Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Dual fluorescence of 2-(2'-hydroxyphenyl) benzoxazole derivatives via the branched decays from upper excited-state

Zhe Tang[a] Haiyun Han,[b] Junxia Ding,[c] and Panwang Zhou[*a]

a Institute of Molecular Sciences and Engineering, Institute of Frontier and Interdisciplinary Science, Shandong University, Qingdao 266237, P.R. China

b Heze Dingtao People's Hospital, Heze, 274199, Shandong, P. R. China

c State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, 116023, Liaoning, P. R. China

E-mail: pwzhou@sdu.edu.cn Tel: +86-532-58632158

Table S1. Comparison of the calculated and the experimental vertical excitation and emission energies for 1H2NBO-enol and 1H2NBO-keto based on CAM-B3LYP/TZVP/IEFPCM levels.

		electronic transition	energy (nm/eV)	f^a	contrib[b]	CI[c]	exp.[d] nm/eV
1H2NBO-enol	VEEs	$S_0 \rightarrow S_1$	324/3.83	0.5649	H→L	0.91	350/3.54
		$S_0 \rightarrow S_2$	282/4.40	0.0568	H-1→L	0.39	
	emission	$S_1 \rightarrow S_0$	363/3.41	0.5946	L→H	0.94	-
1H2NBO-keto	emission	$S_1 \rightarrow S_0$	409/3.03	0.6081	L→H	0.96	470/2.64

Table S2. The primary bond lengths (Å), angles (°) and energy (Hartree) of the S_0, S_1 and S_2 states for 2H3NBO-enol and 2H3NBO-keto.

	2H3NBO-enol			2H3NBO-keto	
	S_0	S_1	S_2	S_1	S_2
O_1-H_2	0.985	1.038	0.987	1.948	2.118
H_2-N_3	1.796	1.584	1.794	1.021	1.007
$\delta(O_1–H_2–N_3)$	146.0	150.6	146.8	125.2	114.2
energy	-859.96890	-859.85798	-859.83947	-859.87013	-859.84180
Dipole moments	3.001516	3.292004	2.689149	8.191112	7.843803

Table S3. Comparison of the calculated and the experimental vertical excitation and emission energies for 2H3NBO-enol and 2H3NBO-keto based on CAM-B3LYP/TZVP/IEFPCM levels.

		electronic transition	energy (nm/eV)	f	contrib	CI	exp. (nm/eV)
2H3NBO-enol	VEEs	$S_0 \rightarrow S_1$	334/3.71	0.1031	H→L	0.84	330/3.76
		$S_0 \rightarrow S_2$	301/4.12	0.8525	H-1→L	0.82	
	emission	$S_1 \rightarrow S_0$	390/3.18	0.1044	L→H	0.92	450/2.76
2H3NBO-keto	emission	$S_1 \rightarrow S_0$	586/2.12	0.1365	L→H	1.00	670/1.85

Fig. S1 Gibbs free-energy profile for the reaction of 1H2NBO and 2H3NBO at the B3LYP-D3/TZVP/IEFPCM levels.

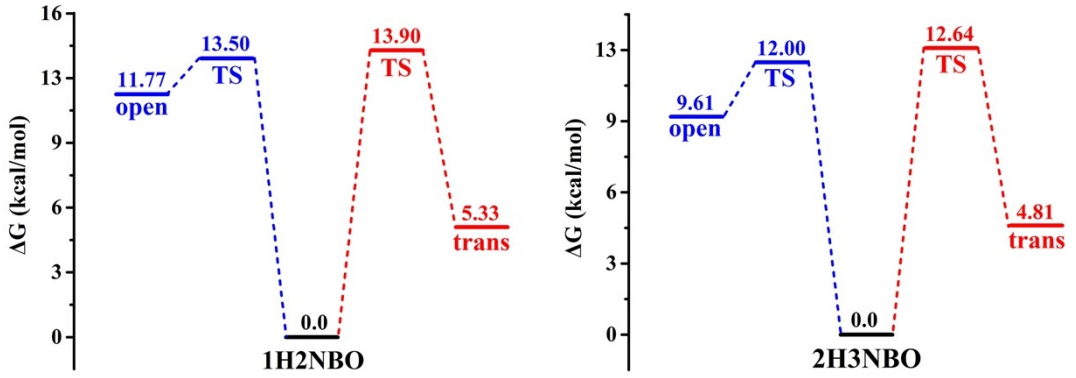


Fig. S2 Orbitals involved in the active space of SA3-CASSCF(12,12)/6-31G(d) calculations.

