Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

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Contents

GENERAL REMARKS

Melting points / Boiling points :

Melting points were recorded on Labhosp or Veego melting point apparatus and are uncorrected. Boiling points refer to the bath temperatures.

Infrared spectra :

Infrared (IR) spectra were recorded on Nicolet Impact-400 FT IR spectrometer. Solid samples were recorded as KBr wafers and liquid samples as their film between NaCl plates.

Nuclear Magnetic Resonance spectra:

Proton Nuclear Magnetic Resonance (^{1}H NMR) spectra were generally recorded Varian VXR 300 (300 MHz) and 400 MHz spectrometers. Carbon Nuclear Magnetic Resonance (^{13}C NMR) spectra were recorded on Varian VXR 300 (75.4 MHz) and 100 MHz spectrometers. NMR samples were generally made in chloroform-d solvent and chemical shifts were reported in δ scale using tetramethylsilane (TMS, or $SiMe_4$) as the internal standard. The standard abbreviations s, d, t, q, m, dd and dq, refer to singlet, doublet, triplet, quartet, multiplet, doublet of doublet, and doublet of quartet respectively. Coupling constants (J) were reported in Hertz.

Mass spectra:

The high-resolution mass measurements were carried out using Micromass Q-Tof micro mass spectrometer instrument.

Chromatography :

Analytical thin-layer chromatography (tlc) were performed on (10×5 cm) glass plates coated with Acme's silica gel G or GF 254 (containing 13% calcium sulfate as a binder) Silica gel is coated on glass plate using 'Sandwich Technique.' In this process, two equally sized clean glass plates are immersed in uniformly stirred silica gel suspension in an organic solvent (usually ethyl acetate). Only the exposed surface of the plate is thus coated with silica gel. The solvent evaporates readily leaving a thin-layer of silica gel and then the plate is ready for the use. Visualization of the spots on tlc plates was achieved either by exposure to iodine vapors or UV light. Flash chromatography

was performed using Acme's silica gel (100-200 mesh) and the column is usually eluted with ethyl acetate-hexane mixture.

Experimental Section

Representative procedure for preparation of Diels-Alder adducts: To a stirred solution of CTAB (0.06 mmol) in 50 mL water was added quinone (3.2 mmol). To this solution, spiroheptadiene 3.5 gm was added slowly and the reaction mixture was stirred at RT for 4 h. At the conclusion of the reaction, (TLC monitoring) the reaction mixture was extracted with ether (3 X 30 mL). The combined organic layers were dried ($MgSO_4$), filtered and concentrated. The product was isolated by column chromatography (SiO_2: hexane/ethyl acetate = 10:1) to afford the colorless Diels–Alder adduct **2a-e.**

Representative procedure for retro Diels–Alder reaction in presence of scavenger

To a solution of the Diels–Alder adduct **2d** (38 mg, 0.15 mmol) in acetonitrile (10 mL) was added *N*-phenylmaleimide (61 mg, 0.35mmol). The reaction mixture was heated under reflux for 10 h. At the conclusion of the reaction, acetonitrile was removed under vacuum and the crude product was charged on a silica-gel column and eluted with ethyl acetate/hexane to afford the desired product **1d** (21 mg, 87 %).

Characterization of the Diels-Alder adducts

2a: colorless solid: mp 110-111 °C; (lit[12] 110 °C)

2b: colorless solid: mp 111-113 °C. δ_H(400 MHz, $CDCl_3$) 0.48-0.61 (m, 4H), 1.93 (s, 6H), 3.04-3.06 (m, 2H), 3.39 (dd, 2H, J_1=2.6, J_2= 1.2 Hz), 6.08 (dd, J_1=J_2=1.8 Hz, 2H); δ_C(100 MHz, $CDCl_3$) 6.8, 7.9, 13.2, 44.7, 49.1, 53.7, 135.4, 147.8, 198.6.; ν_{max}(neat)/cm^{-1}2973, 1675, 1617, 1286, 1195 cm^{-1}; HRMS: m/z for ($C_{15}H_{16}O_2$+H) found 229.1238 (M+1): calculated 229.1229.

2c: colorless solid: mp 142-144 °C, δ_H (400 MHz, $CDCl_3$) 0.55-0.68 (m, 4H), 3.02-3.06 (m, 2H), 3.56-3.66 (m, 2H), 6.11 (dd, J_1=J_2=2 Hz, 2H), 7.11-7.26 (m, 1H), 7.54-7.62 (m, 2H), 12.63 (s, 1H); δ_C (100 MHz, $CDCl_3$) 7.3, 8.3, 45.3, 50.0, 50.4, 54.7, 54.9, 118.5,

118.7, 123.7, 135.3, 136.0, 136.2, 137.1, 162.4, 196.9, 204.7; ν_{max}(neat)/cm^{-1} 3444, 2924, 1674, 1631, 1451, 1266, 1232 cm^{-1}. MS Q-TOf 267.0098 (M+1)

2d: colorless solid: mp 152 °C (lit, [12] 152-153 °C); δ_H (400 MHz, $CDCl_3$) 0.54-0.66 (m, 4H), 3.02-3.04 (m, 2H), 3.62-3.63 (m, 2H), 6.07 (dd, J_1= J_2= 1.8 Hz, 2H), 7.67-7.69 (m, 2H), 8.01-8.06 (m, 2H); ν_{max}(neat)/cm^{-1} 2973, 1675, 1617, 1265, 1195 cm^{-1}.

2e: pale yellow solid: mp 155 °C (decomposed), δ_H (400 MHz, $CDCl_3$) 0.56-0.69 (m, 4H), 3.07-3.09 (m, 2H), 3.71 (dd, J_1= 2.4, J_2= 1.5 Hz, 2H), 6.06 (dd, J_1=J_2= 1.8 Hz, 2H), 7.66 (dd, J_1= 6.2, J_2= 3.3 Hz, 2H), 8.03 (dd, J_1= 6.3, J_2= 3.3 Hz, 2H), 8.59 (s, 2H). δ_C (100 MHz, $CDCl_3$) 7.1, 8.3, 45.3, 50.8, 54.9, 128.9, 129.4, 130.0, 131.9, 135.1, 135.7, 197.9; IR ν_{max}(neat)/cm^{-1} 3060, 2972, 1676, 1617, 1286, 1269, 1194 cm^{-1}; HRMS m/z for $C_{21}H_{16}O_2Na$ found 323.1058 (M+Na) calculated 323.1048.

3a: colorless solid: mp 105-106 °C (lit,[12] 106 °C)

3b: **(**Major diastereomer)
colorless solid: mp 69-71 °C, δ_H (300 MHz, $CDCl_3$) 0.13-0.15 (m, 1H); 0.57-0.59 (m, 1H), 0.98-1.06 (m, 4H), 1.93 (s, 6H), 2.84-2.85 (m, 1H), 3.11-3.13 (m, 1H), 3.36-3.37 (m, 2H), 6.08 (dd, J_1=J_2= 2.0 Hz, 2H). δ_C (100 MHz, $CDCl_3$) 13.3, 14.1, 14.9, 15.8, 48.9, 49.0, 49.6, 50.2, 54.6, 135.5, 147.8, 147.9, 198.8, 198.9; ν_{max}(neat)/cm^{-1} 2997, 2918, 1655, 1611, 1374, 1287 cm^{-1}; HRMS: m/z for ($C_{16}H_{18}O_2$+H) found 243.1384 (M+1), calculated 243.1385.

3d: mp 139-141 °C (lit[12] 140 °C)

3e: (Major diastereomer) mp 130-132 **°C,** δ_H (300 MHz, $CDCl_3$) 0.23-0.25 (m, 1H), 0.70-0.75 (m, 1H), 1.03-1.13(m, 3H), 1.14-1.15 (m, 1H), 3.01-3.05 (m, 1H), 3.30-3.32 (m, 1H), 3.68-3.69 (m, 2H), 6.06 (dd, J_1=J_2= 1.8 Hz, 2H), 7.65-7.67 (m, 2H), 8.02-8.04

(m, 2H), 8.59-8.60 (m, 2H); ν_{max}(neat)/cm^{-1} 3058, 2973, 1675, 1618, 1452, 1265, 1195 cm^{-1}; HRMS: m/z for $C_{22}H_{18}O_2Na$ found 337.1204 (M+Na), calculated 337.1204.

4:

colorless solid: mp 175 °C; δ_H (300 MHz, $CDCl_3$) 0.51-0.67 (m, 4H), 2.88-2.90 (m, 2H), 3.57-3.58 (m, 2H), 6.34 (dd, J_1=J_2=1.8 Hz, 2H), 7.13-7.16 (m, 2H), 7.41-7.45 (m, 3H); δ_C (75 MHz, $CDCl_3$) 6.8, 7.9, 46.3, 48.5, 50.6, 126.7, 128.7, 129.2, 132.0, 134.7, 176.7; ν_{max}(neat)/cm^{-1} 3069, 2999, 1774, 1708, 1596, 1499, 1380, 1192, 1159 cm^{-1}; HRMS m/z for $C_{17}H_{15}O_2NNa$ found 288.1011 (M+Na): calculated 288.1000.

