Routes of π-electron delocalization in 4-substituted-1,2-benzoquinone

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Supporting Information

Figure S1. Relationship between SESE values and substituent constants σ. SI2

Figure S2. Relationship between HOMA (a) of the ring and (b) for transmission paths OC2C3C4 and OC1C6C5C4, and SESE values. SI3

Figure S3. Dependence of electron density at BCP for CO bonds on their bond lengths. SI4

Figure S4. Dependence of electron density at BCP of a1, b1 and c1 CC bonds on their lengths. SI4

Figure S5. Relationship between Mulliken charges on the oxygen atom of the C=O groups values and substituent constants σ SI5

Figure S6. Relationship between frequency values for the C=O groups and substituent constants σ SI5

Table S1. Bond lengths, their mean values and estimated standard deviations for 4-X-*ortho*benzoquinone. SI6

Table S2. Geometrical and energetic parameters of the O···H-F hydrogen bond in 4-X-*ortho*quinone (X = H and NMe_2) complexes optimized without constraints SI7

Table S3. π-electron delocalization: HOMA, MCI, DI and FLU for 4-X-*ortho*-benzoquinone SI8

Cartesian coordinates of optimized 4-X-*ortho*-benzoquinone and H-bonded systems SI9

Application of homodesmotic reaction (Scheme 6) allows us to relate substituent effects stabilization energy, SESE, to substituent constants σ_p^+ for electron donating substituents and for others σ_p (see Fig. S1), changes in aromaticity of the ring (see Fig. S2a) and changes in delocalization in paths OC2C3C4 (*meta* type way) and OC1C6C5C4 (*para* type way). As we see, due to a significant equivalency of SESE and substituent constants σ (σ_p^+ for electron donating substituents and σ_p for others) dependences in Figs S1 and S2b resemble those in Figs 5 and 1.

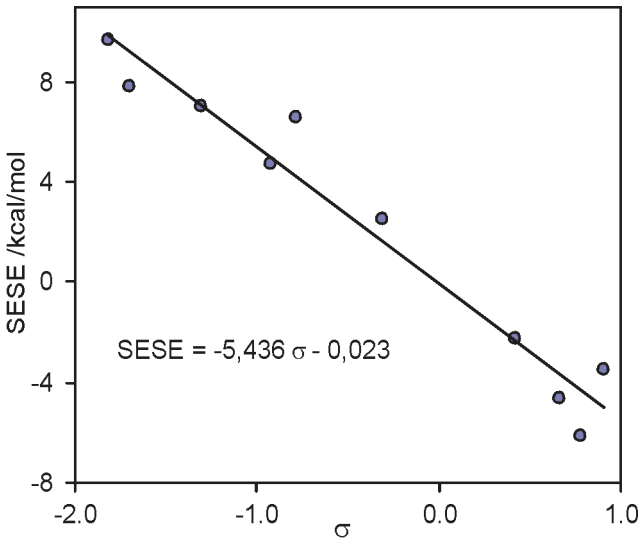

Figure S1. Relationship between SESE values (see Scheme 6) and substituent constants σ (σ_p^+ for electron donating substituents and for others σ_p), *cc* = -0.975.

