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Supporting Information for

Structures and Properties of Ubiquinone-1 and its Radical Anion from Hybrid Hartree-Fock/Density Functional Studies

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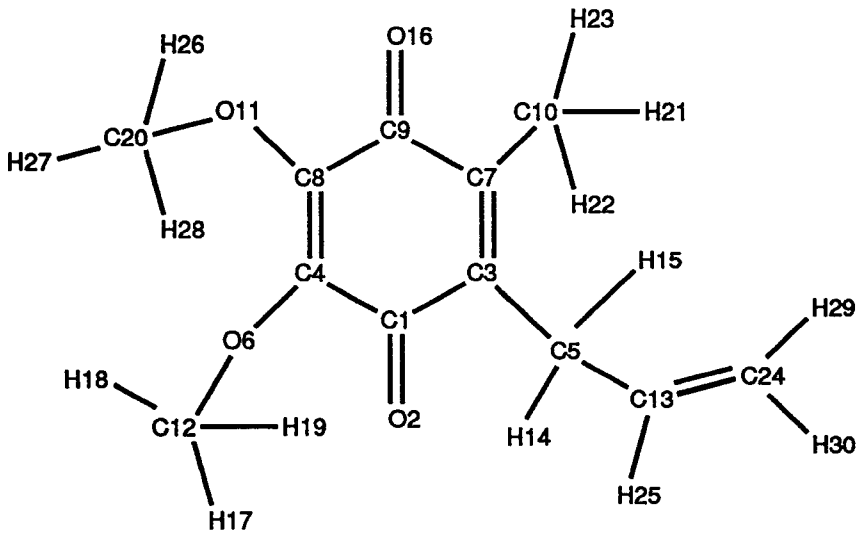
The atom numbering systems and geometries of ubiquinone-1 (UQ_1), the model 5-allyl-2,3-dimethoxy-1,4-benzoquinone (UQ_1 with isoprenyl methyl groups replaced by hydrogens, abbreviated UQ), and their radical anions ($UQ_1^{\bullet -}$ and $UQ^{\bullet -}$)—obtained from B3LYP/6-31G(d) calculations—are provided to show the close structural similarity between the two molecules and the two radical anions. For most bonds between non-hydrogen atoms, for example, bond distances differ by less than 0.002 Å