Computational Methods

Potential energy surfaces have been explored by using the B3LYP/6-31G* level of theory using GAUSSIAN 98 suite of quantum chemical program.[16] All geometries were fully optimized and have been characterized as stationary points on the potential energy surface at the same level of theory by evaluating corresponding Hessian indices. Single point energies have been computed with more flexible basis set, namely, the 6-311+G**. Zero-point vibrational energies (at the B3LYP/6-31G* level) have been scaled by 0.9806 and are included in the reported energies.[17] Transition states of cycloreversion reaction have been characterized by the unique imaginary frequency and subsequently reoptimised using 'calcfc' option. Intrinsic reaction coordinate (IRC) calculations have also been carried out to authenticate the transition state.[18] Wienhold's Natural Bond orbital analysis has been performed using NBO5.0 program to electron delocalization in detail.[19]

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Table S1. Key Structural Parameter of spiro DA adduct obtained at the B3LYP/6-31G* level (bond distance in Å)

Adduct	C_1-C_5	C_2-C_6	C_1-C_7	C_1-C_3	C_3-C_4	C_5-C_6	C_7-C_8	C_8-C_9	C_7-C_9
2a	1.583	1.583	1.532	1.523	1.341	1.562	1.495	1.521	1.499
2b	1.584	1.584	1.532	1.522	1.341	1.553	1.495	1.522	1.500
2c	1.587	1.585	1.532	1.522	1.341	1.556	1.495	1.522	1.500
2d	1.584	1.584	1.532	1.522	1.341	1.559	1.495	1.522	1.500
2e	1.584	1.584	1.532	1.522	1.341	1.560	1.496	1.522	1.499
3a1	1.583	1.584	1.534	1.522	1.341	1.561	1.498	1.522	1.505
3a2	1.583	1.583	1.534	1.522	1.341	1.561	1.500	1.524	1.502
3b1	1.584	1.585	1.534	1.521	1.341	1.552	1.498	1.522	1.505
3b2	1.583	1.584	1.534	1.522	1.341	1.552	1.500	1.524	1.502
3d1	1.584	1.585	1.533	1.522	1.341	1.558	1.498	1.522	1.505
3d2	1.584	1.585	1.533	1.522	1.341	1.558	1.500	1.524	1.502
3e1	1.584	1.585	1.533	1.522	1.341	1.559	1.498	1.522	1.505
3e2	1.584	1.585	1.533	1.522	1.341	1.558	1.500	1.523	1.502

Table S2. Key Structural Parameter obtained at the B3LYP/6-31G* level for the Transition State of rDA reaction of spiro DA adduct. (bond distance in Å)

Adduct	C_1-C_5	C_2-C_6	C_1-C_7	C_1-C_3	C_3-C_4	C_5-C_6	C_7-C_8	C_8-C_9	C_7-C_9
2a	2.173	2.177	1.493	1.413	1.393	1.417	1.532	1.503	1.502
2b	2.178	2.178	1.493	1.412	1.394	1.412	1.532	1.503	1.502
2c	2.231	2.111	1.490	1.410	1.394	1.417	1.533	1.503	1.503
2d	2.170	2.169	1.493	1.413	1.393	1.417	1.532	1.503	1.502
2e	2.167	2.166	1.493	1.414	1.393	1.419	1.533	1.503	1.502
3a1	2.163	2.191	1.494	1.413	1.393	1.416	1.535	1.504	1.510
3a2	2.170	2.177	1.493	1.413	1.393	1.417	1.541	1.504	1.504
3b1	2.167	2.188	1.494	1.413	1.393	1.412	1.535	1.504	1.510
3b2	2.167	2.182	1.493	1.413	1.393	1.412	1.540	1.505	1.504
3d1	2.158	2.180	1.494	1.414	1.392	1.418	1.535	1.504	1.510
3d2	2.167	2.167	1.493	1.414	1.392	1.418	1.541	1.504	1.504
3e1	2.162	2.173	1.494	1.414	1.392	1.418	1.535	1.504	1.510
3e2	2.160	2.169	1.493	1.415	1.392	1.419	1.541	1.504	1.504

Table S3. Energetics of retro Diels-Alder reaction Spiro DA adduct at the B3LYP/6-311+G**//B3LYP/6-31G* level of theory.

Reaction	$\Delta E^{\dagger}$	$\Delta G^{\dagger}$	ΔH_{298}	ΔG_{298}
2a→1a	26.0	23.3	3.4	-11.2
2b→1b	25.9	22.9	2.6	-12.0
2c→1c	24.9	22.3	2.1	-12.5
2d→1d	25.2	22.8	1.6	-12.9
2e→1e	25.0	22.6	0.7	-13.8
$3a_1$→1a	25.8	23.2	3.1	-11.5
$3a_2$→1a	25.6	23.2	3.3	-11.3
$3b_1$→1b	25.8	23.3	2.2	-12.3
$3b_2$→1b	25.7	23.3	2.5	-12.1
$3d_1$→1d	25.0	22.4	1.1	-13.6

$3d_2 \rightarrow 1d$	24.9	22.4	1.5	-13.0
$3e_1 \rightarrow 1e$	24.8	22.3	0.3	-14.3
$3e_2 \rightarrow 1e$	24.7	22.2	0.6	-13.9

Table S4. Major orbital interactions in spiro DA adduct computed at the NBO/B3LYP/6-311+G**//6-31G*

Adduct	$\sigma (C_7\text{-}C_8) \rightarrow \sigma^*(C_1\text{-}C_5)$	$\sigma (C_1\text{-}C_5) \rightarrow \sigma^*(C_7\text{-}C_8)$	$\sigma (C_7\text{-}C_8) \rightarrow \sigma^*(C_2\text{-}C_6)$	$\sigma (C_2\text{-}C_5) \rightarrow \sigma^*(C_7\text{-}C_8)$	Occupancy of $\sigma^*(C_1\text{-}C_5)$	Occupancy of $\sigma^*(C_2\text{-}C_6)$
2a	1.18	4.82	1.18	4.82	0.03306	0.03306
2b	1.15	4.84	1.15	4.84	0.03352	0.03352
2c	1.18	4.85	1.16	4.85	0.03447	0.03316
2d	1.21	4.85	1.21	4.85	0.03328	0.03327
2e	1.16	4.86	1.16	4.86	0.03288	0.03252
3a1	1.10	4.23	1.09	4.38	0.03312	0.03358
3a2	1.15	4.54	1.01	4.74	0.03335	0.03350
3b1	1.21	4.85	1.20	4.96	0.03386	0.03397
3b2	1.11	4.57	1.02	4.77	0.03380	0.03376
3d1	1.20	4.83	1.29	4.96	0.03357	0.03342
3d2	1.13	4.79	1.03	4.56	0.03331	0.03339
3e1	1.23	4.85	1.20	4.95	0.03301	0.03327
3e2	1.13	4.57	1.03	4.81	0.03318	0.03337

Table S5. Major orbital interactions in spiro DA adduct computed at the NBO/B3LYP/6-311+G**//6-31G*

Adduct	$\pi(C_3\text{-}C_4) \rightarrow \sigma^*(C_1\text{-}C_5)$	$\sigma(C_1\text{-}C_5) \rightarrow \pi^*(C_3\text{-}C_4)$	$\pi(C_3\text{-}C_4) \rightarrow \sigma^*(C_2\text{-}C_6)$	$\sigma(C_2\text{-}C_6) \rightarrow \pi^*(C_3\text{-}C_4)$	Sum of delocalization energy of major interactions
2a	3.35	2.73	3.35	2.74	19.35
2b	3.30	2.71	3.30	2.70	19.15
2c	3.32	2.71	3.40	2.68	19.3
2d	3.35	2.70	3.35	2.70	19.37

2e	3.29	2.72	3.29	2.72	19.2
3a1	3.37	2.72	3.37	2.72	18.6
3a2	3.32	2.68	3.35	2.69	18.74
3b1	3.34	2.70	3.32	2.71	19.33
3b2	3.32	2.71	3.34	2.71	18.78
3d1	3.31	2.72	3.37	2.69	19.41
3d2	3.35	2.72	3.32	2.72	19.06
3e1	3.31	2.72	3.32	2.72	19.35
3e2	3.30	2.73	3.35	2.72	18.83

Table S6. Major orbital interactions in Transition state computed at the NBO/B3LYP/6-311+G**//6-31G*