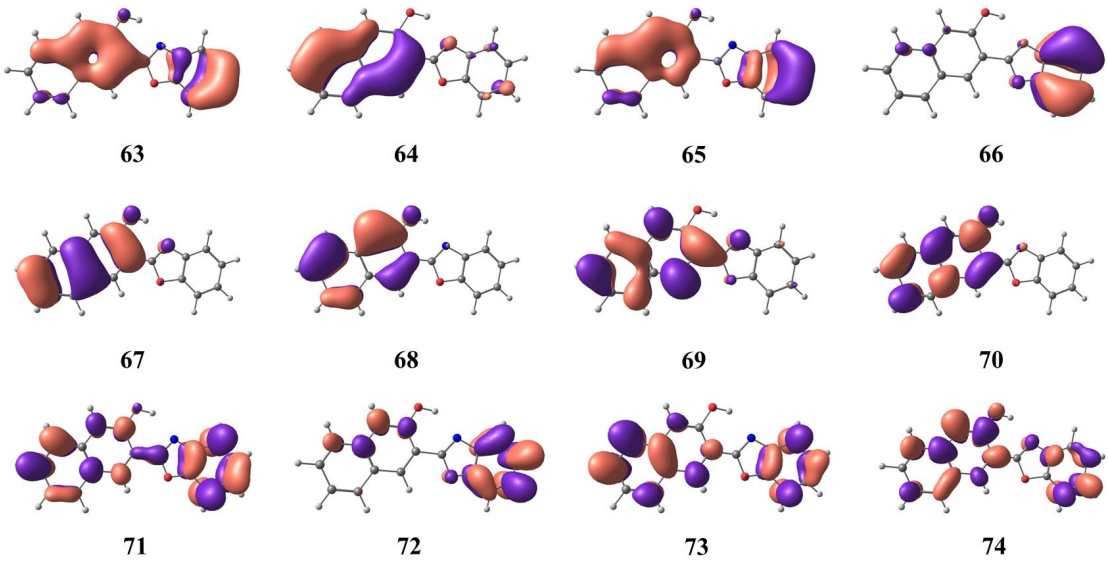


Fig. S3 The calculated IR spectra of 1H2NBO-enol at the spectral region of O_1–H_2 stretching band in the S_0 and S_1 states at the B3LYP-D3/TZVP/IEFPCM levels.

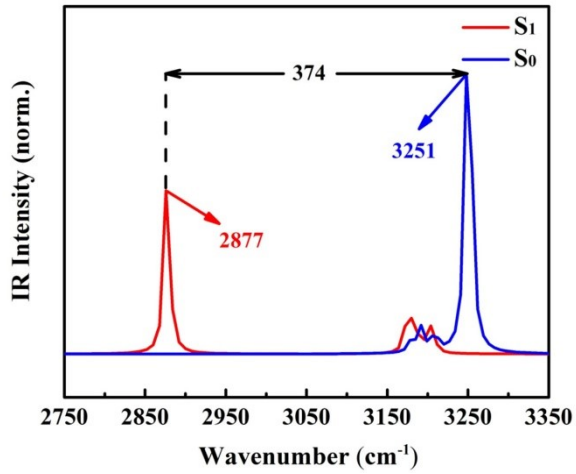
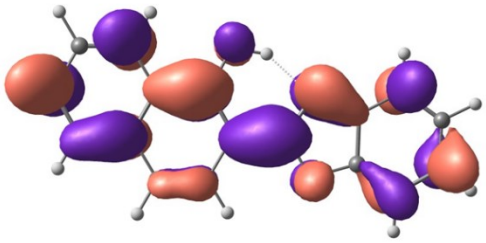
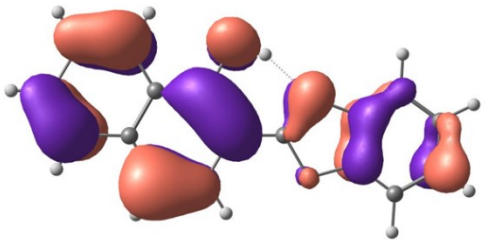


Fig. S4 Calculated frontal MOs of 1H2NBO-enol based on CAM-B3LYP-D3/TZVP/IEFPCM levels.



LUMO



HOMO

Fig. S5 The calculated IR spectra of 2H3NBO-enol at the spectral region of O_1–H_2 stretching band in the S_0 and S_1 states at the B3LYP-D3/TZVP/IEFPCM levels.

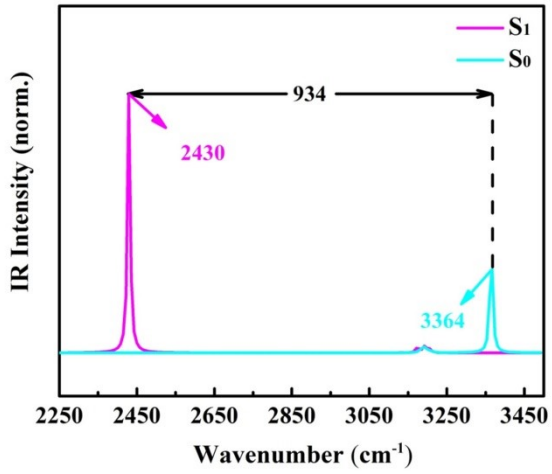


Fig. S6 Natural transition orbitals of 1H2NBO and 2H3NBO in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ based on CAM-B3LYP-D3/TZVP/IEFPCM levels.

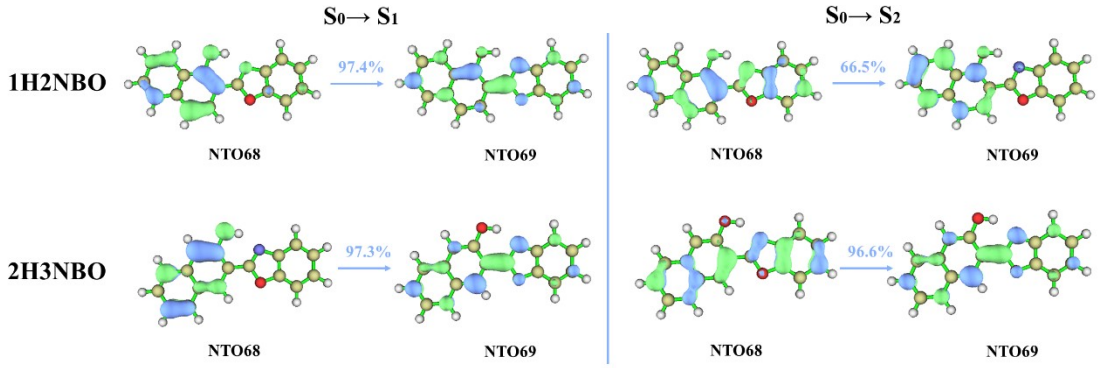
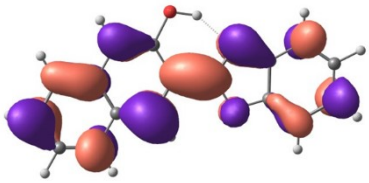
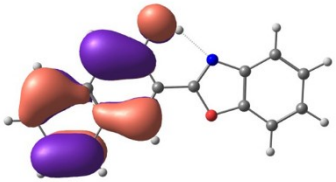


