Supporting Information

Switching between TADF and HLCT Emissions by Connecting Different Donors Based on Theoretical Calculations

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Table S1. Overlap integrals of norm and centroid distances (Å) between the HOMO and LUMO pairs

	Overlap integrals (β)	Centroid distances (Å)
DBFo-Cz	0.43	7.96
DBFo-DMAC	0.23	8.33
DBFo-DHPZ	0.14	4.85
DBFp-Cz	0.39	6.51
DBFp-DMAC	0.12	8.57
DBFp-DHPZ	0.12	4.95

Table S2. The ω values corresponding to the studied molecules were calculated by optDFTω program at the LC-ωPBE/6-31+G* level

	DBFo-Cz	DBFo-DMAC	DBFo-DHPZ	DBFp-Cz	DBFp-DMAC	DBFp-DHPZ
ω	0.152791	0.147428	0.153732	0.155249	0.156932	0.166593

Table S3. Excited state (singlet and triplet) energy data summary of DBFo-Cz, DBFo-DMAC and DBFo-DHPZ

Molecule	States	Singlet states		Triplet states
		Energy level (eV)	Oscillator strength	Energy level (eV)
DBFo-Cz	1	3.3589	0.1480	2.7786
	2	3.3944	0.1728	2.9948
	3	3.9096	0.0287	3.2475
	4	3.9261	0.0206	3.2525
	5	3.9883	0.0014	3.3682
DBFo-DMAC	1	2.7612	0.0108	2.6588
	2	2.8554	0.0112	2.8109
	3	3.7941	0.0867	2.9889
	4	3.9206	0.0823	3.0756
	5	3.9787	0.3267	3.2913
DBFo-DHPZ	1	2.5515	0.0028	2.5204
	2	2.6555	0.0033	2.6323
	3	3.6136	0.0004	2.9231
	4	3.6706	0.0104	2.9544
	5	3.8131	0.0265	2.9686

Table S4. Excited state (singlet and triplet) energy data summary of DBFp-Cz, DBFp-DMAC and DBFp-DHPZ

Molecule	States	Singlet states		Triplet states
		Energy level (eV)	Oscillator strength	Energy level (eV)
DBFp-Cz	**1**	3.5126	0.1243	2.9237
	2	3.7405	0.0858	3.2041
	3	3.9358	0.1115	3.2573
	4	3.9924	0.0361	3.2602
	5	4.0223	0.0274	3.3257
DBFp-DMAC	**1**	3.0205	0.0000	3.0047
	2	3.2069	0.0000	3.0173
	3	3.8544	0.0002	3.1845
	4	3.9251	0.0000	3.1936
	5	3.9800	0.2085	3.2510
DBFp-DHPZ	**1**	2.7743	0.0014	2.7523
	2	2.9714	0.0178	2.8340
	3	3.5760	0.0028	2.8612
	4	3.5817	0.0123	2.8717
	5	3.7084	0.0092	3.0996

Table S5. The main orbital transition contributions in excited state of the designed molecule.

Molecule	States	Orbital transition contribution	
		Singlet states	Triplet states
DBFo-Cz	1	H -> L 94.6%	H -> L 49.7%, H-5 -> L 35.9%
	2	H-1 -> L 91.6%	H-4 -> L 46.0%, H-1 -> L 43.4%
	3	H-4 -> L 66.3%, H-3 -> L 17.7%	H-2 -> L+1 37.5%, H-3 -> L+3 22.3%
	4	H-2 -> L 92.9%	H-3 -> L+1 37.1%, H-2 -> L+3 23.6%
	5	H-3 -> L 75.2%, H-4 -> L 16.6%	H-1 -> L+1 42.9%, H -> L+3 29.0%
DBFo-DMAC	1	H -> L 94.5%	H -> L 78.2%, H-2 -> L 13.6%
	2	H-1 -> L 94.3%	H-1 -> L 89.5%
	3	H-3 -> L 75.5%, H -> L+1 11.4%	H-2 -> L 67.9%, H -> L 15.6%
	4	H -> L+1 57.7%, H-3 -> L 13.9%, H -> L+3 10.1%	H-3 -> L 85.7%
	5	H-2 -> L 70.4%, H-1 -> L+1 16.2%	H -> L+3 39.1%, H-1 -> L+6 30.8%
DBFo-DHPZ	1	H -> L 92.9%	H -> L 92.6%
	2	H-1 -> L 93.0%	H-1 -> L 92.6%
	3	H -> L+2 48.1%, H -> L+1 29.2%, H-1 -> L+6 18.6%	H -> L+2 48.9%, H-1 -> L+6 33.2%
	4	H-1 -> L+2 45.1%, H -> L+6 31.8%, H-1 -> L+1 18.6%	H-1 -> L+2 42.9%, H -> L+6 39.8%
	5	H -> L+1 37.0%, H -> L+5 22.8%, H-1 -> L+6 11.3%, H -> L+2 10.8%	H-4 -> L 81.4%

Table S6. The main orbital transition contributions in excited state of the designed molecule.