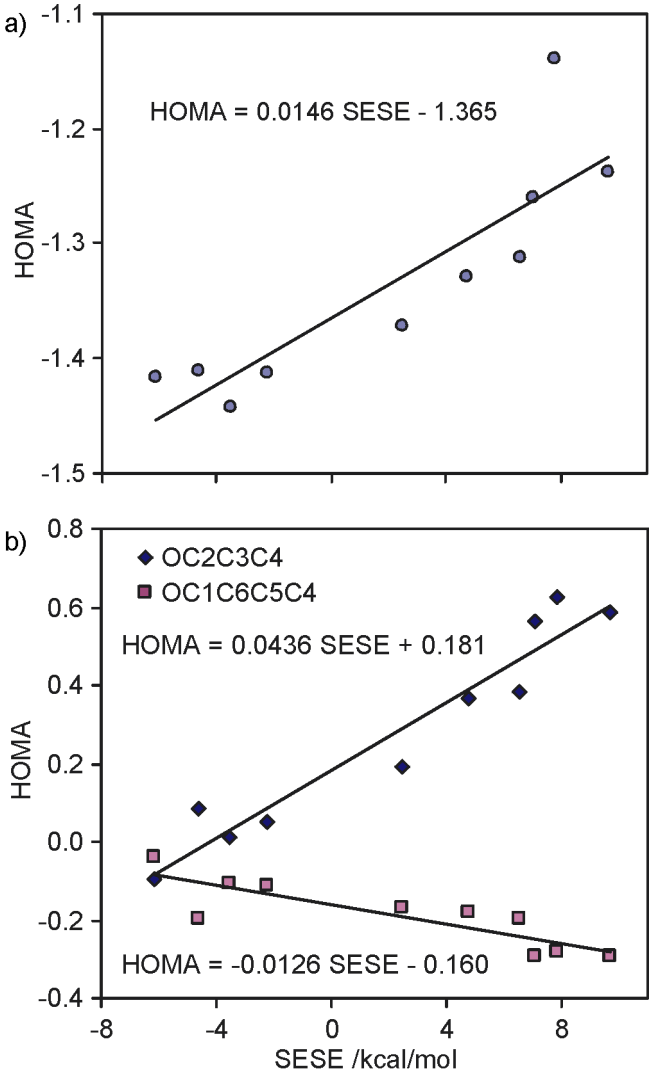

Figure S2. Relationship between HOMA (a) of the ring and (b) for transmission paths OC2C3C4 (*meta* type way) and OC1C6C5C4 (*para* type way), and SESE values (see Scheme 4); *cc* = 0.872, 0.962 and -0.853, respectively.

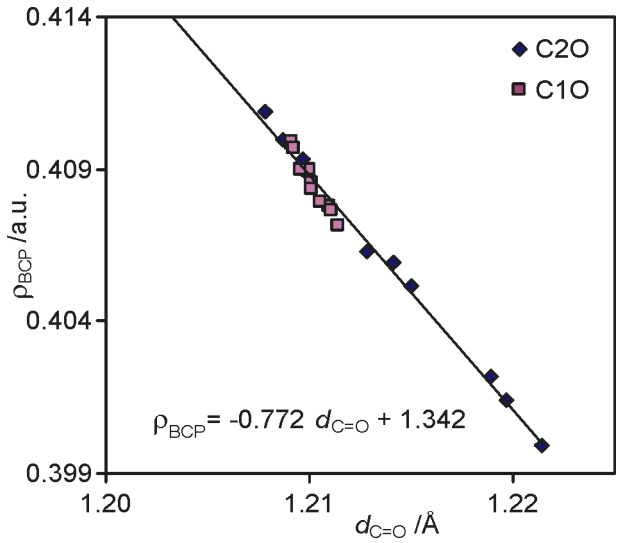

Figure S3. Dependence of electron density at BCP, ρ_{BCP}, for CO bonds on their bond lengths, $d_{C=O}$. The value of *cc* for the regression is equal to -0.994.