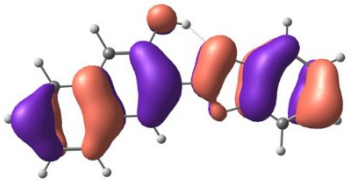
Fig. S7 Calculated frontal MOs of 2H3NBO-enol based on CAM-B3LYP-D3/TZVP/IEFPCM levels.



LUMO

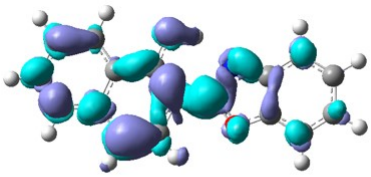


HOMO

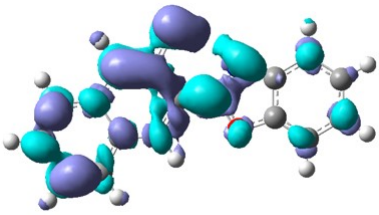


HOMO-1

Fig. S8 The charge density difference (S_1-S_0) maps of 1H2NBO and 2H3NBO based on CAM-B3LYP-D3/TZVP/IEFPCM levels (Blue is negative, purple is positive).

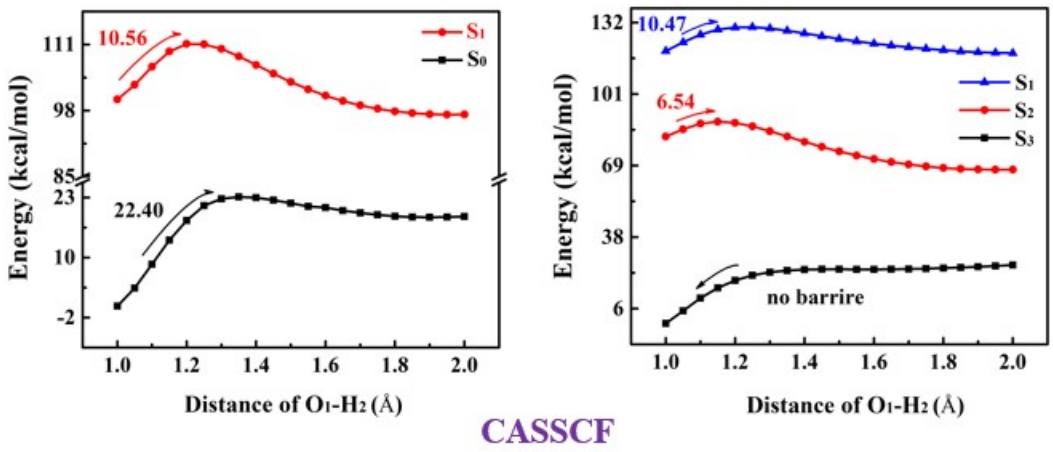


1H2NBO



2H3NBO

Figure S9. The CASSCF(12,12)/6-31G* computed energy profiles along the TD-B3LYP/TZVP determined PECs of the ESIPT process of 1H2NBO (left) and 2H3NBO (right).



S_0 geometry of 1H2NBO-enol in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy= -859.972284

C	2.97296800	-0.69186600	-0.00005200
C	3.13590600	0.69617200	0.00012400
C	4.36362600	1.32598700	0.00010700
C	5.47506000	0.48372900	-0.00010500
C	5.33811000	-0.91195300	-0.00029200
C	4.08859900	-1.52390900	-0.00027100
C	1.01822900	0.20041200	0.00027500
H	4.45511600	2.40338000	0.00025100
H	6.46609600	0.91891400	-0.00013100
H	6.22911700	-1.52684000	-0.00046100
H	3.98094400	-2.60026900	-0.00042000
C	-0.40144600	0.44057700	0.00011200
C	-1.27601100	-0.65204900	0.00015900
C	-0.92381700	1.76406700	-0.00004600
C	-2.68699700	-0.43519000	0.00005100
C	-2.26752100	1.99050000	-0.00014800
H	-0.22695100	2.59121000	-0.00006900
C	-3.18297500	0.90145700	-0.00010800
C	-3.59821000	-1.51718300	0.00009200
H	-2.65351700	3.00222800	-0.00025500
C	-4.58339000	1.10048400	-0.00020500
C	-4.95266200	-1.28684700	-0.00001600
H	-3.20926300	-2.52592200	0.00021000

C	-5.44880200	0.03302200	-0.00016300
H	-4.96489500	2.11485600	-0.00032000
H	-5.64380900	-2.12043300	0.00001900
H	-6.51849900	0.20353000	-0.00024300
N	1.60951400	-0.96522200	0.00000600
O	1.88220800	1.26530900	0.00031200
O	-0.85041700	-1.92477800	0.00022000
H	0.14073500	-1.93279900	0.00003600

S_0 geometry of 1H2NBO-keto in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy=-859.961408