Molecule	States	Orbital transition contribution	
		Singlet states	Triplet states
DBFp-Cz	1	H -> L 57.1%, H-1 -> L 39.4%	H -> L 41.8%, H-5 -> L 33.5%
	2	H-1 -> L 56.3%, H -> L 36.9%	H-4 -> L 84.5%
	3	H-4 -> L 65.4%, H -> L+1 20.5%	H-3 -> L+2 74.9%
	4	H-1 -> L+2 69.0%, H -> L+2 20.8%	H-2 -> L+3 75.5%
	5	H -> L+3 76.2%, H-1 -> L+3 12.9%	H-1 -> L+2 72.7%, H -> L+2 17.7%
DBFp-DMAC	1	H-1 -> L 93.5%	H-1 -> L 93.9%
	2	H -> L 89.0%	H-3 -> L 68.9%, H-2 -> L+1 12.9%
	3	H -> L+3 68.0%, H -> L+1 20.4%	H-2 -> L 85.5%
	4	H-1 -> L+2 91.2%	H -> L 89.5%
	5	H -> L+1 66.1%, H -> L+3 17.5%	H-1 -> L+2 75.9%
DBFp-DHPZ	1	H-1 -> L 94.0%	H-1 -> L 75.4%, H-1 -> L+2 16.8%
	2	H -> L 89.8%	H -> L+3 71.2%, H -> L 10.1%
	3	H -> L+1 88.3%	H-1 -> L+2 68.5%, H-1 -> L 15.9%
	4	H-1 -> L+1 93.0%	H-1 -> L+2 68.5%, H-1 -> L 15.9%
	5	H-2 -> L 81.1%, H-3 -> L+1 12.9%	H-4 -> L 65.8%, H-3 -> L+1 14.3%

Table S7. SOC matrix elements ($<S_1 | H_{soc} | T_n>$, cm^{-1}) of DBFo-Cz, DBFo-DMAC and DBFo-DHPZ at the S_1 state

States	$<S_1 \| H_{soc} \| T_n>$ (cm^{-1})		
	DBFo-Cz	DBFo-DMAC	DBFo-DHPZ
T_1	0.5233	0.1556	0.0200
T_2	0.2200	0.2100	0.2100
T_3	0.4950	1.0748	0.9601
T_4	0.1030	0.3545	0.9025
T_5	0.1838	1.4630	0.0300

Table S8. SOC matrix elements ($<S_1 | H_{soc} | T_n>$, cm^{-1}) of DBFp-Cz, DBFp-DMAC and DBFp-DHPZ at the S_1 state

States	$<S_1 \| H_{soc} \| T_n>$ (cm^{-1})		
	DBFp-Cz	DBFp-DMAC	DBFp-DHPZ
T_1	0.0141	0.0000	0.0000
T_2	0.5829	0.7920	0.0300
T_3	0.0583	0.0141	1.1700
T_4	0.1849	0.4384	0.0400
T_5	0.3535	0.8700	0.1300

Figure S1. Structural changes between two states with RMSDs (S_0, S_1, and T_1 are represented by blue, red, and orange, respectively)

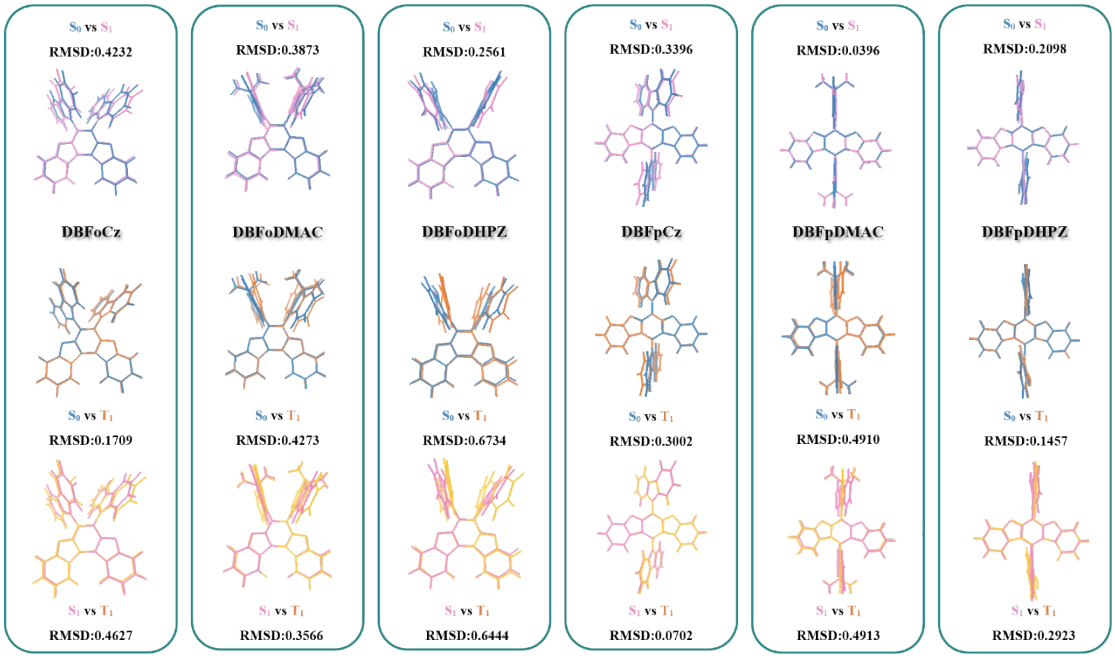


Figure S2. Hole−electron pairs of NTOs with the largest eigenvalues (*v*) in the S_1 and T_1 to T_5 of DBFo-Cz.

