
a_H	-2.8469	-1.02	2.25	2.23
a_H	-2.6189	-0.94	0.91	
a_H	2.2736	0.81	0.85	
a_H	-1.5625	-0.56	0.72	

Fig. S3 The EPR spectrum of 2**c**$^{\bullet}$ **(3c**$^{\bullet}$**) Br;** [**2c**] = [PPh_3] = 0.5 mM, 25°C.



G = 2.0039		2.0034
[MHz]	**[G]**	**[G]**
-20.4897	-7.32	7.59
11.6523	4.16	1.30
-7.39	-2.64	3.30
-4.4005	-1.57	1.81
-4.2085	-1.50	1.74
2.2432	0.80	1.02
-1.4004	-0.50	0.73
		0.64

Fig. S4 The EPR spectrum of **2d$^{\bullet}$ (3d$^{\bullet}$) NO2;** [**2d**] = [PPh_3] = 0.5 mM, 25°C.

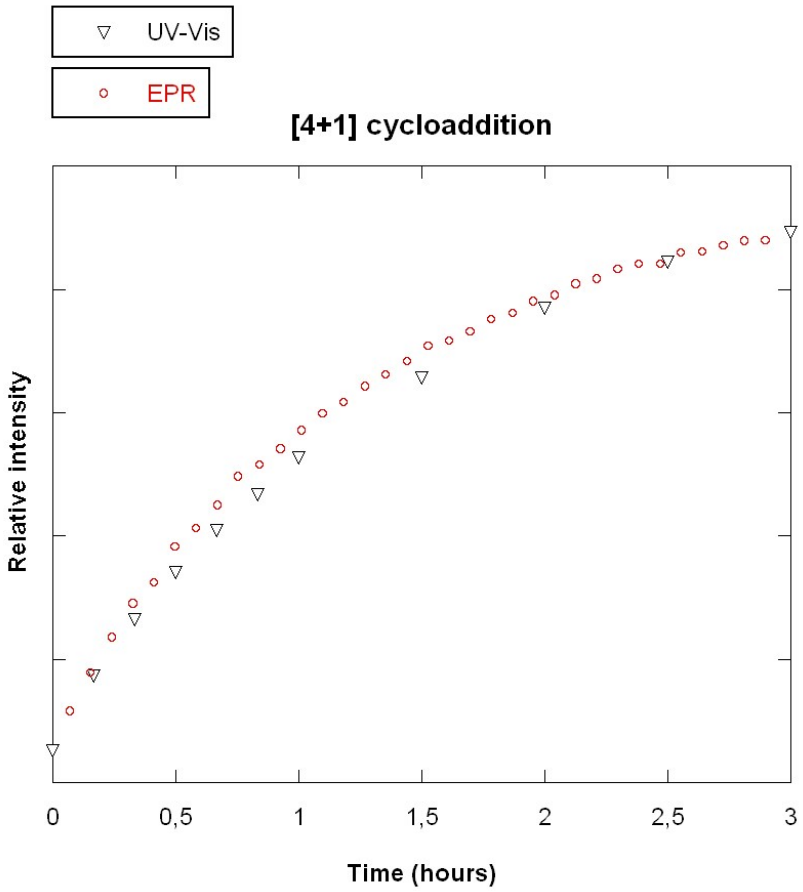


Fig. S5. Time course of the formation of the radical **3b**• by UV-Vis spectroscopy (recorded at 528 nm) and EPR . [**2b**] = [PPh_3] = 0.5 mM, 25°C.

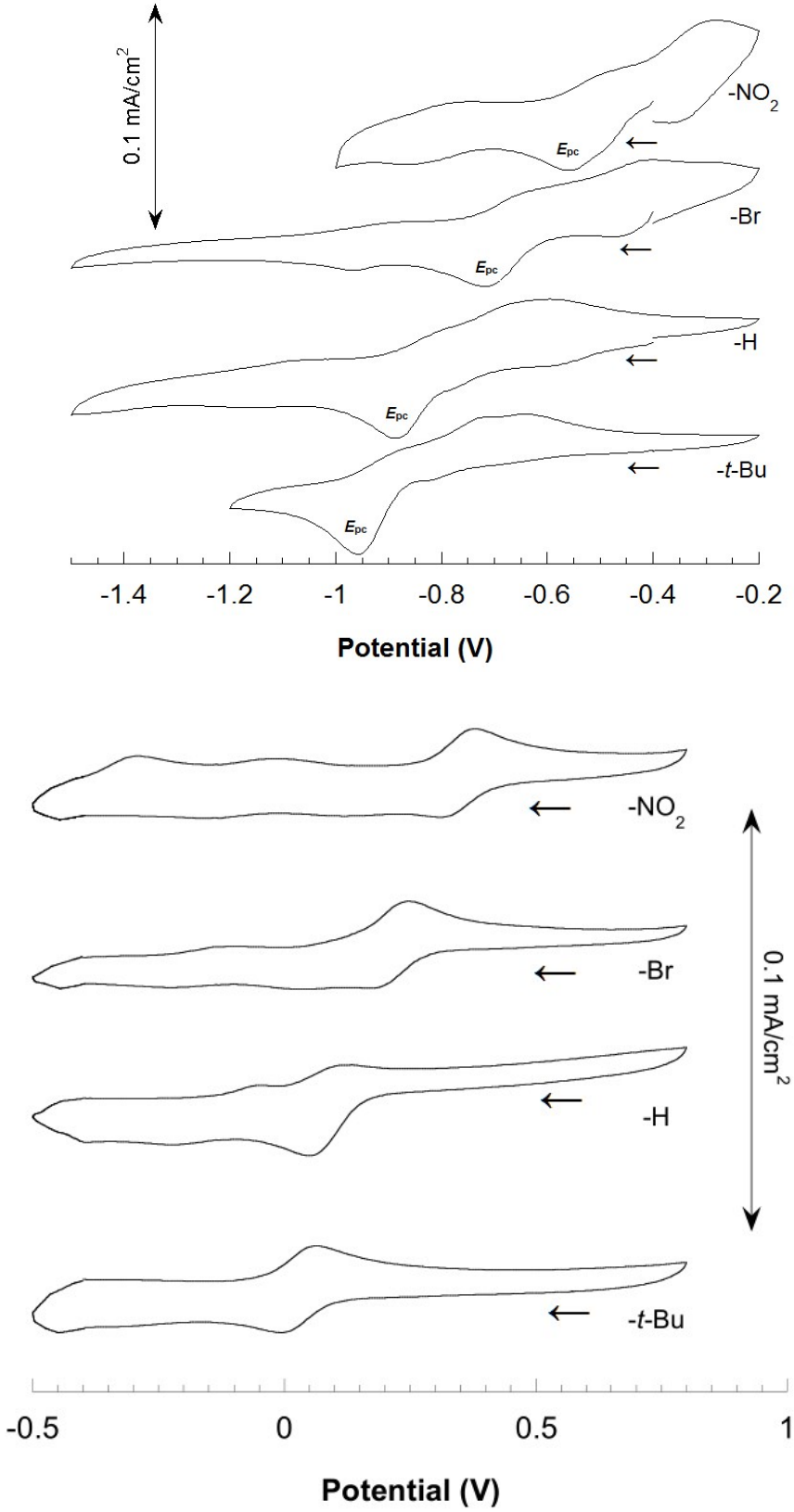


Fig. S6. The CVs of **1a-d** (top) and **2a-d** (bottom) in MeCN.

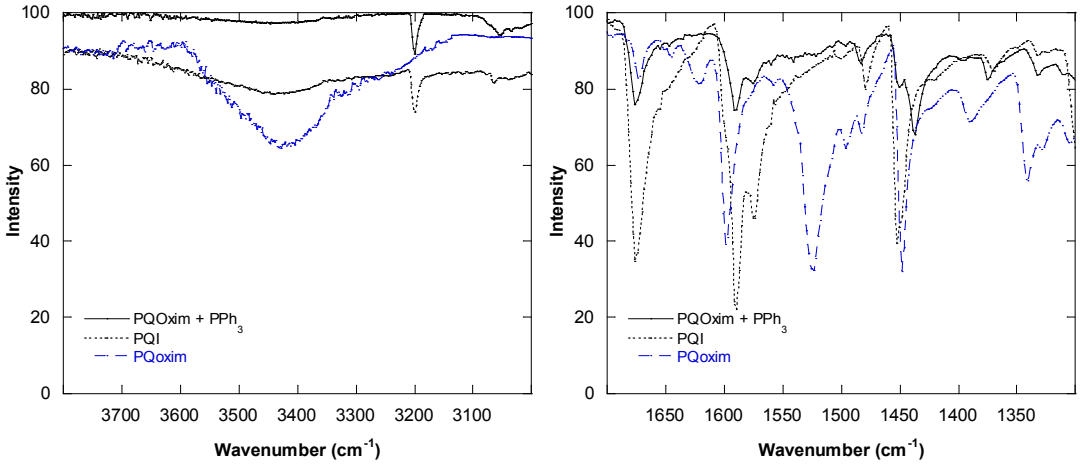


Fig. S7 The IR spectra of 9,10-phenanthrenequinone monoimine, 9,10-phenanthrenequinone oxime and the reaction product between 9,10-phenanthrenequinone oxime and triphenylphosphine under argon in MeCN at 25°C after 2 h reflux. Recorded in KBr.

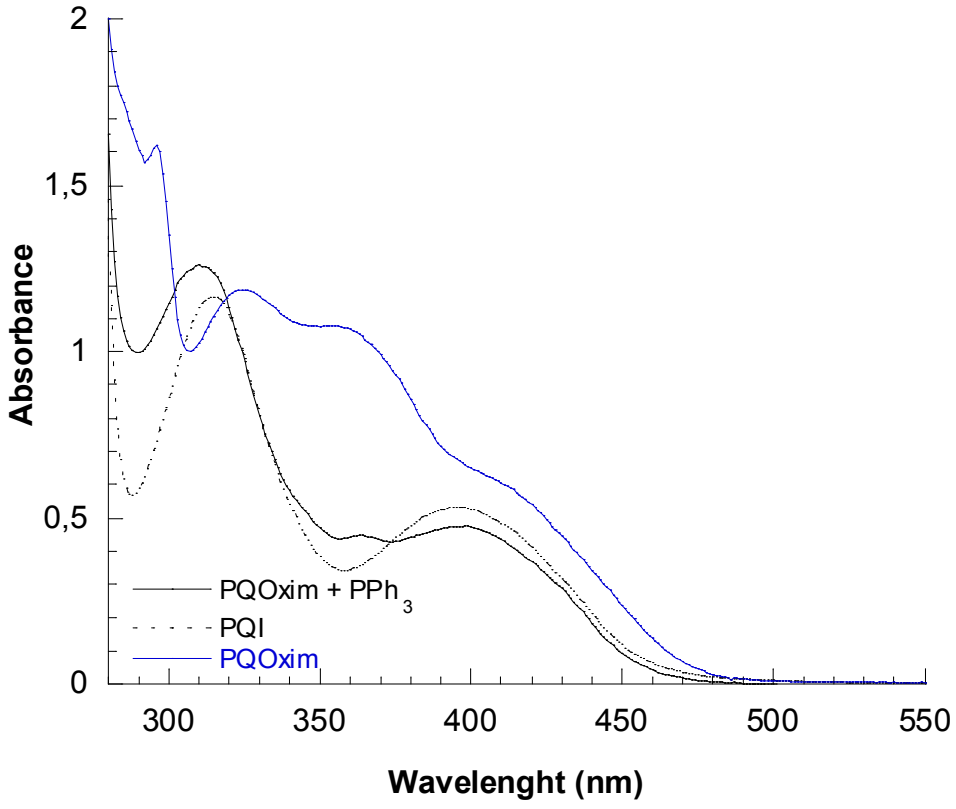


Fig. S8. The UV-Vis spectra of 9,10-phenanthrenequinone monoimine, 9,10-phenanthrenequinone oxime and the reaction product between 9,10-phenanthrenequinone oxime and triphenylphosphine in MeCN after 2 h reflux.