C	-2.97845600	-0.69692600	0.00009000
C	-3.13620200	0.68794500	-0.00005100
C	-4.36417400	1.30847600	-0.00013600
C	-5.47677500	0.46244500	-0.00007100
C	-5.33458700	-0.92786500	0.00007400
C	-4.07981100	-1.53823000	0.00016100
C	-0.96914300	0.27484300	0.00001300
H	-4.45624800	2.38548300	-0.00024000
H	-6.46803600	0.89604200	-0.00012800
H	-6.22051500	-1.54945500	0.00012500
H	-3.97078700	-2.61400200	0.00027800
C	0.40633500	0.47828400	-0.00000800
C	1.25584000	-0.69927300	-0.00012400
C	0.96234700	1.79882200	0.00006100
C	2.70300600	-0.44814100	-0.00004400
C	2.30211000	1.99492000	0.00007800
H	0.28448700	2.64326000	0.00011600
C	3.20758300	0.87776100	0.00005000
C	3.59404400	-1.53274500	-0.00009100
H	2.71194300	2.99732100	0.00013800
C	4.60457700	1.06336500	0.00008400
C	4.95923500	-1.32506400	-0.00005000
H	3.18005600	-2.53247900	-0.00016800
C	5.46477300	-0.01643700	0.00003800
H	4.99894300	2.07314100	0.00014800
H	5.63890800	-2.16819000	-0.00008900
H	6.53579900	0.14767500	0.00006900
N	-1.60726300	-0.91138400	0.00014600
O	-1.88234300	1.28007400	-0.00006900
O	0.79548200	-1.87014900	-0.00018100
H	-1.01302600	-1.75159500	0.00027700

S_0 geometry of 2H3NBO-enol in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy= -859.968897

C	-3.11083100	0.51177400	0.00004500
C	-2.91642000	-0.87191900	-0.00004600
C	-3.94492300	-1.79233800	-0.00007700
C	-5.23243100	-1.25783000	-0.00000700
C	-5.45383100	0.12750600	0.00008400
C	-4.40041800	1.03555400	0.00010900
C	-0.99596000	0.14639100	-0.00000900
H	-3.76146500	-2.85786800	-0.00015100
H	-6.08136100	-1.92930200	-0.00002700
H	-6.47162300	0.49622800	0.00013200
H	-4.56791300	2.10419200	0.00017400
C	0.44430100	0.27297800	-0.00001100
C	1.25886200	-0.84561700	0.00001200
C	1.03598400	1.58245000	-0.00003400
C	2.66053900	-0.73754700	0.00001700
C	2.40677200	1.70256300	-0.00002700
C	3.24590600	0.56959600	-0.00000200
C	3.50655900	-1.87794500	0.00004300
H	2.83569000	2.69670300	-0.00004500
C	4.66151300	0.67566700	0.00000400
C	4.86932900	-1.73829000	0.00004800
H	3.05397700	-2.86295600	0.00005800
C	5.44917000	-0.44667900	0.00002800
H	5.11145500	1.66152400	-0.00001200
H	5.50819800	-2.61247100	0.00006800
H	6.52795800	-0.34828200	0.00003200
N	-1.86082300	1.12176900	0.00003100
O	-1.56009000	-1.10357900	-0.00010900
H	0.80455600	-1.82830500	0.00003000
O	0.28854400	2.70698600	-0.00006900
H	-0.66607500	2.46300400	-0.00010300

S_0 geometry of trans-1H2NBO-enol in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy=-859.962933

C	3.15204500	0.76536300	0.00058000
C	2.97408700	-0.62002000	0.00054300
C	4.00572400	-1.53553400	0.00071200

C	5.29064000	-0.99289500	0.00092200
C	5.50104800	0.39375000	0.00096600
C	4.44070000	1.29407700	0.00079900
C	1.04127500	0.41987600	0.00015700
H	3.83023200	-2.60258800	0.00067900
H	6.14385400	-1.65890500	0.00106200
H	6.51620800	0.76997800	0.00114700
H	4.60019400	2.36398100	0.00085300
C	-0.40567600	0.51059300	-0.00014500
C	-1.24918400	-0.60006200	-0.00018500
C	-0.97825500	1.81738100	-0.00035300
C	-2.66745500	-0.42736200	-0.00044800
C	-2.32601300	2.00499400	-0.00060200
H	-0.30058600	2.65993700	-0.00030900
C	-3.20866900	0.89058300	-0.00065400
C	-3.54555700	-1.53743900	-0.00050700
H	-2.73971300	3.00576500	-0.00076400
C	-4.61416200	1.04638200	-0.00090800
C	-4.90668000	-1.34985800	-0.00075600
H	-3.12870100	-2.53458000	-0.00035500
C	-5.44585200	-0.04733800	-0.00095700
H	-5.02608900	2.04875600	-0.00106300
H	-5.57018700	-2.20564000	-0.00080000
H	-6.52043600	0.08863400	-0.00115300
N	1.90606100	1.38297400	0.00043400
O	1.61659500	-0.85149300	0.00031600
O	-0.82190300	-1.88503800	0.00000500
H	0.14715100	-1.91885700	0.00010800

S_0 geometry of trans-2H3NBO-enol in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy=-859.959818

C	2.93827500	-0.94368300	-0.00001200
C	3.10912800	0.44251400	0.00002400
C	4.33579700	1.07392700	0.00006700
C	5.44514500	0.22927200	0.00007900
C	5.30520700	-1.16673500	0.00004300
C	4.05525300	-1.77614900	-0.00000400
C	0.98121000	-0.08397700	0.00001200
H	4.43045000	2.15110300	0.00009200
H	6.43704000	0.66246600	0.00011000
H	6.19555600	-1.78261000	0.00004300
H	3.94440400	-2.85214400	-0.00004300

