Supplementary Information

Effects of Different Proton donor and acceptor groups on Excited-State Intramolecular Proton Transfers of Amino-type and Hydroxy-type Hydrogen-Bonding Molecules: Theoretical Insights

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Table S1 The intramolecular hydrogen-bonded distances (R1 and R2), the important distances between heavy atoms (Å), and a dihedral angle (°) of compounds (tautomer form) in gas phase computed at B3LYP/TD- B3LYP with TZVP basis set.

Compounds	S_0 state				S_1 state				ΔR1*	ΔR2*
	R1	R2	N1···N2/ N1···O1	N1C1C2C3	R1	R2	N1···N2/ N1···O1	N1C1C2C3		
NH_2-type										
APBI	1.775	1.004	0.010	1.8	1.822	1.037	0.008	0.07	0.033	1.822
APBT	1.869	0.930	0.043	1.9	1.678	1.067	0.056	0.2	0.137	1.678
HNHPIP	1.694	1.006	0.016	1.7	1.710	1.054	0.045	0.0	0.048	1.710
OH-type										
HBI	1.568	1.070	0.014	1.6	1.884	1.023	0.042	0.3	0.047	1.884
HBT	1.738	0.990	0.004	1.7	1.738	1.042	0.002	0.0	0.052	1.738
HPIP	1.658	1.000	0.000	1.7	1.807	1.028	0.012	0.1	0.028	1.807

* ΔR1 = |R1 of S_1 state – R1 of S_0 state|, ΔR1 of all compounds are positive value.

* ΔR2 = |R2 of S_1 state – R2 of S_0 state|, ΔR2 of all compounds are negative value.

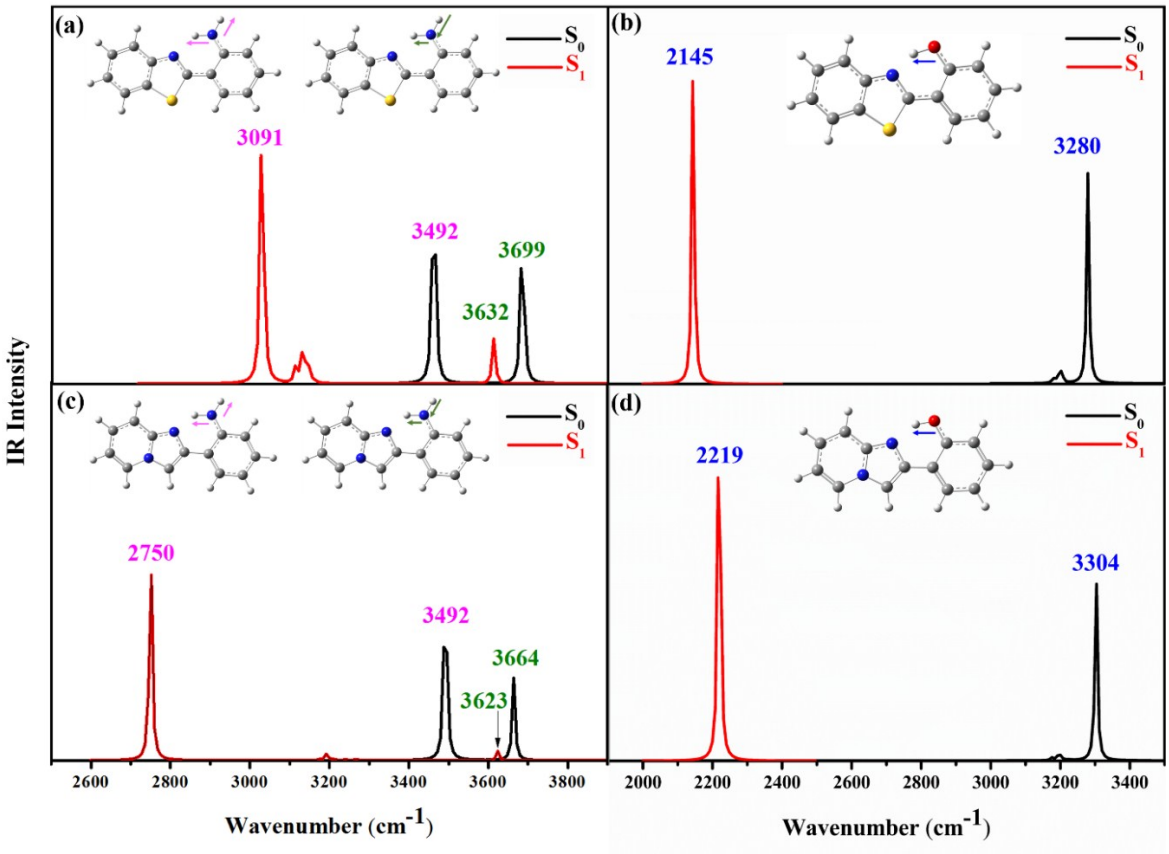

Figure S1. The simulated IR spectra of (a) **APBT**, (b) **HBT**, (c) **HNHPIP**, and (d) **HPIP** both in the ground state (black line) and the excited-state (red line). The stretching vibrational modes of the symmetric and antisymmetric N–H of NH_2-type compounds, and O–H of OH-type compounds are labeled as pink, green and blue, respectively.