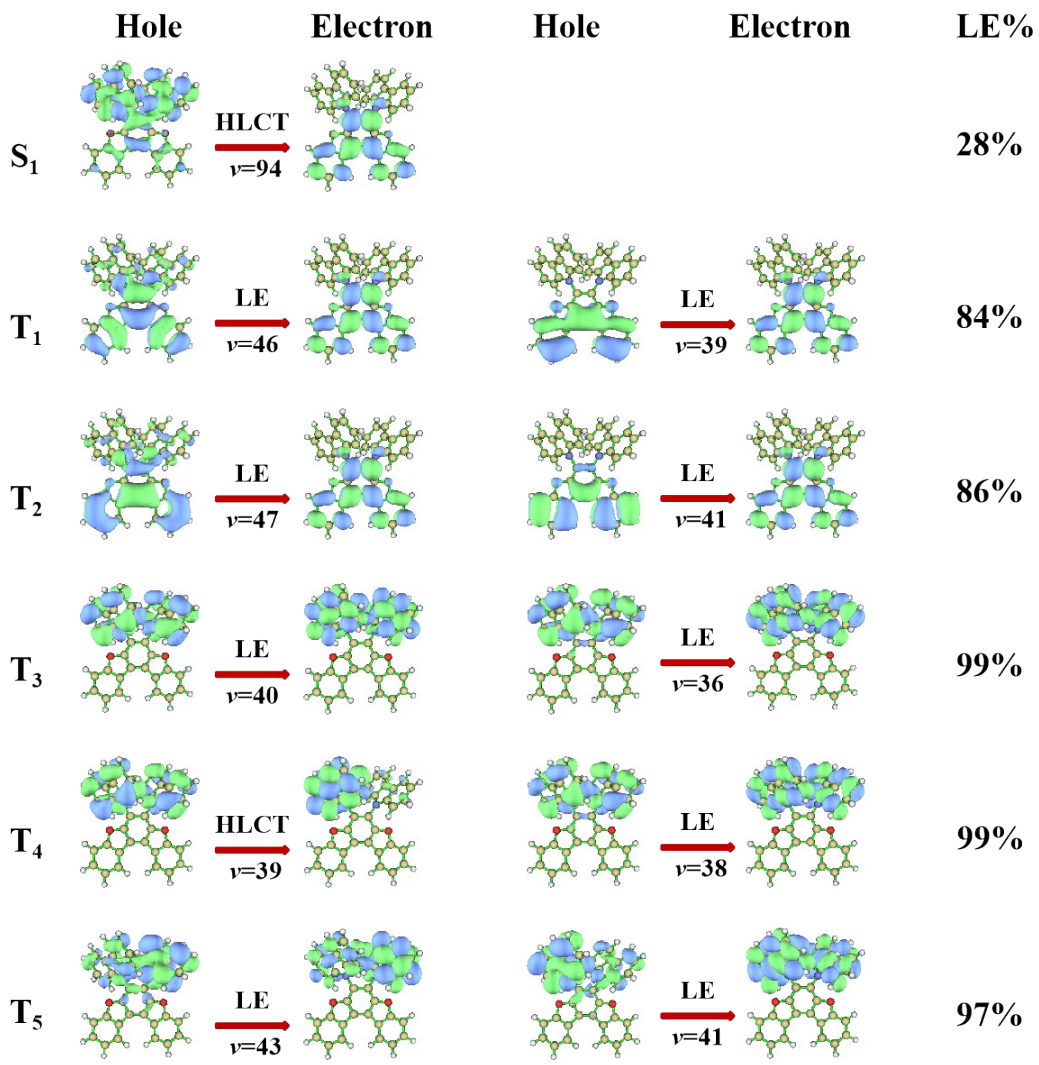
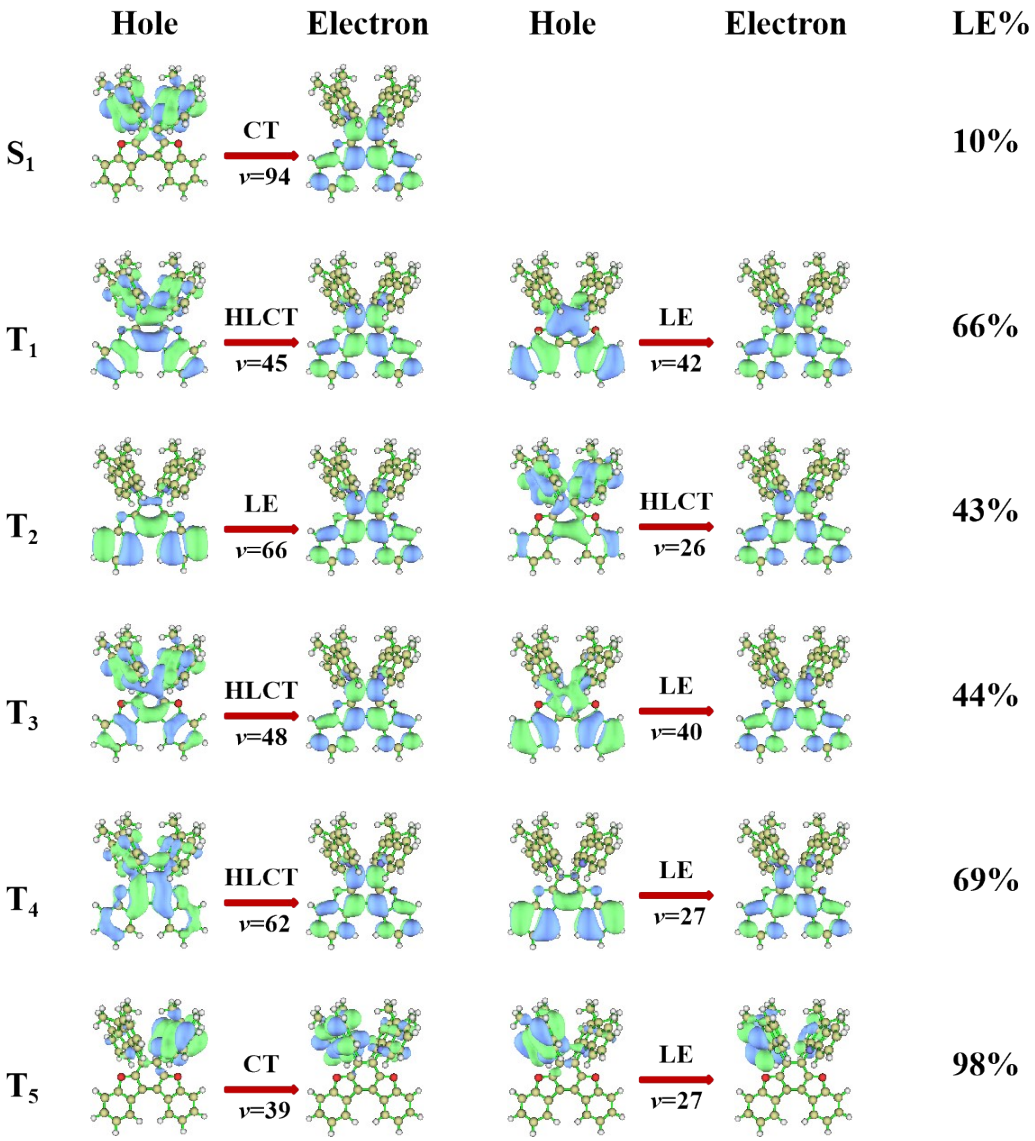