Adduct	σ (C_7-C_8) $\rightarrow$ σ^*(C_1-C_5)	σ (C_1-C_5) $\rightarrow$ σ^*(C_7-C_8)	σ (C_7-C_8) $\rightarrow$ σ^*(C_2-C_6)	σ (C_2-C_5) $\rightarrow$ σ^*(C_7-C_8)	Occupancy of σ^*(C_1-C_5)	Occupancy of σ^*(C_2-C_6)
2a	2.84	7.28	2.85	7.32	0.3577	0.3595
2b	2.81	7.34	2.81	7.34	0.3616	0.3616
2c	-	-	-	-	-	-
2d	2.81	7.33	2.80	7.36	0.3558	0.3555
2e	2.82	7.39	2.82	7.39	0.3535	0.3531
3a1	2.85	6.95	2.85	7.23	0.3543	0.3644
3a2	2.96	6.69	2.62	7.58	0.3566	0.3608
3b1	3.01	7.29	3.01	7.54	0.3574	0.3652
3b2	2.88	6.72	2.58	7.63	0.3568	0.3628
3d1	2.82	7.04	2.83	7.28	0.3511	0.3586
3d2	2.93	6.76	2.58	7.63	0.3544	0.3551
3e1	3.02	7.33	3.02	7.56	0.3523	0.3569
3e2	2.91	6.78	2.60	7.68	0.3513	0.3552

Table S7. Major orbital interactions in Transition state computed at the NBO/B3LYP/6-311+G**//6-31G*

Adduct	$\pi(C_3\text{-}C_4) \rightarrow \sigma^*(C_1\text{-}C_5)$	$\sigma(C_1\text{-}C_5) \rightarrow \pi^*(C_3\text{-}C_4)$	$\pi(C_3\text{-}C_4) \rightarrow \sigma^*(C_2\text{-}C_6)$	$\sigma(C_2\text{-}C_6) \rightarrow \pi^*(C_3\text{-}C_4)$	Sum of delocalization energy of major interactions
2a	17.44	15.87	17.55	15.98	79.81
2b	17.45	16.29	17.45	16.29	80.44
2c	-	-	-	-	
2d	17.33	15.86	17.34	15.83	79.3
2e	17.19	15.81	17.17	15.79	78.99
3a1	17.08	15.83	17.36	16.55	79.47
3a2	17.34	15.72	17.46	16.00	78.79
3b1	17.28	15.96	17.38	16.56	80.49
3b2	17.17	15.92	17.40	16.45	79.12
3d1	16.96	15.75	17.04	16.35	78.79
3d2	17.22	15.68	17.21	15.84	78.22
3e1	17.14	15.62	17.11	15.96	79.2
3e2	17.03	15.54	17.04	15.88	77.78

Table S8.Cartesian Coordinates of the B3LYP/6-31G* Optimized Geometry of Cycloadducts Formed between Spiro Cyclopentadiene and various Quinone and respective Transition states of retro Diels-Alder reaction. The Values in Parenthesis Implies Single-Point Energies Evaluated at the B3LYP/6-311+G**//B3LYP/6-31G* Level

2a HF = -652.9588094 (-653.1349222) Nimag = 0				**2a†** HF = -652.9142084 (-653.0934312) Nimag =1(-460.15)			
6	-1.947612	-.000032	-.098665	6	1.953654	.000446	-.010275
6	-.985256	1.129997	.282519	6	1.158263	-1.149842	.512073
6	-.569291	.670384	1.673149	6	.542865	-.698344	1.701184
6	-.569493	-.670812	1.673113	6	.543323	.694895	1.703245
6	-.985326	-1.130174	.282379	6	1.159896	1.149565	.516247
6	.213140	-.781030	-.691427	6	3.484217	-.000974	.061382
6	.213024	.780950	-.691543	6	2.778767	.002221	-1.265909
6	1.500463	-1.486115	-.300864	6	-.384194	.708823	-.954003
6	2.703421	-.672387	-.000600	6	-1.525379	1.461529	-.388452
6	2.703322	.672778	-.000686	6	-2.531608	.672433	.374359
6	1.500374	1.486302	-.301550	6	-2.531554	-.672495	.374162
8	1.554305	-2.706312	-.234820	6	-1.525222	-1.461026	-.388916
8	1.553638	2.706457	-.234289	6	-.383445	-.707878	-.953752
6	-3.424287	-.000033	.135419	1	1.396517	-2.188143	.304250
6	-2.869544	.000035	-1.281574	1	.037246	-1.332933	2.420252
1	-1.331094	2.159949	.184160	1	.037854	1.327680	2.424003
1	-.242184	1.331075	2.469144	1	1.397244	2.188403	.310248
1	-.242534	-1.331647	2.469047	1	3.970389	.910838	.395593
1	-1.331196	-2.160096	.183828	1	3.968612	-.915055	.391970
1	-.046354	-1.154861	-1.689067	1	2.798582	-.909735	-1.857990
1	3.597394	-1.243535	.239606	1	2.799838	.916627	-1.854156
1	3.597191	1.244086	.239525	1	.152911	1.241276	-1.733186
1	-.046775	1.154644	-1.689149	8	-1.660164	2.673470	-.532320
1	-3.890160	-.912228	.500123	1	-3.295626	1.252872	.886073
1	-3.890153	.912137	.500197	1	-3.295500	-1.253221	.885652
1	-2.967644	.912534	-1.866226	8	-1.659553	-2.672850	-.533472
1	-2.967645	-.912395	-1.866334	1	.152180	-1.239701	-1.734436
2b HF = -731.59905(-731.7938698) Nimag = 0				**2b†** HF= -731.5546893 (-731.7524681) Nimag = -1 (-461.80)			
6	-0.945998	-1.475902	-0.377812	6	2.442569	-0.000109	0.154486
6	0.353187	-0.776504	-0.721780	6	1.585771	-1.150076	0.569543
6	0.353259	0.776433	-0.721792	6	0.817796	-0.697212	1.664552
6	-0.945881	1.475925	-0.377809	6	0.817819	0.696808	1.664679
6	-2.186770	0.680559	-0.132964	6	1.585805	1.149825	0.569759
6	-2.186811	-0.680480	-0.132932	6	0.249444	0.705817	-1.091405
6	1.517541	-1.129783	0.291671	6	-0.958364	1.451282	-0.683938
6	2.492863	-0.000105	-0.056219	6	-2.067502	0.679542	-0.034878
6	1.517621	1.129638	0.291674	6	-2.067560	-0.679456	-0.034951
6	1.055697	0.670551	1.667626	6	-0.958424	-1.451204	-0.683996

6 1.055659 -0.670672 1.667622	6 0.249415 -0.705749 -1.091452
6 3.960931 0.000048 0.226563	6 3.950280 0.000121 0.426937
6 3.453401 0.000031 -1.208117	6 3.425445 0.000150 -0.981682
8 -0.968593 2.699176 -0.309436	6 -3.195415 -1.486470 0.550838
8 -0.968829 -2.699168 -0.309623	6 -3.195308 1.486573 0.550985
1 1.865140 -2.159993 0.203988	1 1.848644 -2.188570 0.395255
1 0.701334 -1.331644 2.451655	1 0.222027 -1.331016 2.311722
1 0.701414 1.331537 2.451666	1 0.222069 1.330511 2.311966
1 1.865321 2.159818 0.204037	1 1.848828 2.188334 0.395777
1 0.645238 1.153970 -1.709132	1 0.880969 1.243281 -1.792366
1 0.645190 -1.154088 -1.709092	8 -1.054656 2.663652 -0.865701
1 4.414405 0.912305 0.606527	1 -3.010235 2.551048 0.398153
1 4.414686 -0.912129 0.606380	1 -4.153768 1.227914 0.083148
1 3.570527 -0.912487 -1.789241	1 -3.306670 1.291591 1.625552
6 -3.439157 1.471622 0.138802	1 -4.154197 -1.226139 0.084627
1 -3.847332 1.235881 1.129871	1 -3.011389 -2.550849 0.396083
1 -3.225506 2.540049 0.092335	1 -3.305305 -1.293227 1.625886
1 -4.222974 1.231626 -0.590671	8 -1.054696 -2.663574 -0.865767
6 -3.439258 -1.471447 0.138979	1 0.880835 -1.243203 -1.792510
1 -3.846926 -1.235948 1.130315	1 4.387837 -0.912904 0.819927
1 -4.223352 -1.231095 -0.590062	1 4.387499 0.913172 0.820235
1 -3.225758 -2.539885 0.092129	1 3.523799 -0.912847 -1.564317
1 3.570268 0.912536 -1.789309	1 3.523258 0.913238 -1.564263
2c HF = -881.8510128 (-882.0881456) Nimag =0	**2c†** HF= -881.808135 (-882.0483477) Nimag = 1 (-460.7393)
6 -0.523814 -1.272974 -0.481253	6 2.924381 -0.168809 0.283738
6 0.849580 -0.704014 -0.753181	6 1.939021 -1.224061 0.650443
6 1.012125 0.843485 -0.756389	6 1.125467 -0.679762 1.666009
6 -0.214834 1.691374 -0.477554	6 1.256947 0.706414 1.649308
6 1.915007 -1.168949 0.326619	6 2.143656 1.065739 0.603447
6 3.020139 -0.151180 0.025341	6 0.943220 0.784246 -1.109748
6 2.153352 1.077807 0.318108	6 -0.199746 1.679278 -0.803129
6 1.573897 0.682443 1.668979	6 -1.445438 1.035947 -0.277814
6 1.432106 -0.651221 1.673869	6 -2.469766 1.844728 0.205143
6 4.463640 -0.303152 0.384969	6 -3.652027 1.257374 0.670735
6 4.034108 -0.260264 -1.074190	6 -3.826338 -0.120152 0.638426
8 -0.112994 2.910463 -0.466403	6 -2.810012 -0.950688 0.134653
8 -0.653246 -2.510150 -0.484049	6 -1.593349 -0.373294 -0.312454
1 2.155638 -2.230803 0.259593	6 -0.520724 -1.238591 -0.833827
1 0.969350 -1.263160 2.441007	6 0.769787 -0.621612 -1.152022
1 1.250330 1.383443 2.431126	6 4.400395 -0.293473 0.678173
1 2.611680 2.064929 0.244921	6 3.991548 -0.284744 -0.767791
1 1.395994 1.177098 -1.727351	1 2.100857 -2.285014 0.491190
1 1.158671 -1.118365 -1.719949	1 0.419512 -1.240989 2.267504
1 4.990103 0.558841 0.787344	1 0.672011 1.404728 2.236733
1 4.798414 -1.255356 0.789202	1 2.531591 2.069644 0.460492

