Supporting Information Accompanying:

***p*-Benzyne Derivatives That Have Exceptionally Small Singlet-Triplet Gaps
And Even A Triplet Ground State**

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Table 1S: Cartesian Coordinates of (6,6)CASSCF / 6-31G* Optimized Structure of 1^1A_g Benzene in Å

C	0.020134	0.00000	-0.02396
C	0.005194	0.00000	1.372365
C	1.208013	0.00000	2.082085
C	2.424226	0.00000	1.396274
C	2.438883	0.00000	0.000243
C	1.236504	0.00000	-0.70979
H	-0.93014	0.00000	1.903402
H	1.196979	0.00000	3.157596
H	3.349318	0.00000	1.944953
H	3.375407	0.00000	-0.52864
H	1.245245	0.00000	-1.78535
H	-0.90516	0.00000	-0.57234

Table 2S: Cartesian Coordinates of (6,6)CASSCF / 6-31G* Optimized Structure of 1^1A Tetramethyl Benzene in Å

C	1.88124	0.00054	-0.49793
C	0.58492	0.00012	0.01387
C	0.30496	-0.0005	1.38793
C	1.38008	-0.00054	2.28666
C	2.68445	-0.00034	1.7718
C	2.96188	0.0001	0.40653
C	-1.13867	-0.00117	1.8461
C	1.20638	-0.00056	3.79167
C	4.39436	0.00002	-0.078
C	2.10451	0.00164	-1.99347
H	5.08412	-0.0004	0.75795
H	4.61167	-0.87432	-0.68482
H	4.61202	0.87465	-0.68427
H	1.15897	0.00241	-2.52315
H	2.66269	0.87631	-2.31486
H	2.66215	-0.87282	-2.31635
H	0.16763	-0.00019	4.09191
H	1.67499	-0.87542	4.23356
H	1.6756	0.87396	4.23356
H	-1.8085	-0.00086	0.9938
H	-1.37216	-0.87747	2.44317
H	-1.37273	0.87425	2.44425
H	-0.24109	0.00028	-0.67731
H	3.50799	-0.00053	2.4673

Table 3S: Cartesian Coordinates of (6,6)CASSCF / 6-31G* Optimized Structure of 1^1A Tetraamino Benzene in Å

C	0.01324	-0.00389	0.02381
C	-0.04311	-0.00033	1.40845
C	1.11846	-0.00094	2.19903
C	2.36465	0.02748	1.5699
C	2.41841	-0.0013	0.16611
C	1.27124	-0.0313	-0.61081
N	0.94681	-0.02417	3.61244
N	3.60181	0.09906	2.27141
N	1.30492	-0.01435	-2.0242
N	-1.14336	-0.05407	-0.78771
H	2.2297	-0.12725	-2.38454
H	0.70995	-0.71862	-2.41467
H	-1.98392	0.06264	-0.2608
H	-1.11179	0.63211	-1.51612
H	3.50349	0.41646	3.21265
H	4.096	-0.77097	2.27262
H	1.76559	-0.3131	4.10482
H	0.64142	0.85556	3.97845
H	3.38576	0.02572	-0.30512
H	-0.99665	-0.02341	1.90722

Table 4S: Cartesian Coordinates of (6,6)CASSCF / 6-31G* Optimized Structure of 1¹A' Tetranitro Benzene in Å

C	-1.19613	-0.69529	0.00634
C	0.00000	-1.4014	0.010725
C	1.195756	-0.69564	0.005963
C	1.195879	0.696831	-0.00956
C	0.000271	1.402748	-0.01427
C	-1.19598	0.696797	-0.00916
N	2.426733	1.471431	-0.14901
O	2.49975	2.469269	0.49158
N	-2.42666	1.472193	-0.14562
O	-2.49412	2.473543	0.490159
N	2.425972	-1.47106	0.146808
O	2.499382	-2.46814	-0.49485
N	-2.42577	-1.47169	0.147194
O	-2.49941	-2.46729	-0.49686
O	3.222973	1.059219	-0.92763
O	-3.22615	1.059467	-0.92051
O	3.216271	-1.06559	0.934943
O	-3.21879	-1.06445	0.931599
H	-0.0002	-2.47219	0.035394
H	0.000218	2.473509	-0.03872

Table 5S: Cartesian Coordinates of (6,6)CASSCF / 6-31G* Optimized Structure of 1^1A_g Tetrafluoro Benzene in Å

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.384034
C	1.146391	0.00000	2.157779
C	2.371319	0.001198	1.50609
C	2.371198	0.002488	0.123435
C	1.224163	0.001358	-0.65078
F	1.080699	0.001476	3.474118
F	3.499731	0.004009	2.188378
F	1.290221	-0.00323	-1.9675
F	-1.12881	-0.00581	-0.68165
H	3.350134	-0.00044	-0.35364
H	-0.9431	-0.00105	1.928534