C	-0.44806500	0.19042000	0.00001400
C	-1.31117700	-0.89429200	-0.00002200
C	-1.00022500	1.51380100	0.00003500
C	-2.70686800	-0.74038500	-0.00003300
C	-2.36570600	1.68194500	0.00002300
C	-3.24821500	0.58400800	-0.00000900
C	-3.59066400	-1.85227200	-0.00006700
H	-2.75560700	2.69205200	0.00004100
C	-4.65872500	0.74076900	-0.00002100
C	-4.94760000	-1.66516200	-0.00007700
H	-3.17138600	-2.85175200	-0.00008500
C	-5.48370200	-0.35445000	-0.00005400
H	-5.07432100	1.74157000	-0.00000300
H	-5.61623300	-2.51681300	-0.00010400
H	-6.55857900	-0.22000000	-0.00006200
N	1.57793200	-1.23152800	-0.00008600
O	1.85170100	1.00261600	0.00000300
H	-0.88499300	-1.88936600	-0.00004300
O	-0.24473600	2.64526300	0.00006800
H	0.69800900	2.42585000	0.00009200

S_0 geometry of open-1H2NBO-enol in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy=-859.951306

C	3.04894800	-0.70167700	-0.11066000
C	3.13011300	0.67882300	0.09209500
C	4.32022700	1.37030500	0.21258400
C	5.47877400	0.60060400	0.12018300
C	5.42526100	-0.78715400	-0.08270800
C	4.21415400	-1.46027800	-0.20102300
C	1.04812000	0.03936100	-0.03700200
H	4.34954300	2.44001000	0.36902600
H	6.44260300	1.08596700	0.20716000
H	6.35158100	-1.34397200	-0.14801600
H	4.16793300	-2.52979300	-0.35749500
C	-0.38499200	0.29358600	-0.04432200
C	-1.32512400	-0.72970600	0.04628700
C	-0.84143200	1.63910300	-0.12927800
C	-2.72515900	-0.43417200	0.02609900
C	-2.16880100	1.95075800	-0.13016000
H	-0.10283400	2.42488600	-0.19338000
C	-3.14599100	0.92764100	-0.05290600
C	-3.71740800	-1.44564300	0.07878100

H	-2.48909700	2.98316700	-0.19373100
C	-4.53148100	1.21702400	-0.05751800
C	-5.05392400	-1.13159700	0.07189400
H	-3.44458400	-2.49482100	0.11124900
C	-5.46660200	0.21474400	0.00627300
H	-4.84265200	2.25343900	-0.11503800
H	-5.79388600	-1.92085700	0.11053200
H	-6.52285500	0.45307500	0.00145600
N	1.70955400	-1.06474100	-0.18786700
O	1.85152800	1.16220600	0.14100700
O	-0.88719600	-2.00565600	0.15249900
H	-1.62538700	-2.60063600	0.32355200

S_0 geometry of open-2H3NBO-enol in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy=-859.952525

C	-3.13930500	0.50590200	0.17451200
C	-2.89171300	-0.83193700	-0.14514300
C	-3.88331700	-1.78060500	-0.30598300
C	-5.18880200	-1.32592000	-0.12781900
C	-5.46470600	0.01225300	0.19374000
C	-4.44859700	0.94857600	0.34947600
C	-1.02458300	0.28321800	0.00240500
H	-3.65963300	-2.80903600	-0.55462800
H	-6.00960500	-2.02282000	-0.24057800
H	-6.49499000	0.31925100	0.32234900
H	-4.65578600	1.98117100	0.59689100
C	0.42963100	0.38837700	-0.01726400
C	1.19180400	-0.76286100	0.06253500
C	1.10369700	1.64731900	-0.11729700
C	2.60053300	-0.73952800	0.06205900
C	2.47820100	1.69329600	-0.11920400
C	3.26227800	0.52218200	-0.02973200
C	3.37612100	-1.92363500	0.15183400
H	2.97643800	2.65425400	-0.19841000
C	4.67937100	0.54976000	-0.02829600
C	4.74614800	-1.86426200	0.15085900
H	2.86655600	-2.87774700	0.22174200
C	5.40108000	-0.61434200	0.05959400
H	5.18666300	1.50503600	-0.09777600
H	5.33178500	-2.77231900	0.21999800
H	6.48370900	-0.57913500	0.05974100
N	-1.92453100	1.17743800	0.25801300

O	-1.53655200	-0.98278200	-0.25914400
H	0.68904900	-1.71784400	0.13531400
O	0.34530600	2.76907500	-0.22420600
H	0.92045600	3.54002300	-0.30158300

S_1 geometry of 1H2NBO-enol in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy= -859.850941

C	-2.95808900	-0.69209100	-0.00000200
C	-3.15636300	0.70671800	0.00000300
C	-4.39480700	1.30567200	0.00002900
C	-5.49856600	0.43858400	0.00005700
C	-5.33114500	-0.95302700	0.00005300
C	-4.07185400	-1.54478200	0.00002200
C	-1.01840600	0.25890600	-0.00006100
H	-4.50784700	2.38113200	0.00002900
H	-6.49754900	0.85501900	0.00008000
H	-6.21064300	-1.58523400	0.00007400
H	-3.94664200	-2.61916500	0.00001700
C	0.37320400	0.49154700	-0.00001800
C	1.28843000	-0.64099800	-0.00001900
C	0.93397400	1.77775300	-0.00001900
C	2.68546900	-0.44777100	-0.00001000
C	2.30613700	1.97653900	-0.00000800
H	0.26931600	2.63141800	-0.00002500
C	3.21850200	0.88901400	-0.00000500
C	3.59587800	-1.53271800	0.00000600
H	2.69538000	2.98742600	-0.00000500
C	4.60582100	1.07868400	0.00001100
C	4.96652300	-1.30676100	0.00002100
H	3.20982300	-2.54280500	0.00000700
C	5.48541400	-0.00702500	0.00002300
H	4.99419100	2.09060100	0.00001500
H	5.64105600	-2.15426000	0.00003200
H	6.55460900	0.15668800	0.00003500
N	-1.61541100	-0.94023100	-0.00004100
O	-1.92268500	1.31219400	-0.00003400
O	0.81303800	-1.88235700	-0.00002200
H	-0.19738500	-1.84736100	-0.00002400