1 4.086007 -1.183869 -1.647186	1 1.678529 1.239191 -1.767238
6 -2.942745 -0.956150 0.032021	8 -0.122349 2.893194 -0.962960
6 -1.662580 -0.387792 -0.223074	1 -2.330467 2.920160 0.200891
6 -1.528579 1.027079 -0.218315	1 -4.451730 1.886304 1.053185
6 -2.630161 1.839868 0.030263	1 -4.744383 -0.586169 0.982246
6 -3.881087 1.262577 0.277919	8 -3.029943 -2.272785 0.095597
6 -4.041737 -0.115188 0.280205	1 -2.226076 -2.674759 -0.337698
1 -2.491184 2.914968 0.025081	8 -0.696629 -2.465585 -0.990896
1 -4.739769 1.900243 0.470569	1 1.404258 -1.224780 -1.793320
1 -5.004955 -0.577820 0.469964	1 4.721576 -1.230422 1.123514
8 -3.152666 -2.277696 0.046329	1 4.883650 0.588046 1.089112
1 -2.273833 -2.705231 -0.148067	1 4.054344 -1.217401 -1.323540
1 4.274300 0.631641 -1.649285	1 4.215561 0.601636 -1.356730
2d HF = -806.6203381(-806.8285449) Nimag = 0	**2d**† HF = -806.5769886 (-806.7882837) Nimag = 1 (-468.58)
6 -.558856 -1.500029 -.451690	6 2.762199 0.000636 0.287153
6 .744896 -.779463 -.744146	6 1.874979 -1.150876 0.627373
6 .744903 .779462 -.744133	6 1.021033 -0.700312 1.659431
6 -.558846 1.500033 -.451689	6 1.018757 0.692617 1.661186
6 1.869442 -1.129727 .315336	6 1.871270 1.148546 0.630167
6 2.856944 -.000027 .005830	6 0.683346 0.708442 -1.130363
6 1.869456 1.129693 .315349	6 -0.543247 1.476063 -0.827193
6 1.352079 .670590 1.671516	6 -1.706050 0.704954 -0.284349
6 1.352065 -.670629 1.671507	6 -2.824845 1.399362 0.191931
6 4.313059 .000030 .346026	6 -3.927430 0.701448 0.676139
6 3.861759 .000012 -1.107358	6 -3.927880 -0.699581 0.675802
8 -.580177 2.723229 -.418455	6 -2.825730 -1.397970 0.191298
8 -.580195 -2.723224 -.418459	6 -1.706527 -0.704059 -0.284764
1 2.220503 -2.159916 .241539	6 -0.544354 -1.475655 -0.828272
1 .965317 -1.331183 2.440387	6 0.682725 -0.708877 -1.131415
1 .965341 1.331140 2.440405	6 4.242447 0.001148 0.683293
1 2.220542 2.159875 .241561	6 3.835767 0.003139 -0.763804
1 1.080657 1.152548 -1.719052	1 2.153303 -2.188773 0.474527
1 1.080635 -1.152537 -1.719076	1 0.372267 -1.334915 2.252285
1 4.751247 .912321 .743431	1 0.368112 1.323595 2.255877
1 4.751371 -.912212 .743406	1 2.146783 2.187779 0.481160
1 4.000779 -.912624 -1.683368	1 1.377088 1.236571 -1.777642
6 -2.996689 -1.396688 .023970	8 -0.609241 2.689702 -1.004079
6 -1.799655 -.704896 -.211776	1 -2.805784 2.484224 0.163588
6 -1.799650 .704905 -.211772	1 -4.792369 1.244070 1.048358
6 -2.996682 1.396701 .023979	1 -4.793154 -1.241831 1.047787
6 -4.178203 .700667 .253161	1 -2.807376 -2.482830 0.162417
6 -4.178207 -.700650 .253157	8 -0.611398 -2.689156 -1.005979
1 -2.968465 -2.481349 .020528	1 1.374770 -1.237296 -1.780351
1 -2.968453 2.481362 .020543	1 4.644985 0.913966 1.112542
1 -5.102042 1.243975 .432433	1 4.646277 -0.912093 1.110391

1 -5.102048 -1.243954 .432426 1 4.000703 .912606 -1.683450	1 3.980355 0.917781 -1.334049 1 3.981099 -0.908778 -1.338099
2e HF = -960.2643334 (-960.5057671) Nimag = 0	**2e**† HF =-960.2210574 (-960.4658534) Nimag = 1 (-469.17)
6 -0.482144 1.506095 -0.538791 6 -1.798829 0.779773 -0.753181 6 -1.798830 -0.779770 -0.753184 6 -0.482146 -1.506093 -0.538785 6 -2.858643 1.129793 0.370817 6 -3.863061 0.000004 0.120171 6 -2.858650 -1.129793 0.370807 6 -2.262183 -0.670604 1.693979 6 -2.262177 0.670588 1.693983 6 -5.297127 -0.000001 0.544409 6 -4.930678 0.000004 -0.932706 8 -0.466504 -2.730236 -0.517508 8 -0.466504 2.730238 -0.517500 1 -3.212934 2.160180 0.317973 1 -1.830232 1.330922 2.438627 1 -1.830243 -1.330946 2.438618 1 -3.212948 -2.160177 0.317955 1 -2.192847 -1.151752 -1.706401 1 -2.192853 1.151759 -1.706394 1 -5.711860 -0.912250 0.966381 1 -5.711866 0.912246 0.966382 1 -5.102403 0.912734 -1.499617 6 1.959993 1.399298 -0.191203 6 0.770040 0.715043 -0.360679 6 0.770039 -0.715042 -0.360679 6 1.959992 -1.399297 -0.191205 1 1.933243 2.485182 -0.193786 1 1.933242 -2.485182 -0.193787 1 - 5.102395 -0.912723 -1.499624 6 4.419261 1.406492 0.152474 6 3.187435 0.718063 -0.019416 6 3.187435 -0.718063 -0.019416 6 4.419260 -1.406493 0.152472 6 5.594279 -0.709231 0.316406 6 5.594280 0.709230 0.316407 1 4.415592 2.493444 0.151788 1 4.415591 -2.493445 0.151786 1 6.530851 -1.244152 0.447050 1 6.530851 1.244150 0.447051	6 3.661804 0.000063 0.557470 6 2.734625 -1.150212 0.769576 6 1.744502 -0.697665 1.671514 6 1.743768 0.694849 1.672070 6 2.733276 1.149153 0.770126 6 1.804111 0.709548 -1.136075 6 0.548740 1.481780 -1.011765 6 -0.679595 0.714897 -0.635519 6 -1.834846 1.401960 -0.319624 6 -3.026100 0.718277 0.024974 6 -4.222550 1.405524 0.366426 6 -5.363688 0.708942 0.693658 6 -5.363654 -0.708982 0.693561 6 -4.222488 -1.405465 0.366215 6 -3.026069 -0.718115 0.024862 6 -1.834797 -1.401698 -0.319873 6 -0.679569 -0.714545 -0.635660 6 0.548685 -1.481362 -1.012331 6 1.803931 -0.709154 -1.136846 6 5.070365 0.000471 1.161919 6 4.874620 0.001087 -0.328523 1 3.031084 -2.188420 0.658971 1 1.017874 -1.330903 2.167554 1 1.016410 1.326875 2.168569 1 3.028808 2.187791 0.660806 1 2.581849 1.235558 -1.682038 8 0.515750 2.695627 -1.198616 1 -1.814615 2.487971 -0.346197 1 -4.219636 2.492630 0.363719 1 -6.272755 1.244435 0.953335 1 -6.272694 -1.244554 0.953168 1 -4.219523 -2.492571 0.363353 1 -1.814543 -2.487703 -0.346695 8 0.515498 -2.695132 -1.199773 1 2.581558 -1.234971 -1.682957 1 5.408428 -0.912547 1.643121 1 5.407505 0.913368 1.644004 1 5.100474 -0.911795 -0.874673 1 5.099371 0.914762 -0.873843
3a1 HF = -692.2742458 (-692.4605824) Nimag = 0	**3a1**† HF = -692.2297917 (-692.4193354) Nimag = 1 (-461.55)
6 -1.856105 -1.282587 -0.618784	6 1.680042 -0.356143 0.356027

