Mechanism and Impact of Mono/bis(iodoimidazolium) Halogen-Bond Donor Catalysts on Michael Addition of Indole with Trans-crotonophenone：DFT Investigations

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1. Structural parameters and energy data

The related configuration parameters along the reaction pathways in CH_3CN solvent are shown in Table S1 and Table S2; Gibbs free energy of the direct hydrogen proton transfer pathway with or without catalyst in CH_3CN solvent are shown in Table S3.

Table S1 C(4)-C(5) distances (in Å) along the reaction pathway in CH_3CN solvent

	uncat	cat1	cat2	cat3	cat4
COM1	3.473	3.892	3.544	3.704	3.345
TS	1.839	1.915	1.937	1.943	1.932
COM2	1.602	1.570	1.589	1.589	1.590

Table S2 O-I distances (in Å) along the reaction pathway in CH_3CN solvent

	cat1	cat2		cat3		cat4	
		O-I(1)	O-I(2)	O-I(1)	O-I(2)	O-I(1)	O-I(2)
COM1	2.772	2.770	3.423	2.806	3.195	2.816	3.215
TS	2.665	2.722	2.625	2.721	2.702	2.736	2.739
COM2	2.503	2.618	2.669	2.624	2.653	2.640	2.679

Table S3 Gibbs free energy of the direct hydrogen proton transfer pathway with and without catalyst in CH_3CN solvent.(unit: kcal·mol^{-1})

	COM1	TS1	COM2	TS2(b)	COM3(b)	P(b)
uncat	-2.1	29.1	28.3	47.3	-14.7	-15.5
cat1	-1.0	27.3	21.0	43.8	-15.9	-12.7
cat2	-1.2	22.0	17.5	40.1	-15.5	-10.0
cat3	-1.0	20.6	17.3	41.3	-16.6	-9.8
cat4	-0.2	22.9	18.4	41.1	-15.5	-11.2

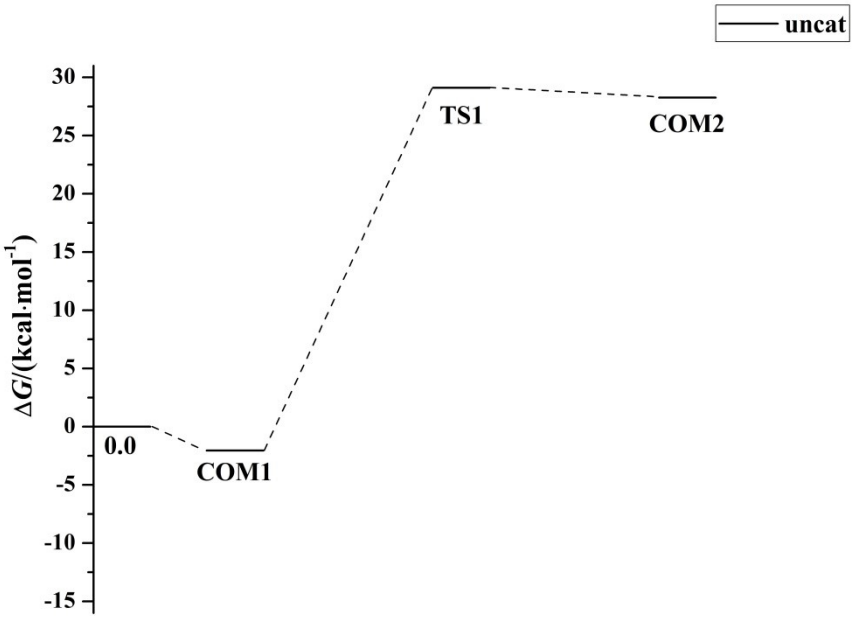

Fig. S1. Potential energy curves of the carbon-carbon coupling process without catalyst.

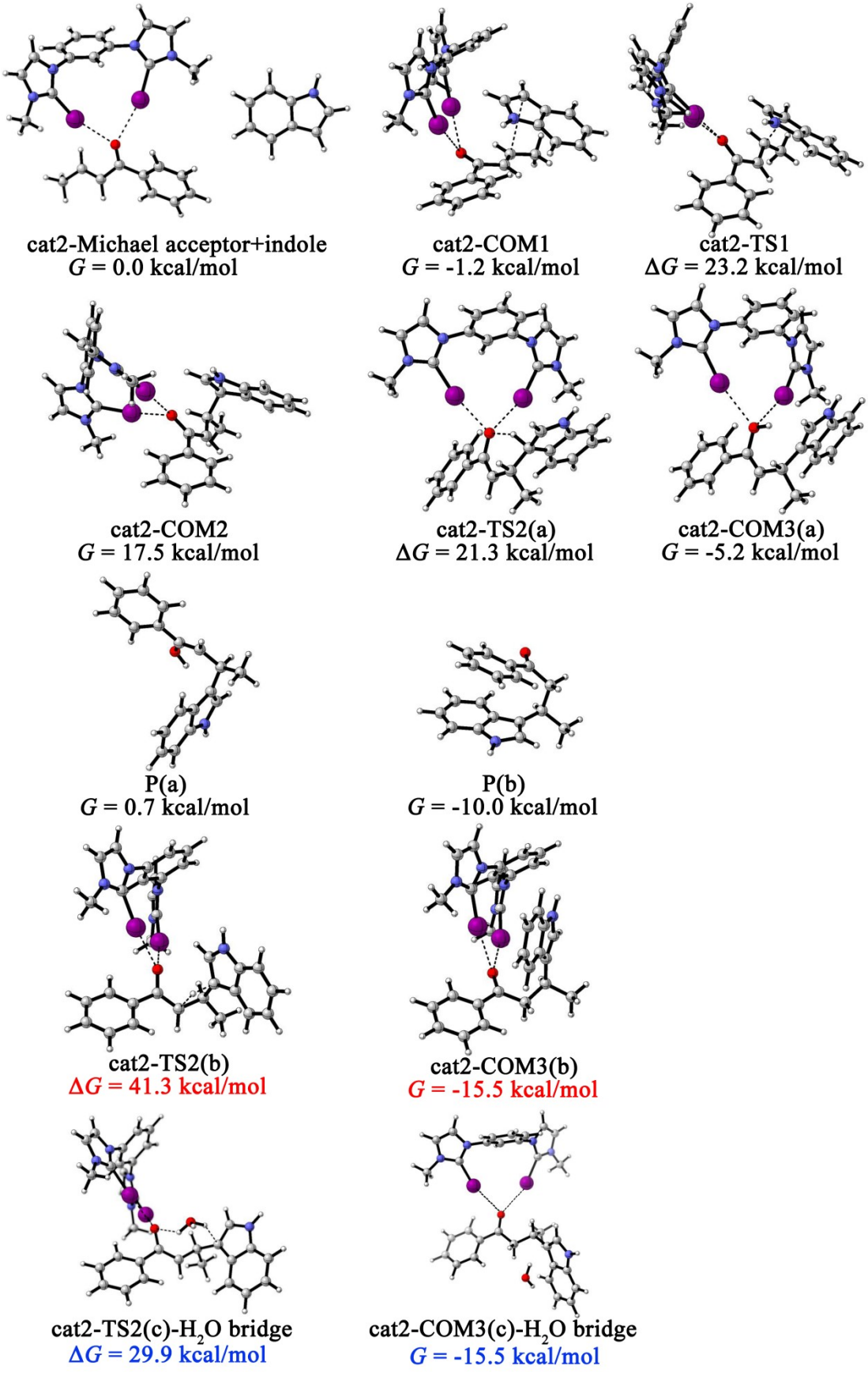

Fig. S2. Representation of the optimized of the saddle points (SMD18(CH_3CN)-M06-2X/6-311+G(d,p) level) for the Michael addition reactions between indole and trans-

crotonophenone catalyzed by cat2. (Graphics by CYLview20; Legault, C. Y., Université de Sherbrooke, 2020,http://www.cylview.org)

2.Calculated Energies and Cartesian Coordinates

2.1 Analysis in the CH_3CN solvent.

2.1.1 Uncatalyzed reaction

Indole

Electronic energy (in solution) = -363.77508 Hartree
Entropic correction (in solution) = -363.66401 Hartree
Sum of electronic and thermal Free Energies (in solution) = -363.67483 Hartree

C	-2.15445600	0.68947800	0.00003600
C	-0.98411200	1.42746600	0.00003500
C	-2.12733000	-0.72137200	0.00001000
C	-0.93111200	-1.41739100	-0.00001500
C	0.25036800	-0.66742500	-0.00001500
C	0.24809300	0.75039700	0.00000900
C	1.62355800	1.16705700	-0.00000800
N	1.56115800	-1.07461800	-0.00003900
C	2.38092000	0.02724300	-0.00000700
H	3.45350800	-0.09464500	-0.00000900
H	1.99808900	2.17925200	-0.00000300
H	-3.11117300	1.19928100	0.00005400
H	-1.01355900	2.51185700	0.00005200
H	-3.06209500	-1.27041900	0.00000900
H	-0.90520600	-2.50128100	-0.00003600
H	1.87675900	-2.03442700	-0.00006400

trans-crotonophenone

Electronic energy (in solution) = -462.22865 Hartree
Entropic correction (in solution) = -462.08230 Hartree
Sum of electronic and thermal Free Energies (in solution) = -462.09290 Hartree

C	3.03932500	0.72421400	0.22583600
C	1.71296500	1.13200800	0.18415100
C	3.35978200	-0.62106800	0.04535900
C	2.35037200	-1.55426700	-0.17170500
C	1.01866700	-1.14941700	-0.19647300
C	0.69205400	0.19800400	-0.02064000
C	-0.72291800	0.69327800	-0.07642800
H	3.82462700	1.45148900	0.39657300
H	1.45169400	2.17549800	0.31567600
H	4.39555900	-0.93991400	0.07329600
H	2.59799500	-2.59871100	-0.32122300
H	0.24442600	-1.88573000	-0.37501200

O	-0.94427800	1.87014500	-0.30445000
C	-1.82001300	-0.27676900	0.16599800
C	-3.09387100	0.05892600	-0.05889300
H	-1.57250700	-1.26418200	0.53955100
C	-4.26224000	-0.83714700	0.16703500
H	-3.30122300	1.05789300	-0.43757600
H	-4.81609900	-0.97641000	-0.76640800
H	-4.95713400	-0.37562800	0.87542200
H	-3.95786200	-1.81204400	0.54985900

COM1

Electronic energy (in solution) = -826.01157 Hartree

Entropic correction (in solution) = -825.74957 Hartree

Sum of electronic and thermal Free Energies (in solution) = -825.75985 Hartree

C	4.19972800	1.59149300	0.60423600
C	3.11660200	0.76228400	0.88253100
C	5.05987800	1.28758900	-0.44683700
C	4.84596600	0.14315200	-1.21454400
C	3.77665400	-0.69446000	-0.92670000
C	2.89960100	-0.38821100	0.11908600
C	1.76530400	-1.33157600	0.39429100
H	4.37009300	2.47510000	1.20818400
H	2.46207400	1.00804200	1.70997600
H	5.89702000	1.93994000	-0.66815000
H	5.51383800	-0.09358500	-2.03472800
H	3.60368000	-1.59028700	-1.51161300
O	1.82136000	-2.48073100	-0.01046300
C	0.58678600	-0.81345200	1.12869100
C	-0.43924500	-1.61118500	1.44130900
C	-1.68478200	-1.15589500	2.11990500
H	-1.69246100	-0.07398700	2.26785000
H	-1.78647300	-1.65022400	3.09182500
H	-2.55996400	-1.44439300	1.52855900
C	-3.50248000	0.43428900	-0.33669000
C	-2.23126600	0.24187300	-0.93229100
C	-1.27691700	1.26987200	-0.84464300
C	-1.60862500	2.43676200	-0.17896500
C	-2.88270100	2.60658000	0.40457500
C	-3.84472200	1.61400200	0.33347000
H	-3.11130400	3.53320900	0.91885300
H	-4.82267800	1.73796300	0.78474300
H	-0.29269600	1.14298900	-1.28415400
H	-0.88095800	3.23668600	-0.10044200
C	-3.45631700	-1.62501700	-1.22003300
N	-4.22393100	-0.71801400	-0.53048500

H	-3.85529000	-2.59761900	-1.46567600
H	-5.17146000	-0.87614300	-0.21733800
H	-0.37126400	-2.66548800	1.17953500
C	-2.22837300	-1.08229300	-1.48826200
H	-1.41826700	-1.56832100	-2.01096400
H	0.54219100	0.24322100	1.36586200

Transition State1 (TS1)

Imaginary frequency -441.23 cm^{-1}

Electronic energy (in solution) = -825.96808 Hartree

Entropic correction (in solution) = -825.69992 Hartree

Sum of electronic and thermal Free Energies (in solution) = -825.71024 Hartree

C	4.02656800	1.73910500	0.59501200
C	2.84097900	1.00894700	0.59553400
C	5.17449900	1.21429400	0.00547100
C	5.12560900	-0.04271500	-0.59376000
C	3.93681300	-0.76528300	-0.60192400
C	2.78223500	-0.25637400	0.00063900
C	1.52226800	-1.09264300	-0.04252000
H	4.05213900	2.72238800	1.05154000
H	1.95549100	1.44076300	1.04793600
H	6.09749200	1.78312200	0.00808900
H	6.01399000	-0.45815100	-1.05676400
H	3.88572400	-1.73856900	-1.07600300
O	1.42162600	-1.95074200	-0.96031300
C	0.53004200	-0.87947500	0.92070900
C	-0.69230900	-1.63720500	0.86232800
C	-1.62858700	-1.47769700	2.04034100
H	-1.89252100	-0.42781100	2.19572700
H	-1.11731400	-1.82537000	2.94231000
H	-2.54577600	-2.05897700	1.93099800
C	-3.38158300	0.28367500	-0.33109100
C	-1.99344000	0.28573000	-0.52950200
C	-1.30468400	1.49670100	-0.47744000
C	-2.02830400	2.65889900	-0.22684700
C	-3.41582500	2.62679100	-0.02684000
C	-4.12135000	1.42995700	-0.07434900
H	-3.94850200	3.55066600	0.16533100
H	-5.19310600	1.38978200	0.07915200
H	-0.23344400	1.53229800	-0.63801900
H	-1.51165000	3.61097800	-0.18835100
C	-2.78667200	-1.84394800	-0.68776800
N	-3.81190700	-1.04679400	-0.43597800
H	-2.92885800	-2.91086700	-0.79543700
H	-4.77044800	-1.35736200	-0.31155500

H	-0.54896500	-2.67316800	0.55869200
C	-1.56065800	-1.11217900	-0.67172000
H	-0.75205200	-1.41097100	-1.33689500
H	0.59454700	-0.05473500	1.61995700

