

Supporting Information

**Competitive excited-state single or double proton transfer
mechanisms for bis-2,5-(2-benzoxazolyl)-hydroquinone and its
derivatives**

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Table S1. Potential energies (Hartree) of stable structures on PESs of the S_0 state the S_1 state for BBHQ, BBHQ-A and BBHQ-B.

	BBHQ		BBHQ-A		BBHQ-B	
	S_0	S_1	S_0	S_1	S_0	S_1
Energy	-1179.830	-1179.728	-1179.811	-1179.732	-	-1179.734

Table S2: The calculated primary bond lengths (Å) and angles (°) of DHBO, DHBO-A and DHBO-B in the S_0 and S_1 states.

	DHBO		DHBO-A		DHBO-B	
Electronic state	S_0	S_1	S_0	S_1	S_0	S_1
O ₁ -H ₂	0.99	1.01	1.75	1.94	-	1.92
H ₂ -N ₃	1.82	1.73	1.04	1.02	-	1.02
O ₄ -H ₅	0.99	1.01	0.99	1.01	-	1.92
H ₅ -N ₆	1.82	1.73	1.82	1.71	-	1.02
$\delta(\text{O}_1\text{-H}_2\text{-N}_3)$	145.2°	147.8°	132.3°	125.3°	-	125.9°
$\delta(\text{O}_4\text{-H}_5\text{-N}_6)$	145.2°	147.8°	145.6°	147.9°	-	125.9°

Table S3. Electronic excitation energy (nm), corresponding oscillator strengths and the corresponding compositions of the low-lying singlet excited states for DHBO.

	Transition	$\lambda(\text{nm})$	f	Composition	CI(%)
DHBO	$S_0 \rightarrow S_1$	415.4	0.9013	H \rightarrow L	98.52%
	$S_0 \rightarrow S_2$	344.4	0.8587	H-1 \rightarrow L	95.22%
	$S_0 \rightarrow S_3$	317.4	0.0000	H-2 \rightarrow L	87.12%

Table S4. Potential energies (Hartree) of stable structures on PESs of the S_0 state the S_1 state for **DHBO**, **DHBO-A** and **DHBO-B**.

	DHBO		DHBO-A		DHBO-B	
	S_0	S_1	S_0	S_1	S_0	S_1
Energy	-1494.348	-1494.247	-1494.331	-1494.253	-	-1494.257

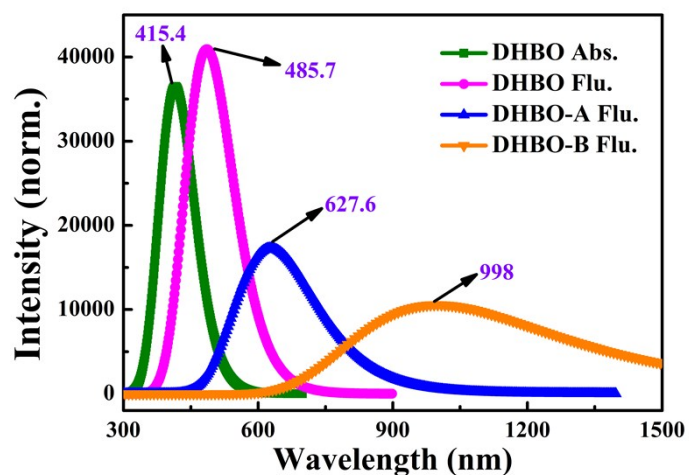


Figure S1 The calculated absorption and fluorescence spectra of DHBO, DHBO-A and DHBO-B forms at the B3LYP/6-31+G(d)/IEF-PCM(heptane) theoretical level.

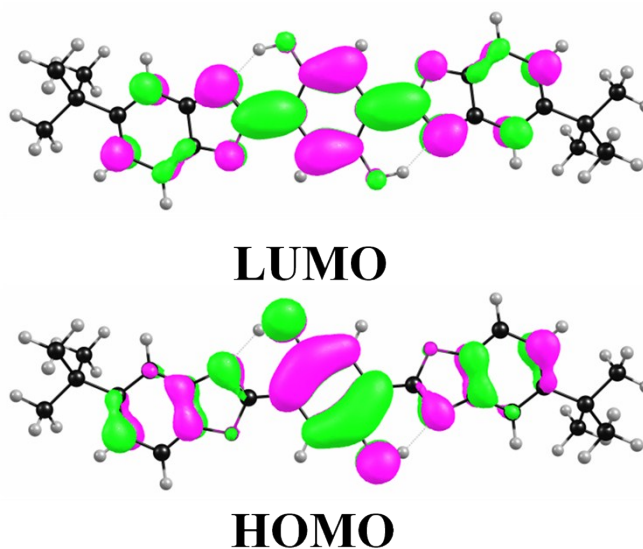


Figure S2 Frontier molecular orbitals, HOMO and LUMO, for the DHBO chromophore based on TDDFT/B3LYP/6-31+G(d)/IEF-PCM(heptane) calculations.