Kinetic measurements

Concentration changes of the red intermediate were followed by UV-visible spectroscopy. As a solvent dried, argon saturated acetonitrile was used. To defend the reaction mixture from air a 1 cm length screw cap cuvette with a septum was used where the volume of the reaction mixture was 4 ml. The measurements were carried out in a thermostable cuvette holder. The molar absorption coefficient of the red intermediate was determined by an instantaneous hydrogen abstraction reaction between TEMPO and oxazaphosphole. In this reaction the absorption immediately reach the maximum at room temperature. 0.1 cm length cuvette was used to determine the calibration line. Therefore the equation of figure below shows the tenth molar absorption coefficient (Fig. S1).

Table S1: Kinetic data for the reaction of PQI (**1b**) with PPh_3.

Exp. entry	$[\mathbf{1b}]_0$ (10^{-3} M)	$[\mathbf{PPh_3}]$ (10^{-3} M)	T (°C)	V_i[a] (10^{-4} M s^{-1})
1	1	2.5	25	2.93 ± 0.05
2	1	3.75	25	3.90 ± 0.15
2	1	5	25	4.83 ± 0.32
3	1	10	25	6.91 ± 0.34
4	1	12.5	25	8.41 ± 0.41
5	1	15	25	8.86 ± 0.39
6	1	17.5	25	9.32 ± 0.46
7	0.75	10	25	4.68 ± 0.27
8	0.5	10	25	3.14 ± 0.09
9	0.25	10	25	1.45 ± 0.02
10	1	10	15	4.63 ± 0.27
11	1	10	20	5.67 ± 0.31
12	1	10	30	9.44 ± 0.42
13	1	10	35	12.2 ± 0.51
14	1	10	40	14.8 ± 0.49
15	1	10	45	18.1 ± 0.57
16	1[a]	10	25	3.83 ± 0.14

[a]with deaturated PQI.

Table S2: Kinetic data for the reaction of PQI (**1d**) with PPh_3.

Exp. entry	$[\mathbf{1b}]_0$ (10^{-3} M)	[$\mathbf{PPh_3}$] (10^{-3} M)	T (°C)	V_i[a] (10^{-3} M s^{-1})
1	1	1	25	2.19 ± 0.02
2	1	2	25	3.34 ± 0.11
2	1	3	25	3.99 ± 0.13
3	1	4	25	5.60 ± 0.24
4	1	5	25	6.54 ± 0.39
5	1	6	25	7.20 ± 0.37
6	1	7	25	7.46 ± 0.40
7	1	8	25	8.48 ± 0.41
8	1	9	25	9.31 ± 0.46
9	1	10	25	9.75 ± 0.43
7	0.75	10	25	7.31 ± 0.27
8	0.5	10	25	4.26 ± 0.12
9	0.25	10	25	1.84 ± 0.03
10	1	10	10	6.69 ± 0.29
11	1	10	15	7.72 ± 0.30
12	1	10	20	8.34 ± 0.35
13	1	10	30	10.5 ± 0.44
14	1	10	35	11.7 ± 0.46

Methods

Density Functional Theory (DFT) calculations were performed with the Gaussian 09 software package[11]. The M06-2X hybrid functional was used[12] together with the TZVP basis set[13]. Geometry optimizations were carried out using the SMD (Solvation Model based on solute electron Density)[14] to account for solvent effects. Frequency calculations were done to verify that the calculated structures are stationary points on the potential energy surfaces (PES). The relative energies are given as Gibbs free energies. TD-DFT simulations were carried out using the B97D functional[15] with the TZVP basis sets and SMD.

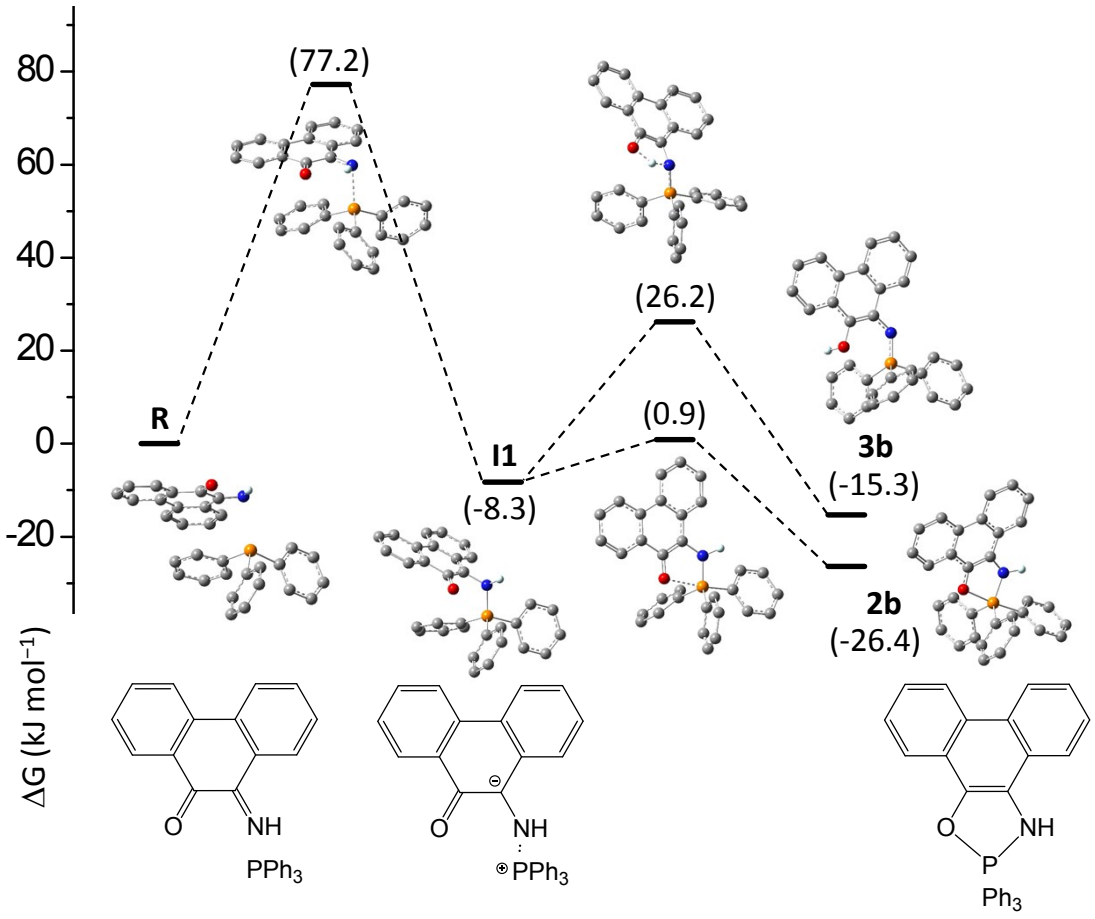


Fig. S9. Reaction pathway of the *Direct Complex formation* of the PQI-PPh_3 complexes. Hydrogen atoms are omitted except the one on the nitrogen atom.

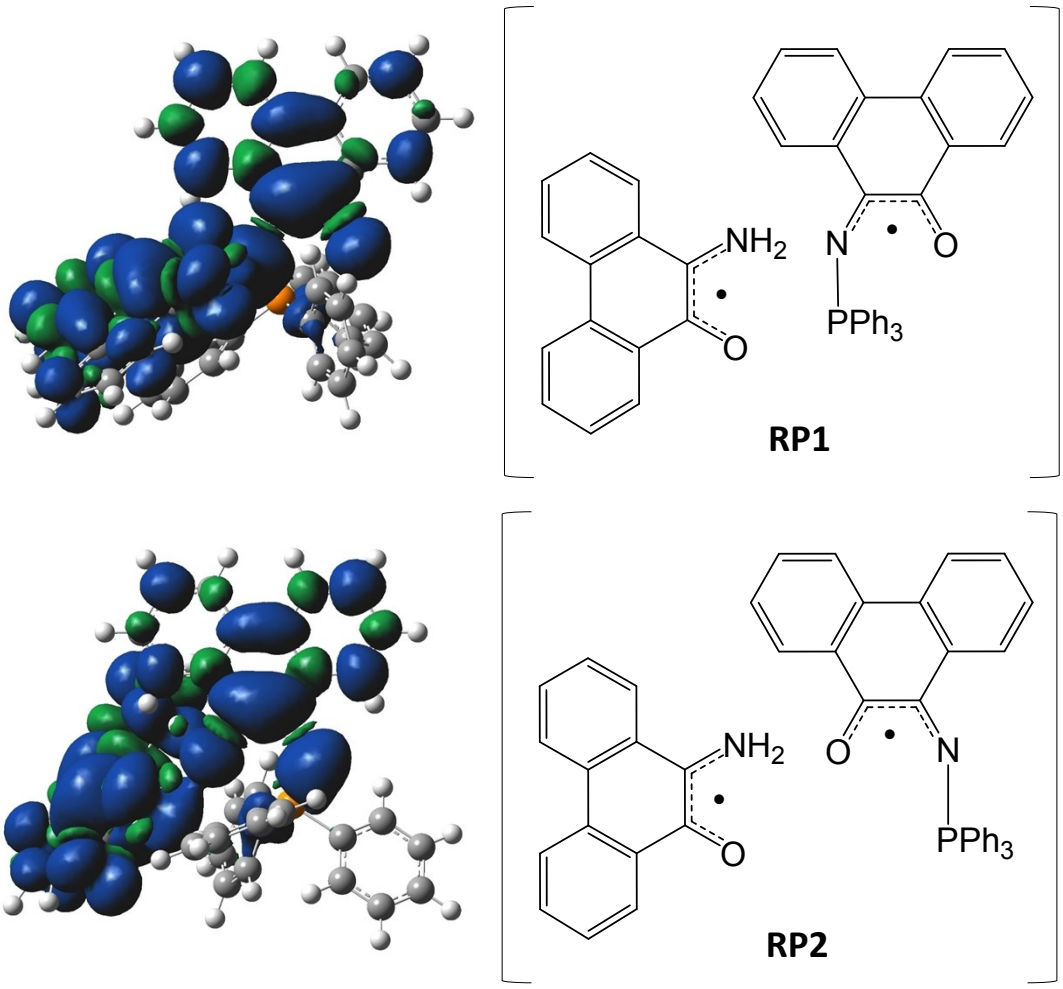


Fig. S10. Structures and spin densities of possible radical pairs in a solvent cage. The unpaired electrons are distributed on the whole aromatic ring and the oxygen and nitrogen atoms as well.