COM2

Electronic energy (in solution) = -825.97093 Hartree

Entropic correction (in solution) = -825.70127 Hartree

Sum of electronic and thermal Free Energies (in solution) = -825.71158 Hartree

C	4.19086100	1.57799400	0.76958800
C	2.97912500	0.89276500	0.76507900
C	5.24455200	1.15089100	-0.03682000
C	5.07082400	0.03612400	-0.85354600
C	3.85526800	-0.64266600	-0.86018500
C	2.79454600	-0.23513100	-0.04481800
C	1.50059600	-1.02201100	-0.10200700
H	4.31038300	2.45328900	1.39888100
H	2.16853200	1.25312700	1.38861400
H	6.18739600	1.68623700	-0.03288100
H	5.88259500	-0.30284000	-1.48826400
H	3.70546000	-1.50350100	-1.50135000
O	1.30260300	-1.73597700	-1.14391300
C	0.61071900	-0.93527700	0.94743300
C	-0.69964900	-1.64302500	0.86887500
C	-1.52265700	-1.50375200	2.14515200
H	-1.71978200	-0.45146400	2.37045400
H	-0.96820700	-1.92575100	2.98710300
H	-2.48123800	-2.02649500	2.07748800
C	-3.39907200	0.27408300	-0.40512100
C	-2.00567100	0.29540500	-0.32374300
C	-1.36587800	1.51942200	-0.16606300
C	-2.14957800	2.67064300	-0.08551900
C	-3.54449300	2.61368300	-0.16649000
C	-4.20292400	1.39841100	-0.33241200
H	-4.12254400	3.52782400	-0.10414100
H	-5.28176500	1.33211900	-0.40284400
H	-0.28575500	1.57819400	-0.11256100
H	-1.66690100	3.63312700	0.03835600
C	-2.75615300	-1.86484100	-0.59881400
N	-3.78832400	-1.07872200	-0.57081900
H	-2.87073700	-2.93634900	-0.70705500
H	-4.75479700	-1.39103900	-0.64959500
H	-0.55167100	-2.70493300	0.64058200
C	-1.50845000	-1.11395200	-0.40819200
H	-0.79585400	-1.30798500	-1.22669600

H	0.79053700	-0.28729400	1.79658300

The indirect hydrogen proton transfer reaction pathway
Transition State2 TS2(a)
Imaginary frequency -140.48 cm^{-1}
Electronic energy (in solution) = -825.96952 Hartree
Entropic correction (in solution) = -825.70009 Hartree
Sum of electronic and thermal Free Energies (in solution) = -825.71040 Hartree

C	4.72892900	0.26224400	1.04858300
C	3.51860000	-0.41193500	0.92192700
C	5.16116400	1.12794000	0.04453600
C	4.37392100	1.30540700	-1.09015800
C	3.16549100	0.62478200	-1.21720800
C	2.71302900	-0.23278300	-0.20966500
C	1.38947800	-0.93025800	-0.39035400
H	5.34153500	0.10512100	1.92965400
H	3.20723400	-1.09483900	1.70448300
H	6.10551200	1.65123100	0.14373100
H	4.70307500	1.97229800	-1.87976600
H	2.55201600	0.74805500	-2.10186700
O	0.93346900	-1.01488600	-1.59913900
C	0.68961300	-1.37487200	0.70090400
C	-0.68173500	-1.95554100	0.51757600
C	-1.41069400	-2.17799300	1.83879200
H	-1.51352700	-1.23744700	2.38767300
H	-0.84632600	-2.87273300	2.46660400
H	-2.40932000	-2.59414100	1.67827600
C	-3.29696800	0.46503700	-0.38656000
C	-1.96330500	0.31323000	0.00670200
C	-1.34016700	1.36770200	0.67116600
C	-2.07776800	2.52202200	0.92182900
C	-3.41083600	2.64427100	0.50963000
C	-4.04947300	1.60777400	-0.16119800
H	-3.95274200	3.55962700	0.71556700
H	-5.07862300	1.68288200	-0.49103800
H	-0.30646300	1.29082300	0.98563400
H	-1.60912600	3.34831500	1.44370600
C	-2.69941200	-1.59144900	-1.03997600
N	-3.68425000	-0.73340400	-1.02190200
H	-2.82388700	-2.57516300	-1.47495600
H	-4.60498800	-0.90040100	-1.42084900
H	-0.62474500	-2.90944000	-0.02385800
C	-1.50368200	-1.03014000	-0.44458800
H	-0.70065700	-0.93239500	-1.27735200

H	1.04592100	-1.20150800	1.70915400

COM3(a)

Electronic energy (in solution) = -826.02516 Hartree

Entropic correction (in solution) = -825.75400 Hartree

Sum of electronic and thermal Free Energies (in solution) = -825.76429 Hartree

C	-4.77641200	-0.02319800	0.83819800
C	-3.55017800	0.60367800	0.65228100
C	-5.10468700	-1.15972000	0.10094600
C	-4.19714000	-1.66077400	-0.82750500
C	-2.96748100	-1.03592200	-1.01464100
C	-2.62488100	0.09670700	-0.26816200
C	-1.30007500	0.73426600	-0.46132800
H	-5.48324900	0.38407500	1.55224900
H	-3.31861200	1.50152600	1.21361400
H	-6.06353100	-1.64461200	0.24434400
H	-4.44483400	-2.54156700	-1.40919600
H	-2.26348300	-1.42991100	-1.73718500
O	-0.78183400	0.48403600	-1.69908200
C	-0.66516600	1.45516000	0.47281400
C	0.68273100	2.12555900	0.28758400
C	1.13876500	2.76022000	1.60768100
H	1.28215400	1.99148800	2.37210900
H	0.38998900	3.46854600	1.97163500
H	2.08320800	3.29107200	1.47244100
C	3.15775400	-0.60390600	-0.51361000
C	2.10697700	-0.10475400	0.29483800
C	1.65337800	-0.88001900	1.37687600
C	2.24941700	-2.10568100	1.61765200
C	3.29453500	-2.58211900	0.79856200
C	3.76222900	-1.84295600	-0.27377100
H	3.73990400	-3.54673500	1.01409500
H	4.56485500	-2.20492600	-0.90628900
H	0.85025600	-0.52209000	2.01196200
H	1.91063900	-2.71371900	2.44868000
C	2.55281000	1.39267000	-1.32551700
N	3.40754000	0.32918500	-1.48819800
H	2.59094300	2.23637300	-1.99975800
H	4.09719300	0.24279200	-2.22138000
H	0.57467900	2.92817400	-0.45399800
C	1.73401500	1.18066200	-0.24520400
H	0.15765600	0.72218100	-1.70841500
H	-1.14540900	1.56151400	1.43898100

The direct hydrogen proton transfer reaction pathway

Transition State2 TS2(b)

Imaginary frequency -1300.49 cm^{-1}

Electronic energy (in solution) = -825.93701 Hartree

Entropic correction (in solution) = -825.67088 Hartree

Sum of electronic and thermal Free Energies (in solution) = -825.68119 Hartree

C	-4.34157000	0.84026000	1.78420600
C	-3.14213400	0.84729100	1.07952200
C	-5.36831700	-0.02605300	1.41472800
C	-5.18309600	-0.89316400	0.34120900
C	-3.98028700	-0.88929500	-0.35735800
C	-2.94996600	-0.01417800	-0.00561500
C	-1.67648400	-0.05716800	-0.82169800
H	-4.47358900	1.50921900	2.62715900
H	-2.34745700	1.51532900	1.39103600
H	-6.30297100	-0.02826400	1.96385400
H	-5.97580100	-1.57322000	0.04983600
H	-3.81639700	-1.56514500	-1.18811600
O	-1.45859100	-1.07937200	-1.51672900
C	-0.77689200	1.01951000	-0.74104900
C	0.48769800	0.96883700	-1.59729400
C	1.12206900	2.33916700	-1.78258400
H	1.22047500	2.86392500	-0.83007800
H	0.48046700	2.94743200	-2.42505900
H	2.10814000	2.27080900	-2.24778300
C	3.08188900	-1.09809700	0.28710000
C	2.56757800	0.18134100	0.00922100
C	3.20896800	1.29155900	0.56727700
C	4.33427000	1.08723700	1.35463800
C	4.82183800	-0.20137700	1.61738900
C	4.19579600	-1.31992100	1.09018300
H	5.69850700	-0.32459900	2.24187700
H	4.55147400	-2.32399900	1.28784400
H	2.84778300	2.29604500	0.39475400
H	4.84472100	1.94308400	1.78031900
C	1.30663100	-1.42663800	-1.03774800
N	2.28431900	-2.03150600	-0.37138100
H	0.58806000	-1.96686900	-1.63330800
H	2.41900200	-3.03560800	-0.32788100
H	0.27525500	0.52568400	-2.57571300
C	1.33686200	-0.02313200	-0.78720600
H	0.36269100	0.07911700	0.03569200
H	-1.07098800	1.96549300	-0.30045200

COM3(b)

Electronic energy (in solution) = -826.04042 Hartree

Entropic correction (in solution) = -825.76971 Hartree
Sum of electronic and thermal Free Energies (in solution) = -825.78000 Hartree

C	4.15443400	1.34174400	1.07920000
C	3.06139100	0.47991300	1.06165000
C	4.87475000	1.57910900	-0.08790800
C	4.50655600	0.94758500	-1.27545100
C	3.42242200	0.08020700	-1.29151600
C	2.68964300	-0.15855700	-0.12458500
C	1.52918400	-1.11173800	-0.19020900
H	4.44101000	1.82915400	2.00381200
H	2.51057700	0.30441100	1.97800100
H	5.72237800	2.25496900	-0.07359200
H	5.06555000	1.13320000	-2.18537900
H	3.12893600	-0.41952300	-2.20723300
O	1.34549700	-1.77478500	-1.18991800
C	0.63242800	-1.24081600	1.02260000
C	-0.68640300	-1.96913100	0.74179100
C	-1.35865500	-2.36867100	2.06055200
H	-1.57817700	-1.49217100	2.67581100
H	-0.70733300	-3.03047100	2.63779800
H	-2.29873700	-2.89191200	1.87040000
C	-2.98583100	0.51209400	-0.93070200
C	-2.19415600	0.14279800	0.18798500
C	-2.14027500	1.01951100	1.28859700
C	-2.85644000	2.20342900	1.24557300
C	-3.63625000	2.54473500	0.12130400
C	-3.71121000	1.70747200	-0.97797900
H	-4.18609000	3.47904400	0.11883600
H	-4.30784600	1.96299100	-1.84652800
H	-1.54549600	0.77529100	2.16181700
H	-2.81945000	2.88282900	2.08957500
C	-2.04807900	-1.47076100	-1.37063600
N	-2.87768700	-0.48897300	-1.86059500
H	-1.82776300	-2.34652200	-1.96328000
H	-3.32821500	-0.50224100	-2.76452100
H	-0.45396400	-2.87984400	0.18335300
C	-1.60154000	-1.13945000	-0.12008800
H	0.44146500	-0.24967100	1.44288000
H	1.21117500	-1.78529000	1.78068700

Product P(b)

Electronic energy (in solution) = -826.04392 Hartree
Entropic correction (in solution) = -825.77107 Hartree
Sum of electronic and thermal Free Energies (in solution) = -825.78153 Hartree

C	1.39189500	1.81678700	-1.92763200

C	0.16083000	1.78602700	-1.27716000
C	2.57190600	1.84080600	-1.19021500
C	2.52182500	1.85354800	0.20397300
C	1.29444600	1.83339800	0.85256500
C	0.10326400	1.78735900	0.11888100
C	-1.18605600	1.67686700	0.88210500
H	1.42712600	1.81583600	-3.01109200
H	-0.74467500	1.75868700	-1.86932700
H	3.52934800	1.85062600	-1.69897700
H	3.43929100	1.87105300	0.78114700
H	1.24351800	1.82716900	1.93504600
O	-1.20720100	1.92144200	2.07354900
C	-2.44252800	1.18744200	0.19479800
C	-2.56940400	-0.35842900	0.27466700
C	-3.87868100	-0.78885400	-0.38553000
H	-3.88174500	-0.52441700	-1.44690100
H	-4.72956200	-0.29231600	0.08710400
H	-4.01781000	-1.86906800	-0.30196000
C	0.77518900	-1.81408800	-0.61729400
C	-0.15243100	-1.37221400	0.35833500
C	0.24694400	-1.31626300	1.70425100
C	1.53700000	-1.69218100	2.03525300
C	2.44694500	-2.12312500	1.04633500
C	2.08174300	-2.19250000	-0.28738900
H	3.45229500	-2.40590800	1.33754700
H	2.77835800	-2.52254100	-1.04986000
H	-0.44228100	-0.97123100	2.46850000
H	1.86103100	-1.65079700	3.06904500
C	-1.14041900	-1.29560200	-1.65804100
N	0.14273000	-1.76153800	-1.83294100
H	0.54582400	-2.03999000	-2.71633600
H	-2.60577300	-0.62514300	1.33650100
C	-1.36869400	-1.03191800	-0.33258800
H	-1.79032100	-1.16893000	-2.51150400
H	-2.47814200	1.48637200	-0.85401100
H	-3.29063100	1.63748200	0.71538700

2.1.2 Cat1 ($C_5H_8N_2I^+$) catalyzed reaction

cat1 ($C_5H_8N_2I^+$)

Electronic energy (in solution) = -602.27768 Hartree

Entropic correction (in solution) = -602.16953Hartree

Sum of electronic and thermal Free Energies (in solution) = -602.18018 Hartree

C	0.00000000	0.67897000	-2.67855800
C	0.00000000	-0.67897000	-2.67855800

C	0.00000000	0.00000000	-0.58501600
H	0.00000000	-1.39189400	-3.48627600
H	0.00000000	1.39189400	-3.48627600
N	0.00000000	-1.08535700	-1.36426500
N	0.00000000	1.08535700	-1.36426500
C	0.00000000	-2.47496100	-0.90481600
H	0.89557200	-2.66303300	-0.31379800
H	-0.89557200	-2.66303300	-0.31379800
H	0.00000000	-3.11102300	-1.78601000
C	0.00000000	2.47496100	-0.90481600
H	-0.89557200	2.66303300	-0.31379800
H	0.89557200	2.66303300	-0.31379800
H	0.00000000	3.11102300	-1.78601000
I	0.00000000	0.00000000	1.46056700

cat1-Michael acceptor

Basis set superposition error correction = 0.000724842 Hartree
Electronic energy (in solution) = -1064.51776 Hartree
Entropic correction (in solution) = -1064.25769 Hartree
Sum of electronic and thermal Free Energies (in solution) = -1064.26775 Hartree