S_1 geometry of 1H2NBO-keto in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy=-859.853939

C	-3.01524100	-0.69960200	0.00564600
C	-3.15867400	0.69475500	-0.00148000
C	-4.37909500	1.33016400	-0.02258700
C	-5.50854400	0.49030200	-0.04057200
C	-5.38114500	-0.89898600	-0.03458700
C	-4.13510400	-1.53277900	-0.01072100
C	-0.99329000	0.25132800	0.05027200
H	-4.45858600	2.40786700	-0.02649600
H	-6.49472200	0.93505800	-0.05831000
H	-6.27592100	-1.50862100	-0.04842300
H	-4.04156500	-2.60957100	-0.00554400
C	0.41204200	0.45541500	0.02317300
C	1.29552600	-0.71370500	0.01878900
C	0.95272700	1.73811400	0.02044900
C	2.72264500	-0.45724200	0.00471200
C	2.33981900	1.96230000	0.00431100
H	0.28512200	2.59094900	0.03176500
C	3.24135600	0.88899400	-0.00436600
C	3.63454600	-1.52478400	-0.01061600
H	2.71198100	2.97911600	0.00021000
C	4.64474600	1.08762000	-0.02201200
C	5.00016200	-1.29619200	-0.02842800
H	3.24223800	-2.53323300	-0.00701400
C	5.51406500	0.01840700	-0.03386500
H	5.02463200	2.10305600	-0.02751200
H	5.68322900	-2.13690300	-0.03799100
H	6.58378200	0.18247600	-0.04769300
N	-1.65988900	-0.92678800	0.03638100
O	-1.90287300	1.27141000	0.02409900
O	0.82042800	-1.88430800	0.02913600
H	-1.10065000	-1.78414400	0.03775700

S_1 geometry of 2H3NBO-enol in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy=-859.857979

C	-3.10502800	0.52497700	-0.00068200
C	-2.97033900	-0.87746700	-0.00107000
C	-4.03318000	-1.74988500	0.00009800
C	-5.31179500	-1.17031300	0.00204500
C	-5.47369200	0.21825800	0.00250900
C	-4.38454900	1.08910400	0.00108700
C	-0.99198600	0.05005900	-0.00427800

H	-3.88820000	-2.82168300	-0.00037200
H	-6.18366500	-1.81138100	0.00313500
H	-6.47564000	0.62994800	0.00397700
H	-4.51732400	2.16270200	0.00134300
C	0.41514700	0.15563400	-0.00272100
C	1.30405600	-0.91226400	0.00311900
C	0.99349800	1.48953600	0.00065900
C	2.72196100	-0.73794500	-0.00137400
C	2.38251700	1.67969800	-0.00288100
C	3.27544400	0.58732700	0.00275700
C	3.60624900	-1.81585700	0.00138000
H	2.74968900	2.69804800	-0.00123300
C	4.67188200	0.76109500	-0.00015400
C	5.00090500	-1.61814500	0.00032400
H	3.21286900	-2.82531300	0.00090400
C	5.53668900	-0.33772900	0.00098700
H	5.07298500	1.76766600	0.00004200
H	5.65526600	-2.48071000	0.00099300
H	6.60787700	-0.18861200	0.00019800
N	-1.85117200	1.08057200	-0.00267900
O	-1.62428200	-1.18141800	-0.00329200
H	0.90864800	-1.92013600	0.00373900
O	0.21919900	2.55264700	0.00251900
H	-0.77030300	2.23914900	0.00137200

S_1 geometry of 2H3NBO-keto in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy= -859.870134

C	-3.15745800	0.52490400	-0.00448900
C	-2.94284900	-0.85882600	0.00686000
C	-3.96331500	-1.78022800	0.00603700
C	-5.26643900	-1.25798300	-0.00937000
C	-5.49565100	0.11826300	-0.02119800
C	-4.44867700	1.04360500	-0.01863200
C	-0.95884900	0.11815200	0.02456400
H	-3.76710900	-2.84306700	0.01607000
H	-6.10688300	-1.93920000	-0.01139200
H	-6.51489300	0.48286000	-0.03250500
H	-4.63045400	2.10927000	-0.02716400
C	0.45578600	0.25886800	0.00871000
C	1.28625600	-0.83188300	0.00385600
C	1.03237000	1.61899200	0.00569700
C	2.72232600	-0.72159200	0.00273600

C	2.43891100	1.71413700	0.00748600
C	3.30269400	0.58376400	-0.00312600
C	3.54595700	-1.84028200	-0.00526600
H	2.85919000	2.71246200	0.00394300
C	4.69944800	0.69442300	-0.00737300
C	4.94624600	-1.70817600	-0.01107700
H	3.10060700	-2.82866000	-0.00373500
C	5.51475700	-0.44487800	-0.01354600
H	5.14994500	1.67992000	-0.00914700
H	5.57038200	-2.59232900	-0.01630800
H	6.59167100	-0.33237800	-0.01827000
N	-1.90353300	1.09132200	0.00462100
O	-1.58129700	-1.09991000	0.02360700
H	0.85674000	-1.82773800	0.00675000
O	0.27309000	2.63616700	0.00492100
H	-1.58788400	2.06197100	-0.00003000