Figure S3. Hole−electron pairs of NTOs with the largest eigenvalues (*v*) in the S_1 and T_1 to T_5 of DBFo-DMAC.



The Cartesian coordinates of the optimized structure of DBFo-Cz

0 1

C	-5.02638300	1.85141100	0.34846200
C	-5.60744800	3.09435700	0.58569700
C	-4.82005700	4.23872300	0.79709900
C	-3.42765900	4.16814400	0.77682200
O	-1.52288700	2.66803000	0.48524600
C	-0.14607600	0.69604600	0.12086200
C	-0.14599500	-0.69610400	-0.12079200
O	-1.52255300	-2.66827100	-0.48508500
C	-3.42713200	-4.16862700	-0.77665500
C	-4.81952300	-4.23938400	-0.79694500
C	-5.60705600	-3.09511500	-0.58555800
C	-5.02614900	-1.85209200	-0.34833200
C	-2.87110000	2.91969500	0.53805800
C	-1.39623200	1.32653400	0.22994100
C	-1.39606400	-1.32676200	-0.22980600
C	-2.87073700	-2.92010800	-0.53790000
C	-3.62746600	-1.75073400	-0.32111300
C	-2.64987900	-0.69513700	-0.11866200
C	-2.64995800	0.69476200	0.11879200
C	-3.62768800	1.75023500	0.32125000
H	-5.65457600	0.98293300	0.18965400
H	-5.65446000	-0.98369900	-0.18952700
H	-5.30142000	-5.19547500	-0.97937000
H	-2.79873800	-5.03793600	-0.93756700
H	-2.79937900	5.03753400	0.93774300
H	-5.30207900	5.19475100	0.97952400
H	-6.68946400	-3.18148200	-0.60809000
H	-6.68986600	3.18059600	0.60822600
C	1.41193000	2.51560400	-0.58761200
C	1.98218900	1.35508200	1.28549100
C	0.78534300	2.99805000	-1.73822300
C	2.61835700	3.07834500	-0.10495700
C	2.00827800	0.49343700	2.38192600
C	2.97886900	2.34253800	1.08991900
C	1.38763800	4.06268200	-2.40653700
H	-0.14278600	2.56681800	-2.09966100
C	3.20358600	4.14582100	-0.79488100
C	3.06709800	0.61953200	3.27912200
H	1.23812400	-0.25409800	2.53437700
C	4.03242100	2.44813800	2.00491500
C	2.58466100	4.63340400	-1.94283000
H	0.91787100	4.45770200	-3.30327200

H	4.13090500	4.58693300	-0.43876400
C	4.07257100	1.58308500	3.09461400
H	3.11256500	-0.04521500	4.13729000
H	4.80530000	3.19998200	1.86791800
H	3.02956900	5.46241100	-2.48585200
H	4.88596200	1.65401300	3.81115800
C	1.41245400	-2.51531100	0.58769900
C	1.98214100	-1.35496400	-1.28568400
C	0.78617300	-2.99770500	1.73850100
C	2.61890900	-3.07787700	0.10490600
C	2.00783900	-0.49348200	-2.38225800
C	2.97905500	-2.34219200	-1.09014700
C	1.38879000	-4.06211800	2.40686400
H	-0.14197300	-2.56658600	2.10003600
C	3.20446500	-4.14514000	0.79488900
C	3.06651300	-0.61948200	-3.27963100
H	1.23747100	0.25384300	-2.53466600
C	4.03245600	-2.44770100	-2.00533200
C	2.58584300	-4.63267300	1.94301900
H	0.91927200	-4.45709300	3.30374800
H	4.13179400	-4.58614500	0.43866600
C	4.07222400	-1.58279900	-3.09516000
H	3.11169200	0.04514600	-4.13790400
H	4.80551600	-3.19937100	-1.86838800
H	3.03101700	-5.46151100	2.48608100
H	4.88550700	-1.65366100	-3.81183300
N	1.03794200	1.45490400	0.25088000
N	1.03812700	-1.45478800	-0.25085500