C	3.45311500	2.96260600	1.06969800
C	3.51763500	1.58572900	0.88068300
C	2.66659500	3.74594000	0.22918200
C	1.93281100	3.15284800	-0.79739300
C	1.97664700	1.77614800	-0.97340700
C	2.77172200	0.98542600	-0.13718500
C	2.77080500	-0.49460800	-0.33640300
H	4.01878900	3.42357200	1.87081300
H	4.12841900	0.98109500	1.54110400
H	2.62722900	4.81990400	0.37153200
H	1.32890100	3.76440700	-1.45755300
H	1.41429000	1.30608700	-1.77227300
O	1.78067900	-1.04539400	-0.80579800
C	3.98424900	-1.25235300	0.02981300
C	3.99346200	-2.58981600	0.00623200
C	5.17069500	-3.43628900	0.34067800
H	6.04116200	-2.83572700	0.60658300
H	5.42240500	-4.07720000	-0.51003800
H	4.92717800	-4.10499700	1.17198400
H	3.07687300	-3.10406700	-0.27594100
H	4.87407100	-0.69747100	0.30608900
H	-1.94019900	0.37605500	2.72401300
H	-3.06282500	0.90645600	-2.45101000
C	-4.79970800	0.06304300	1.26046800
C	-5.07279100	0.18244100	-0.06364200

C	-2.72868900	-0.36981300	2.63337300
H	-5.43584700	0.12197900	2.12772600
N	-3.44832900	-0.17203500	1.37517900
H	-3.44347500	-0.24910200	3.44332400
C	-2.90803400	-0.19622500	0.15167900
H	-5.99533700	0.36827800	-0.58783500
N	-3.88376600	0.01786800	-0.73825200
C	-3.71806000	0.07579200	-2.19118100
H	-4.70053100	0.23121100	-2.63002700
H	-2.30693300	-1.37388600	2.65947400
H	-3.30039100	-0.86444700	-2.54854600
I	-0.91806100	-0.50368000	-0.28711500

COM1

Basis set superposition error correction = 0.002934667 Hartree
Electronic energy (in solution) = -1428.30674 Hartree
Entropic correction (in solution) = -1427.92546 Hartree
Sum of electronic and thermal Free Energies (in solution) = -1427.93545 Hartree

C	2.06130100	4.09555000	1.36736100
C	2.37050200	2.95375200	0.63537100
C	0.88410500	4.79312700	1.10881100
C	0.01023600	4.34710200	0.11861700
C	0.30818800	3.19694100	-0.60073600
C	1.48901300	2.49150600	-0.34647000
C	1.76080600	1.24304500	-1.12329600
H	2.74005300	4.44137200	2.13820000
H	3.28495400	2.41282600	0.84909400
H	0.64962700	5.68749800	1.67495200
H	-0.89932700	4.89739500	-0.09244200
H	-0.36021600	2.85145900	-1.38099800
O	0.82874200	0.61569400	-1.61598300
C	3.16255500	0.81812500	-1.30130800
C	3.46100300	-0.38482700	-1.80638200
C	4.84629700	-0.87139200	-2.05543200
H	5.59431900	-0.16193600	-1.69873900
H	4.99272800	-1.03130800	-3.12904000
H	5.00654200	-1.84002000	-1.57380000
C	3.14573000	-2.36623400	0.65189300
C	1.79150100	-1.95933500	0.75838300
C	1.48261900	-0.84519000	1.55855900
C	2.50781600	-0.18234100	2.20990800
C	3.84871700	-0.60615200	2.08670200
C	4.18559700	-1.70132200	1.31121600
H	4.62759200	-0.06268400	2.60974700
H	5.21355700	-2.03071400	1.20836700

H	0.45699800	-0.50724600	1.66304800
H	2.28143900	0.68139300	2.82508700
C	1.91286300	-3.73431800	-0.62387200
N	3.18498900	-3.44448900	-0.19652200
H	1.74142900	-4.55778200	-1.30051200
H	4.01699400	-3.95412000	-0.45945100
H	2.64104300	-1.05440800	-2.06342400
C	1.02538000	-2.85395200	-0.06540200
H	-0.04149600	-2.84769800	-0.22634400
H	3.95031000	1.50739000	-1.01786500
H	-2.20544300	-0.31306300	2.60823300
H	-4.55681700	1.11545400	-1.92525300
C	-5.09651100	-1.21016700	1.52630700
C	-5.70683400	-0.83804200	0.37244900
C	-2.71443000	-1.24483100	2.36374300
H	-5.49250300	-1.60898200	2.44512300
N	-3.74770200	-0.99023500	1.35932100
H	-3.20562300	-1.63775100	3.25031000
C	-3.53873000	-0.49557200	0.13405600
H	-6.74335900	-0.84626200	0.07972500
N	-4.72184700	-0.39545000	-0.48169400
C	-4.93709700	0.09813800	-1.84181200
H	-6.00752100	0.09011900	-2.03060500
H	-2.00468200	-1.97815900	1.98166400
H	-4.43247700	-0.55506400	-2.55276200
I	-1.70660200	0.03257200	-0.64819200

Transition State1 (TS1)

Imaginary frequency -491.54 cm^{-1}

Basis set superposition error correction = 0.003529659 Hartree

Electronic energy (in solution) = -1428.26646 Hartree

Entropic correction (in solution) = -1427.88104 Hartree

Sum of electronic and thermal Free Energies (in solution)= -1427.89105 Hartree

C	0.35646800	4.00408100	2.29824800
C	1.00339800	3.13695600	1.42223300
C	-0.77341700	4.70591200	1.88464800
C	-1.25939800	4.52920400	0.59068400
C	-0.61878000	3.65464100	-0.28042600
C	0.52611200	2.95713800	0.11923300
C	1.16693900	2.01129900	-0.86157900
H	0.73177800	4.12634300	3.30804800
H	1.87093700	2.58558300	1.76647000
H	-1.27454800	5.38215700	2.56800900
H	-2.13915500	5.07150400	0.26264400
H	-0.99670000	3.50324600	-1.28515500

O	0.42285600	1.52132600	-1.77156300
C	2.51372200	1.68517600	-0.72710100
C	3.13052800	0.73755000	-1.60392400
C	4.61796600	0.53644000	-1.44080800
H	4.85701200	0.14890700	-0.44553500
H	5.11661300	1.50436800	-1.54322500
H	5.03112400	-0.13922700	-2.19047100
C	3.39454100	-2.29415600	0.22112500
C	2.42866000	-1.27853600	0.14953300
C	1.89879000	-0.76124800	1.33249300
C	2.34843800	-1.28200600	2.54178000
C	3.31612600	-2.29685200	2.58435200
C	3.86152800	-2.82116500	1.41840200
H	3.64539700	-2.67911200	3.54333700
H	4.61218500	-3.60229300	1.43861700
H	1.14906800	0.02187600	1.31064400
H	1.94420700	-0.89833200	3.47166100
C	3.05795800	-1.88141100	-1.95310700
N	3.74928700	-2.61990100	-1.09380000
H	3.19936400	-1.99397700	-3.01931300
H	4.45166700	-3.30492400	-1.35372700
H	2.78969100	0.77674400	-2.63575700
C	2.25843600	-0.93293200	-1.26322100
H	1.32001700	-0.58335300	-1.67994300
H	3.08139200	2.04002700	0.12460600
I	-1.55518500	0.03772900	-0.78453100
H	-1.32392200	-1.08037500	2.32031900
H	-4.84994100	0.24505600	-1.43935000
C	-3.92790300	-2.72414700	1.37165300
C	-4.82339200	-2.38568000	0.40979600
C	-1.55271500	-2.06722800	1.91899200
H	-3.99826500	-3.40525700	2.20315900
N	-2.78022400	-2.00410400	1.12503400
H	-1.72324400	-2.76494200	2.73521100
C	-2.96667700	-1.24281200	0.03951000
H	-5.83493100	-2.71028900	0.23164100
N	-4.20789400	-1.46470500	-0.40864000
C	-4.81570300	-0.83447400	-1.58009900
H	-5.82591500	-1.22386600	-1.67807100
H	-0.73180600	-2.42156500	1.29596000
H	-4.23798200	-1.08208900	-2.46981800

COM2

Basis set superposition error correction = 0.001580164 Hartree

Electronic energy (in solution) = -1428.27499 Hartree

Entropic correction (in solution) = -1427.88904 Hartree
Sum of electronic and thermal Free Energies (in solution) = -1427.89906 Hartree

C	0.02569500	4.41291200	2.24017200
C	0.76122900	3.49834700	1.49213000
C	-1.12170200	4.99754100	1.70702300
C	-1.53059300	4.65322600	0.42087900
C	-0.79561000	3.73541500	-0.32403300
C	0.36747700	3.15419500	0.19293100
C	1.12002200	2.16657300	-0.66014400
H	0.34356800	4.66227000	3.24661500
H	1.63886400	3.03857800	1.93274200
H	-1.69465900	5.70832200	2.29178400
H	-2.42441000	5.09902500	-0.00184800
H	-1.11407300	3.45563500	-1.32165300
O	0.43615200	1.57752800	-1.60412900
C	2.44139700	1.92740100	-0.42678900
C	3.22473800	0.91227300	-1.20830300
C	4.67086300	0.81924500	-0.72727000
H	4.71125500	0.53988700	0.32967700
H	5.16265200	1.78875900	-0.83612400
H	5.24312900	0.08314600	-1.29966900
C	3.00152700	-2.45170600	0.04647600
C	2.44442700	-1.17986300	0.18826200
C	1.95116200	-0.80479100	1.43205200
C	2.04271100	-1.71799400	2.48357600
C	2.59924000	-2.98740600	2.30472100
C	3.09464800	-3.38336900	1.06470600
H	2.64661400	-3.67501400	3.14064000
H	3.52945900	-4.36210000	0.90259000
H	1.50059900	0.16869800	1.58171300
H	1.66429700	-1.43979800	3.46050900
C	3.17072600	-1.50864200	-1.98238000
N	3.42615200	-2.57870400	-1.30244800
H	3.43724600	-1.42798200	-3.02922200
H	3.87619700	-3.41004600	-1.68479100
H	3.21726500	1.16470300	-2.27593200
C	2.51446400	-0.48678300	-1.14324400
H	1.51314200	-0.29423600	-1.56203500
H	2.96410100	2.46070600	0.35857900
H	-0.94223400	-1.61954500	2.12381100
H	-4.66897800	0.34497300	-1.08590200
C	-3.60004700	-3.08282600	1.08371000
C	-4.56600200	-2.58002200	0.27450800
C	-1.18463200	-2.51323800	1.54988000

H	-3.61177300	-3.89985300	1.78578300
N	-2.46768700	-2.32683200	0.87314000
H	-1.27939800	-3.36576900	2.21823800
C	-2.72700100	-1.38211000	-0.04125500
H	-5.59289200	-2.86952800	0.12610900
N	-4.00540400	-1.52623400	-0.41410900
C	-4.69859300	-0.69774200	-1.39927200
H	-5.73070000	-1.03585800	-1.45199500
H	-0.40470000	-2.70655300	0.81310500
H	-4.22417900	-0.81118300	-2.37339200
I	-1.34260200	0.03398300	-0.75589400

The indirect hydrogen proton transfer reaction pathway

Transition State2 TS2(a)

Imaginary frequency -295.26 cm^{-1}

Basis set superposition error correction = 0.001783451 Hartree

Electronic energy (in solution) = -1428.27153 Hartree

Entropic correction (in solution) = -1427.88584 Hartree

Sum of electronic and thermal Free Energies (in solution) = -1427.89586 Hartree

C	1.40359500	4.39054000	2.03682200
C	1.90703900	3.24124600	1.43571400
C	0.44976800	5.16715300	1.38128300
C	0.00048100	4.78207600	0.12055000
C	0.50268400	3.63078300	-0.47898400
C	1.46964900	2.85070000	0.16444000
C	1.98635600	1.62530300	-0.52314800
H	1.74844800	4.67495200	3.02481000
H	2.63281200	2.63539000	1.96685300
H	0.05635700	6.06073000	1.85251000
H	-0.74278500	5.37895300	-0.39657900
H	0.15329700	3.32602200	-1.45891900
O	1.17505600	1.06546500	-1.40529300
C	3.21788600	1.12138400	-0.25430900
C	3.70401900	-0.14378700	-0.91143100
C	4.92678000	-0.73034100	-0.20987300
H	4.70007100	-0.96336900	0.83422900
H	5.75025600	-0.01171400	-0.22471800
H	5.25953100	-1.64684500	-0.70443700
C	1.69069100	-3.16213200	-0.13458400
C	2.01215700	-1.84928600	0.22895700
C	1.76995500	-1.43941800	1.53999200
C	1.23019400	-2.36043800	2.43264500
C	0.91283600	-3.66730100	2.03634600
C	1.13503600	-4.09305500	0.73288700
H	0.48551000	-4.35551100	2.75619200

H	0.89482000	-5.09787100	0.40664500
H	2.00176200	-0.42943000	1.85706200
H	1.04505100	-2.06055200	3.45779400
C	2.56556700	-2.21629200	-1.96577400
N	2.04736200	-3.32039700	-1.48705900
H	2.91063400	-2.15792100	-2.99013400
H	1.90474800	-4.17204400	-2.02416600
H	3.96381000	0.05557700	-1.95990500
C	2.54015800	-1.16541300	-0.98016200
H	1.71102400	-0.40061000	-1.36916000
H	3.87187500	1.61432700	0.45511200
I	-1.18421500	0.32131000	-0.64278900
H	-1.63933200	-1.53884600	2.15328100
H	-4.03347800	1.99391400	-1.01826200
C	-4.57962500	-1.68547400	0.92831800
C	-5.21675900	-0.77968500	0.14373700
C	-2.16549100	-2.20020000	1.46530000
H	-4.95749700	-2.46496800	1.56852800
N	-3.22868300	-1.45841400	0.78787900
H	-2.62702600	-3.01612600	2.01651900
C	-3.03857000	-0.43887900	-0.05910200
H	-6.26404300	-0.60750700	-0.04046800
N	-4.24335800	-0.01463600	-0.46013900
C	-4.48817900	1.07995100	-1.39793500
H	-5.56415900	1.21215600	-1.48073300
H	-1.47248400	-2.60014500	0.72547100
H	-4.07087000	0.82779200	-2.37224700

COM3(a)

Basis set superposition error correction = 0.001395283 Hartree
Electronic energy (in solution) = -1428.31823 Hartree
Entropic correction (in solution) = -1427.93245 Hartree
Sum of electronic and thermal Free Energies (in solution) = -1427.94249 Hartree