S_2 geometry of 2H3NBO-enol in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy= -859.839473

C	3.09505300	0.52572200	0.00007600
C	2.89533400	-0.88921300	-0.00020200
C	3.91878600	-1.80503200	-0.00034900
C	5.21548400	-1.27353400	-0.00033500
C	5.44656000	0.12094300	-0.00008800
C	4.41074000	1.03642200	0.00011100
C	0.97021200	0.14931000	0.00019500
H	3.73291000	-2.87005500	-0.00049000
H	6.06213000	-1.94763800	-0.00046900
H	6.46944900	0.47572200	-0.00005200
H	4.58546600	2.10345400	0.00032600
C	-0.41321400	0.27656900	-0.00073600
C	-1.27108800	-0.87502500	-0.00125000
C	-1.02334600	1.59744100	-0.00038800
C	-2.64970300	-0.74831800	-0.00012000
C	-2.38577400	1.71709700	0.00076300
C	-3.24022200	0.57714200	0.00050600
C	-3.52651700	-1.88587800	-0.00032700
H	-2.81575700	2.71054300	0.00104800
C	-4.63686300	0.69096600	0.00124500
C	-4.88831700	-1.72777400	0.00033400
H	-3.08562600	-2.87604400	-0.00085100
C	-5.45337400	-0.43396500	0.00108200

H	-5.08132400	1.67957400	0.00181400
H	-5.53655700	-2.59541700	0.00021400
H	-6.53004500	-0.31745200	0.00164000
N	1.89551500	1.14059600	0.00043900
O	1.55341000	-1.12352300	-0.00005700
H	-0.81574000	-1.85605000	-0.00183800
O	-0.26877900	2.71412200	-0.00081700
H	0.68693700	2.46715700	-0.00052300

S_2 geometry of 2H3NBO-keto in n-hexane solvent, b3lyp-d3/tzvp/iefpcm, empiricaldispersion=gd3bj

Energy= -859.841798

C	3.17783200	0.53070600	0.00005900
C	2.90851300	-0.83879500	-0.00014300
C	3.89314300	-1.79841000	-0.00022600
C	5.21409700	-1.32920300	-0.00005700
C	5.49729100	0.03631900	0.00015100
C	4.48400900	0.99939500	0.00021700
C	0.94907800	0.20799200	-0.00026800
H	3.65455900	-2.85263800	-0.00040400
H	6.02684300	-2.04323400	-0.00010400
H	6.52913300	0.36303700	0.00027200
H	4.70828100	2.05714600	0.00037800
C	-0.45508000	0.32094100	0.00002200
C	-1.27742000	-0.80799000	0.00008200
C	-1.10351300	1.62417700	-0.00003400
C	-2.68795000	-0.72212000	0.00006600
C	-2.45379000	1.73255300	-0.00007000
C	-3.29663200	0.56465900	0.00002400
C	-3.51479500	-1.87050700	0.00016000
H	-2.90252400	2.71675100	-0.00009200
C	-4.69403100	0.65714200	0.00004200
C	-4.88915700	-1.75218200	0.00017700
H	-3.04973800	-2.84986300	0.00020500
C	-5.48403400	-0.48324500	0.00012200
H	-5.15734400	1.63725500	0.00000200
H	-5.50964200	-2.64008900	0.00024500
H	-6.56321700	-0.39161100	0.00013900
N	1.94289900	1.15249500	0.00008500
O	1.54111000	-1.02819000	-0.00031900
H	-0.80927300	-1.78351800	0.00010300
O	-0.27919800	2.67144800	-0.00007200
H	1.77195900	2.14464900	-0.00014700

SA3-CASSCF(12,12)/6-31G(d) optimized S_0-min geometry of 2H3NBO-enol

Energy= -854.492873162663

C	-3.12138167	0.50236725	0.00000388
C	-2.89661962	-0.84907528	-0.00000217
C	-3.89993675	-1.80584153	-0.00009661
C	-5.19979724	-1.30992807	0.00006602
C	-5.45679495	0.07424117	-0.00005765
C	-4.42427912	1.00455062	0.00011470
C	-1.02802512	0.19815880	-0.00002314
C	0.43693864	0.33237519	0.00002972
C	1.23004514	-0.80694210	-0.00005901
C	1.04840658	1.62133145	-0.00001808
C	2.64469976	-0.71989066	-0.00014523
C	2.42507493	1.71955203	0.00004686
C	3.24754507	0.56439650	-0.00011723
C	3.47193120	-1.88126595	0.00021892
C	4.67029461	0.64902967	0.00004801
C	4.81839193	-1.77171349	-0.00012391
C	5.43567733	-0.48909476	-0.00008911
N	-1.88410469	1.14111973	0.00003140
O	-1.54913007	-1.03596966	-0.00005673
O	0.34188363	2.76764732	0.00001298
H	-3.68455071	-2.85715032	-0.00008952
H	-6.02559524	-1.99755680	-0.00007053
H	-6.47606415	0.41509468	0.00024461
H	-4.61246421	2.06142836	0.00007499
H	2.86491363	2.69943534	-0.00009366
H	3.00325282	-2.85012359	-0.00032875
H	5.13542048	1.61879211	-0.00017747
H	5.43490585	-2.65286930	0.00052633
H	6.50837229	-0.41809238	0.00018665
H	0.76375910	-1.77344044	-0.00006537
H	-0.59525343	2.59324611	0.00003310