Cartesian coordinates of the optimized geometries for the ground state S_0 of

HBO-C at B3LYP/6-31+G(d) level

C	1.95792400	-0.75387800	0.00002300
C	1.91033700	0.64686600	0.00001200
C	3.09614900	1.38704200	0.00002000
C	4.29525900	0.67038400	0.00003800
C	4.31530200	-0.73816700	0.00004900
C	3.13328400	-1.48844000	0.00004200
C	-0.11301700	-0.08192000	-0.00001200
H	3.07975000	2.47255600	0.00001200
H	5.23752300	1.21109700	0.00004500
H	5.26988000	-1.25652600	0.00006500
H	3.13661200	-2.57353500	0.00005100
C	-3.56352100	-1.58592700	0.00003800
C	-4.34988200	-0.42233600	0.00000900
C	-3.75756500	0.83581200	-0.00003600
C	-2.36051800	0.96153700	-0.00005300
C	-1.55588000	-0.20915900	-0.00001800
C	-2.17985900	-1.47383500	0.00002400
H	-4.35475200	1.74260000	-0.00006600
H	-1.55776200	-2.36338900	0.00005200
O	-1.84246500	2.20968100	-0.00012300
H	-0.85358200	2.15323700	-0.00016800
N	0.57179400	1.03509100	-0.00000600
O	0.65955700	-1.21629900	0.00001500
H	-5.43393200	-0.50076400	0.00001900
H	-4.03111600	-2.56584000	0.00007300

Cartesian coordinates of the optimized geometries for the ground state S_0 of

HBO-K at B3LYP/6-31+G(d) level

C	-1.95126800	-0.75961700	-0.00003600
C	-1.90342200	0.63810000	0.00001400
C	-3.07328000	1.39349800	0.00003500
C	-4.27922000	0.68224000	0.00000100
C	-4.31018400	-0.72220700	-0.00005100
C	-3.13082900	-1.48095200	-0.00007000
C	0.17343600	-0.17311800	-0.00000200
H	-3.05051500	2.47829200	0.00007600
H	-5.21515000	1.23302700	0.00001500
H	-5.26735500	-1.23479100	-0.00007500
H	-3.13928100	-2.56565000	-0.00010900
C	3.63576300	-1.53025100	-0.00000500
C	4.36761600	-0.30793600	0.00002500
C	3.73884300	0.91527200	0.00003900
C	2.30250300	1.02646700	0.00001900
C	1.57568200	-0.24349900	0.00000200
C	2.26197600	-1.49161500	-0.00001500
H	4.30471100	1.84272600	0.00006200
H	1.68309500	-2.41153300	-0.00003100
O	1.71003600	2.15653200	0.00004100
H	0.00911200	1.83989600	0.00007100
N	-0.55015200	0.95915600	0.00003600
O	-0.65205200	-1.24998000	-0.00004200
H	5.45521400	-0.34658600	0.00003500
H	4.16166100	-2.48018400	-0.00001600

Cartesian coordinates of the optimized geometries for the ground state S_0 of
BBHQ at B3LYP/6-31+G(d) level

C	-4.87594000	0.73494500	0.00004600
C	-4.91536400	-0.66656300	0.00000700
C	-6.14453100	-1.33319600	-0.00000600
C	-7.29621800	-0.54397800	0.00002200
C	-7.22903500	0.86377700	0.00006100
C	-6.00412800	1.54064800	0.00007400
C	-2.85310900	-0.06377200	0.00001400
H	-6.19467300	-2.41758300	-0.00003600
H	-8.27026400	-1.02490500	0.00001400
H	-8.15011800	1.43943200	0.00008200
H	-5.94081900	2.62376100	0.00010400
C	4.87593500	-0.73495200	-0.00004400
C	4.91537300	0.66655500	-0.00000600
C	6.14454600	1.33317800	0.00000300
C	7.29622600	0.54394900	-0.00002800
C	7.22903000	-0.86380500	-0.00006600
C	6.00411600	-1.54066500	-0.00007500
C	2.85311000	0.06378400	-0.00001600
H	6.19469600	2.41756400	0.00003300
H	8.27027600	1.02486800	-0.00002000
H	8.15010700	-1.43946800	-0.00008800
H	5.94079800	-2.62377700	-0.00010300
C	0.67323800	1.24742200	0.00002900
C	1.40417900	0.02729900	-0.00000900
C	0.71749600	-1.19736900	-0.00003700
C	-0.67323900	-1.24740100	-0.00003000
C	-1.40417900	-0.02727900	0.00000700