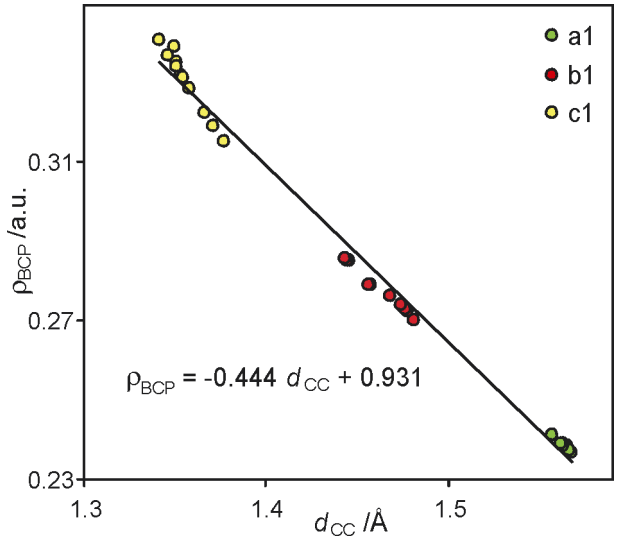

Figure S4. Dependence of electron density at BCP, ρ_{BCP}, of a1 (green), b1 (red) and c1 (yellow) CC bonds on their lengths, d_{CC}. The value of *cc* for the overall regression is equal to -0.996.

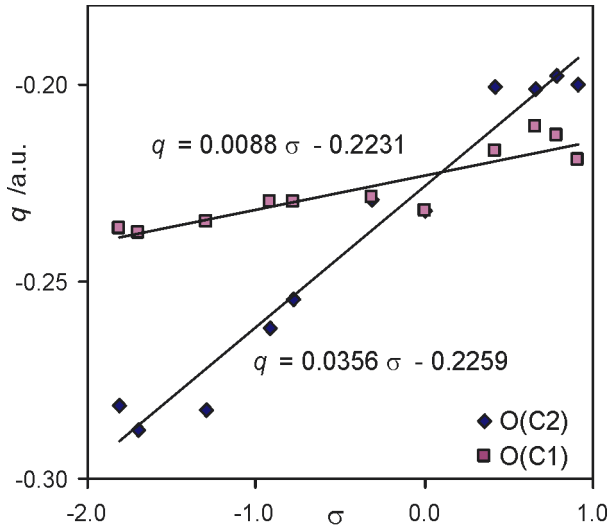

Figure S5. Relationship between Mulliken charges on the oxygen atom of the C=O groups values (O(C1) and O(C2), see Scheme 5) and substituent constants σ (σ_p^+ for electron donating substituents and for others σ_p); *cc* = 0.904 and 0.983, respectively.

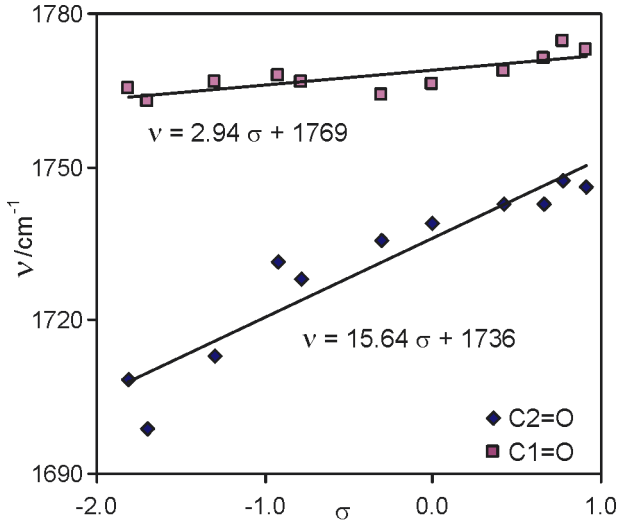

Figure S6. Relationship between frequency values for the C=O groups (C1=O and C2=O, see Scheme 5) and substituent constants σ (σ_p^+ for electron donating substituents and for others σ_p); *cc* = 0.814 and 0.944, respectively.

Table S1. Bond lengths (Å) and their mean values and estimated standard deviations (esd) for 4-X-*ortho*-benzoquinone, see Scheme 5.