SA3-CASSCF(12,12)/6-31G(d) optimized S_1-min geometry of 2H3NBO-enol

Energy= -854.344519176868

C	-3.1187780	0.5027459	0.0266412
C	-2.9042060	-0.8543257	-0.0357533
C	-3.9111493	-1.7993776	-0.0832011
C	-5.2122564	-1.2990800	-0.0647197
C	-5.4597040	0.0823673	-0.0013120
C	-4.4201633	1.0065722	0.0452947

C	-1.0214258	0.1802149	0.0196757
C	0.4047480	0.3060199	0.0315271
C	1.2456025	-0.8265704	-0.0186630
C	1.0376636	1.6146816	0.0960959
C	2.6154792	-0.7274056	-0.0089098
C	2.4335173	1.7395718	0.1070550
C	3.2765535	0.6065407	0.0564615
C	3.4458251	-1.8558058	-0.0593158
C	4.6818747	0.6820180	0.0647073
C	4.8649650	-1.7441459	-0.0496740
C	5.4900849	-0.4832317	0.0118978
N	-1.8866707	1.1345778	0.0607644
O	-1.5577932	-1.0535671	-0.0400716
O	0.3250006	2.7384230	0.1471812
H	-3.7014566	-2.8510191	-0.1312862
H	-6.0407873	-1.9826845	-0.0990911
H	-6.4766599	0.4306742	0.0110880
H	-4.6046004	2.0632118	0.0936764
H	2.8448157	2.7302593	0.1552453
H	2.9982861	-2.8319118	-0.1067046
H	5.1466961	1.6502055	0.1122619
H	5.4568271	-2.6395148	-0.0902309
H	6.5600095	-0.4046088	0.0189171
H	0.7945209	-1.7994860	-0.0663023
H	-0.6142759	2.5497419	0.1338792

SA3-CASSCF(12,12)/6-31G(d) optimized S_2-min geometry of 2H3NBO-enol

Energy= -854.288286599694

C	-3.13527344	0.52076156	0.00000929
C	-2.91014691	-0.83642154	-0.00003486
C	-3.90704549	-1.79122108	-0.00003559
C	-5.21327101	-1.30268629	-0.00000647
C	-5.47218179	0.07736959	0.00006086
C	-4.44051583	1.01258632	0.00005704
C	-1.03637332	0.21660404	-0.00003879
C	0.39925017	0.34491026	-0.00005813
C	1.24658068	-0.83873937	-0.00008853
C	0.99681480	1.59108446	-0.00003051
C	2.68065070	-0.72917652	-0.00004258
C	2.42546354	1.73599051	-0.00003736
C	3.26099974	0.60523505	-0.00002341
C	3.50103453	-1.86780231	0.00000380
C	4.66107407	0.65087770	-0.00002861
C	4.89905660	-1.78948930	0.00010130

C	5.45728852	-0.53873651	0.00002379
N	-1.90695800	1.16344901	0.00000407
O	-1.56035045	-1.02153441	-0.00006635
O	0.32201491	2.73286756	0.00001179
H	-3.68786490	-2.84210048	-0.00008418
H	-6.03559887	-1.99460850	0.00006738
H	-6.49213120	0.41724186	0.00007641
H	-4.63506333	2.06855028	0.00008673
H	2.82956623	2.72875357	-0.00000690
H	3.02368735	-2.83208041	0.00008077
H	5.16219290	1.60147490	-0.00004154
H	5.50199149	-2.67649473	0.00000930
H	6.52683238	-0.42610715	0.00013772
H	0.78879437	-1.80734809	-0.00010085
H	-0.62300246	2.57060202	0.00001843

SA3-CASSCF(12,12)/6-31G(d) optimized MECI geometry of 2H3NBO-enol

Energy= -854.279363957932

C	-3.1408883	0.4901637	0.1189805
C	-2.9290499	-0.8366538	-0.1490209
C	-3.9417906	-1.7699755	-0.3129152
C	-5.2364330	-1.2774025	-0.1871089
C	-5.4802528	0.0817139	0.0882826
C	-4.4394326	0.9886405	0.2460639
C	-1.0513691	0.1810054	0.0118615
C	0.4190572	0.3033154	0.0063244
C	1.2025644	-0.8373962	-0.1930546
C	1.0117742	1.5535000	0.1733067
C	2.6829032	-0.7054155	-0.0852055
C	2.4734739	1.7216906	-0.0004123
C	3.2486417	0.6319986	-0.1510167
C	3.5052146	-1.7827174	0.3294304
C	4.6908924	0.5801896	-0.5177478
C	4.9389984	-1.6303880	0.4608308
C	5.5095108	-0.5029040	0.0224342
N	-1.8987137	1.1109519	0.2152467
O	-1.5841214	-1.0273062	-0.2148499
O	0.3550079	2.6978419	0.4136761
H	-3.7362121	-2.8022351	-0.5225220
H	-6.0685436	-1.9476507	-0.3022512
H	-6.4960870	0.4213235	0.1775812
H	-4.6179926	2.0262596	0.4558134
H	2.8462514	2.7238099	-0.0963526
H	3.0517890	-2.7333979	0.5435206

H	5.0423168	1.1323633	-1.3695819
H	5.5199195	-2.4433446	0.8549333
H	6.5793889	-0.3864556	0.0260527
H	0.7576563	-1.7656837	-0.4911024
H	-0.5869577	2.5479709	0.4488268