C	-0.71749700	1.19738900	0.00003600
H	1.26931300	-2.13081600	-0.00006500
H	-1.26931500	2.13083600	0.00006400
O	-1.26406600	-2.46840200	-0.00005700
H	-2.24621700	-2.35373900	-0.00004700
O	1.26405900	2.46842600	0.00006000
H	2.24621000	2.35377000	0.00005300
N	-3.60430400	-1.13661200	-0.00001400
N	3.60431600	1.13661500	0.00002100
O	-3.55260400	1.11585200	0.00005100
O	3.55259600	-1.11584600	-0.00004500

Cartesian coordinates of the optimized geometries for the S₁ state of BBHQ at
B3LYP/6-31+G(d) level

C	4.90970200	0.74648400	-0.00004700
C	4.92180000	-0.66450300	-0.00000700
C	6.14801500	-1.34740700	0.00000800
C	7.31173200	-0.57502800	-0.00001900
C	7.26988600	0.83276100	-0.00005900
C	6.05009600	1.52900300	-0.00007400
C	2.86399100	-0.01161300	-0.00001700
H	6.18333300	-2.43246300	0.00003900
H	8.27772800	-1.07272600	-0.00000800
H	8.19955500	1.39438000	-0.00007800
H	6.00403600	2.61319700	-0.00010500
C	-4.90970300	-0.74648200	0.00004800
C	-4.92179700	0.66450500	0.00001000
C	-6.14801100	1.34741200	0.00000000
C	-7.31173000	0.57503600	0.00002700

C	-7.26988700	-0.83275300	0.00006400
C	-6.05009900	-1.52899800	0.00007500
C	-2.86399100	0.01161000	0.00001500
H	-6.18332700	2.43246700	-0.00002900
H	-8.27772500	1.07273500	0.00001900
H	-8.19955800	-1.39437000	0.00008400
H	-6.00404200	-2.61319200	0.00010400
C	-0.69637100	1.21566500	-0.00003200
C	-1.44423800	-0.03087500	0.00000700
C	-0.70594300	-1.22401300	0.00003500
C	0.69637100	-1.21567100	0.00002600
C	1.44423800	0.03087000	-0.00001200
C	0.70594200	1.22400700	-0.00004000
H	-1.20890900	-2.18456500	0.00006500
H	1.20890900	2.18456000	-0.00006900
O	1.32301600	-2.39017300	0.00005400
H	2.32141500	-2.23640700	0.00004100
O	-1.32301800	2.39016700	-0.00006100
H	-2.32141600	2.23639800	-0.00005100
N	3.61856900	-1.11061700	0.00001100
N	-3.61856600	1.11061600	-0.00000900
O	3.59560400	1.15906800	-0.00005400
O	-3.59560600	-1.15907000	0.00005100

Cartesian coordinates of the optimized geometries for the ground state S_0 of
 BBHQ-A at B3LYP/6-31+G(d) level

C	-4.86200700	-0.77825800	-0.00005300
C	-4.93853800	0.62155200	0.00000100
C	-6.18475800	1.25630100	0.00002100

C	-7.31521100	0.43737300	-0.00001500
C	-7.21088900	-0.96854200	-0.00007000
C	-5.96910000	-1.61335400	-0.00009000
C	-2.86061700	0.07377500	-0.00001300
H	-6.26298800	2.33907400	0.00006300
H	-8.30173200	0.89227900	-0.00000100
H	-8.11681500	-1.56792100	-0.00009700
H	-5.87742900	-2.69446300	-0.00013200
C	4.90552700	0.70247000	0.00003500
C	4.89414900	-0.69664300	0.00002200
C	6.08378200	-1.42140800	0.00002200
C	7.26986400	-0.67860200	0.00003400
C	7.26393200	0.72675000	0.00004600
C	6.06590200	1.45478200	0.00004700
C	2.80061300	0.06027700	0.00001700
H	6.08926000	-2.50637400	0.00001400
H	8.22013900	-1.20421100	0.00003400
H	8.20754500	1.26381600	0.00005500
H	6.04571500	2.53926400	0.00005700
C	0.71643900	-1.20206000	-0.00004500
C	1.39402800	0.08792300	0.00000900
C	0.67523200	1.31322000	0.00004800
C	-0.70026000	1.32730100	0.00004200
C	-1.40535800	0.07018700	-0.00000600
C	-0.71355500	-1.13397900	-0.00004900
H	1.20774000	2.25918900	0.00008500
H	-1.25405500	-2.07429900	-0.00009000
O	-1.34000900	2.53230500	0.00008100
H	-2.31467400	2.38325500	0.00006900
O	1.34205200	-2.32003900	-0.00009900