The Cartesian coordinates of the optimized structure of DBFo-DMAC

0 1

C	5.40536000	-1.86561900	0.33318200
C	5.98206800	-3.11512700	0.54480900
C	5.19034500	-4.26201900	0.72458200
C	3.79836700	-4.18753200	0.69839100
O	1.89869500	-2.67640700	0.43250500
C	0.52709300	-0.69817100	0.09769900
C	0.52922500	0.70005400	-0.09681500
O	1.90703900	2.67416000	-0.43068300
C	3.81143000	4.17953500	-0.69537700
C	5.20364700	4.24985000	-0.72047600
C	5.99179000	3.10062700	-0.53985100
C	5.41117600	1.85289100	-0.32843500
C	3.24537200	-2.93263100	0.48533900
C	1.77621500	-1.32742700	0.21548600
C	1.78033600	1.32557300	-0.21348300
C	3.25452500	2.92633800	-0.48250900
C	4.01260500	1.75214400	-0.29615600
C	3.03530700	0.69273200	-0.11386600
C	3.03314000	-0.69833200	0.11693200
C	4.00712300	-1.76067900	0.29982500
H	6.03616800	-0.99434000	0.20148700
H	6.03924600	0.97973900	-0.19607900
H	5.68532300	5.20968600	-0.88293300
H	3.18327500	5.05292700	-0.83348600
H	3.16749900	-5.05907500	0.83580800
H	5.66901800	-5.22332500	0.88721900
H	7.07412100	3.18705900	-0.56636400
H	7.06411500	-3.20480600	0.57214600
C	-1.36060000	-1.60055600	1.37687400
C	-1.03582800	-2.25163300	-0.97076900
C	-2.59676100	-2.27480000	1.43342300
C	-0.81023600	-1.05932000	2.55190900
C	-2.25071200	-2.96702600	-0.97442600
C	-0.19652500	-2.31308700	-2.09924200
C	-3.25976500	-2.32026700	2.66763500
C	-1.48886600	-1.13092300	3.76192300
H	0.15713600	-0.57545300	2.51452500
C	-2.58143400	-3.69270900	-2.12719000
C	-0.55018000	-3.05091700	-3.22182800
H	0.74414300	-1.77736000	-2.10180400
C	-2.73228700	-1.75594000	3.82571400
H	-4.22618700	-2.81198200	2.72475500

H	-1.04143500	-0.69318100	4.64997000
H	-3.52500900	-4.22894900	-2.15405000
C	-1.75644600	-3.74686800	-3.24642300
H	0.12264200	-3.07616900	-4.07496600
H	-3.28269600	-1.80969100	4.76048800
H	-2.05328800	-4.32129400	-4.11907700
C	-1.35325000	1.60869900	-1.37918600
C	-1.03182800	2.25766200	0.96915600
C	-2.59093700	2.28009700	-1.43601300
C	-0.79810300	1.07406300	-2.55493200
C	-2.24862200	2.96986800	0.97282000
C	-0.19100000	2.32369100	2.09618000
C	-3.25057000	2.32936400	-2.67184800
C	-1.47355600	1.14929500	-3.76653200
H	0.17061100	0.59287500	-2.51691000
C	-2.57974200	3.69684000	2.12464000
C	-0.54516600	3.06273700	3.21784000
H	0.75127500	1.79077200	2.09840600
C	-2.71833600	1.77147000	-3.83091800
H	-4.21836600	2.81812500	-2.72965700
H	-1.02253700	0.71682100	-4.65535100
H	-3.52490100	4.23012100	2.15224200
C	-1.75330800	3.75536300	3.24264200
H	0.12879300	3.09165500	4.06996600
H	-3.26636500	1.82788400	-4.76693500
H	-2.05064600	4.33053700	4.11463700
N	-0.66729000	-1.47384100	0.15253200
N	-0.66322300	1.47861200	-0.15330100
C	-3.23230700	-2.93599500	0.20411000
C	-3.23237400	2.93048400	-0.20385800
C	-3.64795700	-4.38734300	0.56665700
H	-4.11242500	-4.89427700	-0.28398600
H	-2.77705900	-4.97262600	0.87871700
H	-4.37719600	-4.40032000	1.38181300
C	-4.49337200	-2.13337800	-0.21517000
H	-5.21274700	-2.07944000	0.60993700
H	-4.22537600	-1.11220300	-0.50345000
H	-4.98981100	-2.60577900	-1.07047400
C	-4.48193600	2.11014700	0.21602000
H	-5.20260400	2.04987000	-0.60759400
H	-4.20020600	1.09151400	0.50025100
H	-4.98173100	2.57351700	1.07435000
C	-3.66827900	4.37694800	-0.56122500
H	-4.13760400	4.87526100	0.29174100