X	σ_p	σ_p^+	a1	b1	c1	c2	b2	a2	C1=O	C2=O
4-NO	0.91		1.5668	1.4781	1.3496	1.4623	1.3440	1.4764	1.2091	1.2087
4-NO_2	0.78	0.79	1.5647	1.4809	1.3416	1.4581	1.3449	1.4743	1.2091	1.2079
4-CN	0.66	0.66	1.5632	1.4752	1.3535	1.4725	1.3434	1.4748	1.2092	1.2097
4-CHO	0.42	0.73	1.5656	1.4765	1.3512	1.4665	1.3442	1.4740	1.2100	1.2098
4-H	0.00	0.00	1.5678	1.4739	1.3464	1.4626	1.3464	1.4739	1.2110	1.2110
4-CH_3	-0.17	-0.31	1.5644	1.4678	1.3510	1.4726	1.3445	1.4735	1.2111	1.2129
4-OCH_3	-0.27	-0.78	1.5653	1.4571	1.3579	1.4686	1.3408	1.4774	1.2101	1.2150
4-OH	-0.37	-0.92	1.5667	1.4566	1.3545	1.4659	1.3413	1.4786	1.2096	1.2142
4-NH_2	-0.66	-1.30	1.5629	1.4452	1.3657	1.4731	1.3397	1.4811	1.2101	1.2189
4-NHMe	-0.70	-1.81	1.5619	1.4449	1.3704	1.4736	1.3392	1.4807	1.2106	1.2197
4-$N(Me)_2$	-0.83	-1.70	1.5566	1.4435	1.3774	1.4771	1.3410	1.4776	1.2114	1.2214
		mean val.	1.564	1.464	1.356	1.468	1.343	1.477	1.210	1.214
		esd.	0.003	0.015	0.011	0.006	0.002	0.003	0.001	0.005

Table S2. Geometrical (Å and deg.) and energetic parameters (kcal/mol) of the O···H-F hydrogen bond in 4-X-*ortho*-benzoquinone (X = H and NMe_2) complexes optimized without constraints. For comparison: with O···H-F turned towards the nearest hydrogen atom (a) and with O···H-F turned towards the nearest oxygen atom (b).

4-X-		C1=O	O...H	H-F	C2=O	O···H	H-F	ΔE_{HB} /kcal/mol	angle C=O···H	angle O···H-F
a)										
4-H		1.211			1.211					
	O···HF	1.220	1.704	0.945	1.210			-9.35	118.9	167.0
4-NMe_2		1.211			1.221					
	O1···HF	1.221	1.678	0.948	1.221			-10.58	119.0	168.3
	O2···HF	1.210			1.237	1.609	0.959	-13.41	116.5	170.6
b)										
4-H		1.211			1.211					
	O···HF	1.217	1.797	0.937	1.210			-8.36	134.4	166.7
4-NMe_2		1.211			1.221					
	O1···HF	1.217	1.797	0.938	1.221			-9.58	132.0	162.8
	O2···HF	1.210			1.231	1.709	0.944	-11.36	135.4	168.8

Table S3. π-electron delocalization: HOMA, MCI, DI and FLU for 4-X-*ortho*-benzoquinone, see Scheme 5.

X	HOMA		MCI /a.u.		DI /a.u.		HOMA	MCI/a.u.	FLU /a.u.
	OC2C3C4	OC1C6C5C4	OC2C3C4Y	OC1C6C5C4	C2O	C1O	ring	ring	ring
4-NO	0.009	-0.107	-0.0057	-0.0045	1.464	1.455	-1.442	0.0023	0.0757
4-NO_2	-0.098	-0.040	-0.0031	-0.0046	1.464	1.455	-1.415	0.0023	0.0764
4-CN	0.085	-0.195	-0.0027	-0.0043	1.455	1.456	-1.411	0.0024	0.0760
4-CHO	0.052	-0.115	-0.0042	-0.0045	1.459	1.450	-1.413	0.0024	0.0763
4-H	0.064	-0.059	-0.0016	-0.0046	1.449	1.449	-1.409	0.0024	0.0757
4-CH_3	0.192	-0.169	-0.0006	-0.0045	1.438	1.451	-1.372	0.0024	0.0752
4-OCH_3	0.381	-0.196	0.0052	-0.0045	1.419	1.452	-1.312	0.0024	0.0739
4-OH	0.363	-0.181	0.0049	-0.0047	1.420	1.456	-1.329	0.0024	0.0741
4-NH_2	0.565	-0.294	0.0091	-0.0043	1.398	1.454	-1.260	0.0026	0.0714
4-NHMe	0.588	-0.296	0.0099	-0.0040	1.393	1.451	-1.237	0.0027	0.0710
4-$N(Me)_2$	0.626	-0.284	0.0105	-0.0040	1.388	1.448	-1.139	0.0028	0.0690