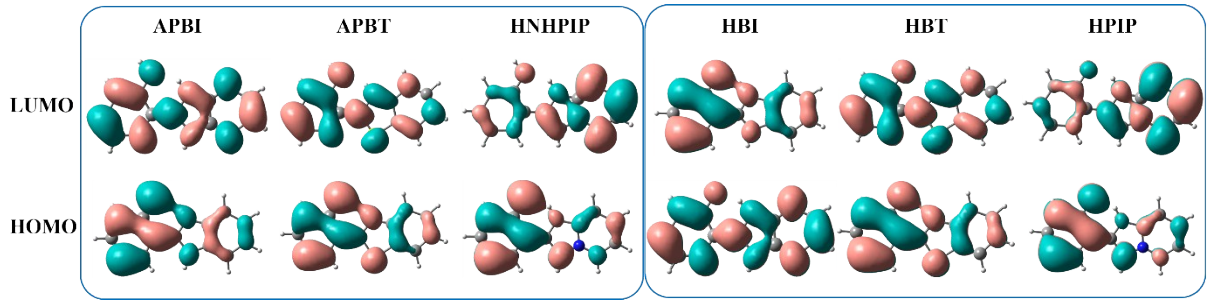

Figure S2. Frontier molecular orbitals of tautomer forms for all compounds (tautomer form**)** computed at B3LYP/TZVP level.

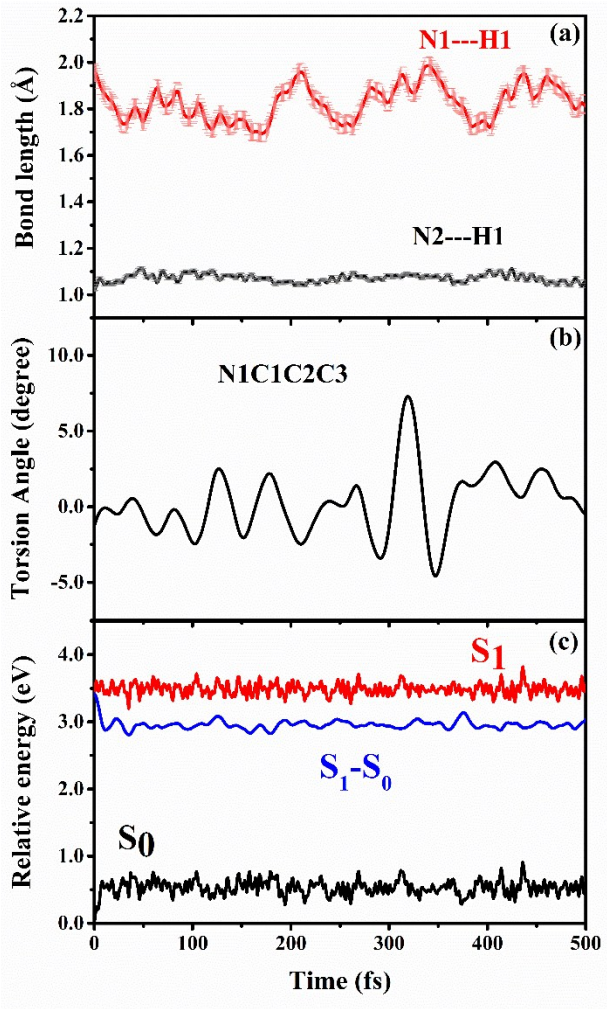

Figure S3. Analyses of all no ESIPT trajectories of **APBT:** (a) Time evolution of average breaking and forming bonds, (b) Average torsion angle (N1C1C2C3), and (c) Average S_1 and S_0 energies and average energy difference between S_1 and S_0 states**.**