H	-2.80634100	4.97495000	-0.87403700
H	-4.40016800	4.38249300	-1.37402600

The Cartesian coordinates of the optimized structure of DBFo-DHPZ

0 1

C	5.01120200	1.88646800	-0.00002300
C	5.59164100	3.15209100	-0.00014800
C	4.80313900	4.31515000	-0.00035000
C	3.41089900	4.24113700	-0.00042600
O	1.50665800	2.71259300	-0.00034900
C	0.13273200	0.70454900	-0.00017400
C	0.13271200	-0.70449200	0.00004000
O	1.50658300	-2.71257400	0.00048900
C	3.41078200	-4.24117100	0.00085800
C	4.80302000	-4.31522200	0.00092900
C	5.59155400	-3.15218500	0.00074600
C	5.01115000	-1.88654500	0.00048900
C	2.85415900	2.96985100	-0.00029200
C	1.38059700	1.34645800	-0.00017500
C	1.38056000	-1.34643600	0.00023100
C	2.85407600	-2.96987000	0.00060500
C	3.61255200	-1.78108300	0.00042400
C	2.63583200	-0.70524600	0.00019700
C	2.63585200	0.70523400	0.00000100
C	3.61260100	1.78104400	-0.00009400
H	5.63972000	1.00371000	0.00015100
H	5.63969200	-1.00380500	0.00033900
H	5.28432400	-5.28889800	0.00112600
H	2.78217500	-5.12509900	0.00098600
H	2.78231700	5.12508300	-0.00058000
H	5.28447000	5.28881300	-0.00044800
H	6.67393900	-3.24198500	0.00080500
H	6.67402900	3.24186100	-0.00008800
C	-1.58624100	1.95440600	-1.22731800
C	-1.58637200	1.95478000	1.22640000
C	-2.86501300	2.55310200	-1.21542400
C	-0.89576600	1.86437200	-2.43491400
C	-2.86513700	2.55348000	1.21419000
C	-0.89602200	1.86510200	2.43409500
C	-3.41539600	3.03985600	-2.39921700
C	-1.46363200	2.33808800	-3.62434900
H	0.08829500	1.41025600	-2.45533000
C	-3.41563300	3.04060800	2.39777600
C	-1.46400400	2.33919100	3.62332600
H	0.08802400	1.41096300	2.45474800
C	-2.72231100	2.92590800	-3.60883000
H	-4.40148500	3.49907100	-2.37170400

H	-0.90989900	2.24111700	-4.55349800
H	-4.40171600	3.49982200	2.37002500
C	-2.72267200	2.92702500	3.60749500
H	-0.91036900	2.24249800	4.55256300
H	-3.17257700	3.29826800	-4.52435800
H	-3.17302600	3.29968100	4.52286000
C	-1.58656200	-1.95395900	1.22711000
C	-1.58607400	-1.95511400	-1.22660700
C	-2.86529800	-2.55272400	1.21509400
C	-0.89637400	-1.86352600	2.43484200
C	-2.86481400	-2.55387300	-1.21451800
C	-0.89544000	-1.86577900	-2.43416300
C	-3.41593900	-3.03914300	2.39890400
C	-1.46450000	-2.33690600	3.62428600
H	0.08765800	-1.40934800	2.45535100
C	-3.41499500	-3.04141100	-2.39808200
C	-1.46310500	-2.34028500	-3.62338000
H	0.08858800	-1.41159700	-2.45472700
C	-2.72314700	-2.92479100	3.60864700
H	-4.40199600	-3.49842300	2.37129600
H	-0.91099300	-2.23962700	4.55353800
H	-4.40106100	-3.50066500	-2.37042200
C	-2.72174500	-2.92818200	-3.60766900
H	-0.90924500	-2.24385900	-4.55251100
H	-3.17361600	-3.29689100	4.52418100
H	-3.17185200	-3.30116200	-4.52302300
N	-1.07473900	1.45153500	-0.00035500
N	-1.07477800	-1.45144500	0.00011300
N	-3.56047600	2.61351900	-0.00066200
N	-3.56045700	-2.61355400	0.00017900
H	-4.40071700	3.17606200	-0.00079300
H	-4.40067300	-3.17613300	0.00027300

The Cartesian coordinates of the optimized structure of DBFp-Cz

0 1

C	1.67150800	-0.00000800	-0.00000300
C	0.90452800	1.16209600	0.12164900
C	-0.51144400	1.19452500	0.11090400
C	-1.23977300	0.00006800	-0.00001200
C	0.36862200	3.28464700	0.30793900
C	0.47772000	4.66132200	0.42891000
C	-0.71919300	5.37884400	0.47167100
C	-1.96161800	4.72839300	0.39569800
C	-2.04782900	3.34225200	0.27667900
C	-0.85886200	2.60204600	0.23169400
H	1.44696800	5.14497100	0.48492400
H	-0.68582000	6.46049100	0.56524600
H	-2.87363600	5.31694000	0.43197100
H	-3.01307100	2.85131200	0.22337300
C	0.36846100	-3.28460600	-0.30782300
C	-0.85899000	-2.60194000	-0.23162600
C	-2.04799400	-3.34208800	-0.27659800
C	-1.96185100	-4.72823700	-0.39556300
C	-0.71945800	-5.37875400	-0.47149000
C	0.47749100	-4.66129100	-0.42873800
C	0.90447100	-1.16207400	-0.12161300
C	-0.51150500	-1.19443100	-0.11088000
H	-3.01321100	-2.85109600	-0.22332400
H	-2.87389800	-5.31674000	-0.43182900
H	-0.68613800	-6.46040600	-0.56502400
H	1.44671500	-5.14499100	-0.48471400
O	1.43887800	2.41478400	0.24374600
O	1.43876000	-2.41479600	-0.24364000
C	3.89869900	0.63160200	-0.94644800
C	3.89868500	-0.63180200	0.94636300
C	3.53888500	1.36236000	-2.07942400
C	5.25380400	0.40109800	-0.60361600
C	3.53884000	-1.36268500	2.07925100
C	5.25379200	-0.40117100	0.60363800
C	4.56559500	1.87511600	-2.86986200
H	2.49820700	1.52730200	-2.33819600
C	6.26577800	0.92748100	-1.41461300
C	4.56552900	-1.87541800	2.86972600
H	2.49815100	-1.52769800	2.33794000
C	6.26574800	-0.92753000	1.41467900
C	5.91592700	1.66359900	-2.54326200
H	4.31329000	2.44934400	-3.75719500