C	-0.17499600	4.29821800	1.74754300
C	0.76875300	3.34207000	1.38835200
C	-1.06391300	4.79943600	0.79889100
C	-1.00305800	4.33719400	-0.51333100
C	-0.05937000	3.38158600	-0.87589500
C	0.84320500	2.88155300	0.06955900
C	1.84033300	1.86120100	-0.33375000
H	-0.22545000	4.64212500	2.77435600
H	1.43607800	2.93605800	2.14027600
H	-1.80239500	5.54045100	1.08266800
H	-1.69228700	4.72043800	-1.25742100
H	-0.01775100	3.02141300	-1.89707900

O	1.37570600	1.08532700	-1.36830700
C	3.04940600	1.72388300	0.22397100
C	4.10883800	0.70199600	-0.13968000
C	5.12621600	0.58268000	1.00460100
H	4.64231000	0.21410700	1.91296300
H	5.57102000	1.55648500	1.22439500
H	5.92476500	-0.11085800	0.73364800
C	2.38855700	-2.63862500	-0.40881500
C	2.65014400	-1.45323900	0.32137600
C	2.05558300	-1.28549700	1.58471200
C	1.24041800	-2.28919600	2.07763200
C	0.99880000	-3.46334400	1.33405800
C	1.56192100	-3.65419900	0.08480600
H	0.35507200	-4.23121600	1.74901800
H	1.37728900	-4.55439700	-0.49060500
H	2.23559100	-0.38494700	2.16233400
H	0.77630400	-2.17503700	3.05094900
C	3.75852700	-1.36311800	-1.63727500
N	3.07570200	-2.55470200	-1.59375800
H	4.36251900	-1.10668500	-2.49576200
H	3.07977700	-3.25516900	-2.32175400
H	4.64671200	1.06078700	-1.02673900
C	3.53307400	-0.64775200	-0.48840400
H	2.04871600	0.42686600	-1.60606900
H	3.31082400	2.43830100	0.99721200
H	-1.76301000	-2.71307500	1.66290500
H	-3.66296500	1.90711700	-0.18395300
C	-4.69875300	-2.06411500	0.62501600
C	-5.19302300	-0.88534000	0.16804400
C	-2.39778700	-3.07443400	0.85478200
H	-5.18703300	-2.92620700	1.04755300
N	-3.33268500	-2.01938500	0.46461700
H	-2.98336700	-3.92547000	1.19412300
C	-2.99962300	-0.84266400	-0.07596400
H	-6.20090400	-0.50994700	0.10995800
N	-4.12146900	-0.13770400	-0.26381900
C	-4.20302200	1.21101300	-0.82526500
H	-5.25405900	1.48541000	-0.86562200
H	-1.79136900	-3.36087100	-0.00362900
H	-3.78198900	1.21520800	-1.82981400
I	-1.10457100	-0.19560000	-0.54861300

P(a)

Electronic energy (in solution) = -826.02488 Hartree

Entropic correction (in solution) = -825.75379 Hartree

Sum of electronic and thermal Free Energies (in solution) = -825.76408 Hartree

C	4.33669500	0.97037700	1.07980100
C	3.07707500	0.38724600	1.01252500
C	5.13564200	1.05369200	-0.05932600
C	4.66048600	0.55365200	-1.26798600
C	3.39948700	-0.03162500	-1.33825900
C	2.59793300	-0.13300600	-0.19596000
C	1.26744500	-0.78211400	-0.28457600
H	4.69087400	1.37223100	2.02232900
H	2.45690000	0.35367900	1.90081400
H	6.11628800	1.51235400	-0.00533700
H	5.27178700	0.61789200	-2.16108500
H	3.03469300	-0.41940100	-2.28143100
O	0.76767200	-0.75285700	-1.55447400
C	0.63980900	-1.35905800	0.74927100
C	-0.71634800	-2.03525500	0.69035000
C	-1.18813100	-2.38179200	2.10906700
H	-1.32422500	-1.47174100	2.69985100
H	-0.45171200	-3.01137700	2.61509900
H	-2.13940300	-2.91668900	2.07669100
C	-3.13586900	0.51509000	-0.66811800
C	-2.10103200	0.17030700	0.23567600
C	-1.63636300	1.14078300	1.14124100
C	-2.20764300	2.40130500	1.12198400
C	-3.23794200	2.72131700	0.21296000
C	-3.71543400	1.78859000	-0.69088200
H	-3.66322200	3.71846700	0.22298300
H	-4.50643700	2.03008300	-1.39177000
H	-0.84287300	0.90389300	1.84195100
H	-1.85981300	3.15940900	1.81434500
C	-2.56509000	-1.61511900	-1.05404300
N	-3.39789900	-0.59086500	-1.43696800
H	-2.61540400	-2.57631000	-1.54521600
H	-4.08174500	-0.64261500	-2.17871400
H	-0.61722200	-2.97514800	0.13104600
C	-1.75011200	-1.20392800	-0.03027000
H	-0.13795000	-1.09660600	-1.55351900
H	1.14972500	-1.36198500	1.70581700

The direct hydrogen proton transfer reaction pathway

Transition State2 TS2(b)

Imaginary frequency -1443.85cm^{-1}

Basis set superposition error correction = 0.001283043 Hartree

Electronic energy (in solution) = -1428.23467 Hartree

Entropic correction (in solution) = -1427.85247 Hartree

Sum of electronic and thermal Free Energies (in solution) = -1427.86245 Hartree

C	-0.88778900	3.98202600	2.30498500
C	0.05757700	3.30163100	1.54332500
C	-2.08488900	4.40087100	1.72789400
C	-2.33490700	4.12927200	0.38459900
C	-1.39378400	3.44024600	-0.37372300
C	-0.18508200	3.02630000	0.19397200
C	0.79009300	2.27851600	-0.67564100
H	-0.69205400	4.17962300	3.35289600
H	0.97668700	2.96509100	2.00956700
H	-2.81946000	4.93196500	2.32262800
H	-3.26374600	4.45324200	-0.07151800
H	-1.58571300	3.21606400	-1.41701400
O	0.32264500	1.58977700	-1.63604800
C	2.15210500	2.31816600	-0.36339600
C	3.16132300	1.56054100	-1.22660200
C	4.59053600	2.03940100	-1.02073200
H	4.83827500	2.11049900	0.03999600
H	4.70447700	3.03712100	-1.45158100
H	5.30837900	1.37187000	-1.50252600
C	3.03865000	-2.03512100	0.04397100
C	3.62065700	-0.75900100	0.16726700
C	4.62152800	-0.57038400	1.12632200
C	5.01210400	-1.65287100	1.90333800
C	4.41118200	-2.91363100	1.76164300
C	3.40599600	-3.12309800	0.83030600
H	4.73658600	-3.73413300	2.39012400
H	2.92468200	-4.08684400	0.71167700
H	5.09005600	0.39432200	1.26807100
H	5.79619400	-1.52106600	2.63975500
C	2.01138000	-0.74037800	-1.46447900
N	2.07665100	-1.97170900	-0.96017700
H	1.36018700	-0.49021200	-2.28733900
H	1.49516000	-2.74886400	-1.25466600
H	2.89641900	1.63365600	-2.28559600
C	2.88655800	0.12476900	-0.76066900
H	2.06566700	0.76455600	0.03826800
H	2.52306600	3.01624300	0.37904900
H	-0.38454700	-3.09372900	0.50846500
H	-4.22458300	0.52552900	0.94513400
C	-3.54792900	-3.60616100	0.71593600
C	-4.53498800	-2.68299900	0.83876700
C	-1.15754100	-3.57627300	-0.08963300
H	-3.52123100	-4.65680800	0.95191000

N	-2.45241700	-2.95719000	0.19160600
H	-1.22852800	-4.62680600	0.18079500
C	-2.75991700	-1.66893200	-0.00373900
H	-5.54588500	-2.76425300	1.20171000
N	-4.02636300	-1.48556700	0.38775200
C	-4.75502400	-0.21778500	0.35068800
H	-5.74119200	-0.39016800	0.77495600
H	-0.92957200	-3.48447500	-1.15127900
H	-4.85164200	0.12124400	-0.68003100
I	-1.47926400	-0.21266500	-0.74237200

COM3(b)

Basis set superposition error correction = 0.000724999 Hartree
Electronic energy (in solution) = -1428.33471 Hartree
Entropic correction (in solution) = -1427.94704 Hartree
Sum of electronic and thermal Free Energies (in solution) = -1427.95707 Hartree

C	-0.84744600	1.78784800	-0.69212100
C	-0.86466200	0.75719100	-1.85602000
H	-1.57521300	1.09687800	-2.61013700
C	-1.19182000	-0.62898400	-1.35433400
C	4.24932000	-0.04725600	0.17933000
N	5.26379100	-0.85636300	0.50265000
I	2.33775800	-0.62574500	-0.33300900
C	5.20681300	-2.31694300	0.55984000
H	6.19103600	-2.67358400	0.85223700
H	4.94877000	-2.71139400	-0.42227400
H	4.46863500	-2.62452400	1.29939300
O	-0.29412500	-1.34282800	-0.92891200
H	6.56765100	2.12348800	0.73485800
C	6.01129400	1.20846000	0.61915700
C	6.37294200	-0.09002700	0.78076000
N	4.68628100	1.21537900	0.24621200
H	7.30922200	-0.53966800	1.06635900
H	-0.07953200	1.46550900	0.02016100
C	-0.45677000	3.15725000	-1.24462900
H	-0.38979100	3.89303300	-0.44017800
H	0.51125700	3.10534100	-1.74957400
H	-1.19678700	3.50791100	-1.96961200
C	-2.60655600	-1.10765600	-1.28890600
C	-2.88675600	-2.21274600	-0.47545400
C	-3.65455400	-0.45523100	-1.94482800
C	-4.19423200	-2.64411800	-0.30221600
H	-2.07096200	-2.70865900	0.03690500
C	-4.96449100	-0.89585500	-1.77836600
H	-3.46458900	0.39625100	-2.58501200

C	-5.23658700	-1.98157100	-0.95116600
H	-4.40498300	-3.48935600	0.34276500
H	-5.77210400	-0.38563500	-2.29030300
H	-6.25929400	-2.31382900	-0.81235700
C	-2.52858000	0.95380500	1.13541500
C	-3.90836900	1.15670900	1.38478900
C	-4.59785100	0.45335000	2.37923800
C	-3.87682800	-0.46122000	3.12802300
C	-2.49983900	-0.67261900	2.90224300
C	-1.82264800	0.02281800	1.91599800
C	-2.16657700	1.80212400	0.03016400
C	-3.30495000	2.48028800	-0.31991900
H	-5.65565300	0.61846000	2.55046800
H	-4.37975400	-1.02598500	3.90488100
H	-1.97015700	-1.39732900	3.51023500
H	-0.76621500	-0.15535200	1.73919500
H	0.12802700	0.71716800	-2.31137500
H	-3.46590100	3.20412300	-1.10535600
H	-5.28944400	2.46386200	0.43852200
N	-4.35012400	2.09534900	0.48776100
C	3.89288900	2.40933000	-0.04601800
H	3.60101600	2.40585100	-1.09579400
H	3.01060400	2.42741300	0.59293400
H	4.51390000	3.27691700	0.16157600

2.1.3 Cat2 ($(C_4H_5N_2I^+)_2C_6H_4$) catalyzed reaction

cat2 ($(C_4H_5N_2I^+)_2C_6H_4$)

Electronic energy (in solution) = -1355.76028 Hartree
Entropic correction (in solution) = -1355.53587 Hartree
Sum of electronic and thermal Free Energies (in solution) = -1355.54598 Hartree

C	0.00000000	1.40679200	0.23094300
C	0.00000000	0.26634100	2.78862200
C	1.18514500	1.11576500	0.88997100
C	-1.18514500	1.11576500	0.88997000
C	-1.20613800	0.55227600	2.15916000
C	1.20613700	0.55227600	2.15916100
H	-2.15169600	0.35224500	2.65001200
H	2.15169500	0.35224500	2.65001300
C	3.31395500	0.51709500	-0.23251400
N	4.32000500	1.18358300	-0.79740600
C	-3.31395500	0.51709500	-0.23251400
N	-4.32000400	1.18358400	-0.79740700
I	3.13876300	-1.51918400	-0.13727900
I	-3.13876400	-1.51918400	-0.13727800

C	5.50335500	0.58847800	-1.42424700
H	6.13694200	1.40363400	-1.76326600
H	5.19735000	-0.02096200	-2.27370800
H	6.03730400	-0.01387100	-0.69058500
C	-5.50335400	0.58847900	-1.42424800
H	-6.13694100	1.40363500	-1.76326800
H	-6.03730400	-0.01387100	-0.69058700
H	-5.19735000	-0.02096100	-2.27371000
H	-0.00000100	-0.16706500	3.78047600
C	2.87898200	2.68277900	-0.07060700
C	4.06619600	2.53519700	-0.70743400
C	-2.87898100	2.68277900	-0.07060800
C	-4.06619400	2.53519800	-0.70743800
N	2.42292300	1.41254500	0.22427600
N	-2.42292200	1.41254600	0.22427400
H	0.00000100	1.83445200	-0.76515300
H	4.75819100	3.26163700	-1.09992600
H	2.31901900	3.55852400	0.21284300
H	-2.31901900	3.55852400	0.21284300
H	-4.75818700	3.26163700	-1.09993300

cat2 -Michael acceptor

Basis set superposition error correction = 0.001242622 Hartree
Electronic energy (in solution) = -1818.00939 Hartree
Entropic correction (in solution) = -1817.62893 Hartree
Sum of electronic and thermal Free Energies (in solution) = -1817.63873 Hartree

C	-2.13117000	-3.27555200	1.92257700
C	-3.11364200	-2.85914300	1.11505600
H	-4.01938300	-3.44334900	0.99516800
C	-3.00647100	-1.58007300	0.39177000
H	2.30796400	1.05859900	-1.08466700
C	2.69824900	1.10191300	-0.07375400
C	3.80760600	1.25833300	2.49464300
C	3.46673800	0.06752900	0.44475500
C	2.47481600	2.20378300	0.74195500
C	3.01920400	2.29824800	2.01655300
C	4.02799500	0.13012600	1.71337100
H	2.82035300	3.17490200	2.62193700
H	4.62265500	-0.69864300	2.07937500
C	2.78727800	-2.00477000	-0.74266000
N	3.41734900	-2.96199300	-1.42326600
C	0.36829500	3.26460000	-0.04710800
N	0.00574800	4.49141100	-0.42172400
I	0.77471900	-1.90900300	-0.32889700
I	-0.85053000	1.61083100	0.05776500