Cartesian coordinates of optimized 4-X-*ortho*-benzoquinone and H-bonded systems

4-NO-*ortho*-benzoquinone
E_{tot}=-510.8722167 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.566844
C	1.318806	0.000000	2.234364
C	2.447832	0.000000	1.494924
C	2.458344	0.000000	0.032666
C	1.314292	0.000000	-0.672581
O	-1.049994	0.000000	-0.599541
O	-1.039831	0.000000	2.183015
H	1.358194	0.000000	3.318147
N	3.678427	0.000000	2.267678
H	3.428507	0.000000	-0.450033
H	1.303212	0.000000	-1.756610
O	4.688792	0.000000	1.603046

4-CN-*ortho*-benzoquinone
E_{tot}=-473.8089935 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.563199
C	1.310869	0.000000	2.239757
C	2.455024	0.000000	1.516569
C	2.454669	0.000000	0.044116
C	1.315146	0.000000	-0.667442
O	-1.046679	0.000000	-0.605529
O	-1.042594	0.000000	2.176602
H	1.311944	0.000000	3.323023
C	3.727451	0.000000	2.173326
H	3.418794	0.000000	-0.451108
H	1.315566	0.000000	-1.751163
N	4.765007	0.000000	2.680942

4-NO_2-*ortho*-benzoquinone
E_{tot}=-586.1034646 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.564701
C	1.316284	0.000000	2.243360
C	2.432966	0.000000	1.499730
C	2.458172	0.000000	0.041851
C	1.315034	0.000000	-0.666602
O	-1.048698	0.000000	-0.601754
O	-1.038673	0.000000	2.181217
H	1.343434	0.000000	3.325271
N	3.755769	0.000000	2.199756
H	3.427706	0.000000	-0.437687
H	1.314230	0.000000	-1.750063
O	3.751387	0.000000	3.418593
O	4.753359	0.000000	1.492186

4-CHO-*ortho*-benzoquinone
E_{tot}=-494.904085 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.565596
C	1.316850	0.000000	2.233365
C	2.458878	0.000000	1.511132
C	2.454556	0.000000	0.044683
C	1.314310	0.000000	-0.667247
O	-1.050226	0.000000	-0.600853
O	-1.041353	0.000000	2.181408
H	1.320621	0.000000	3.319243
C	3.767976	0.000000	2.221075
H	3.424317	0.000000	-0.440099
H	1.310101	0.000000	-1.751287
O	4.835195	0.000000	1.654876
H	3.699733	0.000000	3.326326

ortho-benzoquinone
E_{tot}=-381.5498469 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.567792
C	1.313276	0.000000	2.236854
C	2.449874	0.000000	1.515178
C	2.449861	0.000000	0.052624
C	1.313253	0.000000	-0.669050
O	-1.048731	0.000000	-0.605564
O	-1.048709	0.000000	2.173373
H	1.311434	0.000000	3.320801
H	3.411696	0.000000	2.017308
H	3.411673	0.000000	-0.449529
H	1.311394	0.000000	-1.752999

4-OCH_3-*ortho*-benzoquinone
E_{tot}=-496.1166191 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.565289
C	1.293509	0.000000	2.236000
C	2.442671	-0.000022	1.512627
C	2.449512	-0.000040	0.043999
C	1.315797	-0.000032	-0.671905
O	-1.042636	0.000035	-0.614128
O	-1.060120	-0.000004	2.158966
H	1.277412	0.000003	3.317304
O	3.691252	-0.000014	2.011327
H	3.425941	-0.000056	-0.427600
H	1.315999	-0.000044	-1.755660
C	3.862085	0.000013	3.431670
H	4.936639	0.000051	3.598624
H	3.415326	-0.894837	3.873257
H	3.415261	0.894833	3.873247