H	7.31087000	0.75984400	-1.16753300
C	5.91587000	-1.66375300	2.54324700
H	4.31321100	-2.44972500	3.75700400
H	7.31084500	-0.75981600	1.16767200
H	6.69266700	2.07738200	-3.18006500
H	6.69259500	-2.07752300	3.18007800
C	-3.47758200	-0.19433300	-1.11924200
C	-3.47762700	0.19457300	1.11915200
C	-3.11352600	-0.41526300	-2.44916400
C	-4.83509500	-0.12387300	-0.71425100
C	-3.11360700	0.41569400	2.44905300
C	-4.83512000	0.12374400	0.71417200
C	-4.13811500	-0.57127600	-3.38023200
H	-2.07067500	-0.46400500	-2.74578300
C	-5.84442000	-0.28347800	-1.67188200
C	-4.13822200	0.57152000	3.38012000
H	-2.07076000	0.46467300	2.74565000
C	-5.84447600	0.28315500	1.67180900
C	-5.49001500	-0.50699700	-2.99930600
H	-3.88396900	-0.74561800	-4.42213400
H	-6.89061400	-0.23105700	-1.38184200
C	-5.49011100	0.50686000	2.99921000
H	-3.88411800	0.74598700	4.42201100
H	-6.89066000	0.23047800	1.38178100
H	-6.26448300	-0.63268800	-3.75050900
H	-6.26460200	0.63241100	3.75041400
N	3.08011700	-0.00005100	-0.00001100
N	-2.66012900	0.00010900	-0.00002300

The Cartesian coordinates of the optimized structure of DBFp-DMAC

0 1

C	-1.64516900	0.00017600	-0.00001500
C	-0.87975300	1.16753200	-0.00094800
C	0.53745700	1.19816600	-0.00098200
C	1.26647300	0.00030800	-0.00002000
C	-0.34164100	3.29702300	-0.00266900
C	-0.44712200	4.67932800	-0.00377700
C	0.75157300	5.39545300	-0.00436000
C	1.99324700	4.73892700	-0.00384600
C	2.07567400	3.34759700	-0.00272900
C	0.88551200	2.60942900	-0.00213000
H	-1.41500200	5.16895700	-0.00415800
H	0.72018900	6.48122200	-0.00522300
H	2.90616500	5.32730500	-0.00432200
H	3.03821300	2.84812100	-0.00232900
C	-0.34134000	-3.29655200	0.00264200
C	0.88575100	-2.60884700	0.00209700
C	2.07597700	-3.34691100	0.00269500
C	1.99367500	-4.73824800	0.00381900
C	0.75206000	-5.39488500	0.00434000
C	-0.44669800	-4.67886700	0.00375600
C	-0.87964300	-1.16711400	0.00091300
C	0.53756600	-1.19761700	0.00094500
H	3.03847100	-2.84734800	0.00228600
H	2.90664700	-5.32654300	0.00429400
H	0.72077400	-6.48065700	0.00520900
H	-1.41453600	-5.16858200	0.00414200
O	-1.41300100	2.42593300	-0.00195200
O	-1.41277800	-2.42555800	0.00192400
C	3.38619200	-0.00115200	-1.23138400
C	3.38616300	0.00167600	1.23138000
C	4.79599400	-0.00169600	-1.26726400
C	2.65989700	-0.00209500	-2.43814000
C	4.79596300	0.00140200	1.26729400
C	2.65983800	0.00328400	2.43811800
C	5.41881200	-0.00332300	-2.52317200
C	3.31078100	-0.00366100	-3.66522200
H	1.57716700	-0.00160500	-2.41079100
C	5.41875100	0.00285800	2.52321700
C	3.31069200	0.00467100	3.66521500
H	1.57711000	0.00345000	2.41074100
C	4.70379900	-0.00431700	-3.71702100
H	6.50421800	-0.00382900	-2.56756400