C	2.78628600	-4.13868700	-2.02565300
H	3.56717800	-4.71488100	-2.51486900
H	2.04802600	-3.81837000	-2.75951700
H	2.31709600	-4.73811400	-1.24653500
C	-1.33911300	4.89406300	-0.84059800
H	-1.30332400	5.95217300	-1.08587900
H	-2.03964900	4.72682400	-0.02355900
H	-1.63166700	4.32032300	-1.71905600
O	-1.91511100	-1.04811500	0.18465900
H	4.23689600	1.31962600	3.48649900
H	5.83791800	-0.93681700	-0.58752800
H	3.17858300	4.83882700	0.26222500
C	4.95190800	-1.51509600	-0.79084500
C	4.76559900	-2.67612300	-1.46358800
C	2.14758700	4.58632600	0.07801700
C	1.09841000	5.32913200	-0.34900600
N	3.70741800	-1.10347200	-0.35222300
N	1.67930400	3.29761500	0.25647000
H	5.46145800	-3.32418000	-1.96992000
H	1.02442300	6.37078200	-0.61397100
H	-1.26021400	-2.63525900	2.05098600
C	-2.14662100	-4.54772900	2.69361400
H	-2.06788100	-4.33817900	3.76461700
H	-3.05180200	-5.12560000	2.50529200
H	-1.27235200	-5.15089100	2.42917700
C	-4.24889700	-0.92495400	-0.09992200
C	-4.16327700	-0.03321000	-1.17479400
C	-5.48440500	-1.16176800	0.50965900
C	-5.30199600	0.61226500	-1.63652500
H	-3.20691300	0.12868600	-1.65930900
C	-6.61979700	-0.49831700	0.05709900
H	-5.55814400	-1.84317200	1.34932000
C	-6.53000000	0.38384900	-1.01629800
H	-5.23647000	1.29047100	-2.47917800
H	-7.57380100	-0.67137100	0.54086800
H	-7.41833700	0.89223800	-1.37348700

COM1

Basis set superposition error correction = 0.004371735 Hartree

Electronic energy (in solution) = -2181.80182 Hartree

Entropic correction (in solution) = -2181.29794 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2181.30776 Hartree

C	-2.00865300	-3.17465300	-1.36931900
C	-2.72342500	-2.04360900	-1.32482700
H	-3.73812100	-2.05036100	-0.94257400

C	-2.17131900	-0.77639600	-1.82795800
H	3.00837300	1.41255600	0.04000400
C	2.73509400	0.96937100	0.99158200
C	2.12226800	-0.13812000	3.49253500
C	3.13616100	-0.31713400	1.32882300
C	2.00656700	1.67940700	1.93640200
C	1.69538100	1.14748600	3.18193300
C	2.84119400	-0.88167700	2.56301600
H	1.12570200	1.73690000	3.89088100
H	3.17133200	-1.88991800	2.78537500
C	3.47514400	-1.54315400	-0.80131700
N	4.47842800	-2.21986200	-1.36082500
C	0.68405100	3.40664300	0.72924000
N	0.58365900	4.73507000	0.77985900
I	1.57841100	-1.29686300	-1.56204500
I	-0.42849800	2.19629300	-0.50136900
C	4.43037200	-2.89594700	-2.65919600
H	5.40125700	-3.35481400	-2.82804400
H	4.22473700	-2.16613200	-3.44080600
H	3.65768200	-3.66360700	-2.64008400
C	-0.30699400	5.55773200	-0.04304800
H	-0.15775000	6.59368600	0.24872400
H	-1.34082600	5.26725100	0.14012600
H	-0.05342600	5.42764700	-1.09428200
O	-1.02715700	-0.67486400	-2.26534700
H	1.88252100	-0.56776000	4.45693400
H	5.75704400	-1.21808400	1.47152200
H	2.82412700	4.07114700	3.05903700
C	5.21303000	-1.48509600	0.58072600
C	5.56840700	-2.19600300	-0.51628700
C	2.07594700	4.14746500	2.28740700
C	1.44257900	5.21535900	1.74477100
N	3.90555700	-1.08002400	0.38611900
N	1.59573600	3.02449300	1.63974700
H	6.49256500	-2.68360800	-0.77865400
H	1.52251700	6.27013100	1.94960800
H	-1.00197800	-3.13639100	-1.78104700
C	-2.49917200	-4.50495600	-0.91969700
H	-1.79952700	-4.94048300	-0.20030200
H	-3.48875600	-4.43979500	-0.46485700
H	-2.53910000	-5.19038000	-1.77309000
C	-3.04132600	0.43940000	-1.82498400
C	-2.79293500	1.43738000	-2.77531200
C	-4.03982300	0.62923800	-0.86479100

C	-3.53536200	2.61156600	-2.76414700
H	-2.02117000	1.27962200	-3.52057200
C	-4.75972900	1.81897500	-0.83858500
H	-4.23973600	-0.13486400	-0.12283300
C	-4.51115300	2.80733400	-1.78838400
H	-3.35032200	3.37572000	-3.50995200
H	-5.51832000	1.97220200	-0.07999000
H	-5.08245200	3.72842300	-1.77186300
C	-1.97813700	-2.90808800	2.15475000
C	-2.78669600	-1.75169800	2.02541800
C	-4.16607100	-1.77237800	2.25994800
C	-4.73083100	-2.98144800	2.62796000
C	-3.94510500	-4.14521200	2.76653200
C	-2.58124900	-4.11916300	2.53586300
C	-0.63472200	-2.51422700	1.82981200
C	-0.67699200	-1.17837400	1.53383000
H	-4.76493700	-0.87398600	2.15891800
H	-5.79681800	-3.03490100	2.81767500
H	-4.42362000	-5.07316600	3.05837800
H	-1.98508800	-5.01940100	2.64104500
H	0.24669700	-3.13835300	1.81959000
H	0.12278100	-0.50681800	1.25850300
H	-2.26044000	0.24119600	1.51376000
N	-1.96653300	-0.71749100	1.64173600

Transition State1 (TS1)

Imaginary frequency -431.05 cm^{-1}

Basis set superposition error correction = 0.004505637 Hartree

Electronic energy (in solution) = -2181.76846 Hartree

Entropic correction (in solution) = -2181.26110 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2181.27081 Hartree

C	2.77719800	-2.45117100	-0.24307200
C	3.20032800	-1.44757300	0.68051200
H	4.21825400	-1.47006400	1.05196000
C	2.35133800	-0.41029400	1.04488900
H	-3.53049200	0.53288300	0.59011400
C	-3.65702700	0.33418700	-0.46842500
C	-4.10328400	-0.15785000	-3.18908400
C	-3.96472300	-0.94015900	-0.92862700
C	-3.54115200	1.34805300	-1.41125100
C	-3.76270700	1.12082800	-2.76386800
C	-4.19420500	-1.19991100	-2.27366700
H	-3.66210600	1.93766000	-3.46899800
H	-4.43321300	-2.20740800	-2.59347400
C	-3.05707400	-2.53818000	0.74280000

N	-3.55151100	-3.55620700	1.44765900
C	-2.03875600	3.06137100	-0.41825500
N	-2.10272300	4.37934500	-0.22593400
I	-1.11016300	-1.84166400	0.75189800
I	-0.46863400	1.80627700	0.07659300
C	-2.79314400	-4.38710900	2.38514500
H	-3.47896000	-5.11682600	2.80808100
H	-2.38619500	-3.76033000	3.17759600
H	-1.99145200	-4.89717600	1.85276900
C	-1.04953600	5.20330500	0.37048900
H	-1.41552600	6.22581700	0.40914500
H	-0.15422500	5.15354600	-0.24779400
H	-0.83713300	4.84868400	1.37823500
O	1.14296300	-0.31996400	0.62913100
H	-4.27883900	-0.34717400	-4.24047900
H	-6.14224200	-2.51636500	-0.24433000
H	-4.98118500	3.70864700	-1.61011800
C	-5.21301500	-2.75659200	0.24519200
C	-4.88982200	-3.71044800	1.15084100
C	-4.00148200	3.78921700	-1.16937700
C	-3.31345700	4.85171500	-0.68759800
N	-4.06282800	-2.02714600	0.00593600
N	-3.19796000	2.67775500	-0.98870600
H	-5.48318300	-4.47947300	1.61673700
H	-3.57072900	5.89592300	-0.62338400
H	1.70141900	-2.58807600	-0.30888400
C	3.55078300	-3.74886700	-0.25424300
H	3.30070500	-4.37480500	-1.11183200
H	4.62731200	-3.56848400	-0.24175000
H	3.29433800	-4.30081200	0.65526200
C	2.84040300	0.66414000	1.96908800
C	1.93567900	1.25799700	2.85468200
C	4.16831400	1.10257800	1.95798700
C	2.35163900	2.26173000	3.72317700
H	0.90745100	0.91276700	2.86858500
C	4.58151500	2.11540400	2.81861500
H	4.87578900	0.66406200	1.26217600
C	3.67582700	2.69534100	3.70433300
H	1.64448300	2.70508500	4.41525600
H	5.61053900	2.45586000	2.79421200
H	4.00035000	3.48223500	4.37574200
C	4.38094400	-1.40689100	-2.13759600
C	4.37737500	-0.03020200	-1.87381300
C	5.53474600	0.72755000	-1.74655200

C	6.73943900	0.05255600	-1.90210400
C	6.77156700	-1.32315700	-2.17443700
C	5.60039900	-2.06546600	-2.28727700
C	2.98474400	-1.84995100	-2.07311200
C	2.22591400	-0.64921100	-2.01305200
H	5.49520500	1.79016500	-1.53795600
H	7.67049000	0.60058300	-1.81760900
H	7.72902400	-1.81495200	-2.30094100
H	5.63546100	-3.12877000	-2.49493700
H	2.60394700	-2.73098000	-2.57137600
H	1.15343000	-0.52344900	-2.03075600
H	2.74052900	1.33194000	-1.63956800
N	3.03740700	0.37438000	-1.79735600

COM2

Basis set superposition error correction = 0.002080984 Hartree
Electronic energy (in solution) = -2181.77545 Hartree
Entropic correction (in solution) = -2181.26587 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2181.27557 Hartree

C	2.90233100	-2.40886200	-0.61073500
C	3.15863300	-1.55082600	0.58985400
H	4.08170000	-1.69891200	1.13959400
C	2.28416000	-0.58438000	0.97273400
H	-3.41040300	0.44304700	0.66704900
C	-3.63077000	0.34077800	-0.38949000
C	-4.31486900	0.09102900	-3.09327300
C	-3.98103700	-0.88983600	-0.93234400
C	-3.59334900	1.43587400	-1.24435300
C	-3.93363900	1.32780400	-2.58720100
C	-4.32810500	-1.02879100	-2.27023600
H	-3.89304600	2.20370900	-3.22393700
H	-4.59658900	-2.00491500	-2.65699200
C	-2.93606600	-2.61953000	0.51443000
N	-3.36869200	-3.71612100	1.13843500
C	-2.01679600	3.07128600	-0.22442200
N	-2.06676300	4.37195200	0.06663100
I	-0.99804100	-1.85873900	0.47543700
I	-0.41817300	1.77924500	0.07698600
C	-2.53278000	-4.62619600	1.92389500
H	-3.17762900	-5.39995300	2.33292200
H	-2.05786200	-4.07514600	2.73434400
H	-1.77944700	-5.07600500	1.27821700
C	-0.97382300	5.14991000	0.65277400
H	-1.33015800	6.16754300	0.79001800
H	-0.11983200	5.14431600	-0.02336700

H	-0.69912100	4.72086600	1.61554600
O	1.14805100	-0.36431200	0.34855400
H	-4.58224800	-0.00444900	-4.13801100
H	-6.08334500	-2.56846000	-0.26343200
H	-5.03143900	3.79777600	-1.16942400
C	-5.11969100	-2.83622500	0.13684500
C	-4.72177600	-3.87034900	0.91510900
C	-4.02452100	3.84818700	-0.78981800
C	-3.30402500	4.87456000	-0.27901700
N	-3.99905500	-2.05961400	-0.09820800
N	-3.21399700	2.72786000	-0.74197800
H	-5.27077700	-4.69625600	1.33571800
H	-3.55376300	5.91078900	-0.12281500
H	1.83660200	-2.64790300	-0.67620900
C	3.69977300	-3.70910000	-0.56965300
H	3.56598900	-4.29148600	-1.48438200
H	4.76574200	-3.51472600	-0.43147500
H	3.36296200	-4.31247600	0.27673600
C	2.57630900	0.27872200	2.16232200
C	1.52583000	0.66573800	3.00099800
C	3.87013800	0.72083600	2.45750800
C	1.76358400	1.45843700	4.11959900
H	0.51985900	0.32642000	2.77738000
C	4.10840300	1.51929900	3.57290100
H	4.69117000	0.45062100	1.80154200
C	3.05686600	1.88948300	4.40839500
H	0.94022000	1.73965300	4.76692400
H	5.11556700	1.86087300	3.78451200
H	3.24351400	2.51249800	5.27574500
C	4.56554200	-0.98816000	-2.01221000
C	4.38453800	0.39369000	-2.00312100
C	5.41391400	1.31511800	-1.98171400
C	6.70603500	0.79204300	-1.97508900
C	6.92259900	-0.58676100	-2.00016600
C	5.85817900	-1.49127300	-2.01864400
C	3.20778300	-1.63630400	-1.96578400
C	2.30604400	-0.46202900	-2.07608500
H	5.22322500	2.38129600	-1.97526300
H	7.55290000	1.46758200	-1.96019500
H	7.93852100	-0.96360300	-2.00959800
H	6.04609300	-2.55735800	-2.04947900
H	3.01528200	-2.33487300	-2.78607400
H	1.22960400	-0.46899400	-2.16795900
H	2.57788000	1.57104200	-2.10545500

N	2.98525600	0.63879600	-2.05389700

The indirect hydrogen proton transfer reaction pathway
Transition State2 TS2(a)
Imaginary frequency -290.94 cm^{-1}
Basis set superposition error correction = 0.002514549 Hartree
Electronic energy (in solution) = -2181.76725 Hartree
Entropic correction (in solution) = -2181.26223 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2181.27199 Hartree