Atomic coordinates for all equilibrium geometries

APBI_S_0_Normal				APBI_S_1_Normal			
C	-1.91905700	0.61182800	0.08674900	C	1.91412400	0.61996300	-0.07098600
C	-3.08165500	1.38004400	0.16294200	C	3.08878100	1.39283300	-0.12369400
C	-4.30215600	0.72541600	0.07920300	C	4.30816900	0.73012500	-0.05432700
C	-4.37526200	-0.66825900	-0.07709300	C	4.38797500	-0.66503400	0.06514100
C	-3.22921400	-1.45041700	-0.15300000	C	3.23436100	-1.45588800	0.11727000
C	0.11902700	-0.11381200	0.02159100	C	-0.13133300	-0.13373100	-0.00797200
H	-3.02202200	2.45410100	0.28349400	H	3.03291900	2.47004400	-0.21024900
H	-5.21985600	1.29747600	0.13556700	H	5.22582700	1.30505000	-0.09118900
H	-5.34586400	-1.14428800	-0.13933600	H	5.35952200	-1.13984700	0.11803400
H	-3.29107200	-2.52517700	-0.27191200	H	3.29648600	-2.53315100	0.20977400
N	-0.59235900	0.99373400	0.13550000	N	0.60788500	0.99503300	-0.10757300
C	1.57423000	-0.20443500	0.02761200	C	-1.55577800	-0.23361400	-0.02871400
C	2.38397700	0.96302900	-0.07372000	C	-2.39755500	0.95113600	0.05064900
C	2.20834700	-1.45328500	0.13221100	C	-2.23485400	-1.46456200	-0.11172100
C	3.78437500	0.80351600	-0.08026400	C	-3.79437300	0.85649400	0.05852000
C	3.58388900	-1.58900700	0.12719200	C	-3.64061100	-1.53734100	-0.08526400
H	1.60715700	-2.34717700	0.24931300	H	-1.67569600	-2.38353600	-0.22374500
C	4.37213100	-0.44126700	0.01615400	C	-4.42857000	-0.39539900	-0.00139400
H	4.40349100	1.68987100	-0.16355000	H	-4.37674600	1.76838200	0.12282400
H	4.03850800	-2.56659600	0.21636300	H	-4.11137200	-2.51137600	-0.14037700
H	5.45248800	-0.52225900	0.01122400	H	-5.50714000	-0.46500900	0.01511900
N	1.83976300	2.20794700	-0.19587700	N	-1.77741100	2.15186300	0.13800600
H	0.84483100	2.30778600	-0.02703400	H	-0.74056900	2.15685800	0.07237000
H	2.43975600	3.00821500	-0.10158700	H	-2.31738700	3.00316500	0.14364000
C	-2.00975200	-0.78757200	-0.06800300	C	2.01484300	-0.79650800	0.04507000
N	-0.69964900	-1.22204600	-0.10099900	N	0.71220100	-1.24676800	0.05327000
H	-0.39497200	-2.16406600	-0.27235000	H	0.42435900	-2.18232600	0.28241100
APBI_S_0_Tautomer				APBI_S_1_Tautomer			
C	1.90979000	0.60482200	-0.00003500	C	1.94201400	0.61547000	0.00004400
C	3.04905200	1.39724800	0.00012000	C	3.10469500	1.40165400	0.00009700
C	4.28144100	0.74778200	0.00004900	C	4.32029500	0.71127200	0.00008100
C	4.36943100	-0.64725600	-0.00004600	C	4.38507200	-0.68176600	-0.00002600
C	3.22724000	-1.44617600	-0.00010400	C	3.22182300	-1.47325100	-0.00013700
C	-0.18496400	-0.21463300	0.00014300	C	-0.16298300	-0.16650500	0.00000300
H	2.98048300	2.47697800	0.00023800	H	3.05996700	2.48144100	0.00013700
H	5.18950800	1.33681000	0.00012000	H	5.24313200	1.27827000	0.00012600
H	5.34362400	-1.11891600	-0.00006400	H	5.35236000	-1.16727800	-0.00005800
H	3.29893500	-2.52636100	-0.00015500	H	3.27025300	-2.55374000	-0.00027300
N	0.56119500	0.91647900	0.00030600	N	0.60540900	0.94139900	0.00003100
C	-1.59066800	-0.24362600	-0.00000700	C	-1.61995600	-0.22950600	0.00004200
C	-2.32234900	1.02358000	-0.00021400	C	-2.38530200	1.00031700	-0.00006200
C	-2.29487900	-1.47655900	-0.00006500	C	-2.28133400	-1.44263300	0.00022300
C	-3.76342900	0.89652400	0.00012400	C	-3.78924200	0.88804700	-0.00013600
C	-3.66007700	-1.52988700	-0.00002900	C	-3.70407100	-1.52234700	0.00013200
H	-1.73949200	-2.40933800	-0.00019800	H	-1.72589500	-2.37362800	0.00041000
C	-4.39257800	-0.31135800	0.00015000	C	-4.44096600	-0.36325900	-0.00005000
H	-4.34196000	1.81419300	0.00030700	H	-4.37462800	1.80040100	-0.00025100
H	-4.17824600	-2.47933100	-0.00013800	H	-4.18297600	-2.49230000	0.00022900
H	-5.47645800	-0.34735100	0.00033000	H	-5.52329500	-0.40062100	-0.00009800
N	-1.68232100	2.17402100	-0.00032000	N	-1.70597800	2.16553200	0.00007700
H	0.04867800	1.78024100	-0.00023300	H	0.08706000	1.83981100	-0.00025000
H	-2.33289500	2.95409600	-0.00022400	H	-2.34861600	2.95454100	0.00014800
C	2.00156600	-0.79835600	-0.00010200	C	2.01112100	-0.78892300	-0.00008400
N	0.69424800	-1.27017700	-0.00006500	N	0.69118000	-1.23055500	-0.00020100
H	0.41851100	-2.23591200	0.00065900	H	0.40136900	-2.19293300	-0.00023100