H	3.00365200	-1.94705700	0.00001300
N	-3.64037500	1.12503000	0.00002500
N	3.55038700	-1.05340000	0.00001500
O	-3.53038100	-1.12314600	-0.00006100
O	3.59440100	1.15858500	0.00003500

Cartesian coordinates of the optimized geometries for the S₁ state of BBHQ-A at
B3LYP/6-31+G(d) level

C	-4.93132700	-0.74149900	-0.00002400
C	-4.93444500	0.66745500	0.00004500
C	-6.15552500	1.35672200	0.00012100
C	-7.32595000	0.59183700	0.00012400
C	-7.29358700	-0.81464200	0.00005600
C	-6.07685200	-1.51695500	-0.00002100
C	-2.87898300	0.00153900	-0.00005600
H	-6.18483100	2.44207300	0.00017300
H	-8.28825600	1.09692300	0.00018100
H	-8.22640000	-1.37115900	0.00006100
H	-6.03641400	-2.60146900	-0.00007400
C	4.91065500	0.73683500	0.00008300
C	4.96721800	-0.66439100	0.00006200
C	6.19346500	-1.33087700	0.00010100
C	7.34167600	-0.52851600	0.00014600
C	7.26829200	0.87366600	0.00016000
C	6.03281100	1.54341800	0.00013100
C	2.82945700	-0.00625900	-0.00001300
H	6.25357300	-2.41421000	0.00009600
H	8.31654800	-1.00734400	0.00017600
H	8.18439700	1.45636900	0.00020100

H	5.95972500	2.62558900	0.00014700
C	0.70631900	-1.28883800	-0.00024500
C	1.41961000	0.00019800	-0.00009100
C	0.68903400	1.19657100	-0.00006200
C	-0.71490200	1.19267400	-0.00008100
C	-1.45607300	-0.05254200	-0.00010100
C	-0.72319300	-1.24592400	-0.00017100
H	1.19055100	2.15904200	-0.00000800
H	-1.23891000	-2.20048500	-0.00017800
O	-1.33371200	2.37400100	-0.00003600
H	-2.33246800	2.22190500	-0.00006500
O	1.34941100	-2.38620200	-0.00018200
H	3.20774400	-2.01202500	0.00003200
N	-3.62525800	1.10582400	0.00001800
N	3.64864400	-1.08355100	0.00002400
O	-3.61913600	-1.16340700	-0.00008700
O	3.58154300	1.12886400	0.00005300

Cartesian coordinates of the optimized geometries for the S_1 state of BBHQ-B at
B3LYP/6-31+G(d) level

C	4.92557200	-0.73394700	0.00009200
C	4.97276100	0.66766300	0.00030900
C	6.19485500	1.34084300	0.00046500
C	7.34963100	0.54673900	0.00039000
C	7.28586200	-0.85508500	0.00016700
C	6.05369200	-1.53191800	0.00001500
C	2.83753900	-0.00570200	0.00011800
H	6.24809600	2.42463000	0.00063400
H	8.32090900	1.03303000	0.00050500

H	8.20547100	-1.43235000	0.00011600
H	5.98726800	-2.61458800	-0.00015100
C	-4.92553900	0.73397700	-0.00008700
C	-4.97273700	-0.66763000	-0.00030200
C	-6.19481900	-1.34082400	-0.00044500
C	-7.34960000	-0.54672600	-0.00036500
C	-7.28583300	0.85509800	-0.00014600
C	-6.05366900	1.53193800	-0.00000300
C	-2.83751100	0.00572300	-0.00013100
H	-6.24805300	-2.42461300	-0.00061300
H	-8.32087500	-1.03302300	-0.00047300
H	-8.20544400	1.43236000	-0.00008900
H	-5.98725300	2.61460800	0.00016200
C	-0.72383300	-1.27005700	-0.00023200
C	-1.42865900	0.01994500	-0.00007300
C	-0.70304300	1.21942200	0.00013500
C	0.72374300	1.26997700	0.00021200
C	1.42863100	-0.01999600	0.00005300
C	0.70302200	-1.21947200	-0.00016000
H	-1.21983300	2.17458700	0.00024800
H	1.21980400	-2.17464100	-0.00027800
O	1.35719100	2.37665900	0.00040700
H	3.20402900	2.00316600	0.00042900
O	-1.35731000	-2.37672400	-0.00041800
H	-3.20403100	-2.00305600	-0.00044200
N	3.65202500	1.07872200	0.00032600
N	-3.65199200	-1.07867100	-0.00032800
O	3.60048800	-1.13667500	-0.00002100
O	-3.60046000	1.13670700	0.00001800