C	3.13197400	2.19795300	-2.23734800
C	2.68538200	2.96960700	-1.02009200
H	3.27147800	3.83586700	-0.73687900
C	1.63977700	2.58952400	-0.24630900
H	-2.56343700	-1.33211800	1.12302100
C	-2.72673700	-1.86407100	0.19263800
C	-3.23678800	-3.29942400	-2.15695700
C	-2.05990400	-3.05043900	-0.08493500
C	-3.62996400	-1.39665300	-0.75416700
C	-3.89733100	-2.09910100	-1.92225400
C	-2.30397300	-3.77651800	-1.24401500
H	-4.60936800	-1.70279400	-2.63682300
H	-1.76517800	-4.69917100	-1.42496000
C	0.04237100	-2.98476200	1.24646600
N	0.64913500	-3.81247900	2.09794900
C	-3.76876300	1.06265600	-0.43654200
N	-4.75846100	1.93820900	-0.25391600
I	0.74032800	-1.14829600	0.62412500
I	-1.73339900	1.47180500	-0.53886700
C	1.93543400	-3.56734500	2.75396400
H	1.87503100	-2.65231100	3.34164300
H	2.71768800	-3.48375800	1.99971500
H	2.13760000	-4.41297700	3.40622600
C	-4.58939800	3.38395200	-0.09528800
H	-5.57866200	3.82520100	-0.00412400
H	-4.08361800	3.78886300	-0.97042900
H	-4.00973400	3.58512500	0.80501100
O	0.91419100	1.50200700	-0.49736900
H	-3.43648500	-3.85594100	-3.06386000
H	-2.06577300	-5.44051500	1.30392000
H	-6.34175000	-0.90975100	-0.44092700
C	-1.21460500	-4.80218100	1.47315900
C	-0.11579400	-4.94921100	2.25123300
C	-5.69900500	-0.04605100	-0.40214500
C	-5.96591900	1.27036800	-0.23138900

N	-1.10721800	-3.56883300	0.85707800
N	-4.32559400	-0.16204500	-0.52113000
H	0.19200600	-5.74948700	2.90334100
H	-6.89617900	1.79515800	-0.09095300
H	2.48595500	2.44251900	-3.09120700
C	4.57747400	2.51685100	-2.61552000
H	4.88200000	1.95329300	-3.50115100
H	4.68544200	3.58301000	-2.83014000
H	5.25506100	2.26567000	-1.79476300
C	1.27292600	3.35405700	0.98719700
C	0.65465700	2.69153900	2.05273800
C	1.51598000	4.72799500	1.10822600
C	0.31437200	3.37303800	3.21802700
H	0.44313300	1.63237300	1.96617900
C	1.17169300	5.41104600	2.26966600
H	1.96119000	5.27179200	0.28277200
C	0.57238600	4.73626300	3.33187600
H	-0.15575400	2.83873000	4.03620700
H	1.36223200	6.47608000	2.34160300
H	0.30194200	5.27088100	4.23534200
C	3.74127600	-0.09626300	-1.02594900
C	3.86710700	-1.39166800	-1.53937100
C	4.45384200	-2.44249400	-0.84829300
C	4.95055300	-2.14859000	0.41577600
C	4.85015400	-0.85670300	0.95107400
C	4.24129100	0.17695700	0.24660000
C	2.93429700	0.68894500	-1.99521700
C	2.75934400	-0.22340800	-3.09640100
H	4.51617900	-3.43658100	-1.27441000
H	5.42372900	-2.93155900	0.99655400
H	5.25139100	-0.66272900	1.93912300
H	4.15158000	1.16736600	0.67725000
H	1.85747500	0.74787600	-1.48669900
H	2.25403800	-0.04218900	-4.03652300
H	3.18157000	-2.22101200	-3.40425500
N	3.25554100	-1.40116100	-2.80687000

COM3(a)

Basis set superposition error correction = 0.002092067 Hartree

Electronic energy (in solution) = -2181.80806 Hartree

Entropic correction (in solution) = -2181.30214 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2181.31189 Hartree

C	3.75067100	2.10400700	-2.02684500
C	3.25495000	2.74951800	-0.74855600
H	3.89412800	3.51219400	-0.31716400

C	2.10991200	2.49948300	-0.10553800
H	-2.74395100	-1.15429800	1.08860400
C	-2.85719200	-1.65269300	0.13241900
C	-3.22905900	-2.99300200	-2.29915500
C	-2.22996100	-2.86398400	-0.12621600
C	-3.65738100	-1.11946100	-0.86939700
C	-3.85504200	-1.77129000	-2.07972900
C	-2.40435600	-3.54344200	-1.32481500
H	-4.48790100	-1.32156300	-2.83591900
H	-1.89645300	-4.48706000	-1.48634300
C	-0.22040900	-2.97121000	1.32929900
N	0.24664000	-3.81606900	2.24854100
C	-3.73259900	1.33431800	-0.49841500
N	-4.69231000	2.24377500	-0.33023400
I	0.71368800	-1.26377300	0.68367000
I	-1.70903900	1.68986400	-0.54477400
C	1.50518000	-3.66685600	2.98387700
H	1.49947500	-2.72098500	3.52379300
H	2.34063400	-3.70503600	2.28537700
H	1.57434500	-4.49197400	3.68832100
C	-4.48226500	3.67973200	-0.12877000
H	-5.46030600	4.14960900	-0.06654300
H	-3.92964100	4.08748300	-0.97392900
H	-3.93446600	3.83940400	0.79935400
O	1.20464000	1.53981100	-0.51383100
H	-3.37389100	-3.51152100	-3.23835500
H	-2.56596100	-5.19799000	1.33138300
H	-6.36333500	-0.54111800	-0.66586600
C	-1.66674800	-4.64047700	1.53504300
C	-0.63976700	-4.86274800	2.39047100
C	-5.69311600	0.29758800	-0.57589800
C	-5.92031500	1.61827200	-0.37685100
N	-1.39448700	-3.45217200	0.88342900
N	-4.32219900	0.13386600	-0.64386000
H	-0.45749300	-5.66159600	3.08973200
H	-6.83665500	2.17211500	-0.25856500
H	3.25639800	2.60032800	-2.87200000
C	5.26221200	2.33859600	-2.16680500
H	5.62458500	1.93194500	-3.11292700
H	5.48808900	3.40746200	-2.13720100
H	5.80284600	1.85082400	-1.35125600
C	1.66659400	3.20153200	1.12147900
C	0.84686600	2.55345100	2.05109000
C	2.04984600	4.52526500	1.36949000

C	0.43625200	3.20422000	3.21077400
H	0.53516400	1.53079900	1.87808100
C	1.64100600	5.17263500	2.52902000
H	2.65443200	5.05703100	0.64396400
C	0.83332200	4.51509000	3.45519500
H	-0.19326200	2.68339300	3.92332400
H	1.94287200	6.19909100	2.70330500
H	0.51153800	5.02438400	4.35626900
C	3.79019300	-0.41577000	-1.20879700
C	3.39336500	-1.64162600	-1.79820700
C	3.58886700	-2.87421200	-1.16668600
C	4.18516800	-2.86050600	0.08194000
C	4.57607600	-1.65208000	0.69586800
C	4.38596500	-0.43435200	0.06587500
C	3.43750200	0.63168000	-2.13903200
C	2.84715700	0.00738300	-3.20997200
H	3.28069000	-3.79964500	-1.64009200
H	4.35552400	-3.79744800	0.60011500
H	5.03541400	-1.68258400	1.67745600
H	4.69421700	0.49006100	0.54250900
H	1.55862700	1.09190100	-1.30336600
H	2.44991100	0.43828900	-4.11768000
H	2.43284700	-2.02556800	-3.65485000
N	2.81817200	-1.34991600	-3.00977900

P(a)

Electronic energy (in solution) = -826.02516 Hartree

Entropic correction (in solution) = -825.75399 Hartree

Sum of electronic and thermal Free Energies (in solution) = -825.76429 Hartree

C	0.68276700	2.12563200	0.28735400
C	-0.66517300	1.45531000	0.47258200
H	-1.14563500	1.56225800	1.43857600
C	-1.30004100	0.73406200	-0.46132100
O	-0.78162800	0.48295600	-1.69885000
H	0.57474300	2.92825800	-0.45423200
C	1.13878800	2.76032900	1.60745100
H	2.08319700	3.29121600	1.47215500
H	0.38996200	3.46861500	1.97137600
H	1.28222000	1.99159500	2.37186900
C	-2.62487400	0.09666100	-0.26807300
C	-2.96738900	-1.03624700	-1.01420900
C	-3.55035100	0.60401000	0.65193400
C	-4.19710300	-1.66096100	-0.82714800
H	-2.26328400	-1.43056000	-1.73647800
C	-4.77668700	-0.02276000	0.83780400

H	-3.31899600	1.50205800	1.21302900
C	-5.10486000	-1.15951700	0.10093500
H	-4.44470800	-2.54193300	-1.40859900
H	-5.48362800	0.38487400	1.55155000
H	-6.06377400	-1.64428800	0.24426800
C	2.10699500	-0.10464800	0.29481400
C	3.15785700	-0.60384800	-0.51347100
C	3.76235500	-1.84285800	-0.27348500
C	3.29456500	-2.58195200	0.79885100
C	2.24934400	-2.10547300	1.61778800
C	1.65326600	-0.87986100	1.37684200
C	1.73407100	1.18073400	-0.24536300
C	2.55294000	1.39264800	-1.32561800
H	4.56501200	-2.20487900	-0.90593200
H	3.73991500	-3.54654500	1.01453100
H	1.91047200	-2.71347900	2.44880200
H	0.85012500	-0.52188900	2.01187400
H	0.15777400	0.72138200	-1.70829900
H	2.59110600	2.23627600	-1.99995400
H	4.09752200	0.24281700	-2.22117700
N	3.40745500	0.32900100	-1.48836500

The direct hydrogen proton transfer reaction pathway

Transition State2 TS2(b)

Imaginary frequency -1477.20 cm^{-1}

Basis set superposition error correction = 0.001934023 Hartree

Electronic energy (in solution) = -2181.73002 Hartree

Entropic correction (in solution) = -2181.22970 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2181.23938 Hartree

C	3.10280400	-2.12786400	0.51415800
C	3.28793200	-0.96603600	1.49093900
H	4.17068400	-0.94515600	2.12034900
C	2.25508600	-0.05567000	1.69330000
H	-3.47667900	0.45914100	0.20118800
C	-3.43333100	0.13277000	-0.83173400
C	-3.42497900	-0.69528300	-3.50664400
C	-3.62515800	-1.20023200	-1.17309900
C	-3.20532500	1.03537500	-1.86316900
C	-3.20161800	0.64091500	-3.19530700
C	-3.62686500	-1.62699800	-2.49505600
H	-3.02195700	1.37421900	-3.97273100
H	-3.77952800	-2.67566300	-2.72231600
C	-2.96141300	-2.54091600	0.81089000
N	-3.53748500	-3.48759800	1.55213800
C	-1.94741500	2.93120600	-0.86258000

N	-2.09485800	4.25620100	-0.83521700
I	-1.06439500	-1.75719400	1.04859100
I	-0.42667900	1.82961600	0.00753800
C	-2.92239100	-4.16053000	2.69805300
H	-2.68291800	-3.42552900	3.46526300
H	-2.02196800	-4.68060100	2.37374800
H	-3.64257100	-4.87664600	3.08526300
C	-1.18655600	5.19613700	-0.17475300
H	-0.20138500	5.13500800	-0.63517200
H	-1.12610900	4.95629000	0.88609300
H	-1.59334500	6.19579800	-0.30441800
O	1.13797700	-0.13916000	1.07542400
H	-3.42406700	-1.01494400	-4.54090500
H	-5.84090400	-2.78573600	-0.65157100
H	-4.68244100	3.27244100	-2.56469700
C	-4.99866700	-2.91980300	0.00662600
C	-4.80408200	-3.73922600	1.06747300
C	-3.79087900	3.45815800	-1.98901800
C	-3.23357800	4.60463300	-1.53153800
N	-3.84406900	-2.17231000	-0.13773200
N	-2.98282300	2.42159700	-1.55805400
H	-5.44562400	-4.47246200	1.52724400
H	-3.53995200	5.63285700	-1.62902100
H	2.07133700	-2.48987600	0.53984900
C	4.05313800	-3.28655800	0.77480600
H	4.03322700	-4.00852000	-0.04448100
H	5.07890500	-2.94044400	0.91099800
H	3.75392400	-3.79731900	1.69324500
C	2.45217900	1.10912300	2.61560500
C	1.33546600	1.63588600	3.27159200
C	3.70535900	1.69008000	2.83369100
C	1.46844100	2.71630200	4.13800500
H	0.36445000	1.18106300	3.10786600
C	3.83625800	2.77643000	3.69288200
H	4.57733700	1.30601400	2.31607300
C	2.71949800	3.29154800	4.34820000
H	0.59662000	3.10926200	4.64895900
H	4.81067100	3.22659200	3.84540600
H	2.82405800	4.13775800	5.01770500
C	4.49012400	-1.33182300	-1.70660200
C	4.06725100	-0.67227300	-2.87605500
C	4.92019700	-0.36529900	-3.93283100
C	6.24359000	-0.75527400	-3.80445000
C	6.69288600	-1.41655600	-2.64979600

C	5.83594400	-1.70014800	-1.59565000
C	3.31972700	-1.38623100	-0.81186900
C	2.25341200	-0.85404200	-1.57867700
H	4.55715300	0.15309200	-4.81236000
H	6.94238100	-0.54507500	-4.60545900
H	7.73424100	-1.70833300	-2.57910900
H	6.21285700	-2.19592700	-0.71130100
H	3.51522500	-0.38456500	0.03584600
H	1.21205000	-0.77575800	-1.30552800
H	2.14591600	0.07796000	-3.44043700
N	2.70769900	-0.40744300	-2.74943900

COM3(b)

Basis set superposition error correction = 0.00122609 Hartree
Electronic energy (in solution) = -2181.82586 Hartree
Entropic correction (in solution) = -2181.31770 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2181.32744 Hartree

C	-3.15239000	-2.30719900	0.96482900
C	-2.46389300	-1.29383300	1.92249500
H	-3.11414000	-1.13051700	2.78233400
C	-2.14397900	-0.00625500	1.20801300
C	3.95618400	-0.05364000	-0.20383100
C	5.21141000	-0.19776100	2.29652700
C	4.22651800	-1.27562800	0.39794800
C	4.30551800	1.09470500	0.49444300
C	4.92985800	1.04153900	1.73384900
C	4.85151600	-1.36589100	1.63467600
H	5.18583300	1.96076600	2.24746100
H	5.04524400	-2.33940800	2.06978900
C	2.60766100	-2.91355700	-0.52476000
N	2.69072600	-4.09682300	-1.13257500
C	2.82439100	2.91551200	-0.32204600
N	3.00725800	4.12926800	-0.84153700
I	0.88882900	-1.89614800	-0.02326000
I	1.01835000	2.01485000	0.06824400
C	1.55541700	-4.91350900	-1.56856600
H	1.95535000	-5.80547400	-2.04362100
H	0.95650800	-4.35162000	-2.28388100
H	0.95638400	-5.19212900	-0.70262500
C	1.94577900	5.05330000	-1.24754800
H	1.33294200	4.58541600	-2.01692100
H	2.42268200	5.94458700	-1.64678200
H	1.33984300	5.31314900	-0.38065900
O	-1.08923500	0.08152900	0.58576900
H	5.69773500	-0.25317300	3.26201800