HBI_S_0_Normal				HBI_S_1_Normal			
C	1.89360700	0.60165000	0.00003600	C	-1.87261400	0.60198300	-0.00003200
C	3.03990300	1.39675400	0.00002500	C	-3.02060600	1.41627300	-0.00004500
C	4.27162900	0.75875000	-0.00009000	C	-4.25935800	0.78793600	-0.00002600
C	4.37081300	-0.64209200	-0.00016500	C	-4.38340800	-0.61054700	0.00000500
C	3.24036800	-1.44953300	-0.00015300	C	-3.25777600	-1.44246900	0.00001500
C	-0.13067400	-0.17505500	0.00016700	C	0.15014800	-0.23725800	0.00001000
H	2.95980000	2.47600300	0.00029300	H	-2.92871900	2.49404800	-0.00006300
H	5.17844800	1.35032200	-0.00007900	H	-5.15874600	1.39162600	-0.00003300
H	5.35028400	-1.10347600	-0.00030000	H	-5.37036600	-1.05530800	0.00002000
H	3.32216100	-2.52936100	-0.00009000	H	-3.35587400	-2.52066600	0.00003500
N	0.55749500	0.95414900	0.00037600	N	-0.55546900	0.92555800	-0.00002500
C	-1.58293800	-0.24056400	0.00028700	C	1.56371300	-0.29569400	-0.00001800
C	-2.33172500	0.96389900	-0.00004100	C	2.31549900	0.96225600	0.00004200
C	-2.27566700	-1.46185000	0.00041900	C	2.32160300	-1.48079300	-0.00007400
C	-3.72991800	0.90179100	-0.00041200	C	3.71748400	0.96811400	0.00006600
C	-3.65721000	-1.51123700	0.00009900	C	3.72503700	-1.44369500	-0.00005100
H	-1.72385900	-2.39492000	0.00100700	H	1.82589900	-2.44308100	-0.00014800
C	-4.38277800	-0.31710400	-0.00033300	C	4.42856500	-0.23475400	0.00002400
H	-4.27744200	1.83529600	-0.00070300	H	4.21595600	1.92830300	0.00011700
H	-4.16822600	-2.46495500	0.00025000	H	4.27139800	-2.37885800	-0.00009200
H	-5.46567000	-0.34235900	-0.00065500	H	5.50979300	-0.23110000	0.00004400
C	2.00890400	-0.80416700	-0.00003000	C	-2.01676300	-0.82029600	-0.00000500
N	0.70547700	-1.26820500	-0.00020900	N	-0.73109300	-1.31589400	-0.00002900
H	0.41999000	-2.23183700	-0.00067900	H	-0.47548100	-2.28759700	0.00024100
O	-1.75878400	2.17700500	0.00006400	O	1.67020500	2.11192600	0.00009300
H	-0.77189200	2.06017700	0.00042400	H	0.64129000	1.91324900	0.00004000
HBI_S_0_Tautomer				HBI_S_1_Tautomer			
C	-1.88075200	-0.59108500	0.00009800	C	-1.93838900	0.61109300	0.00036200
C	-3.00641500	-1.40462700	-0.00013000	C	-3.09102300	1.40944600	0.00052500
C	-4.24816300	-0.77739200	-0.00022700	C	-4.31622800	0.72998500	0.00021100
C	-4.36226500	0.61744800	-0.00013900	C	-4.39389800	-0.66045900	-0.00027000
C	-3.23703600	1.43749900	0.00006300	C	-3.23915400	-1.46591500	-0.00047600
C	0.18479900	0.26448800	-0.00001200	C	0.16306800	-0.19590500	0.00024500
H	-2.91694100	-2.48272900	-0.00025000	H	-3.03499600	2.48859300	0.00085600
H	-5.14599200	-1.38187800	-0.00035800	H	-5.23297100	1.30650100	0.00033200
H	-5.34548500	1.06986100	-0.00032500	H	-5.36610500	-1.13625500	-0.00050600
H	-3.32901700	2.51612100	0.00009800	H	-3.29923200	-2.54560100	-0.00090600
N	-0.52769900	-0.87818400	-0.00019300	N	-0.59725100	0.92257500	0.00062100
C	1.60050400	0.27635400	0.00000100	C	1.62169800	-0.24443500	0.00005800
C	2.26595300	-1.01887400	0.00013100	C	2.36211000	1.01378200	-0.00065000
C	2.34980900	1.47553500	-0.00017700	C	2.31350100	-1.43002000	0.00065000
C	3.69923300	-0.97810400	0.00003400	C	3.77994000	0.93115100	-0.00063100
C	3.72040700	1.45406200	-0.00022000	C	3.74645000	-1.47444400	0.00035600
H	1.83769400	2.43319100	-0.00029900	H	1.78698400	-2.37873600	0.00137600
C	4.38743600	0.20592700	-0.00010800	C	4.46073500	-0.30132200	-0.00020000
H	4.21427300	-1.93043000	0.00005400	H	4.32116900	1.86852000	-0.00104500
H	4.28672300	2.37584400	-0.00026000	H	4.24305800	-2.43535600	0.00075100
H	5.47181900	0.18964200	-0.00021200	H	5.54342500	-0.31715900	-0.00025400
C	-1.99974400	0.81108100	0.00038100	C	-2.01954700	-0.79341700	-0.00013500
N	-0.69881000	1.30729700	0.00040300	N	-0.70620900	-1.24944100	-0.00021600
H	-0.43624000	2.27755300	0.00013100	H	-0.43145500	-2.21625900	-0.00054400
O	1.62530100	-2.12033000	0.00021400	O	1.75079000	2.13191200	-0.00045800
H	0.10373700	-1.74219400	0.00007400	H	-0.10754300	1.82128100	0.00050000