6	-0.449365	-0.717769	-0.711460	6	0.672205	-1.443613	0.540487
6	-0.264432	0.813754	-0.471989	6	-0.061479	-1.113159	1.702522
6	-1.503391	1.630880	-0.147962	6	0.111204	0.243493	1.965337
6	-2.825084	0.958345	-0.132343	6	0.960001	0.793974	0.978849
6	-2.984715	-0.360320	-0.345291	6	-0.397660	0.831488	-0.739992
6	0.532159	-1.357561	0.352859	6	- .517982	1.623838	-0.189460
6	1.675222	-0.337475	0.276521	6	-2.711111	0.861392	0.270860
6	0.808528	0.859554	0.691720	6	-2.862410	-0.449724	0.012310
6	0.134958	0.284299	1.930559	6	-1.845140	-1.225657	-0.749032
6	-0.031584	-1.030763	1.728232	6	-0.551616	-0.551678	-1.003339
6	3.081733	-0.597652	0.721350	1	0.813868	-2.456727	0.177087
6	2.776234	-0.350760	-0.749387	1	-0.748580	-1.776380	2.215722
8	-1.421958	2.826794	0.095776	1	- .419871	0.816577	2.717082
8	-2.064795	-2.478645	-0.767520	1	1.340977	1.808955	1.006249
1	0.761095	-2.404446	0.147719	1	0.304858	1.414410	-1.326509
1	-0.553686	-1.736458	2.365932	8	-1.492738	2.849434	-0.113472
1	-0.223917	0.875098	2.766839	1	-3.474327	1.444240	0.781080
1	1.278773	1.837062	0.800185	1	-3.756042	-0.998971	0.299064
1	0.181572	1.280755	-1.358000	8	-2.090113	-2.363522	-1.139583
1	-3.670341	1.609403	0.079222	1	0.034319	-1.011460	-1.794043
1	-3.965717	-0.829136	-0.315251	6	3.159482	-0.626950	0.661947
1	-0.080980	-0.988067	-1.708261	6	2.717456	-0.309843	-0.740403
1	3.599707	0.191016	1.263631	6	3.141040	0.985353	-1.404031
1	3.352900	-1.602465	1.036734	1	3.443604	-1.644023	0.916113
1	2.805458	-1.240777	-1.379900	1	3.697548	0.140073	1.213180
6	3.271058	0.907037	-1.436321	1	2.684058	-1.165216	-1.416050
1	4.314040	0.791416	-1.754961	1	3.144086	1.820807	-0.695386
1	2.677473	1.143473	-2.328413	1	4.156350	0.892067	-1.806872
1	3.226342	1.774044	-0.767741	1	2.477768	1.251717	-2.234756
3a2 HF = -692.2747869 (-692.4610435) Nimag = 0				**3a2**† HF = -692.2307602 (-692.4201354) Nimag = 1 (-461.13)			
6	-2.003296	-1.342563	-.205529	6	1.617765	-.289764	-.119465
6	-.658159	-.821021	-.679630	6	.708481	-1.314944	.472734
6	-.460290	.726115	-.740015	6	.208517	-.757620	1.671526
6	-1.626270	1.603632	-.319441	6	.380461	.623712	1.625093
6	-2.904819	.961743	.070886	6	.992996	.963479	.397247
6	-3.075327	-.371664	.122812	6	-.658619	.671148	-.991032
6	.535264	-1.287535	.249433	6	-1.667687	1.578819	-.402702
6	1.613723	-.303708	-.221397	6	-2.726289	.946296	.431637
6	.820379	.952810	.163184	6	-2.893828	-.387203	.479927
6	.423997	.594085	1.588723	6	-2.032079	-1.319288	-.297990
6	.255316	-.735458	1.639957	6	-.833851	-.733792	-.938980
6	3.091194	-.514665	-.074798	6	2.377876	-.438618	-1.409027
6	2.451602	-.470895	-1.456940	6	3.140834	-.521644	-.115124
8	-1.521975	2.822295	-.300727	1	.809586	-2.380600	.292098
8	-2.209329	-2.543158	-.094215	1	-.337418	-1.303881	2.432360

1	.743650	-2.355836	.174177	1	-.012529	1.335634	2.342272
1	-.110402	-1.323073	2.475538	1	1.332059	1.962210	.144616
1	.224700	1.316112	2.373731	1	-.096936	1.107632	-1.811536
1	1.277086	1.930859	.010566	8	-1.655955	2.793585	-.582374
1	-.205382	1.030431	-1.762137	1	-3.386199	1.633591	.955721
1	-3.705196	1.650583	.331605	1	-3.698385	-.851152	1.045559
1	-4.020559	-.815186	.427629	8	-2.324291	-2.508099	-.392900
1	-.497761	-1.256955	-1.672842	1	-.406895	-1.352717	-1.722577
6	4.025315	.586774	.383219	1	2.510618	.457019	-2.013101
1	3.379368	-1.509427	.265687	1	2.228976	-1.347311	-1.988272
1	2.373393	-1.396496	-2.023997	6	4.112023	.558129	.309276
1	2.644592	.408396	-2.069681	1	3.429393	-1.525327	.192852
1	5.049324	.399588	.038113	1	4.188751	.617361	1.400982
1	3.718890	1.562969	-.008796	1	5.112717	.347955	-.087571
1	4.046957	.659033	1.477160	1	3.808630	1.543443	-.059932
3b1 HF = -770.9145304 (-771.1195574) Nimag =				**3b1'** HF = -770.8702619 (-771.0783511) Nimag = 1 (-458.6466)			
6	-1.258441	-1.411518	-0.547931	6	2.163561	-0.302004	0.457389
6	0.118899	-0.793370	-0.670771	6	1.168594	-1.399373	0.650942
6	0.233292	0.744951	-0.503560	6	0.337270	-1.000248	1.720885
6	-1.039048	1.512623	-0.207814	6	0.459457	0.377493	1.887234
6	-2.350861	0.800366	-0.141224	6	1.371920	0.872974	0.929541
6	-2.452395	-0.547787	-0.300458	6	0.154886	0.740267	-0.883710
6	1.129902	-1.342737	0.417857	6	-1.027053	1.533015	-0.492379
6	2.226702	-0.278305	0.287110	6	-2.248803	0.789151	-0.044285
6	1.308770	0.896975	0.650412	6	-2.350618	-0.555459	-0.213896
6	0.667553	0.351968	1.919218	6	-1.242971	-1.338534	-0.851710
6	0.558553	-0.977248	1.779782	6	0.052453	-0.657691	-1.051858
6	3.646089	-0.452057	0.733178	6	3.620799	-0.507559	0.893074
6	3.321432	-0.291014	-0.745386	6	3.279860	-0.317065	-0.559473
8	-0.979769	2.723393	-0.028239	1	1.359993	-2.432954	0.379776
8	-1.381763	-2.625917	-0.656054	1	-0.373963	-1.640768	2.230140
1	1.402323	-2.387191	0.259290	1	-0.141864	0.992824	2.547105
1	0.070389	-1.674332	2.452918	1	1.728878	1.896774	0.906736
1	0.285880	0.965336	2.728769	1	0.885765	1.301109	-1.456739
1	1.733681	1.899120	0.708676	8	-1.015360	2.762350	-0.529868
1	0.651441	1.195366	-1.411412	6	-3.365685	1.616758	0.533585
1	0.497038	-1.096411	-1.654289	1	-3.076873	2.668876	0.555964
1	4.129638	0.384905	1.233292	1	-4.281129	1.520568	-0.064345
1	3.965654	-1.426924	1.094030	1	-3.617902	1.289717	1.550533
1	3.388158	-1.208662	-1.331878	6	-3.588309	-1.325472	0.162598
6	-3.558499	1.658938	0.127649	1	-3.464294	-2.379036	-0.094118
1	-4.061710	1.352135	1.053414	1	-3.798828	-1.239030	1.236444
1	-3.262210	2.704581	0.218386	1	-4.471181	-0.940413	-0.363551
1	-4.296874	1.566442	-0.678810	8	-1.410785	-2.508603	-1.190470
6	-3.778617	-1.256518	-0.220357	1	0.707935	-1.163205	-1.754923