H	5.81864400	-3.30106900	-0.63788800
H	6.05580400	3.06825400	-0.35292100
C	4.75460800	-3.44014100	-0.73341800
C	4.01852400	-4.44273200	-1.27090200
C	5.00726000	3.29375800	-0.45520600
C	4.35907000	4.38446200	-0.93039400
N	3.86081000	-2.48967800	-0.27756400
N	4.03669200	2.38182300	-0.08497300
H	4.31085200	-5.36585900	-1.74316800
H	4.72896200	5.31437300	-1.32889100
H	-2.45365800	-2.51093000	0.14507000
C	-3.41347300	-3.60853800	1.72071700
H	-3.85836100	-4.35469500	1.05890900
H	-2.48153700	-4.01263000	2.12371400
H	-4.09770100	-3.43954500	2.55691900
C	-3.11754600	1.12116900	1.17397700
C	-2.97986000	2.08397900	0.16539900
C	-4.19245400	1.20825100	2.06371200
C	-3.90409700	3.11129100	0.04342500
H	-2.16770400	1.99617100	-0.54674700
C	-5.11306000	2.24517300	1.94594400
H	-4.32120200	0.47788700	2.85172300
C	-4.97446200	3.19131900	0.93470100
H	-3.80004600	3.84160800	-0.75059400
H	-5.94179100	2.30909300	2.64130300
H	-5.70075900	3.99039600	0.83745300
C	-4.46441800	-0.93959100	-0.84159300
C	-5.77664600	-0.41306700	-0.93185400
C	-6.17409600	0.42255400	-1.98177500
C	-5.22956500	0.72277100	-2.94861200
C	-3.91886700	0.20357500	-2.88170300
C	-3.52902900	-0.62045300	-1.84047800
C	-4.39935300	-1.71308200	0.37046500
C	-5.64466000	-1.64020800	0.93847000
H	-7.18173600	0.81980300	-2.03031600
H	-5.50211300	1.36921100	-3.77519000
H	-3.20874100	0.46133800	-3.65934000
H	-2.51509000	-1.00625900	-1.78947100
H	-1.52088000	-1.71854000	2.27623600
H	-6.01309000	-2.06961500	1.85865300
H	-7.44447900	-0.67296200	0.35747500
N	-6.47130000	-0.86183200	0.16216000
H	3.50909100	-0.00003900	-1.19032500

2.1.4 Cat3 ($(C_4H_5N_2I^+)_2C_6H_3CF_3$) catalyzed reaction

cat3 ($(C_4H_5N_2I^+)_2C_6H_3CF_3$)

Electronic energy (in solution) = -1692.80627 Hartree

Entropic correction (in solution) = -1692.58446 Hartree

Sum of electronic and thermal Free Energies (in solution) = -1692.59449 Hartree

C	-0.01029900	-0.78792200	1.29216200
C	-0.00300600	1.98104500	1.00385600
C	-1.19424600	-0.07120900	1.22309300
C	1.18041700	-0.07793900	1.21891000
C	1.20729700	1.30017700	1.07676900
C	-1.21438400	1.30990100	1.08194700
H	2.15156300	1.83233700	1.03884800
H	-2.15585600	1.84509400	1.05232600
C	-3.33959900	-0.91321900	0.31331600
N	-4.34838700	-1.65098000	0.77188700
C	3.32425000	-0.93141800	0.31368900
N	4.32463600	-1.67957500	0.77390300
I	-3.17984400	-0.16812600	-1.58589900
I	3.18037600	-0.17549100	-1.58246400
C	-5.54270500	-2.03608400	0.01485400
H	-6.18723000	-2.59631700	0.68687300
H	-5.25151100	-2.66118800	-0.82834000
H	-6.05614000	-1.13949300	-0.32958400
C	5.52067100	-2.06906800	0.02184300
H	6.15332300	-2.64482900	0.69194000
H	6.04718200	-1.17427600	-0.30723000
H	5.22951000	-2.68055700	-0.83126300
C	-2.88668200	-1.47378400	2.41049400
C	-4.08473100	-2.01099000	2.07609900
C	2.85535500	-1.49948500	2.40538200
C	4.05092000	-2.04445000	2.07481200
N	-2.43443800	-0.78633900	1.29965600
N	2.41488800	-0.80239900	1.29569200
H	-0.01334400	-1.86732000	1.39206000
H	-4.77924200	-2.60883800	2.64243200
H	-2.31635900	-1.49834300	3.32411400
H	2.27994000	-1.52378700	3.31584800
H	4.73754800	-2.65060900	2.64193100
C	0.02396900	3.47366100	0.82071200
F	-1.16679600	4.03579400	1.04819300
F	0.38411500	3.80828000	-0.42992600
F	0.90625200	4.05810400	1.64369700

cat3 -Michael acceptor

Basis set superposition error correction = 0.001301979 Hartree

Electronic energy (in solution) = -2155.04595 Hartree
Entropic correction (in solution) = -2154.66483 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2154.67463 Hartree

C	-2.82831400	-3.39311700	1.81884100
C	-3.68977200	-2.79891500	0.98472000
H	-4.68788000	-3.19789500	0.84210400
C	-3.31899400	-1.57694100	0.25180900
C	2.58661000	0.99208300	0.33195000
C	2.78333400	0.55942600	3.10109500
C	3.09124600	-0.20491900	0.85042400
C	2.10547600	1.93015200	1.24751600
C	2.21034300	1.72576700	2.61727700
C	3.20154100	-0.42373000	2.21392100
H	1.82109700	2.48158900	3.28912900
H	3.59938800	-1.36829200	2.56533700
C	2.57649400	-2.20814200	-0.48776400
N	3.26620300	-3.09248300	-1.20283300
C	0.13500300	3.12165500	0.37748000
N	-0.17138400	4.37991400	0.07001600
I	0.54967000	-2.17608200	-0.14354700
I	-1.06294800	1.45574800	0.20621100
C	2.70153200	-4.25429600	-1.89467700
H	3.51926800	-4.76975800	-2.39134100
H	1.97398900	-3.91664800	-2.63154800
H	2.23286000	-4.91581900	-1.16729000
C	-1.46683600	4.84355800	-0.43435000
H	-1.37736200	5.90705800	-0.63984500
H	-2.23187200	4.67443400	0.32223100
H	-1.70943800	4.30891700	-1.35169600
O	-2.14718700	-1.21242100	0.14507300
H	2.86908300	0.39907900	4.16810000
H	5.57439400	-1.00780700	-0.19823200
H	2.92427500	4.60705600	1.09306200
C	4.72101700	-1.61278300	-0.45605100
C	4.60177900	-2.74186300	-1.19400200
C	1.91370100	4.39251100	0.78755700
C	0.92013100	5.18659100	0.32052500
N	3.44632500	-1.28313100	-0.03135900
N	1.41021100	3.10672500	0.81127100
H	5.33817300	-3.32962000	-1.71638900
H	0.88437300	6.24806500	0.13998500
H	-1.84803900	-2.94157300	1.96067900
C	-3.11545400	-4.62775800	2.59671100
H	-4.11760700	-5.00860800	2.39862800

H	-2.38067900	-5.40048600	2.34990000
C	-4.39578200	-0.76695200	-0.38137100
C	-4.08179000	0.01827600	-1.49627300
C	-5.69450700	-0.75362700	0.13505000
C	-5.05761000	0.80822600	-2.08849300
H	-3.07963600	-0.01699800	-1.90917300
C	-6.66403400	0.05525900	-0.44808000
H	-5.94356100	-1.35189800	1.00381800
C	-6.34779700	0.83171800	-1.55978700
H	-4.81656700	1.40267000	-2.96194200
H	-7.66611700	0.07727700	-0.03648500
H	-7.10838600	1.45302900	-2.01875400
H	-3.00941300	-4.42854600	3.66741500
C	2.61007800	1.21137400	-1.16824900
F	2.31738200	2.46241200	-1.52550300
F	1.74371100	0.40965000	-1.80594500
F	3.82524400	0.94053800	-1.66231200

COM1

Basis set superposition error correction = 0.004364071 Hartree
Electronic energy (in solution) = -2518.83756 Hartree
Entropic correction (in solution) = -2518.33347 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2518.34327 Hartree

C	-3.08705300	-2.67250600	-1.24043900
C	-3.52001100	-1.41286600	-1.37306700
H	-4.56725900	-1.17373900	-1.22396400
C	-2.60360600	-0.32528900	-1.74210700
C	2.82813200	0.28730900	1.13972700
C	1.44976200	-0.74847900	3.35982500
C	2.78381000	-1.08706300	1.39703400
C	2.08998700	1.11701400	1.98654100
C	1.41745400	0.61190400	3.09201400
C	2.11309600	-1.60688800	2.49263700
H	0.86220200	1.29607200	3.72288400
H	2.10885200	-2.67946200	2.64773900
C	2.78766200	-2.50703400	-0.61610400
N	3.61294100	-3.39274900	-1.16692800
C	1.17865900	3.06747200	0.77860400
N	1.30787500	4.38998900	0.85505300
I	0.92796800	-1.92928700	-1.28086400
I	0.00823600	2.02777600	-0.55184300
C	3.34375900	-4.16195200	-2.38454800
H	4.22669500	-4.75801700	-2.59878600
H	3.15084900	-3.47697500	-3.20889800
H	2.48698200	-4.81368600	-2.21876800

C	0.62561100	5.36808100	0.00262000
H	0.91354600	5.20642600	-1.03534100
H	0.94029800	6.35720200	0.32491600
H	-0.45196900	5.26338400	0.12365400
O	-1.39743200	-0.49453000	-1.91924500
H	0.92630200	-1.14423300	4.22076600
H	5.28134300	-2.37492500	1.45270500
H	3.27002600	3.31575000	3.23738800
C	4.62763900	-2.62153600	0.63271600
C	4.76203200	-3.48013800	-0.40574700
C	2.59217800	3.53193700	2.42838000
C	2.18240700	4.69947000	1.87581600
N	3.39444800	-2.01220300	0.48268600
N	1.96029300	2.52217100	1.72873000
H	5.56539400	-4.14384200	-0.67870700
H	2.42845000	5.72185400	2.11011800
H	-2.03431200	-2.88130900	-1.41792200
C	-3.94707700	-3.83251900	-0.88379700
H	-3.52089600	-4.36599300	-0.02915500
H	-4.96576900	-3.52375800	-0.64433600
H	-3.97339500	-4.54357100	-1.71646000
C	-3.16154000	1.04882500	-1.92420300
C	-2.54566100	1.90086800	-2.84782200
C	-4.23377700	1.51358200	-1.15820300
C	-2.99727600	3.20532000	-3.00216800
H	-1.72311900	1.52851500	-3.44940800
C	-4.66432300	2.82943200	-1.29497100
H	-4.71662600	0.86136400	-0.43939800
C	-4.05007800	3.67327900	-2.21747300
H	-2.52838400	3.85788700	-3.72937400
H	-5.48236400	3.19432400	-0.68492200
H	-4.39619300	4.69441200	-2.32973900
C	-3.31355900	-2.15304300	2.13894100
C	-3.74067900	-0.82490700	1.89286300
C	-5.07028900	-0.42256200	2.05919400
C	-5.97871900	-1.38311400	2.47025100
C	-5.57780600	-2.71310800	2.71576800
C	-4.25990100	-3.10426300	2.55661900
C	-1.90276100	-2.19301700	1.86648000
C	-1.54042400	-0.93009500	1.48359900
H	-5.37242800	0.60260600	1.87564100
H	-7.01791700	-1.10770200	2.60941700
H	-6.31812900	-3.43684200	3.03716300
H	-3.95990800	-4.12896400	2.74864900

H	-1.24403700	-3.04560100	1.94287800
H	-0.56965500	-0.54725900	1.20724800
H	-2.63752500	0.88305600	1.28160000
N	-2.64003800	-0.10705900	1.48724400
C	3.69566500	0.79251500	0.00280400
F	3.82936300	2.11948100	-0.01248900
F	3.21178000	0.43535800	-1.19616500
F	4.92897600	0.27832800	0.09217200

Transition State1 (TS1)

Imaginary frequency -429.60 cm^{-1}

Basis set superposition error correction = 0.004681476 Hartree

Electronic energy (in solution) = -2518.80498 Hartree

Entropic correction (in solution) = -2518.29946 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2518.30917 Hartree

C	3.29594100	-2.16578400	-0.82290100
C	3.47677800	-1.45503600	0.40312900
H	4.39565400	-1.59191800	0.96128300
C	2.52814800	-0.53888900	0.83631000
C	-3.55011700	0.22469500	-0.67461400
C	-3.24061000	-0.29090800	-3.41826700
C	-3.58080600	-1.07960000	-1.17975100
C	-3.26563000	1.25292400	-1.57642600
C	-3.12379000	1.00381100	-2.93537500
C	-3.44050000	-1.34205300	-2.53300900
H	-2.90186400	1.83243100	-3.59742000
H	-3.47199100	-2.36929900	-2.87596100
C	-2.62766600	-2.77943300	0.32814800
N	-3.08598200	-3.83477500	0.99676300
C	-1.86245400	2.99289600	-0.55298800
N	-1.98025900	4.29319400	-0.29276500
I	-0.69750600	-2.03834100	0.26254500
I	-0.26512900	1.73851100	-0.13552700
C	-2.27290200	-4.73095800	1.82293100
H	-1.51607300	-5.20892500	1.20262700
H	-2.93409500	-5.48360400	2.24475300
H	-1.80558300	-4.15820900	2.62286300
C	-0.95529600	5.12494100	0.34133000
H	-1.34281100	6.13865300	0.39790100
H	-0.04914800	5.10717800	-0.26240900
H	-0.75378400	4.74838600	1.34337700
O	1.42665400	-0.33944300	0.20904400
H	-3.13487200	-0.48685000	-4.47755700
H	-5.78458600	-2.64857700	-0.41432300
H	-4.85334200	3.56890600	-1.67006200