Cartesian coordinates of the optimized geometries for the ground state S_0 of

DHBO at B3LYP/6-31+G(d) level

C	4.77560800	1.23429300	0.00020600
C	4.96034400	-0.15331600	0.00019500
C	6.24622200	-0.69416000	-0.00002200
C	7.34720200	0.17886500	-0.00026700
C	7.11000300	1.57405100	-0.00024500
C	5.82537100	2.13403800	0.00000300
C	2.84542900	0.23436900	0.00048900
H	6.37469200	-1.77176300	-0.00004300
H	7.94997300	2.25832200	-0.00040900
H	5.67176800	3.20821600	0.00003100
C	-4.77562100	-1.23430600	0.00021700
C	-4.96034300	0.15330600	0.00020100
C	-6.24621400	0.69416200	-0.00002000
C	-7.34720300	-0.17885100	-0.00025600
C	-7.11002000	-1.57403900	-0.00024000
C	-5.82539300	-2.13404100	0.00001100
C	-2.84543300	-0.23440200	0.00049700
H	-6.37467600	1.77176700	-0.00004500
H	-7.94999500	-2.25830400	-0.00043000
H	-5.67180200	-3.20822000	0.00003600
C	-0.79958900	1.16903800	0.00064200
C	-1.39992500	-0.11976900	0.00061500
C	-0.58855700	-1.26582200	0.00062000
C	0.79958400	-1.16908000	0.00064400
C	1.39992100	0.11972800	0.00060900
C	0.58855200	1.26578100	0.00061000
H	-1.04088400	-2.25147300	0.00059300

H	1.04087700	2.25143200	0.00057800
O	1.51822100	-2.32161300	0.00063700
H	2.48302800	-2.09954500	0.00052000
O	-1.51822900	2.32156900	0.00064100
H	-2.48303500	2.09949500	0.00053500
N	3.70233600	-0.75637200	0.00036500
N	-3.70233000	0.75635000	0.00037100
O	3.41839000	1.47901200	0.00045000
O	-3.41840500	-1.47903900	0.00047000
C	-8.77349500	0.41026100	-0.00063800
C	8.77350600	-0.41022200	-0.00064000
C	9.86511600	0.67811600	-0.00090500
H	10.85218200	0.20144900	-0.00117500
H	9.80898500	1.31733900	-0.89002000
H	9.80944100	1.31729400	0.88827100
C	8.97043900	-1.28409600	1.26223500
H	8.25796100	-2.11534800	1.30131200
H	9.98123700	-1.71061400	1.27248400
H	8.84344500	-0.68891600	2.17453300
C	8.96970500	-1.28401500	-1.26369100
H	8.84208800	-0.68880500	-2.17588000
H	9.98052000	-1.71047400	-1.27460600
H	8.25724200	-2.11530300	-1.30233900
C	-8.97021300	1.28463300	1.26192300
H	-8.25766500	2.11584100	1.30060700
H	-9.98098000	1.71122600	1.27212700
H	-8.84315600	0.68978600	2.17443100
C	-9.86513600	-0.67804600	-0.00031700
H	-10.85218900	-0.20135100	-0.00099000
H	-9.80892600	-1.31783800	-0.88902100

H	-9.80958300	-1.31665700	0.88927000
C	-8.96985400	1.28357000	-1.26400000
H	-8.84241100	0.68800500	-2.17598100
H	-9.98065100	1.71007300	-1.27491700
H	-8.25736200	2.11481300	-1.30308000

Cartesian coordinates of the optimized geometries for the S₁ state of DHBO at
B3LYP/6-31+G(d) level