Table 6S: Cartesian Coordinates of (8,8)CASSCF / 6-31G* Optimized Structure of 1^1A_g *p*-Benzyne in Å

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.41129
C	1.221219	0.00000	2.059417
C	2.442154	0.00000	1.410137
C	2.441957	0.00000	-0.00075
C	1.220654	0.00000	-0.6493
H	3.370396	0.00000	-0.54156
H	3.371534	0.00000	1.949318
H	-0.92825	0.00000	1.952424
H	-0.92897	0.00000	-0.53978

Table 7S: Cartesian Coordinates of (8,8)CASSCF / 6-31G* Optimized Structure of 1¹A Tetramethyl *p*-Benzyne in Å

C	0.624229	-7.1E-05	0.041018
C	0.298793	-0.00063	1.393088
C	1.382282	-0.00051	2.298858
C	2.655203	-0.0003	1.73757
C	2.97851	0.000049	0.39338
C	1.889845	0.000447	-0.51663
C	-1.14881	-0.00127	1.836497
C	1.215919	-0.00043	3.803363
C	4.41508	-4.8E-05	-0.07763
C	2.097914	0.001751	-2.01396
H	5.094669	-0.00048	0.765418
H	4.633159	-0.87513	-0.68243
H	4.633587	0.875266	-0.68193
H	1.147438	0.002634	-2.53276
H	2.654233	0.877131	-2.33548
H	2.653624	-0.87335	-2.3373
H	0.175424	-2.5E-05	4.098613
H	1.684409	-0.87546	4.242263
H	1.685023	0.874336	4.242133
H	-1.80636	-0.00086	0.976134
H	-1.38335	-0.87808	2.431727
H	-1.38384	0.874622	2.43291

Table 8S: Cartesian Coordinates of (8,8)CASSCF / 6-31G* Optimized Structure of 1¹A Tetraamino *p*-Benzyne in Å

C	0.05659	0.046752	0.048054
C	-0.0268	0.006297	1.441242
C	1.188774	-0.00535	2.143524
C	2.354034	-0.04698	1.375403
C	2.431931	-0.04327	-0.00283
C	1.211681	0.041955	-0.70783
N	-1.30603	-0.02337	2.053352
N	1.297634	0.025032	3.557568
N	3.64537	-0.04124	-0.72306
N	1.22946	0.038767	-2.11877
H	4.436106	-0.18709	-0.1304
H	3.641189	-0.72933	-1.45036
H	0.321283	0.185558	-2.50792
H	1.862696	0.725539	-2.47903
H	0.463271	0.331486	4.010439
H	1.585726	-0.84996	3.946223
H	-1.28111	-0.32522	3.003821
H	-1.78826	0.850425	1.993581

Table 9S: Cartesian Coordinates of (8,8)CASSCF / 6-31G* Optimized Structure of 1¹A' Tetranitro *p*-Benzyne in Å

C	-1.33917	-0.13579	0.00000
C	1.339374	0.143923	0.00000
C	0.693453	0.07339	1.220779
C	0.693453	0.07339	-1.22078
C	-0.69358	-0.0657	1.220831
C	-0.69358	-0.0657	-1.22083
N	1.498742	0.03809	2.437299
N	1.498742	0.03809	-2.4373
N	-1.49862	-0.02935	2.437144
N	-1.49862	-0.02935	-2.43714
O	-1.19622	0.793662	3.23761
O	-1.19622	0.793662	-3.23761
O	1.196202	-0.78488	3.237958
O	1.196202	-0.78488	-3.23796
O	-2.40158	-0.79628	2.49177
O	-2.40158	-0.79628	-2.49177
O	2.401504	0.805001	2.491608
O	2.401504	0.805001	-2.49161

Table 10S: Cartesian Coordinates of (8,8)CASSCF / 6-31G* Optimized Structure of 1^1A_g Tetrafluoro *p*-Benzyne in Å

C	0.049601	0.001636	0.028867
C	0.001051	-0.00109	1.411086
C	1.202889	-0.00101	2.104438
C	2.375321	0.001955	1.371546
C	2.423944	0.003543	-0.01147
C	1.223259	0.00333	-0.70467
F	-1.15002	-0.00113	2.053031
F	1.22235	-0.00079	3.422945
F	3.575543	0.000439	-0.6533
F	1.203022	0.000104	-2.02318

Table 11S: Cartesian Coordinates of (8,8)CASSCF / 6-31G* Optimized Structure of 1^3B_2 *m*-Quinone in Å