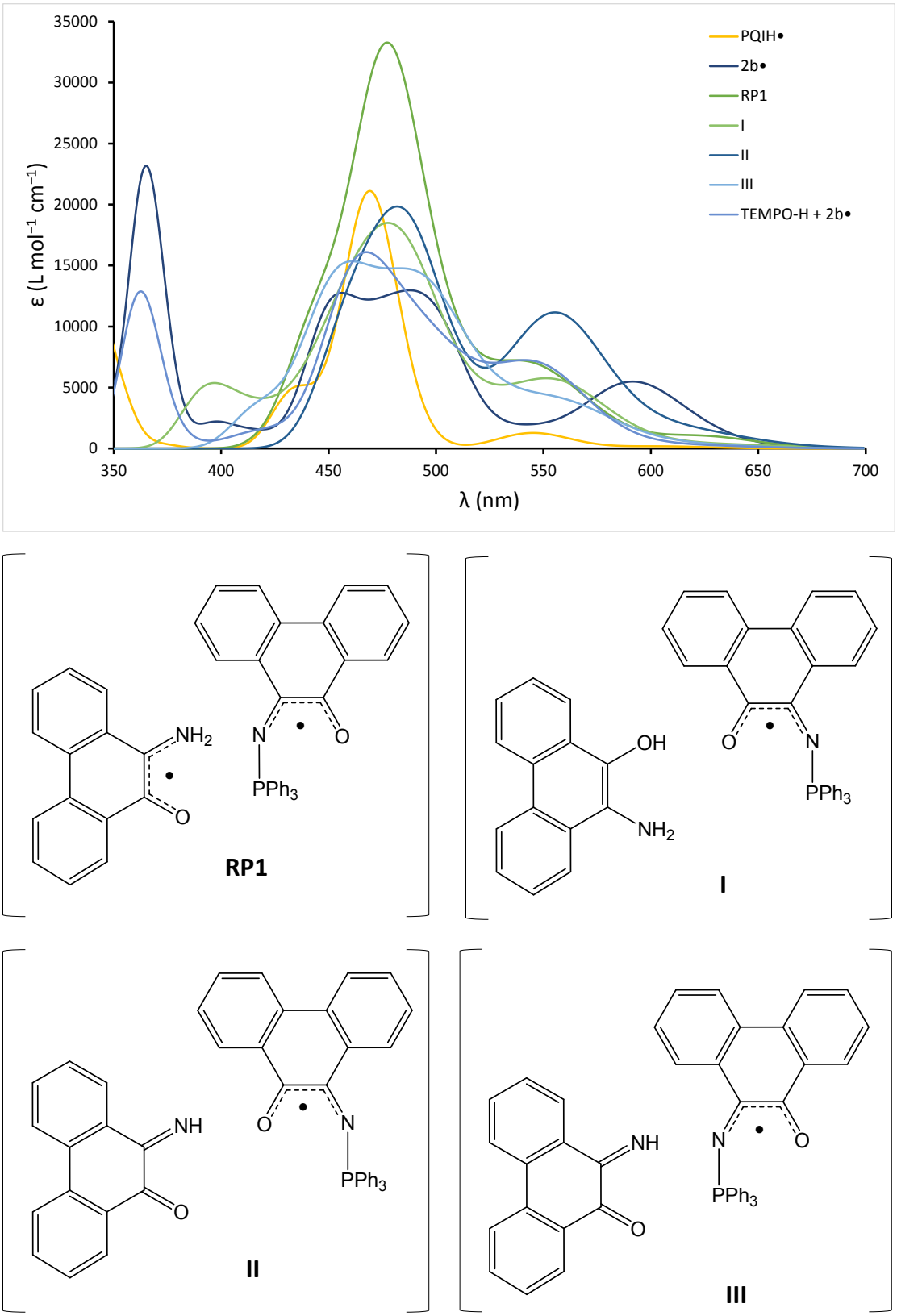


Fig. S11. Simulated UV-VIS spectra at the B97D/TZVP theoretical level and the related structures. The half widths values of the peaks are 0.1 eV.

NUMBER OF ATOMS, ENERGIES, AND COORDINATES OF THE STRUCTURES OPTIMIZED BY M062X/TZVP/SMD METHOD

Number of atoms: 25
Name of the species: PhenQ
Energies in an atomic unit (Hartree):
Electronic energy:
E(SCF) = -668.853237912
Zero-point corrected energy:
E(ZPE) = -668.660358
Gibbs free energy:
E(G) = -668.698461 a.u.
Cartesian coordinates:

C	-3.55328100	-0.78052600	0.01888300
C	-2.85602100	0.41146400	-0.02876400
C	-1.46033600	0.41450400	-0.02672300
C	-0.73089600	-0.78651600	0.01103000
C	-1.45710600	-1.97981800	0.06796900
C	-2.84341300	-1.97653200	0.06984700
C	-0.76969700	1.71616900	-0.06701800
C	0.75472700	-0.77776100	-0.00397300
C	1.46614000	0.43310400	0.02026800
C	0.75029500	1.72493500	0.06066300
C	2.86125400	0.43307100	0.01080500
H	3.38143300	1.38206600	0.03067100
C	3.56710600	-0.75548000	-0.02942800
C	2.87203100	-1.95991600	-0.06382000
C	1.48687800	-1.96875600	-0.05425200
H	-4.63566700	-0.78374500	0.02071700
H	-3.37799900	1.35955700	-0.06263000
H	-0.94893600	-2.93212400	0.11495600
H	-3.37476100	-2.91941700	0.11477000
H	4.64971000	-0.74652900	-0.03884400
H	3.41090000	-2.89858000	-0.10289000
H	0.98098100	-2.92286200	-0.09075500
O	-1.35290200	2.77309700	-0.16905600
N	1.36159900	2.82793000	0.18329700
H	0.68028200	3.59369900	0.17044800

24
PhenQ-N-rad, E(SCF) = -668.192943427, E(ZPE) = -668.013244, E(G) = -668.051693 a.u.

C	-3.52174700	-0.80911600	0.05274700
C	-2.84836400	0.39263600	-0.06213400
C	-1.45356700	0.42044200	-0.06273100
C	-0.70227500	-0.76374100	0.03277900
C	-1.40369300	-1.96565700	0.15420000
C	-2.79011000	-1.98726700	0.16500400
C	-0.79482000	1.73832800	-0.16553700
C	0.78109700	-0.72977900	-0.01096800
C	1.46833900	0.49065600	0.05179900
C	0.70376000	1.75553300	0.16790100
C	2.86100800	0.53648200	0.01725600
H	3.36204000	1.49604100	0.06065500
C	3.59260900	-0.63340300	-0.08567300
C	2.92534400	-1.85135700	-0.15924900
C	1.54058200	-1.89778900	-0.12553500
H	-4.60383600	-0.83160300	0.06302400
H	-3.38830400	1.32785900	-0.14208100
H	-0.87456300	-2.90326700	0.24840000
H	-3.30362600	-2.93559300	0.26614200
H	4.67407900	-0.59709700	-0.11744700
H	3.48597600	-2.77336600	-0.25085400
H	1.05557100	-2.86096200	-0.19997400
O	-1.36769100	2.75849000	-0.45506900
N	1.19788900	2.83346700	0.55621900

26
PhenQ-NH2-rad, E(SCF) = -669.466929201, E(ZPE) = -669.263688, E(G) = -669.302526 a.u.

C	-3.58397100	-0.68454400	0.00365700
C	-2.84112300	0.47698200	0.00890200
C	-1.44097400	0.43002700	0.00915400

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C -0.76987700   -0.80703500   -0.00595600
C -1.54824700   -1.97655600   -0.00988200
C -2.92825000   -1.91810100   -0.00772600
C -0.70104900    1.69781900   -0.00073800
C  0.69916400   -0.84155800    0.00580100
C  1.43814300    0.36686700   -0.00845100
C  0.74211600    1.62953300    0.00159800
C  2.84566700    0.31734400   -0.00578700
H  3.42672400    1.23048000   -0.01101300
C  3.51401100   -0.88682300   -0.00167400
C  2.78905700   -2.08021800    0.00705200
C  1.40811200   -2.05090100    0.00781300
H -4.66611100   -0.64225900    0.00564100
H -3.32239200    1.44677000    0.01539900
H -1.07672200   -2.94907100   -0.02165000
H -3.50164200   -2.83700800   -0.01342300
H  4.59661600   -0.90442000   -0.00229200
H  3.30675700   -3.03127700    0.01148500
H  0.87595900   -2.99154100    0.01747200
O -1.27140600    2.80525000   -0.00384800
N  1.37365200    2.80709500    0.00057800
H  0.80386900    3.64321700    0.00359700
H  2.37594800    2.90643800   -0.00106400


52
phenQ-reduced_phenQ_DIMER, E(SCF) = -1338.95824323, E(ZPE) = -1338.548011, E(G) = -
1338.600676 a.u.
C   -2.49688200    1.40093000    2.48090400
C   -2.11777200    0.09194200    2.25877200
C   -0.80284900   -0.21149200    1.89779400
C    0.16554900    0.79827300    1.76567300
C   -0.24655800    2.11877700    1.97425800
C   -1.55372800    2.41469600    2.32577300
C   -0.47358600   -1.61717600    1.61374000
C    1.57138400    0.46460800    1.42841500
C    1.94282000   -0.85968100    1.13649200
C    0.93618100   -1.93746100    1.13997900
C    3.26527800   -1.17011400    0.82016400
H    3.52230800   -2.19887700    0.60063700
C    4.23622100   -0.18328900    0.79880100
C    3.88208600    1.12633100    1.10132400
C    2.56847200    1.44405800    1.41226300
H   -3.51721400    1.63808200    2.75495700
H   -2.83098600   -0.71737300    2.35289200
H    0.45087100    2.93656400    1.86161600
H   -1.83952600    3.44821000    2.48013600
H    5.26184000   -0.43265400    0.55699500
H    4.63177200    1.90835500    1.09659700
H    2.33317800    2.47277000    1.64631400
O   -1.28001700   -2.52123900    1.70192300
N    1.21226500   -3.11431200    0.74022500
H    0.38457900   -3.71024700    0.84235200
C   -4.19973700   -0.11969000   -0.77453400
C   -3.19972800   -1.04614300   -0.97180300
C   -1.87860400   -0.63900700   -1.23756700
C   -1.57585800    0.74122100   -1.31204400
C   -2.61909500    1.66356300   -1.10363200
C   -3.90591900    1.24626900   -0.84338300
C   -0.83564400   -1.62363300   -1.44164300
C   -0.21344200    1.16365000   -1.60673100
C    0.76905700    0.17989000   -1.85688200
C    0.43597700   -1.20930000   -1.72898700
C    2.08810400    0.56684000   -2.16963100
H    2.82477500   -0.20337600   -2.35553100
C    2.43083400    1.89669500   -2.22933000
C    1.46598400    2.88033600   -1.96641800
C    0.17192400    2.51720400   -1.66565400
H   -5.21227500   -0.44993300   -0.57715900
H   -3.44395300   -2.10019900   -0.94016700
H   -2.42018300    2.72529500   -1.15633100
H   -4.68909500    1.97910800   -0.69223400
H    3.44776400    2.18476700   -2.46791300
H    1.73572500    3.92874800   -2.00354300
H   -0.55218000    3.29631300   -1.46898200
H   -0.37106300   -3.59917000   -1.52008800
O    1.42937500   -2.12662000   -1.95677800
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N   -1.15507800   -2.97181100   -1.40576700
H   -1.76105400   -3.26322500   -0.64806700
H    1.58672700   -2.64722200   -1.14153900