4-CH_3-*ortho*-benzoquinone
E_{tot}=-420.8813657 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.564385
C	1.306059	0.000000	2.234241
C	2.464092	0.001632	1.538500
C	2.447931	0.002047	0.065945
C	1.316940	0.002066	-0.661023
O	-1.044613	-0.002459	-0.612729
O	-1.052694	0.001246	2.166787
H	1.290594	0.000347	3.318878
C	3.808978	0.002686	2.206581
H	3.410554	0.002143	-0.437152
H	1.323451	0.002037	-1.745105
H	3.720195	0.000742	3.293073
H	4.390251	-0.875092	1.903814
H	4.387116	0.883782	1.907262

4-OH-*ortho*-benzoquinone
E_{tot}=-456.8047924 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.566708
C	1.297968	0.000000	2.227755
C	2.440933	0.000000	1.500998
C	2.451976	0.000000	0.035169
C	1.314881	0.000000	-0.676239
O	-1.043116	0.000000	-0.612403
O	-1.057805	0.000000	2.162755
H	1.304239	0.000000	3.312952
O	3.685982	0.000000	2.026708
H	3.426579	0.000000	-0.439900
H	1.310719	0.000000	-1.759892
H	3.644737	0.000000	2.991290

4-NH_2-*ortho*-benzoquinone
E_{tot}=-436.9374779 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.562917
C	1.288031	0.000000	2.218344
C	2.454892	0.000905	1.508670
C	2.452789	0.002308	0.035595
C	1.317820	-0.000721	-0.676132
O	-1.036418	0.001406	-0.624735
O	-1.067122	-0.004336	2.151860
H	1.289234	-0.001592	3.302977
N	3.688203	0.032281	2.095320
H	3.416357	0.009640	-0.466269
H	1.314609	0.000122	-1.760148
H	3.772733	-0.068108	3.093817
H	4.517290	-0.138352	1.551660

4-$N(CH_3)_2$-*ortho*-benzoquinone
E_{tot}=-515.5650977 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.556621
C	1.283942	0.000000	2.216376
C	2.474432	0.000237	1.523487
C	2.457633	-0.001315	0.046485
C	1.320154	-0.001538	-0.663704
O	-1.033231	0.001260	-0.632398
O	-1.068694	-0.000553	2.147994
H	1.249786	-0.000625	3.296319
N	3.692446	0.003078	2.146024
H	3.402537	-0.002029	-0.480498
H	1.323884	-0.002349	-1.747939
C	3.735815	0.004612	3.603960
H	3.249322	-0.886809	4.014441
H	4.771883	0.016516	3.934571
H	3.230788	0.886889	4.010911
C	4.956135	-0.012861	1.408577
H	5.061132	-0.911354	0.792886
H	5.070149	0.869188	0.771435
H	5.774002	-0.007975	2.125576

4-$NHCH_3$-*ortho*-benzoquinone
E_{tot}=-476.2559526 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.561897
C	1.286096	0.000000	2.220507
C	2.457580	0.000327	1.509375
C	2.451772	0.000826	0.035747
C	1.317370	0.000781	-0.675915
O	-1.036170	-0.000739	-0.625998
O	-1.068911	-0.000084	2.149388
H	1.275109	-0.000381	3.302653
N	3.691494	0.000456	2.082235
H	3.415192	0.001319	-0.467509
H	1.314349	0.001154	-1.759983
C	3.919727	-0.000188	3.514243
H	4.993044	0.000972	3.699989
H	3.482726	0.887140	3.983814
H	3.484700	-0.888991	3.982905
H	4.493898	0.000007	1.475081