C	-0.02683	0.00000	-0.0154
C	-0.04802	0.00000	1.431851
C	1.233055	0.00000	2.128385
C	2.432484	0.00000	1.419169
C	2.459006	0.00000	0.025543
C	1.222214	0.00000	-0.74661
O	-1.11671	0.00000	2.051466
O	1.235459	0.00000	-1.98217
H	-0.95301	0.00000	-0.55636
H	3.383028	0.00000	-0.52005
H	1.211705	0.00000	3.201261
H	3.361272	0.00000	1.959911

Table 12S: Cartesian Coordinates of (10,10)CASSCF / 6-31G* Optimized Structure of 1^3B_2 2,6-Quinone p -Benzyne in Å

C	0.00000	0.00000	1.64213
C	0.00000	0.00000	-1.03286
C	0.00000	1.315488	-0.36347
C	0.00000	-1.31549	-0.36347
C	0.34332	1.180227	1.08883
C	-0.34332	-1.18023	1.08883
H	1.020979	1.887372	1.52968
H	-1.02098	-1.88737	1.52968
O	-0.08582	2.363398	-0.9637
O	0.085815	-2.3634	-0.9637

Table 13S: Cartesian Coordinates of (10,10)CASSCF / 6-31G* Optimized Structure of 1^1B_2 2,6-Quinone p -Benzyne in Å

C	0.00000	0.00000	1.6906
C	0.00000	0.00000	-1.07956
C	0.00000	1.302799	-0.4014
C	0.00000	-1.3028	-0.4014
C	0.00000	1.237279	1.083955
C	0.00000	-1.23728	1.083955
H	0.00000	2.163493	1.624207
H	0.00000	-2.16349	1.624207
O	0.00000	2.358981	-0.99904
O	0.00000	-2.35898	-0.99904

Table 14S: Cartesian Coordinates of (10,10)CASSCF / 6-31G* Optimized Structure of 2^3B_2 2,6-Quinone *p*-Benzyne in Å

C	0.00000	0.00000	1.680719
C	0.00000	0.00000	-1.07493
C	0.234622	1.286647	-0.40398
C	-0.23462	-1.28665	-0.40398
C	0.247783	1.217244	1.078897
C	-0.24778	-1.21724	1.078897
H	0.448907	2.115637	1.629234
H	-0.44891	-2.11564	1.629234
O	0.40397	2.322718	-1.01108
O	-0.40397	-2.32272	-1.01108

Table 15S: Cartesian Coordinates of (10,10)CASSCF / 6-31G* Optimized Structure of 1^5B_2 2,6-Quinone *p*-Benzyne in Å

C	0.00000	0.00000	1.698286
C	0.00000	0.00000	-1.03624
C	0.00000	1.294513	-0.37436
C	0.00000	-1.29451	-0.37436
C	0.020117	1.241325	1.093689
C	-0.02012	-1.24133	1.093689
H	0.042657	2.161148	1.644594
H	-0.04266	-2.16115	1.644594
O	-0.02033	2.351512	-0.99334
O	0.020325	-2.35151	-0.99334

Table 16S: Total CASSCF / 6-31G* Energies, Number and Magnitude of Imaginary Vibrations for Benzene, Tetrasubstituted Benzene, *p*-Benzyne, Tetrasubstituted Benzyne, *m*-Quinone, 2,6-quinone *p*-Benzyne.

Molecule	State	Total Energy	Imaginary Vibrations
Benzene	1^1A_g	-230.776449743865	0
Tetramethyl Benzene	1^1A	-386.919640650495	-122 cm ⁻¹
Tetraamino Benzene	1^1A	-450.873284815801	-90 cm ⁻¹
Tetranitro Benzene	$1^1A'$	-1044.5902306552	0
Tetrafluoro Benzene	1^1A_g	-626.161190628874	0
<i>p</i> -Benzyne	1^1A_g	-229.480808359	0
Tetramethyl <i>p</i> -Benzyne	1^1A	-385.626011640	-113
Tetraamino <i>p</i> -Benzyne	1^1A	-449.573107586	-100
Tetranitro <i>p</i> -Benzyne	$1^1A'$	-1043.271895491079	0
Tetrafluoro <i>p</i> -Benzyne	1^1A_g	-624.847238538	0
<i>m</i> -Quinone	1^3B_2	-379.297475277795	0
2,6-Quinone <i>p</i> -Benzyne	1^3B	-378.015629554714	0
2,6-Quinone <i>p</i> -Benzyne	1^1B_2	-377.989407136	0
2,6-Quinone <i>p</i> -Benzyne	2^3B	-377.990332382	0
2,6-Quinone <i>p</i> -Benzyne	1^5B_2	-378.00101175	0