H26
O16
H23
O11
C10
H21
C20
C9
H27
C8
C7
H22
H28
C4
C3
H15
H29
C1
O6
C5
C24
H18
C13
C12
H19
O2
H14
H30
H25
H17

Zmatrix for ubiquinone (UQ) and ubisemiquinone $(UQ)^{\bullet-}$ models

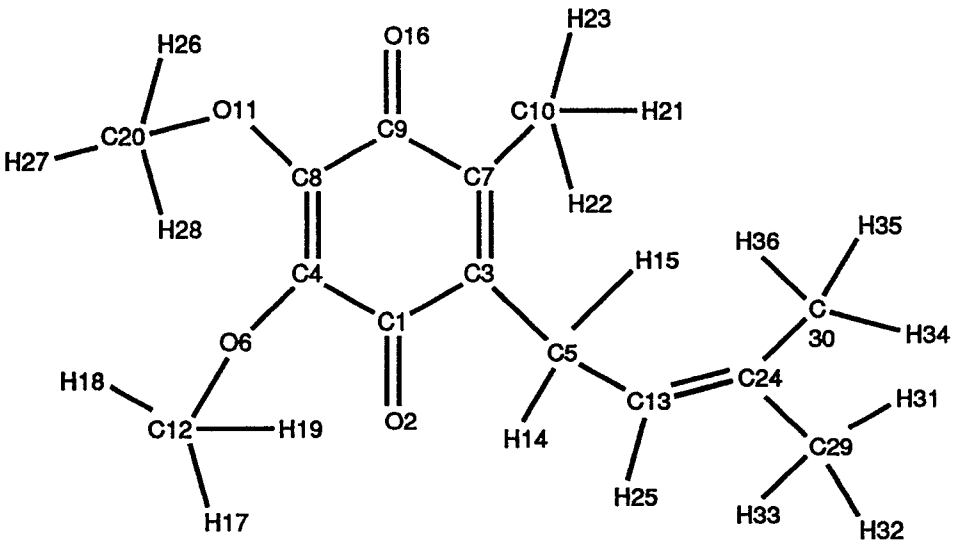
C1
O2,1,R2
C3,1,R3,2,A3
C4,1,R4,2,A4,3,D4
C5,3,R5,1,A5,2,D5
O6,4,R6,1,A6,2,D6
C7,3,R7,1,A7,5,D7
C8,4,R8,1,A8,6,D8
C9,7,R9,3,A9,1,D9
C10,7,R10,3,A10,9,D10
O11,8,R11,4,A11,1,D11
C12,6,R12,4,A12,1,D12
C13,5,R13,3,A13,1,D13
H14,5,R14,3,A14,13,D14
H15,5,R15,3,A15,13,D15
O16,9,R16,7,A16,3,D16
H17,12,R17,6,A17,4,D17
H18,12,R18,6,A18,17,D18
H19,12,R19,6,A19,17,D19
C20,11,R20,8,A20,4,D20
H21,10,R21,7,A21,3,D21
H22,10,R22,7,A22,21,D22
H23,10,R23,7,A23,21,D23
C24,13,R24,5,A24,3,D24
H25,13,R25,5,A25,24,D25
H26,20,R26,11,A26,8,D26
H27,20,R27,11,A27,26,D27
H28,20,R28,11,A28,26,D28
H29,24,R29,13,A29,5,D29
H30,24,R30,13,A30,29,D30

TABLE S1: Bond Distances, Bond Angles, and Torsional Angles for the Models of ubiquinone (UQ) and ubisemiquinone $(UQ)^{\bullet-}$ Using the Becke3LYP Hartree-Fock/Density Functional Method and a 6-31G(d) Basis Set. Variables are in regard to the above zmatrix.

Variables	UQ 6-31G(d)	$UQ^{\bullet-}$ 6-31G(d)
R2	1.23083744	1.27186192
R3	1.49589068	1.45742714
R4	1.48175163	1.45316574
R5	1.51494183	1.52021454
R6	1.36832226	1.38242428
R7	1.35157006	1.38101427
R8	1.36292682	1.37810267
R9	1.49554731	1.46020014
R10	1.50557384	1.51082573
R11	1.33950874	1.3825469
R12	1.43557474	1.42112052
R13	1.51274075	1.5078966
R14	1.0959195	1.09807177

R15	1.09459423	1.09633673
R16	1.22168287	1.26877112
R17	1.09198569	1.09619163
R18	1.09080323	1.09311926
R19	1.09850086	1.10254638
R20	1.43131831	1.42081081
R21	1.09754459	1.09285837
R22	1.09527939	1.10066239
R23	1.09085709	1.09796072
R24	1.33344733	1.33550109
R25	1.08923349	1.08975733
R26	1.09154989	1.09623054
R27	1.0909227	1.10253368
R28	1.09502185	1.09304846
R29	1.08667173	1.08839978
R30	1.08836868	1.08939174
A3	119.76921041	121.19302542
A4	120.34999302	122.25346456
A5	115.64742469	115.17652805
A6	117.90532259	119.79898703
A7	20.67040621	122.11163426
A8	19.95049703	121.56249104
A9	19.80344459	121.15763326
A10	123.86879517	122.60323149
A11	129.25991782	118.33666984
A12	117.06672918	115.29181374
A13	111.74420936	112.0183889
A14	108.05537037	107.16273704
A15	110.18847253	111.42240858
A16	121.16959515	122.15740175
A17	105.56908407	106.1895296
A18	111.0949662	111.01205671
A19	110.53996653	111.06588804
A20	122.18951995	115.317965
A21	111.15869095	108.52397265
A22	110.80346366	112.20672881
A23	110.04854153	111.88943977
A24	124.74802409	125.92489816
A25	115.25565725	114.17601195
A26	104.59079318	106.20158617
A27	111.54435469	111.09036632
A28	110.9816579	111.01314614
A29	121.62544646	121.95058665
A30	121.83078817	121.66178483
D4	179.2144328	-179.69231434
D5	-2.8257268	-1.25411356
D6	-2.74943565	-2.03527343
D7	176.80933947	178.1290838
D8	-172.78307619	-175.62218415
D9	3.79026645	1.62483157
D10	179.28904986	-179.3992999
D11	177.90632472	175.68249114
D12	64.32206482	59.23341511
D13	6.61047096	83.21582004