C	4.79316400	-1.26251100	0.00008700
C	4.96044600	0.13835300	-0.00001700
C	6.24899200	0.68793000	-0.00005000
C	7.35754000	-0.17485000	0.00002400
C	7.13649200	-1.57318200	0.00012700
C	5.85258400	-2.14597500	0.00016000
C	2.84175500	-0.28691900	0.00000600
H	6.36837600	1.76657000	-0.00012800
H	7.98289800	-2.24931300	0.00018400
H	5.71054700	-3.22190400	0.00023900
C	-4.79316500	1.26251200	-0.00010800
C	-4.96044500	-0.13835200	0.00001400
C	-6.24899000	-0.68793100	0.00006500
C	-7.35753900	0.17484700	-0.00000500
C	-7.13649300	1.57318000	-0.00014100
C	-5.85258600	2.14597500	-0.00018900
C	-2.84175500	0.28692300	-0.00002600
H	-6.36837200	-1.76657100	0.00015300
H	-7.98290100	2.24930900	-0.00021400
H	-5.71055100	3.22190400	-0.00029000
C	-0.81577700	-1.14327900	0.00007700

C	-1.42971500	0.17887000	-0.00002300
C	-0.57238200	1.29495400	-0.00011400
C	0.81577700	1.14328400	-0.00010500
C	1.42971500	-0.17886500	-0.00000300
C	0.57238200	-1.29494900	0.00008400
H	-0.97840300	2.30020900	-0.00019200
H	0.97840300	-2.30020400	0.00016000
O	1.56623000	2.24678500	-0.00019400
H	2.54020800	1.98802200	-0.00016900
O	-1.56623100	-2.24677900	0.00016200
H	-2.54020800	-1.98801600	0.00015300
N	3.71455800	0.72440000	-0.00006900
N	-3.71455700	-0.72439700	0.00005800
O	3.44357500	-1.53151200	0.00010200
O	-3.44357600	1.53151500	-0.00013100
C	-8.77786400	-0.42796400	0.00003400
C	8.77786500	0.42795900	0.00000500
C	9.88124000	-0.64869400	0.00016300
H	10.86323000	-0.16149600	0.00009900
H	9.83207600	-1.28840500	0.88931900
H	9.83208100	-1.28865400	-0.88881500
C	8.96615500	1.30394900	-1.26294500
H	8.24505400	2.12764900	-1.30169600
H	9.97279000	1.74040300	-1.27328400
H	8.84495400	0.70744600	-2.17517900
C	8.96606300	1.30422700	1.26277600
H	8.84479900	0.70792300	2.17513300
H	9.97269500	1.74068800	1.27309100
H	8.24495300	2.12793100	1.30129500
C	-8.96608700	-1.30422400	-1.26273900

H	-8.24499500	-2.12794300	-1.30126500
H	-9.97272800	-1.74066400	-1.27304800
H	-8.84481800	-0.70792000	-2.17509400
C	-9.88124100	0.64868900	-0.00009900
H	-10.86323000	0.16148900	-0.00014500
H	-9.83214400	1.28856900	0.88893900
H	-9.83201400	1.28847900	-0.88919400
C	-8.96613000	-1.30396200	1.26298300
H	-8.84492400	-0.70746100	2.17521800
H	-9.97275900	-1.74042800	1.27333200
H	-8.24501700	-2.12765300	1.30172000

Cartesian coordinates of the optimized geometries for the ground state S_0 of
DHBO-A at B3LYP/6-31+G(d) level

C	4.75415400	-1.23606900	0.00016100
C	4.96851800	0.14714200	-0.00003400
C	6.26529200	0.66167300	-0.00008300
C	7.34763400	-0.23390700	0.00007000
C	7.08109100	-1.62420700	0.00027000
C	5.78540800	-2.15753600	0.00031600
C	2.84537000	-0.19492200	-0.00002100
H	6.41543700	1.73645100	-0.00022900
H	7.90697800	-2.32553500	0.00039200
H	5.60958400	-3.22829500	0.00046700
C	-4.80753200	1.25138400	-0.00016100
C	-4.96143800	-0.13678700	-0.00003100
C	-6.22106100	-0.72291100	0.00003800
C	-7.34787500	0.12227300	-0.00002800
C	-7.15172600	1.52030700	-0.00014800