1	-4.241402	-1.117181	0.765147	1	3.906902	-1.492407	1.250977
1	-4.484608	-0.858240	-0.959751	1	4.100022	0.316121	1.416232
1	-3.644325	-2.324429	-0.396228	1	3.313368	-1.225074	-1.162458
6	3.751862	0.952951	-1.497731	6	3.727362	0.929803	-1.295851
1	3.669463	1.849104	-0.872586	1	3.654612	1.821541	-0.663595
1	4.797136	0.871517	-1.819612	1	4.773793	0.832468	-1.608114
1	3.141430	1.115756	-2.394846	1	3.127595	1.106570	-2.195866
3b2 HF = -770.9150397 (-771.1199896) Nimag = 0				**3b2**† HF = -770.8711118 (-771.0790078) Nimag = 1(-460.52)			
6	-1.384776	-1.458864	-0.320027	6	2.136417	-0.258673	-0.028006
6	-0.047394	-0.884530	-0.738915	6	1.205993	-1.304522	0.491808
6	0.081877	0.660730	-0.800810	6	0.549957	-0.734837	1.606345
6	-1.138488	1.480234	-0.434363	6	0.671261	0.651132	1.532676
6	-2.429505	0.802650	-0.108160	6	1.408706	0.981188	0.373737
6	-2.543536	-0.552854	-0.056952	6	-0.063051	0.572944	-1.184141
6	1.125405	-1.295703	0.242064	6	-1.175285	1.442025	-0.752300
6	2.177977	-0.267004	-0.189671	6	-2.307323	0.805576	-0.003311
6	1.312697	0.953730	0.151989	6	-2.422698	-0.546263	0.074330
6	0.874511	0.585349	1.562523	6	-1.423515	-1.445299	-0.589689
6	0.763517	-0.750201	1.615953	6	-0.182366	-0.831707	-1.103492
6	3.655837	-0.410001	0.020505	6	3.657200	-0.425742	0.148550
6	3.074186	-0.401630	-1.387680	6	3.037870	-0.412296	-1.222564
8	-1.056386	2.702779	-0.415194	1	1.369955	-2.369559	0.360324
8	-1.507219	-2.672788	-0.205733	1	-0.057894	-1.281768	2.318249
1	1.382825	-2.354122	0.182111	1	0.170502	1.366447	2.175524
1	0.389305	-1.349787	2.439196	1	1.734218	1.985713	0.126815
1	0.609874	1.302003	2.333019	1	0.568615	1.015368	-1.948460
1	1.728832	1.951112	0.010577	8	-1.177162	2.648095	-0.993591
1	0.362421	0.975853	-1.812964	6	-3.326906	1.738784	0.593380
1	0.172545	-1.321108	-1.720452	1	-3.058683	2.773250	0.372658
1	3.974163	-1.389044	0.379356	1	-4.328494	1.544181	0.189233
1	3.062486	-1.332396	-1.951571	1	-3.395503	1.609494	1.681334
6	-3.598072	1.706595	0.183681	6	-3.579029	-1.220031	0.763791
1	-3.983732	1.538319	1.197297	1	-3.629360	-0.938361	1.823436
1	-3.296647	2.750636	0.091482	1	-3.479476	-2.303829	0.684857
1	-4.428891	1.512579	-0.506383	1	-4.535749	-0.925661	0.313487
6	-3.845289	-1.224683	0.292245	8	-1.633846	-2.652110	-0.697082
1	-4.190395	-0.923391	1.289541	1	0.354562	-1.456643	-1.810777
1	-4.636194	-0.942347	-0.414016	1	3.949681	-1.407235	0.518406
1	-3.724356	-2.308430	0.275512	6	4.534806	0.704985	0.639442
1	3.253190	0.482748	-1.997387	1	2.987059	-1.343171	-1.782987
6	4.519482	0.734343	0.510556	1	3.199204	0.470332	-1.838536
1	4.492577	0.811243	1.604069	1	4.488741	0.799551	1.730446
1	5.564434	0.592839	0.209061	1	5.580388	0.524275	0.361443
1	4.185827	1.694397	0.101356	1	4.238073	1.666151	0.206595
3d1 HF = -845.9358462 (-846.1540822)				**3d1**† HF = -845.8925771 (-846.1141837)			

Nimag = 0				Nimag = 1(-465.91)			
6	-.857357	-1.473757	-.571566	6	2.478540	-0.277164	0.532576
6	.504093	-.811585	-.679383	6	1.485192	-1.381762	0.688344
6	.589740	.735705	-.518900	6	0.592322	-0.973129	1.705842
6	-.691104	1.503132	-.243947	6	0.690463	0.407600	1.852979
6	1.510688	-1.334051	.426972	6	1.648972	0.896869	0.935755
6	2.589401	-.250828	.306823	6	0.542037	0.719945	-0.933856
6	1.646226	.909482	.650235	6	-0.656190	1.526436	-0.622193
6	.993753	.359824	1.911518	6	-1.895072	0.777580	-0.240148
6	.910697	-.971887	1.777699	6	-3.002422	1.486923	0.240808
6	4.004794	-.397414	.775555	6	-4.173217	0.813075	0.575983
6	3.699781	-.248942	-.708568	6	-4.253567	-0.576916	0.419426
8	-.647876	2.716521	-.090022	6	-3.162634	-1.288324	-0.071499
8	-.950594	-2.688225	-.690677	6	-1.975914	-0.620360	-0.397457
1	1.804425	-2.374208	.278410	6	-0.824034	-1.401871	-0.948501
1	.422928	-1.673666	2.446149	6	0.464105	-0.687831	-1.081929
1	.586909	.970288	2.710897	6	3.909886	-0.458162	1.057535
1	2.052473	1.919291	.709700	6	3.653509	-0.297778	-0.415656
1	1.017256	1.183554	-1.423596	1	1.702460	-2.418043	0.448592
1	.904632	-1.109230	-1.655603	1	-0.142200	-1.610773	2.184347
1	4.465735	.450293	1.278881	1	0.043946	1.027149	2.464099
1	4.335705	-1.364846	1.146015	1	1.995889	1.924167	0.914634
1	3.791405	-1.167946	-1.289506	1	1.302820	1.270114	-1.477852
6	4.119543	.999206	-1.460054	8	-0.642252	2.754037	-0.668383
1	5.170397	.934166	-1.767129	1	-2.919878	2.565128	0.334517
1	3.518900	1.148308	-2.366077	1	-5.029016	1.366816	0.952968
1	4.013515	1.896225	-.839707	1	-5.171491	-1.099480	0.675289
6	-3.312973	-1.269127	-.240443	1	-3.204233	-2.362815	-0.219417
6	-2.065857	-.632733	-.322504	8	-0.946804	-2.582245	-1.264797
6	-1.987609	.766470	-.167727	1	1.169364	-1.189031	-1.738621
6	-3.157863	1.503059	.066723	1	4.183762	-1.433027	1.450457
6	-4.389138	.861956	.144362	1	4.347809	0.380371	1.593061
6	-4.466926	-.528668	-.009859	1	3.731584	-1.216261	-0.998302
1	-3.345109	-2.346850	-.362158	6	4.130283	0.940633	-1.147869
1	-3.069585	2.578268	.182715	1	3.578826	1.097224	-2.081921
1	-5.291543	1.439960	.324262	1	4.016440	1.842166	-0.535839
1	-5.429622	-1.029022	.050724	1	5.192809	0.847380	-1.401418
3d2 HF = -845.9363213 (-846.15466) Nimag = 0				**3d2†** HF = -845.8934873 (-846.1149238) Nimag = 1 (-467.14)			
6	0.969235	1.535356	-0.403771	6	-2.474390	0.226559	0.065787
6	-0.363330	0.913499	-0.779777	6	-1.537096	1.283279	0.547999
6	-0.461357	-0.639937	-0.847577	6	-0.781538	0.698386	1.590409
6	0.781472	-1.455319	-0.540286	6	-0.868808	-0.686734	1.478964
6	-1.508416	1.289523	0.248501	6	-1.680732	-1.002075	0.364476
6	-2.551714	0.237317	-0.144698	6	-0.358238	-0.508243	-1.279323
6	-.645216	-0.963074	0.155458	6	0.792835	-1.383119	-0.972050