APBT_S_0_Normal				APBT _S_1_Normal			
C	-1.85636900	0.63461900	0.00647600	C	1.84693300	0.64380800	-0.09173900
C	-2.89148700	1.57415800	0.01628500	C	2.90310100	1.57776000	-0.19044100
C	-4.20398400	1.12995100	0.01513500	C	4.20979900	1.12912700	-0.14190100
C	-4.49926500	-0.23898800	0.00416500	C	4.51249600	-0.23295100	0.00473500
C	-3.48442900	-1.18732700	-0.00588600	C	3.48764900	-1.17604500	0.10844400
C	0.24511600	-0.12810000	-0.00357300	C	-0.24563400	-0.15705200	0.01463300
H	-2.65330700	2.62998100	0.02452500	H	2.67316600	2.62943000	-0.30476500
H	-5.01298500	1.84960400	0.02268800	H	5.01958300	1.84512600	-0.21821500
H	-5.53176500	-0.56513400	0.00340400	H	5.54452700	-0.55721900	0.03848500
H	-3.71687200	-2.24442400	-0.01444800	H	3.71867200	-2.22741900	0.22560200
N	-0.50881100	0.93277000	0.00633700	N	0.52622600	0.92890600	-0.12867300
C	1.69975000	-0.13455500	-0.00317800	C	-1.69177900	-0.17043500	-0.03247100
C	2.44943600	1.08006500	-0.00982200	C	-2.46242800	1.05464300	0.09152800
C	2.40208700	-1.35340200	0.00946000	C	-2.43065100	-1.33785900	-0.18273600
C	3.85790600	0.99496600	0.00185100	C	-3.86506900	1.03875500	0.05673300
C	3.78003600	-1.41446700	0.01813700	C	-3.84820000	-1.34149000	-0.18831400
H	1.84006400	-2.27946300	0.01502500	H	-1.91208500	-2.27986000	-0.30339700
C	4.50800500	-0.22010000	0.01537900	C	-4.56908600	-0.16476800	-0.07890800
H	4.42933700	1.91652300	-0.00293900	H	-4.39651400	1.97780600	0.16205000
H	4.28599300	-2.37047600	0.02838600	H	-4.36457000	-2.28814200	-0.28565200
H	5.59114000	-0.24418700	0.02368400	H	-5.65010200	-0.16881700	-0.08932600
N	1.84908200	2.29951000	-0.03876400	N	-1.78323200	2.21063100	0.27514800
H	0.83925100	2.34731600	0.00227300	H	-0.75077800	2.16178100	0.18868800
H	2.40644900	3.13186000	0.02540800	H	-2.27285700	3.09183700	0.28885800
C	-2.16697800	-0.74052100	-0.00469900	C	2.17528500	-0.73611500	0.06048900
S	-0.68113400	-1.67346000	-0.01621200	S	0.69096900	-1.68284700	0.16825200
APBT _S_0_ Tautomer				APBT _S_1_ Tautomer			
C	-1.85376600	0.63356000	0.00023100	C	-1.85656500	0.63518600	0.00035600
C	-2.87247100	1.58296800	0.00025300	C	-2.88747700	1.59051500	0.00056900
C	-4.18862700	1.13720900	0.00014800	C	-4.19716400	1.13694100	0.00042000
C	-4.48747000	-0.22667800	-0.00008900	C	-4.50154800	-0.22896500	0.00002900
C	-3.47000900	-1.17703800	-0.00024400	C	-3.48029600	-1.18490100	-0.00024700
C	0.31515300	-0.21286900	0.00014400	C	0.28590600	-0.22099500	0.00000300
H	-2.63810400	2.63967400	0.00040600	H	-2.65570900	2.64743400	0.00086500
H	-4.99323600	1.86133600	0.00020600	H	-5.00415200	1.85924900	0.00059800
H	-5.51968800	-0.55202600	-0.00015100	H	-5.53421100	-0.55159100	-0.00008000
H	-3.70137000	-2.23428900	-0.00048300	H	-3.71285400	-2.24184400	-0.00060900
N	-0.49184300	0.87438800	0.00039500	N	-0.51060900	0.86038700	0.00047600
C	1.70714000	-0.16243900	0.00034500	C	1.73821900	-0.17318900	0.00009000
C	2.39387400	1.13844500	-0.00009600	C	2.41709600	1.11360100	-0.00050000
C	2.47531500	-1.36607200	0.00094000	C	2.48849600	-1.33313400	0.00079200
C	3.84307600	1.07467800	-0.00086600	C	3.82897200	1.09471300	-0.00048900
C	3.83587500	-1.35363800	0.00061300	C	3.91303100	-1.31521600	0.00070200
H	1.95341700	-2.31683800	0.00174000	H	1.98769900	-2.29471200	0.00141300
C	4.52097600	-0.10163300	-0.00042700	C	4.56700300	-0.10601500	0.00010300
H	4.37859700	2.01799600	-0.00167000	H	4.34983800	2.04562500	-0.00101300
H	4.39685300	-2.27858800	0.00123500	H	4.45750800	-2.24976700	0.00116300
H	5.60524500	-0.09428900	-0.00094400	H	5.64920000	-0.06564900	0.00004800
N	1.71160800	2.25653100	0.00015300	N	1.66727600	2.22816400	-0.00105100
H	-0.07375100	1.70511000	0.00055200	H	0.05298700	1.76658900	0.00018200
H	2.33497300	3.05983800	-0.00042900	H	2.24125500	3.06682300	-0.00112900
C	-2.15542400	-0.73412400	-0.00015600	C	-2.16883900	-0.74221800	-0.00008400
S	-0.66644600	-1.69491000	-0.00056800	S	-0.67557700	-1.69999700	-0.00049200

HBT_S_0_Normal			
C	-1.83206600	0.62608800	-0.00004100
C	-2.85143000	1.58219900	-0.00008400
C	-4.16918500	1.15526600	-0.00006200
C	-4.48344000	-0.20995100	0.00000400
C	-3.48350300	-1.17327500	0.00004800
C	0.25512000	-0.18053100	-0.00000300
H	-2.59760300	2.63422100	-0.00013400
H	-4.96824200	1.88571100	-0.00009500
H	-5.52038300	-0.52129900	0.00002000
H	-3.73107300	-2.22684100	0.00009900
N	-0.47835800	0.89692000	-0.00005500
C	1.70771200	-0.16320000	-0.00000900
C	2.39969000	1.07648600	0.00004200
C	2.45954300	-1.35064300	-0.00006900
C	3.79905800	1.08173100	0.00002600
C	3.84007000	-1.33307600	-0.00008300
H	1.94160900	-2.30247600	-0.00010800
C	4.50812400	-0.10473900	-0.00003500
H	4.30159200	2.04014000	0.00006700
H	4.39631200	-2.26102700	-0.00013000
H	5.59099700	-0.07806100	-0.00004500
C	-2.15993400	-0.74440800	0.00002600
S	-0.68575300	-1.70121100	0.00006700
O	1.77161500	2.26267100	0.00011500
H	0.79587300	2.09752200	0.00015400