C	-5.88176300	2.11680800	-0.00022400
C	-2.79235600	0.37062100	-0.00009800
H	-6.31966900	-1.80295700	0.00014400
H	-8.00981500	2.18098000	-0.00018800
H	-5.75617000	3.19421200	-0.00032200
C	-0.84417800	-1.10499800	0.00009600
C	-1.38748200	0.24475300	-0.00009200
C	-0.54902100	1.39032900	-0.00025200
C	0.82160400	1.26591000	-0.00024000
C	1.39685000	-0.05323600	-0.00005400
C	0.58454900	-1.18123400	0.00010800
H	-0.98487500	2.38461200	-0.00038800
H	1.02941000	-2.17058200	0.00025900
O	1.58137200	2.40198200	-0.00040300
H	2.53633000	2.15059300	-0.00036000
O	-1.58204700	-2.15546600	0.00027300
H	-3.24519000	-1.59919000	0.00008100
N	3.72372600	0.77576000	-0.00014200
N	-3.66507500	-0.64708600	0.00000300
O	3.39339100	-1.45135000	0.00016300
O	-3.45057200	1.55187000	-0.00021000
C	-8.75426500	-0.51069400	0.00007800
C	8.78613300	0.32488500	0.00004600
C	9.85420100	-0.78642300	0.00038200
H	10.85126900	-0.33109100	0.00030000
H	9.78431000	-1.42401600	0.88968300
H	9.78437400	-1.42448700	-0.88858500
C	9.00137300	1.19416400	-1.26306600
H	8.30677900	2.04040000	-1.30229600
H	10.02096200	1.59930100	-1.27355800

H	8.86169000	0.60163100	-2.17522600
C	9.00117600	1.19474300	1.26279300
H	8.86136900	0.60262400	2.17520200
H	10.02075600	1.59990300	1.27325000
H	8.30655800	2.04098300	1.30153300
C	-8.92207700	-1.38988100	-1.26344800
H	-8.18459300	-2.19903400	-1.30205400
H	-9.91900400	-1.84719100	-1.27354300
H	-8.81352200	-0.79111000	-2.17564800
C	-9.87767100	0.54482900	0.00011300
H	-10.84954300	0.03832200	0.00018800
H	-9.84126100	1.18508600	0.88942300
H	-9.84136600	1.18503000	-0.88924100
C	-8.92191100	-1.38979100	1.26368900
H	-8.81323800	-0.79095500	2.17583100
H	-9.91883500	-1.84710400	1.27394600
H	-8.18441700	-2.19893800	1.30225400

Cartesian coordinates of the optimized geometries for the S_1 state of DHBO-A at

B3LYP/6-31+G(d) level

C	4.83403400	-1.26488500	0.00013300
C	4.98363800	0.13345200	-0.00002300
C	6.26326800	0.69731500	-0.00008000
C	7.38491800	-0.15235300	0.00002400
C	7.18256200	-1.55022200	0.00017900
C	5.90413800	-2.13606500	0.00023400
C	2.86867400	-0.31621000	0.00002600
H	6.37100600	1.77738000	-0.00019600
H	8.03607500	-2.21738800	0.00025800
H	5.77359300	-3.21362300	0.00035300

C	-4.79691300	1.22098700	-0.00013600
C	-5.01143500	-0.16358100	0.00000500
C	-6.29820400	-0.69402000	0.00006000
C	-7.38701100	0.20140200	-0.00003200
C	-7.13129100	1.58905900	-0.00017400
C	-5.83342400	2.13009600	-0.00022800
C	-2.81215600	0.25173700	-0.00004000
H	-6.44434900	-1.76859700	0.00016900
H	-7.95999300	2.28638500	-0.00024700
H	-5.66123100	3.20107500	-0.00033800
C	-0.82427200	-1.24439200	0.00011600
C	-1.40780600	0.11120800	-0.00002300
C	-0.56180200	1.22804800	-0.00013400
C	0.83496300	1.08434000	-0.00011300
C	1.44837400	-0.22692300	0.00001800
C	0.59975800	-1.34432100	0.00012800
H	-0.96516400	2.23554600	-0.00023500
H	1.01992700	-2.34475800	0.00022800
O	1.56955700	2.19949300	-0.00021100
H	2.54724400	1.94785300	-0.00015200
O	-1.57642700	-2.27222100	0.00022100
H	-3.42826000	-1.70068600	0.00015800
N	3.72391000	0.70564600	-0.00008900
N	-3.74723700	-0.72720100	0.00005800
O	3.48492300	-1.55162800	0.00016000
O	-3.43274500	1.46362200	-0.00016100
C	-8.81947900	-0.36952900	0.00002400
C	8.79675600	0.47115600	-0.00001600
C	9.91520900	-0.58998000	0.00018800
H	10.89075700	-0.08968900	0.00010000