52
phenQ-NH2-rad_DIMER_stacking, E(SCF) = -1338.95208289, E(ZPE) = -1338.540482, E(G) = -
1338.592329 a.u.
C   -3.95512900   -1.16245300   -1.17177000
C   -3.35246000    0.07401500   -1.07359800
C   -1.96846600    0.20896800   -1.23545300
C   -1.16731700   -0.91378100   -1.51193600
C   -1.80067000   -2.16318700   -1.59997400
C   -3.16741300   -2.28626400   -1.42997800
C   -1.38752200    1.55136400   -1.13253200
C    0.27896100   -0.74958500   -1.72270100
C    0.85096700    0.54452200   -1.72885400
C    0.04503200    1.68578200   -1.35778000
C    2.20723200    0.70438300   -2.05899600
H    2.64537500    1.69342100   -2.10590400
C    3.00249000   -0.39077000   -2.32546200
C    2.45799400   -1.67383900   -2.26549500
C    1.11462600   -1.84188200   -1.98360500
H   -5.02586900   -1.26339200   -1.04370700
H   -3.93249400    0.96442600   -0.86538400
H   -1.22731100   -3.05466700   -1.81382300
H   -3.62723300   -3.26401600   -1.51007100
H    4.04852600   -0.25183600   -2.56974900
H    3.07912900   -2.53952200   -2.46005600
H    0.71499800   -2.84647400   -1.96536600
O   -2.07031900    2.55728600   -0.88596400
N    0.49996200    2.94307300   -1.44030500
H   -0.15595500    3.66332600   -1.16101900
H    1.48024800    3.14354900   -1.28617900
C   -3.00252700   -0.35701400    2.33196900
C   -2.20630500    0.73422800    2.05244400
C   -0.85063400    0.56918400    1.72288500
C   -0.27957100   -0.72532800    1.73178000
C   -1.11621500   -1.81374500    2.00521200
C   -2.45933900   -1.64113800    2.28580100
C   -0.04384300    1.70514600    1.33712700
C    1.16657600   -0.89330500    1.52270400
C    1.96868800    0.22546500    1.23314900
C    1.38870700    1.56666000    1.11293400
C    3.35262400    0.08766500    1.07329900
H    3.93334600    0.97511100    0.85468500
C    3.95432200   -1.14800100    1.18607700
C    3.16557800   -2.26818400    1.45685800
C    1.79885300   -2.14215000    1.62515900
H   -4.04814100   -0.21417400    2.57577500
H   -2.64326300    1.72416200    2.08898300
H   -0.71755100   -2.81884800    1.99861400
H   -3.08116900   -2.50403600    2.49026800
H    5.02501000   -1.25136200    1.05953000
H    3.62458200   -3.24536500    1.54798300
H    1.22465500   -3.03063800    1.84900400
H    0.15936700    3.68052700    1.11738000
H   -1.47803400    3.16462000    1.25438300
O    2.07172200    2.56902200    0.85287400
N   -0.49723000    2.96323900    1.40227500

27
phenQ_reduced, E(SCF) = -670.082181011, E(ZPE) = -669.866349, E(G) = -669.904371 a.u.
C    3.54345900   -0.78147400   -0.06067600
C    2.82682300    0.39131400   -0.09024600
C    1.41664200    0.38020100   -0.02053600
C    0.73323300   -0.85899500    0.02807700
C    1.49818300   -2.04106300    0.06676400
C    2.87376300   -2.00889900    0.02666700
C    0.66292300    1.59964300   -0.00167200
C   -0.72172000   -0.86360300    0.03622300
C   -1.42279900    0.36439000   -0.02150300
C   -0.69841000    1.61300800    0.01697100
C   -2.83226100    0.35504400   -0.07717200
H   -3.37435600    1.28908500   -0.14967000
C   -3.53334900   -0.82753800   -0.06578500
C   -2.84488900   -2.04557000    0.00391700
C   -1.46970200   -2.05843300    0.04511300
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H    4.62493300   -0.75476900   -0.11351600
H    3.36356000    1.32794000   -0.18193200
H    1.00602800   -3.00222200    0.12316800
H    3.43663500   -2.93347700    0.05610100
H   -4.61522800   -0.81626800   -0.11541900
H   -3.39355200   -2.97920800    0.01407900
H   -0.96345000   -3.01296700    0.08521300
O    1.29218700    2.82043000   -0.01878100
N   -1.38939000    2.82505700   -0.01461300
H   -0.79136300    3.61292200    0.20169100
H    2.12938000    2.77539100    0.46076500
H   -2.22572900    2.84658900    0.55520500
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DIRECT COMPLEX FORMATION:

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59
Reactant, E(SCF) = -1705.09532932, E(ZPE) = -1704.627151, E(G) = -1704.693088 a.u.
C   4.36653700   -3.27734900   -0.59685000
C   3.33370800   -2.66512800   -1.28155500
C   3.05259500   -1.31399600   -1.07679900
C   3.80733400   -0.54251600   -0.17655300
C   4.84998700   -1.18138600    0.50192200
C   5.12501300   -2.52456600    0.29473200
C   1.93396000   -0.71882200   -1.83238100
C   3.46715300    0.88046100    0.07589200
C   2.40982500    1.50063900   -0.61083700
C   1.62841100    0.75812500   -1.62054800
C   2.06654300    2.82453600   -0.33157800
H   1.23688100    3.27027100   -0.86611300
C   2.76559300    3.55167500    0.61485800
C   3.82142900    2.94985600    1.29235400
C   4.16496000    1.63511900    1.02557900
H   4.58365500   -4.32612000   -0.75400500
H   2.72520800   -3.22169400   -1.98329600
H   5.46412300   -0.63839600    1.20565100
H   5.93962200   -2.98859700    0.83744600
H   2.49095700    4.57728800    0.82769700
H   4.37832300    3.50558000    2.03678400
H   4.98466700    1.19975600    1.57899600
O   1.26316700   -1.34799700   -2.62161500
N   0.71095200    1.30943000   -2.30061600
P  -1.89003000   -0.30971700   -0.71116400
C  -0.68529900   -0.07744000    0.66954600
C  -0.63116800    1.06220600    1.46908900
C   0.24822900   -1.09791700    0.87999600
C   0.33405600    1.17758300    2.46655900
H  -1.34300800    1.86590000    1.32311900
C   1.20042200   -0.98868300    1.88440400
H   0.22038700   -1.99206400    0.26367500
C   1.24951200    0.15424300    2.67754000
H   0.36532500    2.07044300    3.08005100
H   1.91353800   -1.79038200    2.03881500
H   1.99968700    0.24659500    3.45387400
C  -2.94603800    1.20001700   -0.54721200
C  -2.55370000    2.33118900   -1.26696200
C  -4.09007600    1.26482000    0.24721700
C  -3.28342300    3.51074700   -1.18027500
H  -1.66629600    2.29100100   -1.89087400
C  -4.82602600    2.44239900    0.32433100
H  -4.41197300    0.39748800    0.81148500
C  -4.42345900    3.56717300   -0.38618800
H  -2.96697100    4.38262900   -1.74029600
H  -5.71497100    2.47920100    0.94280300
H  -4.99842500    4.48333600   -0.32574000
C  -2.99539400   -1.61591500   -0.01092200
C  -3.06745600   -1.93650400    1.34508100
C  -3.80974400   -2.30196000   -0.91360900
C  -3.94249400   -2.92176700    1.78843700
H  -2.44397900   -1.41398200    2.06152000
C  -4.69191500   -3.27967300   -0.46907800
H  -3.75355400   -2.07090900   -1.97238400
C  -4.75784000   -3.59230200    0.88372200
H  -3.98966100   -3.16233200    2.84388100
H  -5.32030300   -3.80233700   -1.18013900
H  -5.43929200   -4.35895700    1.23225500
H   0.28708400    0.61081000   -2.91998400
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59
TS1, E(SCF) = -1705.07008023, E(ZPE) = -1704.601155, E(G) = -1704.663699 a.u.
C  -4.46899300   -2.81516700    0.18875700
C  -3.26153800   -2.59305500   -0.44049600
C  -2.82614400   -1.29196300   -0.71594500
C  -3.60777400   -0.18024100   -0.34494800
C  -4.83584800   -0.43211200    0.28890400
C  -5.25801600   -1.72157500    0.55150100
C  -1.50470600   -1.11621800   -1.34731300
C  -3.11980600    1.18926700   -0.58683900
C  -1.83934300    1.38340500   -1.14678900
C  -1.03720600    0.24188200   -1.56206900
C  -1.34862700    2.68813400   -1.31191000
H  -0.36294500    2.82129800   -1.74035400
C  -2.10005300    3.78296800   -0.93502400
C  -3.37365600    3.59799000   -0.39347100
C  -3.86965900    2.31857800   -0.22516900
H  -4.80131000   -3.82380500    0.40085800
H  -2.62386400   -3.41834600   -0.73197600
H  -5.47130400    0.38746300    0.59379300
H  -6.20883000   -1.88011500    1.04611300
H  -1.70331300    4.78279700   -1.06497600
H  -3.97365500    4.45162100   -0.10332100
H  -4.85739500    2.20253600    0.19975200
O  -0.78272700   -2.07838500   -1.64199600
N   0.20048200    0.40796300   -2.01306400
P   1.61905400   -0.06597700   -0.27251600
C   2.45272600    1.48169700    0.19639500
C   2.72619200    1.80837200    1.52555400
C   2.84110100    2.34520300   -0.82754100
C   3.38483200    2.99374300    1.82341100
H   2.42854500    1.13773900    2.32338600
C   3.50588900    3.52714400   -0.52377500
H   2.61704900    2.09656700   -1.85886000
C   3.77548500    3.85168500    0.80018800
H   3.59646300    3.24616000    2.85529300
H   3.80650600    4.19584600   -1.32091400
H   4.28922400    4.77554400    1.03690900
C   0.48007500   -0.48657700    1.07154100
C  -0.40324000    0.50307300    1.50873600
C   0.33513000   -1.79358400    1.54511700
C  -1.40942500    0.19395400    2.41744800
H  -0.30391900    1.52082400    1.14810500
C  -0.66892300   -2.09623000    2.45190600
H   1.00295300   -2.57648800    1.20705600
C  -1.54854300   -1.10586500    2.88388100
H  -2.08861300    0.97040600    2.74868300
H  -0.77027900   -3.10997400    2.81980200
H  -2.33862900   -1.35022200    3.58374400
C   2.90510800   -1.35686800   -0.36665600
C   4.21795100   -1.13949200    0.05337400
C   2.54927500   -2.58161100   -0.93859000
C   5.15922800   -2.15315600   -0.07478400
H   4.50658600   -0.18775700    0.48346500
C   3.49340400   -3.59355000   -1.05094100
H   1.53269000   -2.73553500   -1.28848500
C   4.79855100   -3.37960800   -0.62159800
H   6.17705800   -1.98353900    0.25490100
H   3.21177800   -4.54492800   -1.48545100
H   5.53687200   -4.16616500   -0.71947400
H   0.51028100   -0.47227400   -2.43003600