HBT_S_1_Normal			
C	1.80114600	0.63108800	-0.00005100
C	2.81972900	1.60869800	-0.00011200
C	4.14109700	1.20160500	-0.00008300
C	4.49068400	-0.15658000	0.00000900
C	3.50025600	-1.14161800	0.00007500
C	-0.26342700	-0.27845800	0.00000100
H	2.55313400	2.65765600	-0.00018500
H	4.92516800	1.94918300	-0.00013000
H	5.53327600	-0.44649800	0.00002900
H	3.76858400	-2.19048600	0.00015000
N	0.46847700	0.85377500	-0.00008100
C	-1.70351500	-0.23594800	0.00000000
C	-2.36500300	1.06219700	0.00000200
C	-2.52842600	-1.34466400	-0.00001300
C	-3.77197000	1.15998000	-0.00004400
C	-3.94814500	-1.22783100	-0.00003600
H	-2.09211900	-2.33567200	-0.00001500
C	-4.56854600	0.01239500	-0.00005200
H	-4.20059700	2.15359800	-0.00004500
H	-4.54142800	-2.13327000	-0.00003900
H	-5.64667300	0.09299300	-0.00007800
C	2.17415500	-0.74537000	0.00004800
S	0.72351500	-1.76087400	0.00012000
O	-1.65106500	2.16345400	0.00005200
H	-0.61461400	1.86947000	0.00006700

HBT_S_0_Tautomer			
C	1.83317500	0.62708700	-0.00002600
C	2.84003200	1.58901700	-0.00004300
C	4.16002100	1.15761500	-0.00002800
C	4.47417200	-0.20375600	-0.00000200
C	3.46965500	-1.16646100	0.00000900
C	-0.31757100	-0.24572100	0.00000200
H	2.59261800	2.64266800	-0.00006100
H	4.95692100	1.89005700	-0.00003800
H	5.51024000	-0.51651300	0.00000500
H	3.71391800	-2.22071600	0.00002000
N	0.46813500	0.84767100	-0.00002700
C	-1.71616500	-0.18440500	0.00001900
C	-2.34904200	1.14123500	0.00010200
C	-2.51607300	-1.36120900	-0.00002400
C	-3.79118500	1.14115100	0.00003900
C	-3.87829700	-1.29105000	-0.00003000
H	-2.02908200	-2.33087200	-0.00006100
C	-4.51113500	-0.01702500	-0.00001400
H	-4.27371600	2.11030600	0.00005500
H	-4.47626400	-2.19265600	-0.00007000
H	-5.59466400	0.02912000	-0.00003300
C	2.14968600	-0.73801200	-0.00000500
S	0.67096100	-1.71467100	-0.00002400
O	-1.68439400	2.21129100	0.00010200
H	-0.02078500	1.70851800	-0.00005400

HBT_S_1_Tautomer			
C	-1.84810700	0.63283900	0.00001700
C	-2.86591400	1.59982400	0.00002300
C	-4.18195400	1.16292300	0.00002700
C	-4.50231000	-0.19820700	0.00001900
C	-3.49298800	-1.16619500	0.00000400
C	0.28616200	-0.25978900	0.00000200
H	-2.62092900	2.65380000	0.00002800
H	-4.97951500	1.89546600	0.00003400
H	-5.53868100	-0.50870600	0.00002100
H	-3.73874900	-2.22011500	-0.00001100
N	-0.49915500	0.83851800	0.00001600
C	1.74058400	-0.18666000	-0.00000900
C	2.38611800	1.12361500	-0.00005100
C	2.52132400	-1.31664500	0.00004100
C	3.80946100	1.13526600	-0.00003400
C	3.95543500	-1.26531100	0.00002300
H	2.05149500	-2.29474600	0.00009100
C	4.58094000	-0.04451400	-0.00000700
H	4.28306900	2.10887300	-0.00005400
H	4.51630500	-2.18993100	0.00005200
H	5.66175000	0.02229900	-0.00000200
C	-2.17591300	-0.74074100	0.00000200
S	-0.69598700	-1.72294600	-0.00003600
O	1.71003500	2.20500900	0.00000000
H	0.03783800	1.73206500	-0.00004000