6	-1.156623	-0.589947	1.548103	6	1.968072	-0.742999	-0.300879
6	-1.076206	0.747750	1.603733	6	3.005294	-1.551402	0.180162
6	-4.022776	0.343520	0.128730	6	4.117973	-0.975052	0.785946
6	-3.501057	0.352999	-1.302721	6	4.211061	0.417881	0.904179
8	0.724499	-2.677704	-0.562602	6	3.191341	1.229724	0.415893
8	1.065716	2.751978	-0.312207	6	2.061783	0.657944	-0.182224
1	-1.793760	2.341551	0.204057	6	0.990310	1.551665	-0.725790
1	-0.680976	1.352672	2.413068	6	-0.262867	0.901433	-1.162917
1	-0.841271	-1.302753	2.302896	6	-3.980798	0.338262	0.370559
1	-2.042990	-1.969585	0.026072	6	-3.475254	0.389602	-1.045343
1	-0.783042	-0.950407	-1.848688	1	-1.739350	2.346550	0.464772
1	-0.633146	1.347489	-1.749862	1	-0.133960	1.239706	2.270632
1	-4.349053	1.313735	0.504004	1	-0.297260	-1.405252	2.055495
1	-3.537094	1.284827	-1.863945	1	-1.996712	-2.007998	0.110768
6	3.375035	1.254916	0.157495	1	-1.042701	-0.932020	-2.008151
6	2.147452	0.652432	-0.153927	8	0.788265	-2.580890	-1.244669
6	2.058964	-0.753244	-0.217565	1	2.916184	-2.626428	0.059652
6	3.199726	-1.530162	0.031713	1	4.919012	-1.606152	1.161708
6	4.412369	-0.922149	0.336279	1	5.084298	0.865385	1.371429
6	4.500355	0.474994	0.399273	1	3.247049	2.311948	0.477607
1	3.415058	2.338314	0.201873	8	1.149690	2.767577	-0.796893
1	3.103818	-2.609631	-0.021813	1	-0.873864	1.527071	-1.806781
1	5.292304	-1.530999	0.525528	1	-4.270957	1.296937	0.797560
1	5.448521	0.949529	0.637191	6	-4.780779	-0.836211	0.890123
1	-3.683759	-0.534409	-1.906945	1	-3.499356	1.338983	-1.575924
6	-4.837506	-0.822532	0.650401	1	-3.660349	-0.477853	-1.676151
1	-4.763932	-0.901110	1.741677	1	-5.850312	-0.681362	0.702157
1	-5.897078	-0.705725	0.392382	1	-4.644314	-0.964121	1.970053
1	-4.497759	-1.773328	0.224790	1	-4.490070	-1.772286	0.401849
3e1 HF = -999.5798199 (-999.8314113) Nimag = 0				**3e1†** HF = -999.5366638 (-999.8319376) Nimag = 1 (-468.72)			
6	-0.193220	1.531374	-0.572890	6	3.385141	-0.224387	0.699163
6	-1.540966	0.837758	-0.668342	6	2.398253	-1.339735	0.812901
6	-1.590594	-0.715530	-0.545377	6	1.404860	-0.899923	1.717783
6	-0.289699	-1.468227	-0.323801	6	1.467879	0.487854	1.805387
6	-2.532603	1.310302	0.472716	6	2.502169	0.951261	0.959344
6	-3.589742	0.206067	0.353187	6	1.589166	0.666698	-0.992435
6	-2.612853	-0.940342	0.644985	6	0.358781	1.472459	-0.841051
6	-1.940764	-0.405891	1.902601	6	-0.905210	0.726247	-0.551448
6	-1.891194	0.930215	1.799481	6	-2.046034	1.431469	-0.223472
6	-4.995750	0.309855	0.860342	6	-3.270681	0.769672	0.036042
6	-4.725074	0.202694	-0.634056	6	-4.453983	1.475108	0.386120
8	-0.312599	-2.686613	-0.204079	6	-5.629010	0.799984	0.626898
8	-0.136816	2.751410	-0.659998	6	-5.677581	-0.613633	0.527679
1	-2.852977	2.346722	0.356774	6	-4.550148	-1.327269	0.189789
1	-1.402070	1.626919	2.472221	6	-3.319801	-0.662355	-0.064118

1	-1.499764	-1.025743	2.676252	6	-2.141372	-1.363697	-0.417367
1	-2.994995	-1.960260	0.690207	6	-0.953683	-0.698976	-0.649633
1	-2.033495	-1.148336	-1.450012	6	0.259693	-1.482589	-1.040286
1	-1.969801	1.150066	-1.627908	6	1.542714	-0.747933	-1.081946
1	-5.425269	-0.559320	1.354830	6	4.759474	-0.349572	1.371750
1	-5.338447	1.260796	1.261579	6	4.649066	-0.266007	-0.126056
1	-4.851594	1.132620	-1.190544	1	2.652610	-2.381795	0.646009
6	2.256356	1.367518	-0.310254	1	0.636855	-1.527983	2.154562
6	1.039317	0.713921	-0.377018	1	0.756098	1.122844	2.320526
6	0.993748	-0.710554	-0.259265	1	2.834614	1.982902	0.921978
6	2.167313	-1.420309	-0.080523	1	2.393664	1.201896	-1.486333
1	2.264116	2.449915	-0.401056	8	0.372143	2.697113	-0.941739
1	2.105936	-2.501322	0.006370	1	-1.987978	2.515340	-0.174873
6	4.726559	1.316261	-0.062861	1	-4.413860	2.559038	0.459120
6	3.467459	0.659721	-0.130313	1	-6.527711	1.349304	0.893688
6	3.421920	-0.770836	-0.012630	1	-6.612903	-1.132213	0.719624
6	4.637394	-1.485848	0.167032	1	-4.584250	-2.411017	0.111353
6	5.839754	-0.819189	0.227861	1	-2.157004	-2.445465	-0.517823
6	5.884655	0.593798	0.112027	8	0.192364	-2.680406	-1.305226
1	4.757396	2.399129	-0.152059	1	2.317264	-1.265733	-1.640382
1	4.599309	-2.568579	0.255001	1	5.008206	-1.298413	1.838186
1	6.763540	-1.374280	0.365193	1	5.127745	0.522830	1.905606
1	6.842269	1.104526	0.162349	1	4.800388	-1.209812	-0.650964
6	-5.136007	-1.036994	-1.404142	6	5.176211	0.945763	-0.868245
1	-6.195120	-0.988287	-1.684868	1	6.261676	0.868378	-1.001564
1	-4.554075	-1.152424	-2.327124	1	4.977410	1.873756	-0.320965
1	-4.995687	-1.945091	-0.807154	1	4.725706	1.039842	-1.862823
3e2 HF = -999.5802808 (-999.8319376) Nimag = 0				**3e2†** HF = -999.5375967 (-999.7925511) Nimag = 1 (-469.37)			
6	-0.115841	1.602022	-0.537075	6	-3.405996	0.147248	0.290863
6	-1.450720	0.936652	-0.824325	6	-2.447913	1.222814	0.683261
6	-1.506682	-0.619261	-0.896821	6	-1.530978	0.627536	1.580953
6	-0.223078	-1.404004	-0.690780	6	-1.582335	-0.753926	1.417118
6	-2.529851	1.271491	0.286320	6	-2.533430	-1.056951	0.414737
6	-3.565156	0.187838	-0.035287	6	-1.476897	-0.433710	-1.374112
6	-2.601344	-0.983978	0.189877	6	.261452	-1.269685	-1.273877
6	-2.023773	-0.600693	1.545182	6	0.972312	-0.605489	-0.749004
6	-1.982462	0.738698	1.603170	6	2.083682	-1.373650	-0.463940
6	-5.014833	0.244762	0.346432	6	3.280424	-0.786762	0.014300
6	-4.600759	0.275416	-1.119506	6	4.432502	-1.559590	0.323898
8	-0.250676	-2.627205	-0.740826	6	5.581126	-0.955532	0.782543
8	-0.055587	2.822419	-0.457746	6	5.633314	0.451202	0.952460
1	-2.850807	2.314022	0.269579	6	4.535898	1.229149	0.660851
1	-1.547974	1.352772	2.385024	6	3.333253	0.638252	0.186622
1	-1.630949	-1.305641	2.270470	6	2.186685	1.407705	-0.127375
1	-2.975247	-2.002356	0.083614	6	1.024870	0.812553	-0.577213