59
I1, E(SCF) = -1705.10492592, E(ZPE) = -1704.635388, E(G) = -1704.696241 a.u.
C  -4.90952100    2.71842300   -0.31921000
C  -3.56648800    2.56262200   -0.58124400
C  -2.99065700    1.28623900   -0.68529300
C  -3.78705700    0.13715800   -0.50005300
C  -5.16088900    0.32242700   -0.23680500
C  -5.71111800    1.58240000   -0.14781200
C  -1.53854100    1.19636300   -0.95707900
C  -3.17865200   -1.18558500   -0.58605800
C  -1.79157400   -1.27780000   -0.89161400
C  -1.02340000   -0.09550500   -1.10956500
C  -1.20557100   -2.56723700   -0.94621900
H  -0.15024000   -2.64770000   -1.17047500
C  -1.94604600   -3.70350600   -0.71412500
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C  -3.31205000   -3.60982800   -0.41545100
C  -3.90540900   -2.36619300   -0.35543500
H  -5.34466500    3.70786700   -0.24504500
H  -2.91694000    3.41824100   -0.71762400
H  -5.80766300   -0.53359300   -0.09871900
H  -6.76981600    1.69174300    0.05559800
H  -1.46719500   -4.67498200   -0.76177600
H  -3.89592100   -4.50256300   -0.22931600
H  -4.95914700   -2.30905500   -0.11530500
O  -0.82955800    2.23918800   -1.01693600
N   0.38673500   -0.23635300   -1.36263400
P   1.49560100    0.06011300   -0.15073000
C   0.68938400   -0.37786700    1.39732700
C  -0.26728100    0.49406800    1.92292000
C   0.94346500   -1.60694100    2.00019000
C  -0.97420900    0.12274000    3.05610300
H  -0.45797800    1.44928000    1.44493500
C   0.23347400   -1.96584500    3.14022600
H   1.68312300   -2.28179300    1.58508400
C  -0.72479900   -1.10598100    3.66121500
H  -1.72047700    0.79155800    3.46615500
H   0.42596300   -2.91975200    3.61480600
H  -1.28082700   -1.39181900    4.54588100
C   2.14272400    1.75084600   -0.05175900
C   2.39687300    2.35718600    1.17508400
C   2.45270400    2.40532700   -1.24341400
C   2.94913500    3.63308200    1.20694300
H   2.16823800    1.84498800    2.10196300
C   3.00262000    3.67664100   -1.20272100
H   2.25902100    1.93167700   -2.19971400
C   3.24718300    4.29213300    0.02210500
H   3.14203400    4.10926500    2.16025000
H   3.23777300    4.19114000   -2.12605000
H   3.67252300    5.28793100    0.05050500
C   2.92052600   -1.01102200   -0.46806500
C   4.10086900   -0.80697700    0.24861800
C   2.83418500   -2.03119900   -1.41183600
C   5.19123600   -1.63281000    0.02049700
H   4.17209700   -0.00913800    0.97975500
C   3.93616000   -2.84617500   -1.64197500
H   1.91853700   -2.18378000   -1.96790200
C   5.10969000   -2.64929700   -0.92655500
H   6.10769900   -1.47850700    0.57605900
H   3.87314700   -3.63496700   -2.38119900
H   5.96632700   -3.28674200   -1.10881300
H   0.69788400    0.08266800   -2.27783900

59
TS2, E(SCF) = -1705.10420804, E(ZPE) = -1704.633916, E(G) = -1704.692735 a.u.
C   4.52797500   -2.95270600    0.26621100
C   3.22799300   -2.51527300    0.16440800
C   2.93866700   -1.15651600   -0.05489200
C   3.98845800   -0.21552100   -0.16875500
C   5.31196500   -0.69457800   -0.06041300
C   5.57772800   -2.02867800    0.15282500
C   1.54450600   -0.74263000   -0.16656500
C   3.67730100    1.18831900   -0.39903400
C   2.31194800    1.58490200   -0.48127200
C   1.29493300    0.59524200   -0.40529700
C   2.01118200    2.95744000   -0.66515500
H   0.97742900    3.27843900   -0.71348900
C   3.01024200    3.89661600   -0.76439900
C   4.35552800    3.50754200   -0.69086800
C   4.67086300    2.17851100   -0.50621200
H   4.74302000   -4.00098000    0.43507400
H   2.39556700   -3.20289200    0.24942100
H   6.14477000   -0.00892400   -0.14147200
H   6.60463500   -2.36452100    0.23315400
H   2.75554700    4.94134000   -0.89894400
H   5.14286400    4.24634900   -0.77343400
H   5.71484600    1.89996500   -0.44677300
O   0.56566700   -1.56342900   -0.05813100
N  -0.07432000    0.95698600   -0.52556900
P  -1.36542400    0.01605100   -0.05711300
C  -1.35444400   -0.43265500    1.70577700
C  -1.22326900   -1.75985500    2.11104400
C  -1.49933600    0.57940300    2.65282200
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C  -1.25831400   -2.07044100    3.46241600
H  -1.07079900   -2.53614700    1.37516400
C  -1.50686600    0.26262200    4.00598900
H  -1.60166700    1.61360900    2.34787100
C  -1.39680800   -1.06116500    4.40995600
H  -1.16595200   -3.10246400    3.77723500
H  -1.60882600    1.05170400    4.74041700
H  -1.41406000   -1.30812900    5.46462700
C  -1.92113000   -1.33911400   -1.13057700
C  -2.88536200   -2.24607700   -0.70204500
C  -1.41083600   -1.40965200   -2.42388500
C  -3.33233900   -3.23506200   -1.57193700
H  -3.29771900   -2.18408200    0.29819600
C  -1.86716800   -2.39449000   -3.28831900
H  -0.65122400   -0.70851100   -2.75107800
C  -2.82520700   -3.30924900   -2.86229800
H  -4.07899500   -3.94390600   -1.23603000
H  -1.46917400   -2.45287500   -4.29379900
H  -3.17565100   -4.07956700   -3.53831400
C  -2.69924400    1.27788100   -0.22505300
C  -3.99301400    0.90913100   -0.59517000
C  -2.42837200    2.62272300    0.04696500
C  -4.99574200    1.86634400   -0.69023000
H  -4.23305200   -0.12119100   -0.82086700
C  -3.43234600    3.57613300   -0.05367400
H  -1.43313400    2.93180900    0.34231400
C  -4.71824800    3.20014000   -0.42225500
H  -5.99409600    1.56531800   -0.98257400
H  -3.20670200    4.61420500    0.15734500
H  -5.50035800    3.94514800   -0.50390300
H  -0.30848400    1.65835300   -1.22005000

59
TS3, E(SCF) = -1705.09062605, E(ZPE) = -1704.623647, E(G) = -1704.683123 a.u.
C   5.37716200   -2.53738100   -0.41372100
C   4.03281800   -2.49660100   -0.69466200
C   3.32868400   -1.27791800   -0.64965800
C   3.99678100   -0.07274400   -0.32267500
C   5.37654100   -0.15207500   -0.03546000
C   6.05057000   -1.35162600   -0.07834400
C   1.91580100   -1.25059300   -0.90354900
C   3.25938400    1.18349300   -0.31931600
C   1.85990000    1.17968500   -0.59069600
C   1.20560900   -0.07076600   -0.77800800
C   1.18340800    2.41449100   -0.71322700
H   0.13947100    2.41381100   -0.99666200
C   1.83707000    3.60613700   -0.51103700
C   3.20179800    3.61282100   -0.18431400
C   3.89243300    2.42418500   -0.10631800
H   5.91633000   -3.47631000   -0.44625300
H   3.48602500   -3.39563200   -0.95103100
H   5.92807500    0.74036600    0.22775100
H   7.10954800   -1.37843600    0.14839300
H   1.29925000    4.54130000   -0.61502200
H   3.71705300    4.55064000   -0.01789600
H   4.95176200    2.45580000    0.11133400
O   1.19885700   -2.29909000   -1.23673200
N  -0.15693000   -0.34477600   -1.10082800
P  -1.44769300   -0.16180400   -0.09776500
C  -1.99594800    1.55406600    0.10413200
C  -1.51584400    2.34276800    1.14955900
C  -2.82493100    2.10774400   -0.87083100
C  -1.87225400    3.68188300    1.21970700
H  -0.85122800    1.92287700    1.89552200
C  -3.17332100    3.44967700   -0.79687200
H  -3.19572500    1.49778300   -1.68688200
C  -2.69867700    4.23462500    0.24727300
H  -1.49885500    4.29517400    2.03018400
H  -3.81812100    3.87983200   -1.55290700
H  -2.97397700    5.28078800    0.30388200
C  -1.21881300   -0.86387300    1.56602900
C  -2.01342400   -0.47143400    2.64511400
C  -0.25802100   -1.86211100    1.72885200
C  -1.84164000   -1.07691600    3.88206100
H  -2.76652000    0.29809800    2.52460000
C  -0.08772300   -2.45676600    2.97307100
H   0.34538800   -2.18710400    0.88867200
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C  -0.87597000   -2.06416200    4.04740500
H  -2.45982300   -0.77470600    4.71818600
H   0.66210000   -3.22763900    3.10031300
H  -0.74039700   -2.52914700    5.01642200
C  -2.79186000   -1.06579500   -0.91743900
C  -4.00127500   -1.24087200   -0.24458300
C  -2.62442700   -1.56823000   -2.20522500
C  -5.03899800   -1.92397000   -0.86133500
H  -4.13993000   -0.84519200    0.75539400
C  -3.66850700   -2.25457600   -2.81462900
H  -1.68970500   -1.42288600   -2.73097900
C  -4.87209900   -2.43235900   -2.14567000
H  -5.97772500   -2.06061600   -0.33934600
H  -3.53833000   -2.64770100   -3.81515800
H  -5.68355100   -2.96624900   -2.62505300
H   0.13658600   -1.53647800   -1.31113900