D14	-119.63756675	-117.94789281
D15	22.34600792	123.41240922
D16	178.14361489	-179.37645006
D17	78.33510883	-179.60267124
D18	119.16891582	119.91494593
D19	-118.11295834	-117.8172108
D20	10.2784089	123.32905953
D21	-65.442793	175.17592824
D22	119.28172839	119.45627973
D23	-119.77301939	-120.4729943
D24	121.12633143	123.07125046
D25	79.74545592	-179.59676181
D26	175.06114276	179.84847204
D27	119.37620472	117.83606721
D28	-118.10599554	-119.85860412
D29	179.40381439	-179.35442896
D30	-179.08698966	179.61119549


H23
H26
O16
O11
C10
H21
C20
C9
H27
C8
C7
H22
H28
H36
H35
C4
C3
H15
C
30
H34
O6
C1
C5
C24
H18
C13
H31
C12
H19
O2
H14
C29
H25
H33
H17
H32

Zmatrix for ubiquinone-1 $(UQ)_1$ and ubisemiquinone-1 $(UQ)_1^{\bullet-}$

C1
O2,1,R2
C3,1,R3,2,A3
C4,1,R4,2,A4,3,D4
C5,3,R5,1,A5,2,D5
O6,4,R6,1,A6,2,D6
C7,3,R7,1,A7,5,D7
C8,4,R8,1,A8,6,D8
C9,7,R9,3,A9,1,D9
C10,7,R10,3,A10,9,D10
O11,8,R11,4,A11,1,D11
C12,6,R12,4,A12,1,D12
C13,5,R13,3,A13,1,D13
H14,5,R14,3,A14,13,D14
H15,5,R15,3,A15,13,D15
O16,9,R16,7,A16,3,D16
H17,12,R17,6,A17,4,D17
H18,12,R18,6,A18,17,D18
H19,12,R19,6,A19,17,D19
C20,11,R20,8,A20,4,D20
H21,10,R21,7,A21,3,D21
H22,10,R22,7,A22,21,D22
H23,10,R23,7,A23,21,D23
C24,13,R24,5,A24,3,D24
H25,13,R25,5,A25,24,D25
H26,20,R26,11,A26,8,D26
H27,20,R27,11,A27,26,D27
H28,20,R28,11,A28,26,D28
C29,24,R29,13,A29,5,D29
C30,24,R30,13,A30,29,D30
H31,29,R31,24,A31,13,D31
H32,29,R32,24,A32,31,D32
H33,29,R33,24,A33,31,D33
H34,30,R34,24,A34,13,D34
H35,30,R35,24,A35,34,D35
H36,30,R36,24,A36,34,D36

TABLE S2: Bond Distances, Bond Angles, and Torsional Angles for Ubiquinone-1 $(UQ)_1$ and Ubisemiquinone-1 $(UQ)_1^{\bullet-}$ Using the Becke3LYP Hartree-Fock/Density Functional Method and a 6-31G(d) Basis Set. Variables are in regard to the above zmatrix.