1	-1.895756	-0.933089	-1.872510	6	-0.152432	1.670855	-0.918181
1	-1.802687	1.367226	-1.769279	6	-1.425046	0.973524	-1.202974
1	-5.344442	1.202648	0.749484	6	-4.854254	0.181184	0.816785
1	-4.708952	1.206725	-1.672298	6	-4.564786	0.314623	-0.653393
6	2.307298	1.386424	-0.113311	1	-2.700271	2.278617	0.681917
6	1.100399	0.756531	-0.357098	1	-0.812207	1.167383	2.186711
6	1.049510	-0.670726	-0.430597	1	-0.907499	-1.470544	1.871330
6	2.207681	-1.406674	-0.257539	1	-2.845053	-2.063923	0.159885
1	2.319329	2.471352	-0.061682	1	-2.240561	-0.857327	-2.019754
1	2.142435	-2.489287	-0.317498	8	-0.263770	-2.455244	-1.597103
1	-4.797817	-0.616285	-1.712833	1	2.024733	-2.447042	-0.621747
6	4.751479	1.284235	0.313497	1	4.389848	-2.637674	0.190663
6	3.502813	0.651970	0.064683	1	6.456052	-1.556013	1.016066
6	3.451678	-0.781348	-0.009501	1	6.547683	0.913438	1.314214
6	4.651252	-1.523167	0.168332	1	4.573117	2.308169	0.788012
6	5.843758	-0.879562	0.407864	1	2.207233	2.489143	-0.024427
6	5.894282	0.536101	0.481098	8	-0.065159	2.895999	-0.951195
1	4.786647	2.369232	0.368672	1	-2.149570	1.593058	-1.723359
1	4.608905	-2.607823	0.111482	1	-5.112911	1.107069	1.328006
1	6.755401	-1.455054	0.542403	6	-5.524238	-1.048618	1.389409
1	6.844049	1.028386	0.670817	1	-4.700277	1.284076	-1.127912
6	-5.749270	-0.949519	0.920692	1	-4.811478	-0.531590	-1.292042
1	-5.592068	-1.028856	2.003077	1	-5.222400	-1.218282	2.429316
1	-6.828421	-0.868150	0.742441	1	-6.614826	-0.932489	1.370284
1	-5.409822	-1.886777	0.465791	1	-5.276027	-1.948503	0.816842

Table S9. Cartesian Coordinates of the B3LYP/6-31G* Optimized Geometry of Spiro cyclopentadiene and various quinones. The Values in Parenthesis Implies Single-Point Energies Evaluated at the B3LYP/6-311+G**//B3LYP/6-31G* Level

1a HF = -381.4516858 (-381.5616335) Nimag = 0				**1b** HF = -460.0930138 (-460.2219625) Nimag = 0			
6	1.268886	0.671718	0.000000	6	-1.436266	-0.603235	-0.000016
6	1.268886	-0.671770	0.000000	6	-0.678575	0.687022	0.000047
6	-0.000007	-1.445182	0.000000	6	0.678565	0.687018	0.000042
6	-1.268886	-0.671718	0.000000	6	1.436274	-0.603236	0.000019
6	-1.268886	0.671770	0.000000	6	0.669820	-1.873843	0.000092
6	0.000007	1.445182	0.000000	6	-0.669827	-1.873839	0.000077
8	-0.000007	-2.670347	0.000000	6	-1.493541	1.951513	0.000048
8	0.000007	2.670347	0.000000	6	1.493538	1.951502	-0.000006
1	-2.183095	-1.258539	0.000000	8	2.662925	-0.628870	-0.000132
1	-2.183186	1.258447	0.000000	8	-2.662917	-0.628883	-0.000141
1	2.183095	1.258539	0.000000	1	1.263888	-2.783342	0.000123
1	2.183186	-1.258447	0.000000	1	-1.263885	-2.783345	0.000113
				1	1.268983	2.566110	-0.880841
				1	1.269815	2.565602	0.881404
				1	2.558417	1.713919	-0.000537

	1 -1.269396 2.565865 0.881167 1 -1.269400 2.565866 -0.881078 1 -2.558422 1.713937 0.000016
1c HF = -610.3459704 (-610.5171171) Nimag = 0	**1d** HF = -535.1159458 (-535.2582862) Nimag = 0
6 -2.276694 -1.253855 0.000023 6 -1.399719 -2.327352 0.000032 6 -1.781745 0.065140 -0.000002 6 -0.010813 -2.126263 0.000013 6 0.493161 -0.832124 -0.000003 6 -0.382184 0.282991 -0.000014 6 0.148017 1.648450 -0.000018 6 1.616249 1.828455 0.000062 6 2.458270 0.781678 0.000058 6 1.970888 -0.621386 -0.000017 1 0.683434 -2.959329 0.000007 1 1.961352 2.858609 0.000109 1 3.537877 0.902799 0.000096 8 -0.590644 2.649859 -0.000047 8 2.767825 -1.552669 -0.000074 1 -1.795515 -3.339186 0.000051 1 -3.352544 -1.396075 0.000038 8 -2.665302 1.070769 -0.000021 1 -2.142209 1.915109 0.000032	6 2.677864 0.699637 -0.000020 6 2.677886 -0.699520 0.000024 6 1.472727 1.400226 -0.000022 6 1.472773 -1.400206 0.000052 6 0.260161 -0.704410 0.000019 6 0.260127 0.704375 0.000061 6 -1.025135 1.463078 0.000235 6 -2.281301 0.671539 0.000041 6 -2.281252 -0.671941 0.000090 6 -1.024972 -1.463031 -0.000041 1 1.447353 2.485298 -0.000020 1 1.447337 -2.485251 0.000062 1 -3.199444 1.253151 -0.000055 1 -3.199235 -1.253700 0.000216 8 -1.061831 2.688227 -0.000199 8 -1.061585 -2.688000 -0.000154 1 3.619055 -1.242227 0.000022 1 3.618986 1.242431 -0.000031
1e HF = -688.7611014 (-688.9369829) Nimag = 0	2de HF = -271.490377 (-271.5634367) Nimag = 0
6 4.001677 0.708329 -0.000018 6 2.813787 1.405636 -0.000027 6 1.571608 0.717741 -0.000005 6 1.571605 -0.717773 0.000026 6 2.813804 -1.405623 0.000028 6 4.001684 -0.708290 0.000012 6 0.330520 1.403012 -0.000007 6 0.330499 -1.403069 0.000034 6 -0.864916 -0.714794 0.000012 6 -0.864918 0.714747 0.000070 6 -2.149474 1.470448 0.000267 6 -3.400921 0.672008 0.000045 6 -3.400901 -0.672304 0.000097 6 -2.149375 -1.470352 -0.000060 1 0.305904 2.489277 0.000003 1 4.946938 1.243951 -0.000034 1 2.810223 2.492664 -0.000036 1 2.810269 -2.492652 0.000043 1 4.946949 -1.243901 0.000011 1 0.305761 -2.489305 0.000038	6 0.433177 0.000212 -0.000148 6 -0.468235 1.175973 -0.000244 6 -1.747208 0.732888 -0.000067 6 -1.746952 -0.733243 0.000151 6 -0.467757 -1.175778 0.000016 6 1.777719 0.000343 0.743034 6 1.778034 -0.000261 -0.742845 1 -0.124797 2.204609 -0.000352 1 -2.640299 1.348736 0.000071 1 -2.639771 -1.349458 0.000226 1 -0.124170 -2.204381 0.000070 1 2.044173 0.913591 1.266898 1 2.043827 -0.912673 1.267505 1 2.043961 -0.913831 -1.266406 1 2.044406 0.912614 -1.267398

1	-4.321315	1.250281	-0.000066
1	-4.321160	-1.250686	0.000241
8	-2.194532	2.696208	-0.000217
8	-2.194424	-2.695948	-0.000164

3de HF = -310.8065322 (-310.8897259)
Nimag = 0

6	0.018651	-0.256533	0.162865
6	-0.598744	1.056609	0.465080
6	-1.909070	0.999777	0.126831
6	-2.212128	-0.330677	-0.405235
6	-1.084707	-1.079844	-0.384434
6	1.130610	-0.867671	1.034528
6	1.467793	-0.426083	-0.343907
1	-0.072224	1.900659	0.894476
1	-2.632549	1.801478	0.231362
1	-3.188549	-0.647926	-0.755594
1	-0.968741	-2.107236	-0.712159
1	1.472915	-0.259660	1.868158
1	1.054438	-1.928562	1.255003
1	1.568875	-1.220497	-1.081478
6	2.353613	0.773538	-0.603403
1	3.407403	0.469323	-0.632463
1	2.111883	1.246918	-1.561702
1	2.250434	1.530809	0.180454