H	9.87425600	-1.23050600	0.88920900
H	9.87426100	-1.23083700	-0.88859500
C	8.97400800	1.34960900	-1.26266400
H	8.24069600	2.16249200	-1.30207800
H	9.97423200	1.80094000	-1.27302100
H	8.86166100	0.75118200	-2.17485600
C	8.97390100	1.34998500	1.26238600
H	8.86147300	0.75183000	2.17474600
H	9.97412400	1.80131900	1.27269600
H	8.24058300	2.16287900	1.30149300
C	-9.02617800	-1.24095400	-1.26332700
H	-8.32644100	-2.08298400	-1.30181300
H	-10.04285800	-1.65267900	-1.27376700
H	-8.89033200	-0.64782600	-2.17555500
C	-9.89606900	0.73337700	-0.00019100
H	-10.88908500	0.26966200	-0.00010800
H	-9.83147300	1.37158600	0.88893600
H	-9.83146500	1.37124900	-0.88956100
C	-9.02624800	-1.24052900	1.26365700
H	-8.89045100	-0.64709400	2.17569200
H	-10.04292800	-1.65225000	1.27417900
H	-8.32651200	-2.08254700	1.30246300

Cartesian coordinates of the optimized geometries for the S_1 state of DHBO-B at
B3LYP/6-31+G(d) level

C	-4.82458200	1.22659100	0.00025400
C	-5.02216200	-0.15962400	-0.00002000
C	-6.30240200	-0.70414300	-0.00009400
C	-7.40317100	0.17777400	0.00012400

C	-7.16475700	1.56716900	0.00040900
C	-5.87232500	2.12241500	0.00047400
C	-2.82600500	0.28244500	0.00000300
H	-6.43622900	-1.78045100	-0.00031000
H	-8.00108200	2.25535100	0.00058700
H	-5.71261000	3.19541600	0.00069000
C	4.82457400	-1.22658200	-0.00023600
C	5.02216400	0.15963100	-0.00006800
C	6.30240900	0.70413700	0.00001000
C	7.40317200	-0.17779200	-0.00009000
C	7.16474500	-1.56718400	-0.00022600
C	5.87230700	-2.12241600	-0.00031700
C	2.82600400	-0.28242200	-0.00013500
H	6.43625000	1.78044100	0.00016000
H	8.00106100	-2.25537600	-0.00027200
H	5.71257800	-3.19541600	-0.00043700
C	0.84062900	1.19476000	0.00011000
C	1.42159500	-0.15628100	-0.00011200
C	0.58403400	-1.28071500	-0.00026700
C	-0.84063200	-1.19472800	-0.00030700
C	-1.42159700	0.15631100	-0.00006100
C	-0.58403700	1.28074600	0.00010100
H	1.00849600	-2.28042800	-0.00036900
H	-1.00850100	2.28045900	0.00023000
O	-1.57824200	-2.23685400	-0.00026500
H	-3.41661600	-1.67756100	-0.00040200
O	1.57823400	2.23688900	0.00014200
H	3.41663000	1.67758000	0.00012100
N	-3.75059000	-0.70917900	-0.00017100
N	3.75059600	0.70919500	0.00000000

O	-3.46337800	1.48776900	0.00025700
O	3.46336800	-1.48775000	-0.00028700
C	8.82822600	0.41191800	0.00007100
C	-8.82821700	-0.41194700	0.00005300
C	-9.91925600	0.67681000	0.00023200
H	-10.90632900	0.20033600	0.00029700
H	-9.86273200	1.31572900	0.88943300
H	-9.86291000	1.31584800	-0.88889400
C	-9.02439600	-1.28550000	-1.26339300
H	-8.31335800	-2.11801000	-1.30251400
H	-10.03561900	-1.71069100	-1.27398900
H	-8.89640900	-0.69021300	-2.17539800
C	-9.02435600	-1.28587800	1.26324400
H	-8.89630600	-0.69087100	2.17542300
H	-10.03558900	-1.71104500	1.27376200
H	-8.31333800	-2.11841900	1.30207600
C	9.02462000	1.28549700	-1.26332400
H	8.31363000	2.11804200	-1.30252400
H	10.03586200	1.71064300	-1.27376700
H	8.89673400	0.69024100	-2.17536400
C	9.91926100	-0.67685200	0.00040500
H	10.90633700	-0.20038700	0.00046200
H	9.86270400	-1.31568400	0.88966600
H	9.86294300	-1.31597900	-0.88866000
C	9.02416100	1.28582100	1.26331200
H	8.89597500	0.69079300	2.17546000
H	10.03538600	1.71100400	1.27399900
H	8.31312500	2.11835000	1.30205000