59
2b, E(SCF) = -1705.11277779, E(ZPE) = -1704.642919, E(G) = -1704.703144 a.u.
C  -4.11983500   -3.19768800   -0.08117300
C  -2.88022500   -2.60898400   -0.14286000
C  -2.75903200   -1.20770000   -0.22316500
C  -3.91352800   -0.38491400   -0.23501800
C  -5.16928200   -1.02524300   -0.17226400
C  -5.27294100   -2.39543200   -0.09539800
C  -1.47066700   -0.58842900   -0.28067000
C  -3.76970400    1.06146200   -0.32320300
C  -2.47041500    1.64019400   -0.36478300
C  -1.34702100    0.76689500   -0.35217200
C  -2.33308500    3.04389800   -0.44268900
H  -1.34456200    3.48587800   -0.48281200
C  -3.43947500    3.85812600   -0.46756200
C  -4.72458200    3.29659900   -0.41982300
C  -4.87854400    1.93083700   -0.34696200
H  -4.21093200   -4.27542000   -0.01972700
H  -1.97631100   -3.20545600   -0.13179300
H  -6.07776900   -0.43830900   -0.17846500
H  -6.25171800   -2.85668300   -0.04460300
H  -3.31865600    4.93310900   -0.52580200
H  -5.59743500    3.93730400   -0.43870100
H  -5.88095600    1.52585300   -0.31336500
O  -0.32589400   -1.25343400   -0.28739500
N   0.00322600    1.14251300   -0.39043900
P   1.17355800   -0.03999200   -0.03504800
C   1.24839900   -0.69341900    1.66881200
C   0.63657600    0.04836400    2.67657200
C   1.85122200   -1.91238100    1.96441100
C   0.63156500   -0.43101000    3.98147200
H   0.16858100    1.00082500    2.44815700
C   1.85311300   -2.38034400    3.27287400
H   2.31293300   -2.50199100    1.18111300
C   1.24398900   -1.64195800    4.28142500
H   0.15161300    0.14452200    4.76359100
H   2.32868400   -3.32612000    3.50265200
H   1.24317000   -2.01214500    5.29930200
C   2.53624200    1.26467800    0.08552900
C   3.26989600    1.52871800    1.23998900
C   2.83273100    1.99447300   -1.07196200
C   4.26887100    2.50046200    1.24166400
H   3.07866800    0.97766900    2.15231900
C   3.82199900    2.96712200   -1.07187500
H   2.28908600    1.79212400   -1.99024100
C   4.54528900    3.22237900    0.08985000
H   4.82961400    2.68980900    2.14931600
H   4.03607200    3.52017200   -1.97869300
H   5.32273100    3.97710500    0.09255500
C   2.02873300   -1.04241000   -1.31393300
C   3.36839900   -1.38215200   -1.13008500
C   1.37841200   -1.39876100   -2.49198600
C   4.04136600   -2.10676700   -2.10543100
H   3.89173300   -1.08596700   -0.22748500
C   2.06741400   -2.08868400   -3.48231900
H   0.33789900   -1.13834500   -2.63538500
C   3.39408500   -2.45225900   -3.28644800
H   5.07547100   -2.38733600   -1.94754500
H   1.56188200   -2.34857600   -4.40430100
H   3.92472400   -3.00125400   -4.05493200
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H   0.26689600    2.10896700   -0.26210900

59
3b, E(SCF) = -1705.10683351, E(ZPE) = -1704.637960, E(G) = -1704.698926 a.u.
C   4.84814300   -2.75430200   -0.06743500
C   3.51455900   -2.41892700   -0.04972500
C   3.10859900   -1.06658800   -0.00340400
C   4.09067900   -0.04852500    0.01778800
C   5.44702100   -0.42511900   -0.00339100
C   5.82442800   -1.74944400   -0.03930600
C   1.71898200   -0.72255300    0.05299800
C   3.65142600    1.33838200    0.02949700
C   2.26834900    1.63341300    0.05195600
C   1.26361800    0.57050200    0.06879300
C   1.85237800    2.97945300    0.06054700
H   0.79045800    3.18513100    0.07181000
C   2.76550600    4.00808600    0.05406800
C   4.13664800    3.72042800    0.03744500
C   4.56460400    2.41295200    0.02627200
H   5.14306500   -3.79610700   -0.10643200
H   2.76631100   -3.20056100   -0.08677800
H   6.22056900    0.33082800    0.01271400
H   6.87526500   -2.01123600   -0.05200900
H   2.42585000    5.03680200    0.06002700
H   4.86146500    4.52545300    0.03193900
H   5.62803800    2.21817000    0.01042700
O   0.78488500   -1.74049200    0.02497400
N  -0.04776200    0.97163800    0.12808800
P  -1.38437100    0.09605000    0.01832000
C  -1.61974600   -0.87387200   -1.51318000
C  -1.59900600   -0.16289700   -2.71290800
C  -1.78811500   -2.25518700   -1.52602900
C  -1.75066700   -0.83228000   -3.91993500
H  -1.46420600    0.91386000   -2.70521000
C  -1.94676000   -2.92061300   -2.73531200
H  -1.78388400   -2.81659200   -0.60025100
C  -1.92939300   -2.21117800   -3.93075300
H  -1.73222400   -0.27706400   -4.84956800
H  -2.08091200   -3.99531600   -2.74310000
H  -2.05232100   -2.73295500   -4.87208400
C  -2.74860700    1.30975200   -0.00053200
C  -3.98726300    0.97573500   -0.54678200
C  -2.56348600    2.55853200    0.58945200
C  -5.03341000    1.88855300   -0.50440500
H  -4.13847200    0.00863100   -1.01330200
C  -3.61258500    3.46862000    0.62795000
H  -1.59826100    2.81447400    1.00890200
C  -4.84701800    3.13464600    0.08317900
H  -5.99247200    1.62698500   -0.93441200
H  -3.46476900    4.44020500    1.08364400
H  -5.66340400    3.84610900    0.11362400
C  -1.76221200   -0.96903100    1.45707000
C  -2.96616000   -1.66571200    1.54940900
C  -0.85387500   -1.00544600    2.51183700
C  -3.24693500   -2.41429600    2.68497900
H  -3.68458400   -1.63100300    0.73773200
C  -1.14045300   -1.75216000    3.64850200
H   0.07583600   -0.45053400    2.44331100
C  -2.33470800   -2.45832700    3.73364000
H  -4.17951000   -2.96095900    2.75159100
H  -0.43181600   -1.78055700    4.46709200
H  -2.55789500   -3.04078000    4.61932400
H   0.91146600   -2.32685300    0.78609900

84
RP1, E(SCF) = -2373.97352359, E(ZPE) = -2373.309395, E(G) = -2373.386900 a.u.
C  -6.71381500   -1.27714700    1.97521900
C  -5.57377400   -0.55482000    1.69309000
C  -4.56800000   -1.09404200    0.87993900
C  -4.70339100   -2.38815800    0.34652900
C  -5.87381200   -3.10490200    0.64559100
C  -6.86037200   -2.56201300    1.44570100
C  -3.36886500   -0.28374400    0.62653300
C  -3.63832300   -2.93214800   -0.50532100
C  -2.49087400   -2.15328600   -0.78774300
C  -2.33295700   -0.81668100   -0.23124200
C  -1.49370400   -2.68225400   -1.62692500
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H  -0.63353300   -2.06867000   -1.85362600
C  -1.60276700   -3.94817100   -2.16050000
C  -2.72658000   -4.72456000   -1.86978600
C  -3.72323100   -4.21841100   -1.05840600
H  -7.48847600   -0.85418100    2.60284300
H  -5.43250600    0.44193600    2.09112600
H  -6.02210000   -4.10134700    0.25327300
H  -7.75162300   -3.13869000    1.66139000
H  -0.82226500   -4.33574300   -2.80374000
H  -2.82298000   -5.72188800   -2.28088900
H  -4.58340100   -4.84062400   -0.85418600
O  -3.22785900    0.84259200    1.14478100
N  -1.21404100   -0.13167300   -0.51825700
P  -0.91681400    1.44097900   -0.14344200
C   0.59988400    1.84949600   -1.08186800
C   0.49890300    2.11083600   -2.45086100
C   1.85035100    1.88061200   -0.46749100
C   1.63470100    2.40967800   -3.18913400
H  -0.46554200    2.09111400   -2.94481300
C   2.98553900    2.18753200   -1.21064100
H   1.95221500    1.66270400    0.58898400
C   2.87918600    2.45583600   -2.56801300
H   1.54699300    2.61380400   -4.24917300
H   3.95241600    2.21294300   -0.72234400
H   3.76421100    2.69775800   -3.14434200
C  -2.19377200    2.58287000   -0.77198900
C  -2.92708300    2.18795300   -1.89034900
C  -2.44231800    3.81383400   -0.17229000
C  -3.90181700    3.03076600   -2.40936700
H  -2.74591300    1.22304900   -2.35091000
C  -3.41816800    4.65139300   -0.69730200
H  -1.89906600    4.12256900    0.71103000
C  -4.14692800    4.26311700   -1.81506700
H  -4.47183600    2.72131100   -3.27680400
H  -3.61187300    5.60692700   -0.22557500
H  -4.90816300    4.91868900   -2.21994400
C  -0.48267200    1.77070400    1.59422500
C   0.08713400    2.98713700    1.96823000
C  -0.64686800    0.75779000    2.53550800
C   0.45813200    3.19790100    3.29015800
H   0.26018500    3.76529000    1.23347700
C  -0.25755100    0.96719600    3.85140100
H  -1.07763000   -0.19201400    2.24144800
C   0.28671900    2.18906200    4.23044100
H   0.89242200    4.14646000    3.58054000
H  -0.38160700    0.17642700    4.58078000
H   0.58498200    2.35266900    5.25890700
H   0.63439500   -1.13441600   -0.07143300
C   7.07042800   -1.00550200    2.57331200
C   5.70202200   -1.15054900    2.65937100
C   4.90828900   -1.14769500    1.50449400
C   5.49956100   -1.00581200    0.23443200
C   6.89485300   -0.85560000    0.17276600
C   7.66684300   -0.85748200    1.31837700
C   3.45562100   -1.29829700    1.65548100
C   4.65516200   -0.99869000   -0.96776900
C   3.25350200   -1.15483500   -0.84964600
C   2.65184500   -1.25900300    0.45522000
C   2.45467000   -1.14709100   -2.00869100
H   1.38059100   -1.25020400   -1.92825900
C   3.01555000   -1.00489200   -3.25798600
C   4.39854800   -0.85093300   -3.37974700
C   5.19750700   -0.85202400   -2.25266300
H   7.67841700   -1.00616800    3.46960500
H   5.21230600   -1.26605500    3.61811700
H   7.39131900   -0.73759900   -0.78034900
H   8.74089500   -0.74103800    1.23860800
H   2.38465400   -1.00144800   -4.13827300
H   4.84963500   -0.73253800   -4.35727100
H   6.26410400   -0.73128200   -2.38132400
O   2.90884500   -1.42272500    2.76777300
N   1.33061100   -1.33837100    0.63988800
H   1.01325700   -1.37289600    1.60157200