H-bonded complexes

ortho-benzoquinone O...HF linear

E_{tot}= -482.043692799 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.566968
C	1.313289	0.000000	2.234956
C	2.447252	0.000000	1.510099
C	2.439965	0.000000	0.047181
C	1.302266	0.000000	-0.675137
O	-1.056126	0.000000	-0.599289
O	-1.050784	0.000000	2.166149
H	1.311982	0.000000	3.318656
H	3.411242	0.000000	2.007333
H	3.399706	0.000000	-0.458684
H	1.299150	0.000000	-1.758840
H	-2.617907	0.000000	-1.485507
F	-3.428655	0.000000	-1.945558

ortho-benzoquinone O...HF -> O

E_{tot}= -482.045518547 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.564300
C	1.310951	0.000000	2.234210
C	2.444443	-0.000483	1.508322
C	2.436899	-0.000923	0.045141
C	1.299263	-0.000728	-0.677510
O	-1.056774	0.000572	-0.603587
O	-1.055166	-0.000002	2.156521
H	1.309493	0.000281	3.317809
H	3.408601	-0.000584	2.005067
H	3.396642	-0.001402	-0.460512
H	1.294580	-0.000999	-1.761100
H	-2.785299	0.001523	-0.111524
F	-3.721014	0.002082	-0.069227

ortho-benzoquinone O...HF -> H

E_{tot}= -482.047100292 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.564811
C	1.313896	0.000000	2.230735
C	2.446362	-0.001040	1.503608
C	2.435261	-0.001782	0.040868
C	1.297019	-0.001274	-0.681431
O	-1.068757	0.000565	-0.588339
O	-1.049914	0.000182	2.165594
H	1.313833	0.000533	3.314354
H	3.411429	-0.001375	1.998724
H	3.393578	-0.002758	-0.467585
H	1.292696	-0.001673	-1.765464
H	-1.071068	0.003018	-2.291934
F	-0.860233	0.004764	-3.212881

NMe2-ortho-benzoquinone O1...HF linear

E_{tot}= -616.060475740 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.555079
C	1.283141	0.000000	2.211441
C	2.471455	0.000195	1.513993
C	2.447524	-0.001256	0.036613
C	1.308824	-0.001461	-0.672926
O	-1.040811	0.001217	-0.626256
O	-1.071881	-0.000563	2.139079
H	1.251469	-0.000659	3.291195
N	3.691031	0.002914	2.129245
H	3.390190	-0.001898	-0.494173
H	1.309130	-0.002198	-1.756896
C	3.740556	0.004630	3.587796
H	3.255597	-0.886946	3.999242
H	4.777810	0.016409	3.913930
H	3.237274	0.887253	3.995689
C	4.952875	-0.012560	1.386543
H	5.055229	-0.911173	0.771027
H	5.064083	0.870234	0.750335
H	5.772829	-0.007952	2.100816
H	-2.561906	0.002995	-1.541498
F	-3.362171	0.003931	-2.023017

NMe2-ortho-benzoquinone O1...HF -> O

E_{tot}= -616.062711893 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.551888
C	1.279730	0.000000	2.210923
C	2.467698	-0.003895	1.511805
C	2.443635	-0.005722	0.033898
C	1.305129	-0.003875	-0.676168
O	-1.043262	0.002373	-0.626942
O	-1.077828	0.003533	2.126462
H	1.248156	0.006277	3.290582
N	3.687262	-0.013858	2.125939
H	3.386556	-0.012215	-0.496274
H	1.303906	-0.007321	-1.759975
C	3.738524	-0.029842	3.584566
H	3.203080	-0.897375	3.982118
H	4.774983	-0.085937	3.908701
H	3.287887	0.874803	4.007531
C	4.948073	0.051720	1.383727
H	5.090490	-0.822014	0.741178
H	5.018436	0.957962	0.775258
H	5.767468	0.070995	2.098388
H	-2.761715	0.009658	-0.101462
F	-3.699898	0.013640	-0.104321