H	2.72283200	-0.00436600	-4.57903300
H	6.50415600	0.00266400	2.56763800
C	4.70371000	0.00448600	3.71704900
H	2.72272000	0.00589900	4.57901100
H	5.22675700	-0.00557500	-4.66880400
H	5.22664600	0.00557700	4.66884400
C	-3.75239100	0.00111000	1.23212200
C	-3.75240900	-0.00126900	-1.23212600
C	-5.16100400	0.00096000	1.26753600
C	-3.02667900	0.00228500	2.43816500
C	-5.16102300	-0.00164000	-1.26751700
C	-3.02672300	-0.00227000	-2.43818500
C	-5.78411000	0.00208000	2.52281100
C	-3.67702700	0.00334300	3.66586300
H	-1.94365200	0.00236700	2.41221200
C	-5.78415400	-0.00313900	-2.52277900
C	-3.67709500	-0.00370900	-3.66587000
H	-1.94369500	-0.00191300	-2.41226100
C	-5.06968800	0.00326000	3.71733400
H	-6.86953000	0.00201900	2.56661900
H	-3.08888400	0.00423600	4.57968000
H	-6.86957500	-0.00346800	-2.56656000
C	-5.06975600	-0.00418800	-3.71731700
H	-3.08896800	-0.00445400	-4.57969800
H	-5.59314400	0.00410400	4.66892200
H	-5.59322800	-0.00534200	-4.66889600
N	2.69744700	0.00036000	-0.00001000
N	-3.06568200	0.00010000	-0.00000700
C	5.65997900	-0.00062500	0.00002600
C	-6.02396900	-0.00031100	0.00001500
C	-6.92158800	1.26720600	-0.00129200
H	-7.56753200	1.29275900	-0.88511400
H	-7.56754500	1.29457400	0.88246700
H	-6.30825700	2.17406700	-0.00222300
C	-6.92172300	-1.26772500	0.00134200
H	-7.56767400	-1.29506500	-0.88242100
H	-6.30848100	-2.17464500	0.00232800
H	-7.56772400	-1.29318200	0.88512500
C	6.56110400	1.26456300	-0.00154800
H	5.95191000	2.17464200	-0.00284400
H	7.20675600	1.29114700	0.88233000
H	7.20697800	1.28879100	-0.88533500
C	6.55964100	-1.26685000	0.00162000
H	7.20548500	-1.29179000	0.88541300

H	5.94941400	-2.17624100	0.00294900
H	7.20523300	-1.29419500	-0.88228300

The Cartesian coordinates of the optimized structure of DBFp-DHPZ

0 1

C	1.66683900	-0.02271100	0.00001400
C	0.89261900	-1.18501000	-0.00019900
C	-0.52543300	-1.20758000	-0.00020200
C	-1.24661900	-0.00267800	0.00000900
C	0.34323500	-3.31129300	-0.00062700
C	0.44236700	-4.69422800	-0.00088700
C	-0.75936700	-5.40502500	-0.00100000
C	-1.99801000	-4.74279600	-0.00085400
C	-2.07450900	-3.35107700	-0.00058900
C	-0.88078700	-2.61784300	-0.00048100
H	1.40826700	-5.18776900	-0.00098800
H	-0.73292900	-6.49094800	-0.00120500
H	-2.91375400	-5.32676000	-0.00094800
H	-3.03564200	-2.84903800	-0.00048000
C	0.38127500	3.28297300	0.00057500
C	-0.84939500	2.60178500	0.00047000
C	-2.03635700	3.34563100	0.00060300
C	-1.94563800	4.73670800	0.00084500
C	-0.70065500	5.38687200	0.00094800
C	0.49446100	4.66460100	0.00081300
C	0.90830800	1.15015400	0.00019500
C	-0.50816800	1.18879100	0.00020000
H	-3.00146300	2.85109200	0.00052300
H	-2.85550300	5.32987100	0.00095300
H	-0.66358900	6.47251100	0.00113700
H	1.46498500	5.14899300	0.00088300
O	1.41836500	-2.44639100	-0.00045800
O	1.44859100	2.40584000	0.00041300
C	-3.38111800	-0.04405800	-1.22847600
C	-3.38113900	-0.04450100	1.22851000
C	-4.76632900	0.23127500	-1.21676200
C	-2.76426500	-0.35563000	-2.44027700
C	-4.76634700	0.23085000	1.21684000
C	-2.76429000	-0.35650900	2.44018900
C	-5.49611900	0.17576700	-2.40204500
C	-3.50099900	-0.38727500	-3.63102600
H	-1.70129800	-0.56733000	-2.45830800
C	-5.49613300	0.17491900	2.40211500
C	-3.50103100	-0.38857200	3.63092700
H	-1.70132400	-0.56821600	2.45814400
C	-4.86555400	-0.12486600	-3.61423500
H	-6.56285200	0.38857700	-2.37532500

H	-2.99484800	-0.62172300	-4.56269100
H	-6.56287000	0.38773600	2.37546500
C	-4.86558400	-0.12614600	3.61419700
H	-2.99489600	-0.62335700	4.56251400
H	-5.44700100	-0.15097700	-4.53105300
H	-5.44705200	-0.15256500	4.53099400
C	3.78325200	0.03286600	1.23238200
C	3.78322200	0.03357800	-1.23236200
C	5.18608100	-0.13329800	1.21981100
C	3.14131500	0.24994000	2.45060300
C	5.18605100	-0.13259500	-1.21990200
C	3.14124200	0.25139600	-2.45041700
C	5.90213500	-0.07147000	2.41351400
C	3.86670600	0.29435700	3.64846800
H	2.06508100	0.37996600	2.47049600
C	5.90205300	-0.07005400	-2.41360500
C	3.86658900	0.29653600	-3.64828400
H	2.06500600	0.38145100	-2.47017500
C	5.24649600	0.13595800	3.63196200
H	6.98218700	-0.20058800	2.38598000
H	3.33907800	0.45641600	4.58368700
H	6.98210800	-0.19918900	-2.38618800
C	5.24637900	0.13810800	-3.63190200
H	3.33893400	0.45917800	-4.58338600
H	5.82108500	0.17145100	4.55286000
H	5.82095300	0.17414600	-4.55278900
N	-2.67322700	0.03873000	0.00002000
N	3.08348300	-0.04841600	-0.00000100
N	5.82087000	-0.39023300	-0.00013300
H	6.83056000	-0.34901000	-0.00015800
N	-5.36081400	0.60056500	0.00010900
H	-6.37172400	0.63888300	0.00012800