HNHPIP_S_0_Normal				HNHPIP_S_1_Normal			
C	-1.88191200	0.59891800	0.13912600	C	1.87822300	0.58481700	-0.12287900
C	-3.06021100	1.35868300	0.27252800	C	3.02803300	1.40168800	-0.22360000
C	-4.27878200	0.74321600	0.15162700	C	4.28504000	0.76797600	-0.09873600
C	-4.35573800	-0.64956100	-0.10808100	C	4.38257600	-0.60851000	0.11143800
C	-3.21982500	-1.39072800	-0.23742900	C	3.26178700	-1.41617500	0.20566300
C	-0.72152800	-1.27241500	-0.20250800	C	0.73793800	-1.32392400	0.14120800
C	0.12760100	-0.19542600	0.00704500	C	-0.12382500	-0.27651200	-0.02978300
H	-2.96559100	2.41734300	0.46992200	H	2.91714700	2.46028500	-0.39323900
H	-5.19027300	1.31710300	0.25337100	H	5.18994100	1.35752100	-0.16589600
H	-5.31460200	-1.13895300	-0.20523600	H	5.35646100	-1.07159200	0.20635800
H	-3.20920500	-2.45305900	-0.43377500	H	3.24836000	-2.47686000	0.38520400
H	-0.53341300	-2.30786400	-0.42138700	H	0.58877800	-2.37404900	0.31681900
N	-0.60529800	0.94776900	0.20995400	N	0.57375600	0.90255300	-0.18983900
N	-2.00014100	-0.77766000	-0.11441200	N	2.00882900	-0.77069600	0.07780600
C	1.59387600	-0.22320200	0.03169100	C	-1.60289800	-0.29148700	-0.04764900
C	2.38004700	0.95000900	-0.12150200	C	-2.35663400	0.93297500	0.10805200
C	2.25342800	-1.44949400	0.20036500	C	-2.32846400	-1.45082100	-0.20293300
C	3.78170600	0.82417300	-0.10687400	C	-3.77624300	0.90601400	0.13660400
C	3.63334700	-1.55746400	0.21078300	C	-3.73588700	-1.46563300	-0.16453700
H	1.65773900	-2.34162000	0.35084400	H	-1.80182600	-2.38275200	-0.35656000
C	4.39873100	-0.40189800	0.05329700	C	-4.45884200	-0.28477500	0.00687300
H	4.38167300	1.71958900	-0.22893200	H	-4.30923700	1.84094400	0.26208800
H	4.10669100	-2.52051800	0.35096300	H	-4.25772600	-2.40683500	-0.27683600
H	5.48079500	-0.45786500	0.06327500	H	-5.53997800	-0.30142700	0.03106100
N	1.81187800	2.18530400	-0.33361700	N	-1.68558800	2.08648400	0.21336800
H	0.83562800	2.28100300	-0.08242600	H	-0.63275200	2.01086900	0.08560500
H	2.40104700	2.98808100	-0.19050100	H	-2.18297600	2.96170900	0.27772600
HNHPIP_S_0_ Tautomer				HNHPIP_S_1_ Tautomer			
C	-1.86849500	0.58195700	-0.00004100	C	-1.89173100	0.57151700	-0.00031500
C	-3.00070700	1.39212100	-0.00020700	C	-3.01257000	1.42180600	-0.00060000
C	-4.24536200	0.79244200	-0.00007200	C	-4.26413800	0.79693400	-0.00036900
C	-4.34893500	-0.61127900	0.00016200	C	-4.37630000	-0.60626400	0.00012500
C	-3.22633200	-1.39400200	0.00025300	C	-3.26710600	-1.41324900	0.00041100
C	-0.73008100	-1.36088800	0.00006000	C	-0.72714300	-1.37200700	0.00046700
C	0.19156900	-0.31702900	-0.00016600	C	0.15063600	-0.33541500	0.00008500
H	-2.87864100	2.46603800	-0.00038300	H	-2.88484300	2.49264900	-0.00095500
H	-5.13928000	1.40050600	-0.00017800	H	-5.16320200	1.39814400	-0.00055100
H	-5.31668400	-1.09261700	0.00027900	H	-5.35448200	-1.06788400	0.00031900
H	-3.23903100	-2.47337000	0.00042000	H	-3.26465800	-2.49012900	0.00087800
H	-0.59180400	-2.42549800	0.00027900	H	-0.60225800	-2.43705300	0.00091000
N	-0.55369600	0.85342200	-0.00030600	N	-0.57062100	0.83446500	-0.00038100
N	-1.98902300	-0.80317300	0.00013300	N	-2.02159600	-0.77829600	0.00015300
C	1.61510900	-0.27608100	-0.00013500	C	1.64437900	-0.27466600	-0.00000800
C	2.29860200	1.01077300	0.00009600	C	2.33442600	0.99747800	0.00039200
C	2.35865400	-1.47701000	-0.00023400	C	2.35815600	-1.44426100	-0.00048800
C	3.73852800	0.94017300	0.00022000	C	3.76055700	0.93305000	0.00034000
C	3.73060600	-1.48569900	-0.00013200	C	3.77333200	-1.47128600	-0.00050500
H	1.82498200	-2.42174300	-0.00044300	H	1.82777400	-2.38944600	-0.00088000
C	4.41557500	-0.24673000	0.00010400	C	4.45769200	-0.26943500	-0.00006400
H	4.28360000	1.87844000	0.00039900	H	4.30491100	1.87098000	0.00065300
H	4.27988300	-2.41777900	-0.00020600	H	4.29739000	-2.41720700	-0.00086300
H	5.50031600	-0.23968600	0.00017700	H	5.54123600	-0.25775400	-0.00007600
N	1.61309900	2.14636800	0.00015400	N	1.64867500	2.14628000	0.00067400
H	-0.02281400	1.70785700	-0.00010800	H	-0.00851500	1.72603400	-0.00014800
H	2.23443900	2.94905400	0.00045400	H	2.27029600	2.94931100	0.00076800