Variables	UQ_1 6-31G(d)	$UQ_1^{\bullet-}$ 6-31G(d)
R2	1.23065673	1.2705849
R3	1.49651227	1.4552446
R4	1.48225604	1.457014
R5	1.51521474	1.5213635
R6	1.36869773	1.38239831
R7	1.35168505	1.38092277
R8	1.36265217	1.37794896

R9	1.4945272	1.46050933
R10	1.50556044	1.51087391
R11	1.33977913	1.38271754
R12	1.4353775	1.42116583
R13	1.51413603	1.50982775
R14	1.09619028	1.09840246
R15	1.09285483	1.09425882
R16	1.22203124	1.26886347
R17	1.0920395	1.09619887
R18	1.0908083	1.09308917
R19	1.09853685	1.10256759
R20	1.4311116	1.42069774
R21	1.09769253	1.0928894
R22	1.0950669	1.10057481
R23	1.090923	1.09825663
R24	1.34201578	1.34246626
R25	1.08947304	1.08973555
R26	1.09160877	1.09625327
R27	1.09093875	1.10254345
R28	1.09506404	1.09311732
R29	1.51113714	1.5119364
R30	1.50944924	1.51042188
R31	1.09428437	1.10120909
R32	1.0991644	1.09496515
R33	1.09918373	1.10169191
R34	1.0925229	1.10131468
R35	1.09891465	1.09230621
R36	1.09876352	1.1004599
A3	119.86873309	121.48687132
A4	120.22788557	121.99153498
A5	115.73804301	115.06997387
A6	117.87439571	119.82406127
A7	120.52626577	122.14177015
A8	119.98818161	121.53529144
A9	119.96036243	121.20715823
A10	123.75715799	122.72228328
A11	129.30325473	118.36090195
A12	117.00724966	115.31144458
A13	111.46565453	111.93590748
A14	107.81592419	106.99194741
A15	109.65020883	110.83960793
A16	121.22161507	122.17220583
A17	105.58295963	106.18615922
A18	111.0944217	111.00423595
A19	110.55470241	111.07382578
A20	122.22126541	115.27066097
A21	111.18659456	108.47268537
A22	110.78722216	112.28606189
A23	110.05637205	111.99400752
A24	128.39312832	129.45332521
A25	113.73720467	112.61135172
A26	104.58689373	106.20842318
A27	111.56602717	111.08127148
A28	111.02839269	111.01608684

A29	120.3382158	120.71994823
A30	125.34598016	125.03880546
A31	111.95132721	111.44281106
A32	111.05710479	111.62933215
A33	111.0913829	111.5810864
A34	113.5898642	111.00896027
A35	110.42289746	112.8315421
A36	110.74553344	111.00055251
D4	179.250506	-179.55693694
D5	-2.66197028	-1.33143117
D6	-2.77235791	-2.21074134
D7	177.02643787	178.51058612
D8	-172.90063735	-175.64595931
D9	3.50650096	1.41678789
D10	179.32561231	-179.39470763
D11	177.8152219	175.73459272
D12	64.38320457	59.26848084
D13	87.68508984	81.47876413
D14	-119.04509529	-117.16380426
D15	123.87342597	125.21533142
D16	178.13610452	-179.33121678
D17	178.16310424	-179.25038181
D18	119.18381637	119.89920013
D19	-118.11836734	-117.81171338
D20	9.72127233	123.10920919
D21	-66.59154871	176.40013262
D22	119.31318761	119.53673602
D23	-119.68719421	-120.25851562
D24	126.88286083	125.15109341
D25	179.00297333	-179.88758354
D26	175.66682092	179.9103472
D27	119.37110253	117.83575524
D28	-118.09761127	-119.84994956
D29	179.20326507	-179.55088044
D30	-178.78652885	-179.71881253
D31	0.74985711	120.47030754
D32	120.92374373	-120.65754937
D33	-120.88165323	118.49094074
D34	-2.7940445	119.24884822
D35	120.96103479	-121.1498143
D36	-121.58533063	117.90893397