NMe2-ortho-benzoquinone O1...HF -> H

E_{tot}= -616.064308651 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.553337
C	1.283511	0.000000	2.207383
C	2.470381	-0.001542	1.507009
C	2.442454	0.000851	0.029958
C	1.303553	0.001457	-0.679695
O	-1.054468	-0.000610	-0.614649
O	-1.071417	-0.000949	2.138584
H	1.253643	-0.002788	3.287113
N	3.691152	-0.003578	2.118745
H	3.383571	0.003909	-0.503449
H	1.303413	0.003975	-1.763893
C	3.745085	0.006473	3.577094
H	3.263232	-0.883845	3.994828
H	4.783319	0.021769	3.899929
H	3.241475	0.890486	3.981529
C	4.951185	-0.015709	1.372219
H	5.044163	-0.904726	0.742044
H	5.067346	0.876522	0.750054
H	5.772913	-0.030192	2.084300
H	-1.019577	-0.000406	-2.291909
F	-0.807763	-0.000049	-3.216116

NMe2-ortho-benzoquinone O2...HF -> O

E_{tot}= -616.065551986 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.550062
C	1.265601	0.000000	2.216080
C	2.462669	0.001471	1.524085
C	2.454523	0.002353	0.046183
C	1.318917	0.001812	-0.665295
O	-1.037394	-0.002185	-0.623012
O	-1.077575	0.000566	2.145283
H	1.228225	0.001139	3.295516
N	3.670364	-0.000567	2.152451
H	3.401417	0.001362	-0.476418
H	1.320749	0.001162	-1.749206
C	3.708684	-0.012268	3.613196
H	3.198349	-0.895309	4.009685
H	4.743491	-0.031823	3.946027
H	3.225642	0.879183	4.025901
C	4.941671	0.021873	1.423271
H	5.071069	-0.869210	0.802650
H	5.034848	0.912183	0.795654
H	5.753132	0.041655	2.146680
H	-2.723575	0.009996	1.684693
F	-3.664595	0.015409	1.611650

NMe2-ortho-benzoquinone O2...HF
linear

E_{tot}= -616.063653854 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.552866
C	1.268270	0.000000	2.217267
C	2.465180	0.000077	1.525407
C	2.456609	-0.001477	0.047721
C	1.320781	-0.001583	-0.663402
O	-1.033934	0.001293	-0.628644
O	-1.078152	-0.000509	2.139321
H	1.232294	-0.000666	3.296853
N	3.673208	0.002479	2.153648
H	3.403372	-0.002272	-0.475196
H	1.323531	-0.002357	-1.747394
C	3.711726	0.004327	3.614398
H	3.224398	-0.887528	4.020998
H	4.746659	0.016190	3.947245
H	3.205925	0.887124	4.017401
C	4.944201	-0.010964	1.423993
H	5.051518	-0.908884	0.809111
H	5.058813	0.872561	0.790150
H	5.756343	-0.006249	2.146897
H	-2.583458	-0.001220	2.958124
F	-3.407577	-0.001609	3.406399

NMe2-ortho-benzoquinone O2...HF -> H

E_{tot}= -616.068828294 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.548305
C	1.260271	0.000000	2.217500
C	2.459933	0.008703	1.527683
C	2.457319	0.018759	0.050280
C	1.322205	0.015644	-0.661713
O	-1.031897	-0.012518	-0.632133
O	-1.093605	-0.001474	2.125240
H	1.224115	-0.004275	3.297216
N	3.661635	0.008775	2.163071
H	3.405243	0.028506	-0.470524
H	1.324866	0.022069	-1.745594
C	3.690292	-0.005126	3.625943
H	3.188167	-0.894527	4.017844
H	4.723360	-0.010117	3.964463
H	3.191033	0.878104	4.035320
C	4.937737	0.021636	1.442103
H	5.058816	-0.865127	0.813895
H	5.045950	0.916552	0.823335
H	5.744635	0.023863	2.170717
H	-1.055967	-0.004519	3.733683
F	-0.876947	-0.006369	4.675584