84
RP2, E(SCF) = -2373.98024235, E(ZPE) = -2373.316806, E(G) = -2373.395706 a.u.
C  -0.24318700    4.36867300    2.37019800
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C	0.06288900	3.08438100	1.97342800
C	1.12460200	2.84106700	1.08893400
C	1.89406600	3.91087300	0.59360700
C	1.56482000	5.20944400	1.01367800
C	0.51429400	5.43635900	1.88192300
C	1.38937300	1.46216400	0.67398100
C	3.01512100	3.63586100	-0.31378700
C	3.29796900	2.30718600	-0.70273000
C	2.49747300	1.19205300	-0.20966900
C	4.37855500	2.05483200	-1.56620600
H	4.58463700	1.03019200	-1.84645200
C	5.16186500	3.08238400	-2.04521000
C	4.88232700	4.39780800	-1.66714300
C	3.82616400	4.66358400	-0.81786400
H	-1.06249500	4.54875600	3.05504000
H	-0.50926900	2.24078000	2.34079700
H	2.13093600	6.05959300	0.65878600
H	0.28241800	6.44976500	2.18621900
H	5.99095200	2.86982600	-2.70895800
H	5.49231000	5.21291300	-2.03667200
H	3.63541400	5.69079200	-0.54010700
O	0.67364300	0.50927500	1.07316600
N	2.80984600	-0.03765900	-0.61832800
P	2.14282600	-1.45289800	-0.13950600
C	2.28673600	-1.84626700	1.63165100
C	1.18030200	-2.09871500	2.43583600
C	3.57160800	-1.88172900	2.17219900
C	1.35946900	-2.39931100	3.77929700
H	0.18306100	-2.05695200	2.01904400
C	3.74410200	-2.16893700	3.51992300
H	4.43534500	-1.68557600	1.54546700
C	2.63940100	-2.43270500	4.32134300
H	0.49806700	-2.60375300	4.40313200
H	4.74158700	-2.19188400	3.94082800
H	2.77650100	-2.66360600	5.37076000
C	3.16915300	-2.70892700	-0.97349500
C	3.82261500	-2.38641300	-2.16109800
C	3.24433900	-4.00551500	-0.46541900
C	4.55422000	-3.35756300	-2.83310300
H	3.76284100	-1.37803600	-2.55130000
C	3.97636700	-4.97227600	-1.14237200
H	2.74033300	-4.26361500	0.45923900
C	4.63177300	-4.64904400	-2.32492600
H	5.06637300	-3.10365900	-3.75300800
H	4.03863600	-5.97682000	-0.74261200
H	5.20457600	-5.40435700	-2.84914800
C	0.45748600	-1.75334100	-0.75888000
C	-0.19186600	-2.95812600	-0.49745400
C	-0.14605300	-0.78715500	-1.55938600
C	-1.46223600	-3.18001600	-1.01556800
H	0.28431600	-3.71906300	0.11123700
C	-1.40466300	-1.02565500	-2.09372800
H	0.36054800	0.15005900	-1.76168900
C	-2.06730800	-2.21555100	-1.81380100
H	-1.97571900	-4.10884800	-0.79949300
H	-1.87490200	-0.27348100	-2.71586700
H	-3.05685500	-2.39131600	-2.21949200
C	-7.78294000	-1.65190200	-0.01852500
C	-6.55786500	-1.81635700	0.59215400
C	-5.50463100	-0.92890400	0.33368800
C	-5.68559200	0.15143700	-0.55090100
C	-6.94217200	0.29768100	-1.16167000
C	-7.97240100	-0.58480400	-0.90047700
C	-4.22413900	-1.14938200	1.01568500
C	-4.57089400	1.07120900	-0.81727400
C	-3.33371300	0.89447500	-0.15400000
C	-3.14961700	-0.22485900	0.73491100
C	-2.27299200	1.78310700	-0.41310100
H	-1.31753600	1.64400200	0.07752500
C	-2.42516600	2.83465500	-1.28934200
C	-3.64621000	3.01517700	-1.94457900
C	-4.69576300	2.14883200	-1.70603100
H	-8.59271700	-2.34185800	0.18434800
H	-6.38298900	-2.63223300	1.28197700
H	-7.12525200	1.11343500	-1.84703700
H	-8.93158900	-0.44455600	-1.38389900
H	-1.59903300	3.51153500	-1.47191400

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H  -3.77519300    3.83522800   -2.63993400
H  -5.62722400    2.31456900   -2.22916200
O  -4.03891900   -2.10085200    1.79963900
N  -1.99615400   -0.47450300    1.35442400
H  -1.97914000   -1.29760300    1.94416300
H  -1.12106900    0.01824300    1.18749400

83
A1, E(SCF) = -2372.66210771, E(ZPE) = nofreq, E(G) = nofreq a.u.
C   -0.25167400    4.36840300    2.36913300
C    0.05556200    3.08386600    1.97405500
C    1.11665600    2.84046600    1.08884100
C    1.88429600    3.91043500    0.59104300
C    1.55389700    5.20925900    1.00942400
C    0.50399400    5.43624800    1.87840300
C    1.38268400    1.46124000    0.67577000
C    3.00474600    3.63537300   -0.31708300
C    3.28881700    2.30643800   -0.70424100
C    2.49019700    1.19110100   -0.20860600
C    4.36881600    2.05405400   -1.56844200
H    4.57586100    1.02922900   -1.84729900
C    5.15037100    3.08181100   -2.04986500
C    4.86961500    4.39748300   -1.67356600
C    3.81400800    4.66329700   -0.82360800
H   -1.07049200    4.54855600    3.05454300
H   -0.51518200    2.24014300    2.34333600
H    2.11860400    6.05954200    0.65261600
H    0.27119300    6.44984500    2.18135400
H    5.97902900    2.86922800   -2.71414000
H    5.47821700    5.21275300   -2.04500200
H    3.62228900    5.69070400   -0.54726000
O    0.66853400    0.50810300    1.07718800
N    2.80365200   -0.03886700   -0.61566500
P    2.13886000   -1.45416900   -0.13393900
C    2.28508600   -1.84458900    1.63768100
C    1.17979600   -2.09713000    2.44340800
C    3.57056000   -1.87763500    2.17695000
C    1.36072200   -2.39540400    3.78715100
H    0.18207300   -2.05723800    2.02758600
C    3.74480200   -2.16252200    3.52494200
H    4.43340700   -1.68140700    1.54901600
C    2.64125500   -2.42638500    4.32791900
H    0.50021800   -2.59992200    4.41219800
H    4.74275000   -2.18359100    3.94484700
H    2.77972500   -2.65547500    5.37755300
C    3.16585900   -2.71024600   -0.96702700
C    3.81769500   -2.38879300   -2.15581100
C    3.24315800   -4.00594500   -0.45700200
C    4.54979200   -3.36009900   -2.82705500
H    3.75628300   -1.38110200   -2.54752700
C    3.97566700   -4.97286900   -1.13320200
H    2.74042700   -4.26321300    0.46858100
C    4.62945100   -4.65068700   -2.31694000
H    5.06068000   -3.10700900   -3.74788700
H    4.03957900   -5.97670900   -0.73193600
H    5.20263500   -5.40611900   -2.84057400
C    0.45324900   -1.75764000   -0.75109200
C   -0.19435700   -2.96280700   -0.48710900
C   -0.15230100   -0.79344700   -1.55248200
C   -1.46499100   -3.18706000   -1.00355600
H    0.28338600   -3.72220800    0.12227700
C   -1.41117200   -1.03432100   -2.08514300
H    0.35294200    0.14406800   -1.75677600
C   -2.07207000   -2.22458600   -1.80266800
H   -1.97711300   -4.11618000   -0.78549600
H   -1.88297500   -0.28369700   -2.70796900
H   -3.06182000   -2.40219500   -2.20705600
C   -7.78652400   -1.66511400   -0.00234400
C   -6.56061700   -1.82711500    0.60731900
C   -5.50873800   -0.93878100    0.34637300
C   -5.69193700    0.13995200   -0.53971700
C   -6.94932700    0.28370400   -1.14940900
C   -7.97820400   -0.59963000   -0.88576700
C   -4.22727100   -1.15662700    1.02738400
C   -4.57864200    1.06066700   -0.80868500
C   -3.34055900    0.88648400   -0.14641900
C   -3.15417300   -0.23123200    0.74404900
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C   -2.28119600    1.77600500   -0.40801100
H   -1.32506200    1.63883600    0.08184000
C   -2.43556400    2.82599300   -1.28573700
C   -3.65750600    3.00399700   -1.93998800
C   -4.70575000    2.13674500   -1.69899600
H   -8.59524500   -2.35574000    0.20244800
H   -6.38402800   -2.64169600    1.29823500
H   -7.13411500    1.09816000   -1.83586100
H   -8.93806400   -0.46131100   -1.36841200
H   -1.61044900    3.50359600   -1.47022400
H   -3.78821300    3.82280100   -2.63649000
H   -5.63795500    2.30052400   -2.22141800
O   -4.04007500   -2.10664100    1.81263200
N   -1.99976400   -0.47849600    1.36275500
H   -1.12545600    0.01505700    1.19414600
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RADICAL COMPLEX FORMATION:

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58
R_N-Rad, E(SCF) = -1704.43395958, E(ZPE) = -1703.978495, E(G) = -1704.044465 a.u.
C    4.61126900   -3.14911900   -0.78543000
C    3.51588500   -2.57387100   -1.40161600
C    3.15323500   -1.25783400   -1.11236200
C    3.87833400   -0.49279400   -0.18357500
C    4.98860200   -1.09105300    0.41919200
C    5.34871300   -2.39673200    0.12365100
C    1.97654400   -0.70733600   -1.81693100
C    3.45423300    0.88442300    0.16631100
C    2.38965100    1.50200700   -0.50530800
C    1.69522000    0.78665400   -1.60258500
C    1.96687600    2.78464300   -0.15402700
H    1.13120600    3.23171100   -0.67997300
C    2.59843300    3.47327500    0.86636400
C    3.65407500    2.87136900    1.54352000
C    4.07215300    1.59661600    1.19971600
H    4.89414700   -4.16903500   -1.01260200
H    2.92655200   -3.13049400   -2.11934700
H    5.59168600   -0.54121300    1.12734700
H    6.21523200   -2.83019400    0.60784000
H    2.26580500    4.46663100    1.13940700
H    4.15174200    3.39509300    2.35035500
H    4.88351300    1.15342300    1.75937000
O    1.27980400   -1.35715400   -2.55643400
N    0.89565300    1.33840900   -2.38883600
P   -1.91816600   -0.40492600   -0.75451100
C   -0.71102900   -0.17234200    0.62454500
C   -0.69631900    0.93894200    1.46475500
C    0.24528000   -1.17639900    0.81215700
C    0.25222500    1.04281800    2.47900600
H   -1.42627800    1.72948000    1.33708200
C    1.18276800   -1.07814100    1.83182200
H    0.24666100   -2.04856900    0.16496900
C    1.19059800    0.03605500    2.66642900
H    0.25415100    1.91441800    3.12311400
H    1.91389400   -1.86671200    1.96847500
H    1.92757600    0.11955600    3.45623200
C   -2.89719900    1.16127400   -0.65765200
C   -2.44665300    2.23974800   -1.42231500
C   -4.03395200    1.32000400    0.13408200
C   -3.10931900    3.46083500   -1.38028800
H   -1.56979900    2.12405200   -2.05156500
C   -4.70323700    2.53856400    0.16649400
H   -4.40180100    0.49462900    0.73253700
C   -4.24083300    3.61132800   -0.58671100
H   -2.74769500    4.29085200   -1.97546400
H   -5.58673000    2.64884500    0.78409600
H   -4.76390800    4.55959200   -0.55936100
C   -3.09864000   -1.61224000    0.00034100
C   -3.13373800   -1.93217700    1.35739100
C   -4.01730300   -2.21522700   -0.86164700
C   -4.07615100   -2.83277800    1.84303500
H   -2.42995300   -1.47649000    2.04431700
C   -4.96657400   -3.10512100   -0.37427600
H   -3.99233200   -1.98482600   -1.92194200
C   -4.99621500   -3.41688800    0.98061800
H   -4.09329700   -3.07324700    2.89945800
H   -5.67715200   -3.56006500   -1.05392400
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H -5.73031900 -4.11620100 1.36231500