HPIP_S_0_Normal				HPIP _S_1_Normal			
C	-1.85794400	0.59385500	-0.00000300	C	1.84559000	0.58179300	0.00004600
C	-3.01786300	1.39082000	-0.00000700	C	2.97247000	1.43280700	0.00009200
C	-4.24835100	0.78706600	-0.00000400	C	4.24504200	0.81830000	0.00006600
C	-4.35307600	-0.62730500	0.00000200	C	4.37950200	-0.57152000	-0.00000200
C	-3.23243400	-1.40210200	0.00000500	C	3.28087900	-1.41371000	-0.00004800
C	-0.73221700	-1.33488100	0.00000500	C	0.75777200	-1.37977900	-0.00005300
C	0.13872100	-0.25829400	0.00000100	C	-0.13493400	-0.34009700	-0.00001100
H	-2.90117800	2.46545400	-0.00001100	H	2.83433700	2.50155500	0.00014500
H	-5.14800800	1.38785300	-0.00000700	H	5.13448600	1.43437000	0.00009900
H	-5.32157500	-1.10708200	0.00000400	H	5.36593000	-1.01696000	-0.00002000
H	-3.24258200	-2.48230000	0.00001000	H	3.29405000	-2.48938900	-0.00010100
H	-0.57062600	-2.39735300	0.00000900	H	0.63848200	-2.44830100	-0.00010800
N	-0.57162400	0.91776200	-0.00000500	N	0.53190400	0.86665500	0.00005500
N	-2.00052200	-0.80102100	0.00000300	N	2.01031900	-0.78754600	-0.00002200
C	1.60079700	-0.25854600	0.00000000	C	-1.59872200	-0.33571000	-0.00001800
C	2.32991600	0.95490500	0.00000300	C	-2.29839300	0.93658400	-0.00004700
C	2.32073600	-1.46336300	-0.00000400	C	-2.37956900	-1.47409800	0.00003000
C	3.72905400	0.92132500	0.00000100	C	-3.71747200	0.98979200	-0.00001200
C	3.70373400	-1.48915700	-0.00000500	C	-3.78023900	-1.40704900	0.00005600
H	1.77702000	-2.40050100	-0.00000600	H	-1.90165800	-2.44432800	0.00005800
C	4.40833900	-0.28348700	-0.00000300	C	-4.45004600	-0.17139600	0.00004200
H	4.25694000	1.86631700	0.00000300	H	-4.18040000	1.96722600	-0.00003600
H	4.23098800	-2.43440100	-0.00000800	H	-4.35248100	-2.32546100	0.00009700
H	5.49167600	-0.28687600	-0.00000400	H	-5.53103900	-0.13981400	0.00006600
O	1.74178700	2.16823600	0.00000800	O	-1.64423000	2.06713900	-0.00012900
H	0.76160800	2.04079200	0.00001300	H	-0.67471000	1.87471800	-0.00024900
HPIP_S_0_Tautomer				HPIP_S_1_Tautomer			
C	1.85346900	0.57535500	0.00000900	C	1.89735100	0.57673000	-0.00012100
C	2.97917400	1.39699800	0.00001900	C	3.00938700	1.42312400	-0.00013600
C	4.22596600	0.80676900	0.00001000	C	4.27055800	0.80091700	0.00003400
C	4.34262400	-0.59717000	-0.00001000	C	4.38055700	-0.60122500	0.00018200
C	3.22686100	-1.38797400	-0.00001900	C	3.27482800	-1.41059000	0.00015600
C	0.72907000	-1.37775200	-0.00001400	C	0.72785400	-1.36915900	-0.00009500
C	-0.19644900	-0.34329400	-0.00000100	C	-0.15015800	-0.34068200	-0.00012800
H	2.84815100	2.46984700	0.00003600	H	2.88104600	2.49404000	-0.00028000
H	5.11522700	1.42175400	0.00001800	H	5.16711500	1.40467300	0.00003000
H	5.31467800	-1.06944800	-0.00001700	H	5.35869700	-1.06345700	0.00029000
H	3.24775300	-2.46728700	-0.00003400	H	3.27515000	-2.48727700	0.00023000
H	0.59893400	-2.44343000	-0.00002800	H	0.60088900	-2.43414800	-0.00004700
N	0.53730700	0.83349000	0.00001600	N	0.56846800	0.83399900	-0.00030000
N	1.98645000	-0.80674300	-0.00001000	N	2.02347400	-0.77750800	0.00000700
C	-1.62276800	-0.29154200	0.00000000	C	-1.64470700	-0.27725600	-0.00011800
C	-2.26401600	1.01438500	-0.00000100	C	-2.32260900	1.00635900	-0.00001600
C	-2.39561800	-1.47237900	0.00000300	C	-2.37402700	-1.43179300	-0.00017200
C	-3.69881900	0.99870300	0.00000100	C	-3.75928800	0.96431200	0.00018200
C	-3.76835200	-1.42958500	0.00000700	C	-3.79827100	-1.43394800	-0.00011700
H	-1.89307800	-2.43455200	0.00000300	H	-1.86479000	-2.38866600	-0.00028500
C	-4.41234000	-0.17175000	0.00000600	C	-4.47312200	-0.22906500	0.00008000
H	-4.19520400	1.96128900	-0.00000300	H	-4.26504400	1.92140000	0.00041500
H	-4.34928200	-2.34259600	0.00001000	H	-4.33084000	-2.37522700	-0.00017300
H	-5.49654100	-0.13353900	0.00000900	H	-5.55625200	-0.20917100	0.00019900
O	-1.60551100	2.10661400	-0.00001600	O	-1.71144800	2.11919600	0.00048000
H	-0.00566100	1.67324300	0.00003300	H	0.05190200	1.72248800	-0.00056400