58
TS1_N-Rad, E(SCF) = -1704.42197304, E(ZPE) = -1703.966194, E(G) = -1704.027695 a.u.
C -3.50085300 -3.34951700 0.21407200
C -2.45013900 -2.74383500 -0.44906100
C -2.46052300 -1.36737300 -0.68469300
C -3.53868800 -0.57168100 -0.26220200
C -4.58927200 -1.20386400 0.41328600
C -4.57032700 -2.56920000 0.64726400
C -1.28885000 -0.76828900 -1.35776600
C -3.54146600 0.88490900 -0.52412700
C -2.38994700 1.51845300 -1.02117900
C -1.16055800 0.73356900 -1.31964400
C -2.38918900 2.89784500 -1.24195700
H -1.49030600 3.36273900 -1.62721400
C -3.51679200 3.65587800 -0.98592700
C -4.66775600 3.03417000 -0.50842600
C -4.67716800 1.66864300 -0.28398400
H -3.48780900 -4.41533700 0.40383900
H -1.59666300 -3.32031800 -0.78434200
H -5.43180000 -0.63148500 0.77565400
H -5.39610500 -3.02961200 1.17606300
H -3.50640700 4.72351700 -1.16688300
H -5.56191300 3.61405000 -0.31544600
H -5.58882200 1.21117200 0.07492700
O -0.41234600 -1.44483800 -1.86333100
N -0.03897400 1.30437300 -1.49663700
P 1.59855600 0.11653900 -0.35248700
C 2.42807600 1.61495800 0.28067900
C 2.63867000 1.86151400 1.63683200
C 2.88487300 2.53256300 -0.66688800
C 3.30248800 3.01477700 2.03858500
H 2.28899400 1.15438000 2.37994400
C 3.55587300 3.67928500 -0.26237500
H 2.71162900 2.35023500 -1.72203700
C 3.76302000 3.92196200 1.09107000
H 3.46374300 3.20180300 3.09334400
H 3.91207000 4.38553800 -1.00242700
H 4.28140600 4.81914600 1.40725200
C 0.61687300 -0.53776700 1.03773500
C -0.32874400 0.30528500 1.63204000
C 0.65464900 -1.88425100 1.40563100
C -1.21439200 -0.18992800 2.58157000
H -0.36857000 1.35500900 1.36157400
C -0.23482300 -2.37478100 2.35288300
H 1.37506100 -2.55512100 0.95318600
C -1.17641400 -1.53307900 2.93625900
H -1.94009700 0.47530400 3.03409100
H -0.19635200 -3.42133900 2.63065400
H -1.87469500 -1.92322100 3.66688300
C 2.97029400 -1.08193500 -0.61180700
C 4.25642800 -0.86985200 -0.11245600
C 2.70817500 -2.21990100 -1.37836600
C 5.25964200 -1.79960500 -0.35913400
H 4.47969500 0.01398300 0.47293700
C 3.71277200 -3.15014800 -1.61335300
H 1.71665000 -2.37382600 -1.78790500
C 4.99006500 -2.94040400 -1.10645800
H 6.25425700 -1.63126200 0.03605000
H 3.49811000 -4.03341600 -2.20264900
H 5.77517900 -3.66234300 -1.29568900

58
P_N-Rad (**oxazaphospholyl radical**), E(SCF) = -1704.49678358, E(ZPE) = -1704.039252,
E(G) = -1704.100380 a.u.
C -4.74326700 2.81017800 -0.05448600
C -3.41575900 2.43941900 -0.08980400
C -3.04891100 1.08656000 -0.06854500
C -4.03605600 0.08439400 -0.02464800
C -5.38133800 0.48625400 0.01479200
C -5.73045700 1.82258000 -0.00196700
C -1.62035700 0.74978100 -0.11933200
C -3.63487400 -1.32761800 -0.00192400
C -2.26314600 -1.66988400 -0.03699000
C -1.23278300 -0.64147700 -0.07542000
C -1.88972000 -3.02629800 -0.01447500

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H   -0.83532100   -3.26920300   -0.03325600
C   -2.83741400   -4.02542000    0.03021700
C   -4.19388400   -3.69116800    0.05857900
C   -4.57883300   -2.36499100    0.04081200
H   -5.01978800    3.85737500   -0.06825300
H   -2.63004500    3.18307100   -0.13280500
H   -6.17206500   -0.24981200    0.05628200
H   -6.77673100    2.10192400    0.02732400
H   -2.53136300   -5.06445900    0.04559000
H   -4.94671900   -4.46906900    0.09539100
H   -5.63571100   -2.13777900    0.06435600
O   -0.74181600    1.63486400   -0.19716100
N    0.04602500   -1.02778100   -0.09228100
P    1.36916500   -0.07304800   -0.00620300
C    1.51771300    0.99501200    1.46090100
C    1.64865100    2.37697400    1.36385400
C    1.48779200    0.37624000    2.70946800
C    1.76332400    3.13821100    2.51920900
H    1.64474500    2.85784800    0.39400300
C    1.58839800    1.14486200    3.86217600
H    1.38802300   -0.70182800    2.78440300
C    1.73203700    2.52403000    3.76654200
H    1.86946800    4.21358100    2.44517600
H    1.55877000    0.66518900    4.83265400
H    1.81499300    3.12201100    4.66602600
C    1.77193200    0.84817100   -1.52488400
C    2.98447300    1.52768100   -1.62558300
C    0.90066700    0.79982800   -2.60859200
C    3.31270200    2.17845700   -2.80785400
H    3.67107300    1.55705100   -0.78606500
C    1.23946100    1.44322100   -3.79192800
H   -0.03936300    0.26678700   -2.52811100
C    2.44143000    2.13527700   -3.89021800
H    4.25031100    2.71501600   -2.88361000
H    0.56243600    1.40665100   -4.63644000
H    2.70041600    2.64070300   -4.81263100
C    2.73752200   -1.27200700    0.15322500
C    3.92076100   -0.92934100    0.80606400
C    2.61783100   -2.51932900   -0.45860300
C    4.97402700   -1.83428600    0.85338200
H    4.02455300    0.03815300    1.28370000
C    3.67375900   -3.41967700   -0.40878700
H    1.69789900   -2.78410900   -0.96539100
C    4.85148100   -3.07868200    0.24698400
H    5.88844100   -1.56648100    1.36813200
H    3.57489900   -4.38945600   -0.88098800
H    5.67298200   -3.78359500    0.28782000

88
RP_1_TEMPO-H, E(SCF) = -2188.23605160, E(ZPE) = nofreq, E(G) = nofreq a.u.
C    2.93950200    3.62736800    0.34158700
C    2.08407000    2.54574900    0.31245900
C    0.70041600    2.73409100    0.17974100
C    0.16400300    4.03363800    0.09106900
C    1.05631700    5.11706700    0.12029900
C    2.41845200    4.92044300    0.24419600
C   -0.16889600    1.55643100    0.16857900
C   -1.28774300    4.21324100   -0.03523200
C   -2.13946600    3.08590500   -0.03143200
C   -1.59750700    1.73662300    0.06993700
C   -3.52909900    3.26723800   -0.14574200
H   -4.16349100    2.39078600   -0.14571800
C   -4.07478000    4.52776900   -0.25581800
C   -3.23660000    5.64556500   -0.25803000
C   -1.86940100    5.48543200   -0.14832900
H    4.00768500    3.47406700    0.44150200
H    2.47364700    1.53528500    0.37965200
H    0.68690800    6.13092000    0.05300400
H    3.08141700    5.77688300    0.26585400
H   -5.14749000    4.65089900   -0.34251300
H   -3.65520700    6.64057100   -0.34660200
H   -1.24616800    6.36884400   -0.15450800
O    0.28639100    0.39098900    0.26554600
N   -2.45185600    0.71275600    0.07347800
P   -2.10643800   -0.88674100    0.04909100
C   -3.74827400   -1.65577800   -0.16462900
C   -4.03621100   -2.51312000   -1.22177100
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C	-4.73078700	-1.36362400	0.78387400
C	-5.30686100	-3.07069000	-1.33416900
H	-3.28200700	-2.74876500	-1.96277100
C	-5.99402100	-1.92307100	0.66838000
H	-4.50599500	-0.69952400	1.61176400
C	-6.28275300	-2.77755000	-0.39289400
H	-5.52925500	-3.73399400	-2.16084000
H	-6.75392400	-1.69625600	1.40605900
H	-7.27039200	-3.21340900	-0.48303300
C	-1.13469100	-1.45724700	-1.38039600
C	-1.24861500	-0.72992900	-2.56421200
C	-0.38997600	-2.63216700	-1.34687500
C	-0.62206500	-1.18679800	-3.71648100
H	-1.83143300	0.18426900	-2.58993800
C	0.22556700	-3.08864800	-2.50716700
H	-0.28228500	-3.19460100	-0.42798300
C	0.10595900	-2.37128100	-3.69122300
H	-0.70893700	-0.62062000	-4.63566700
H	0.80184400	-4.00537700	-2.48254000
H	0.58682500	-2.73050800	-4.59309500
C	-1.51067800	-1.58931400	1.62205900
C	-1.63384000	-2.96058100	1.84672200
C	-1.02349100	-0.75679700	2.62639300
C	-1.22114400	-3.50180200	3.05733100
H	-2.05361100	-3.60786700	1.08439800
C	-0.62831700	-1.30207900	3.84073500
H	-0.95382500	0.31104700	2.46545100
C	-0.71591200	-2.67316700	4.05241800
H	-1.30515400	-4.56824300	3.22556300
H	-0.25109100	-0.65337800	4.62147800
H	-0.39907800	-3.09521900	4.99851400
C	6.27495300	-0.63791900	-0.76256700
C	5.12143000	-0.29061200	-1.69379700
C	3.80876300	-0.97574800	-1.29722600
C	4.60451400	-0.95232100	1.13666400
C	5.89488000	-0.27012400	0.66555900
H	4.96402900	0.79355700	-1.67043400
H	5.34899600	-0.56385100	-2.72790200
H	6.51806000	-1.70114000	-0.83211900
H	7.17220800	-0.09076800	-1.06056800
H	5.75280800	0.81473300	0.72439100
H	6.69221300	-0.53155900	1.36646300
C	3.84456000	-2.47656000	-1.62279100
H	3.05133500	-2.99544200	-1.08295600
H	3.67697200	-2.61873000	-2.69338800
H	4.79822500	-2.94071800	-1.37542800
C	2.66637300	-0.33317100	-2.08820700
H	2.83372800	-0.46879100	-3.15935400
H	1.70755500	-0.78304800	-1.82648500
H	2.61150900	0.73693400	-1.87608300
C	4.83850700	-2.44741100	1.39837600
H	5.41538800	-2.56365000	2.31902700
H	3.88495000	-2.96074200	1.52775000
H	5.39159300	-2.93527000	0.59782100
C	4.16058000	-0.29810600	2.44613400
H	3.28218200	-0.79716300	2.85677600
H	4.96658800	-0.35893300	3.18106100
H	3.91865800	0.75447700	2.28145300
N	3.55297500	-0.66267200	0.13341900
O	2.37168100	-1.34510700	0.54356200
H	1.67188600	-0.66791100	0.48328500

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