C	-4.82562800	-2.93251900	-0.01399800
C	-4.44813100	-3.94940800	0.79613700
C	-3.87159300	3.67037900	-1.23822300
C	-3.21961800	4.73465500	-0.71096900
N	-3.68251400	-2.20208900	-0.28726200
N	-3.01514500	2.59179300	-1.12639400
H	-5.01702300	-4.74302800	1.25115500
H	-3.51768500	5.76341400	-0.59473000
H	2.26391100	-2.25077000	-1.15353300
C	4.10113500	-3.42937600	-1.01246900
H	4.04947800	-3.80711900	-2.03430400
H	5.14629500	-3.27865800	-0.73576600
H	3.68837300	-4.19438100	-0.34755300
C	2.76424400	0.25347500	2.08589600
C	1.66803800	0.62281200	2.87182000
C	4.04647100	0.65079000	2.47872900
C	1.84941100	1.36321400	4.03529000
H	0.67301700	0.30947700	2.57401800
C	4.22646700	1.40189900	3.63630600
H	4.90390900	0.38878200	1.86804900
C	3.12963900	1.75808400	4.41811800
H	0.99302000	1.63204200	4.64344300
H	5.22366700	1.71394700	3.92556400
H	3.27212700	2.34098000	5.32098300
C	5.23022800	-0.66437500	-1.95179700
C	5.09254000	0.58706800	-1.33476200
C	6.14747600	1.26487300	-0.73689600
C	7.38948700	0.64293900	-0.77917800
C	7.55686900	-0.60453800	-1.39837700
C	6.48464800	-1.27144400	-1.98223100
C	3.88176500	-1.09444100	-2.33371100
C	3.06490900	0.05078300	-2.12923500
H	6.00443500	2.22831100	-0.26195300
H	8.24511900	1.13359100	-0.33032200
H	8.54235800	-1.05483400	-1.42221400
H	6.62320100	-2.23642100	-2.45616200
H	3.67086700	-1.80268700	-3.12306400
H	2.01852300	0.18643900	-2.35890900
H	3.36592300	1.84186200	-1.11757800
N	3.74996000	0.96874600	-1.46554600
C	-3.85469200	0.45417500	0.79313900
F	-4.03864000	1.73984000	1.09763700
F	-2.88070900	-0.00238300	1.59357100
F	-4.97638700	-0.19129700	1.14293800

COM2

Basis set superposition error correction = 0.002311476 Hartree

Electronic energy (in solution) = -2518.81248 Hartree

Entropic correction (in solution) = -2518.30230 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2518.31200 Hartree

C	3.37715700	-2.36854700	-0.55080200
C	3.44292100	-1.53904000	0.69471200
H	4.29581900	-1.66459100	1.35274000
C	2.48001100	-0.62987500	0.99381600
C	-3.44482000	0.31634200	-0.71634300
C	-3.10955000	-0.12306700	-3.47027800
C	-3.50889600	-0.97027400	-1.26238800
C	-3.11453900	1.36283300	-1.58080800
C	-2.95938700	1.15135800	-2.94474200
C	-3.35603200	-1.19411000	-2.62127500
H	-2.70168400	1.99320100	-3.57640100
H	-3.41375500	-2.20895200	-2.99659400
C	-2.62046000	-2.75852200	0.17951400
N	-3.11744900	-3.83404500	0.78637200
C	-1.66660500	3.02729400	-0.49819200
N	-1.74813000	4.32273800	-0.20096600
I	-0.66918000	-2.02936300	0.19155800
I	-0.12079800	1.69255200	-0.09064500
C	-2.34295300	-4.79683600	1.57279400
H	-1.51439100	-5.16998600	0.97285000
H	-3.00567900	-5.61738500	1.83585400
H	-1.97231500	-4.31407600	2.47609100
C	-0.70032500	5.10375100	0.45930000
H	-1.05990700	6.12504500	0.55323100
H	0.20410800	5.08372700	-0.14692800
H	-0.50626600	4.68614500	1.44644500
O	1.41984000	-0.44191800	0.23664700
H	-2.99394000	-0.28919800	-4.53362800
H	-5.77052400	-2.49481300	-0.57158100
H	-4.63455800	3.72772300	-1.61147500
C	-4.82326100	-2.82631600	-0.18038300
C	-4.48174900	-3.89545600	0.57609600
C	-3.65270100	3.78577500	-1.17208100
C	-2.97194800	4.81395700	-0.61093800
N	-3.65588200	-2.11875400	-0.40972200
N	-2.82864900	2.67940700	-1.08809100
H	-5.07655900	-4.69524600	0.98492400
H	-3.23923200	5.84751800	-0.46580800
H	2.34058800	-2.66137200	-0.74568800

C	4.23609900	-3.62544300	-0.44994500
H	4.23656000	-4.18712300	-1.38710900
H	5.26819500	-3.38019200	-0.18948600
H	3.84207800	-4.27043400	0.33899400
C	2.57288000	0.19824500	2.23860800
C	1.40816500	0.48423200	2.95898800
C	3.79172000	0.70478100	2.70138600
C	1.46107700	1.24337900	4.12368900
H	0.45873500	0.09369000	2.60679400
C	3.84497100	1.46993700	3.86336200
H	4.69956700	0.51100100	2.13943000
C	2.68073900	1.74086400	4.57880100
H	0.55105300	1.44698900	4.67726400
H	4.79593800	1.86252900	4.20586600
H	2.72284500	2.33817900	5.48252300
C	5.10313400	-0.80807500	-1.70811200
C	4.83666800	0.55973700	-1.69610700
C	5.79638100	1.54000700	-1.53041800
C	7.10805600	1.09501100	-1.37452200
C	7.41173700	-0.26725000	-1.39925600
C	6.41594800	-1.23281600	-1.56553000
C	3.79222900	-1.53722900	-1.83926200
C	2.83840100	-0.41559600	-2.03344800
H	5.54057300	2.59243600	-1.52732600
H	7.90278200	1.81939300	-1.24282400
H	8.44289400	-0.58240000	-1.29106100
H	6.67192500	-2.28469700	-1.59328300
H	3.74324100	-2.21938400	-2.69401600
H	1.78271400	-0.48387600	-2.25298400
H	2.98672900	1.63055400	-1.99502400
N	3.44117200	0.72261800	-1.91312900
C	-3.77325900	0.50824000	0.75145300
F	-3.88656400	1.78992700	1.10414800
F	-2.85446300	-0.03842000	1.55939600
F	-4.94294200	-0.07990000	1.04304400

The indirect hydrogen proton transfer reaction pathway

Transition State2 TS2(a)

Imaginary frequency -261.33 cm^{-1}

Basis set superposition error correction = 0.002762404 Hartree

Electronic energy (in solution) = -2518.80422 Hartree

Entropic correction (in solution) = -2518.29760Hartree

Sum of electronic and thermal Free Energies (in solution) = -2518.30735 Hartree

C	-3.71952900	-2.30083700	-1.79288400
C	-3.22623400	-2.88615600	-0.49207500

H	-3.85808700	-3.61970900	-0.00566200
C	-2.08338000	-2.47954600	0.11242900
C	2.81690700	1.51498400	-0.26368800
C	2.50112200	2.42434400	-2.90370100
C	2.04348100	2.64213500	-0.56085600
C	3.35257700	0.80666500	-1.34211300
C	3.21086300	1.26104600	-2.64699400
C	1.88921700	3.10339900	-1.85849700
H	3.64524000	0.67976900	-3.45169800
H	1.28233400	3.98349200	-2.03596200
C	0.10871200	2.98936000	0.93233100
N	-0.26835000	3.91278400	1.81343900
C	3.34198700	-1.61450100	-0.92041900
N	4.26113200	-2.57443600	-0.82558600
I	-0.93092700	1.29930000	0.38565100
I	1.27283800	-1.76537600	-0.69723300
C	-1.52621700	3.90817000	2.56478200
H	-1.54320700	4.80304700	3.18166700
H	-1.56650500	3.02154500	3.19642900
H	-2.36393200	3.91996400	1.86837600
C	3.98377800	-3.98666800	-0.55502600
H	3.59090100	-4.09211800	0.45550700
H	4.91945300	-4.53199700	-0.64827800
H	3.26586500	-4.36012500	-1.28339200
O	-1.30119800	-1.53044000	-0.39634300
H	2.39302000	2.78088800	-3.91997800
H	2.66750100	4.97942500	0.85386700
H	6.06524800	0.08826300	-1.40145000
C	1.72011700	4.51866500	1.07979700
C	0.71804200	4.87310000	1.91833000
C	5.35721600	-0.70311800	-1.22040400
C	5.51778900	-2.03111200	-1.00878300
N	1.33270600	3.33347900	0.47994700
N	3.99823900	-0.45957300	-1.15537000
H	0.61276600	5.71490000	2.58231700
H	6.40456300	-2.64185600	-0.97393300
H	-3.17014400	-2.74464300	-2.63383700
C	-5.21201200	-2.55250800	-2.00090200
H	-5.55078500	-2.12649200	-2.94885500
H	-5.41593100	-3.62612600	-2.01157200
H	-5.79500700	-2.10436700	-1.19148300
C	-1.66264400	-3.03531200	1.43781100
C	-0.85289100	-2.26691000	2.28116700
C	-2.04179100	-4.31453800	1.86457700

C	-0.45658900	-2.74706000	3.52638900
H	-0.53365400	-1.28370500	1.95687200
C	-1.64278300	-4.79702300	3.10616500
H	-2.63824600	-4.94639000	1.21637200
C	-0.85148200	-4.01417000	3.94550700
H	0.16394200	-2.13049900	4.16743100
H	-1.94200400	-5.79229100	3.41554100
H	-0.53904200	-4.39324300	4.91186900
C	-4.04142900	0.20850300	-0.95821800
C	-4.12094100	1.40624800	-1.67742600
C	-4.56415400	2.60394400	-1.13508500
C	-4.96387600	2.56857300	0.19540100
C	-4.91183300	1.37949100	0.93586900
C	-4.44471000	0.19427900	0.37647300
C	-3.39049500	-0.79580600	-1.83935100
C	-3.25917400	-0.09929000	-3.09448300
H	-4.59338500	3.51467000	-1.72103700
H	-5.32404100	3.47530700	0.66685900
H	-5.23671800	1.38730900	1.96983200
H	-4.39049400	-0.71521100	0.96309900
H	-2.27748000	-0.86015500	-1.42576400
H	-2.86198600	-0.47848700	-4.02721700
H	-3.56166800	1.84821800	-3.70916800
N	-3.63685000	1.14941100	-2.97398200
C	3.05999900	1.14629500	1.18749000
F	4.01125900	0.22469300	1.34405900
F	1.95655800	0.67543600	1.78646400
F	3.44704900	2.22394700	1.88470200

COM3(a)

Basis set superposition error correction = 0.001329101 Hartree

Electronic energy (in solution) = -2518.84619 Hartree

Entropic correction (in solution) = -2518.33777 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2518.34753 Hartree

C	-3.82522900	-2.87581500	-1.18290900
C	-3.21302800	-2.97716100	0.19960500
H	-3.82996100	-3.37194500	0.99921200
C	-1.96400800	-2.61373200	0.50628000
C	2.61864800	1.65123600	-0.19329300
C	2.33310900	2.70977800	-2.78237500
C	1.75257100	2.71683500	-0.45850400
C	3.30289900	1.10188200	-1.27929500
C	3.16935900	1.62686500	-2.55861600
C	1.60684200	3.24917600	-1.72904300
H	3.71807700	1.16455900	-3.37047400

H	0.92188600	4.07558600	-1.87815900
C	-0.29516800	2.89480800	0.90845600
N	-0.74339600	3.70006500	1.86800700
C	3.69750100	-1.31671600	-0.99468000
N	4.76112800	-2.11433900	-0.94031900
I	-1.33783400	1.34928700	0.05918100
I	1.72378700	-1.84905200	-0.78072300
C	-2.06514800	3.62226100	2.49742400
H	-2.14195000	4.44550500	3.20286200
H	-2.16127400	2.67216000	3.02146800
H	-2.83451300	3.71704300	1.73166500
C	4.72910600	-3.56989400	-0.77509600
H	4.27370700	-3.81496400	0.18360200
H	5.75621600	-3.92402700	-0.79976800
H	4.16428700	-4.01439500	-1.59320700
O	-1.11102100	-2.05227100	-0.41942200
H	2.23025700	3.11849800	-3.77928900
H	2.26062100	4.84816000	1.28805400
H	6.08369300	0.85098300	-1.30848200
C	1.29853300	4.37191400	1.37765100
C	0.23400100	4.62607800	2.17452100
C	5.52068300	-0.05975100	-1.18914800
C	5.90537000	-1.35264500	-1.06064400
N	0.95768600	3.28004000	0.59769200
N	4.14003800	-0.05406500	-1.13998200
H	0.07694500	5.37652700	2.93124000
H	6.88306900	-1.80468100	-1.04642300
H	-3.26098100	-3.53143900	-1.85924800
C	-5.27851400	-3.36544800	-1.15235900
H	-5.70903700	-3.34786300	-2.15533100
H	-5.32982400	-4.38736900	-0.76835100
H	-5.88416400	-2.72499400	-0.50548200
C	-1.34800400	-2.74122100	1.84578000
C	-0.37277400	-1.82964600	2.26275600
C	-1.72852900	-3.76881500	2.71657200
C	0.19995200	-1.93146500	3.52663900
H	-0.07159000	-1.02771500	1.60142200
C	-1.15889200	-3.86647300	3.98061900
H	-2.45892300	-4.50325100	2.39689700
C	-0.19286500	-2.94921100	4.39083900
H	0.95102600	-1.21284700	3.83494200
H	-1.46026900	-4.67012000	4.64273100
H	0.25380600	-3.03265200	5.37488600
C	-4.22127400	-0.25785400	-1.15851900

C	-4.04189900	0.77129000	-2.11745600
C	-4.41928900	2.09644500	-1.87224700
C	-4.97634900	2.38042000	-0.63854300
C	-5.15937000	1.37434000	0.33464900
C	-4.79116100	0.06404700	0.08795700
C	-3.74451500	-1.48121800	-1.75996200
C	-3.29590000	-1.14093500	-3.01176000
H	-4.27387900	2.86626800	-2.62156800
H	-5.27833600	3.39695900	-0.41273700
H	-5.59830700	1.63768300	1.29029300
H	-4.93748700	-0.70371300	0.84007200
H	-1.60564500	-1.83789300	-1.22834000
H	-2.87105600	-1.77059500	-3.78048600
H	-3.21442800	0.69646000	-4.07283400
N	-3.46800500	0.20462200	-3.22725700
C	2.77389400	1.19189100	1.24231400
F	3.65932900	0.20873500	1.40198600
F	1.60720000	0.75178600	1.74401300
F	3.17183000	2.20591400	2.02125100

P(a)

Electronic energy (in solution) = -826.02516 Hartree

Entropic correction (in solution) = -825.75400 Hartree

Sum of electronic and thermal Free Energies (in solution) = -825.76429 Hartree

C	0.68283700	2.12562900	0.28720900
C	-0.66510500	1.45533700	0.47256100
H	-1.14541600	1.56229300	1.43862300
C	-1.30003300	0.73401400	-0.46123800
O	-0.78167200	0.48300800	-1.69879500
H	0.57481000	2.92812700	-0.45450600
C	1.13885800	2.76052500	1.60720800
H	2.08328000	3.29137300	1.47184200
H	0.39004700	3.46887500	1.97103400
H	1.28227100	1.99189500	2.37173700
C	-2.62493000	0.09663600	-0.26798800
C	-2.96809200	-1.03536800	-1.01515600
C	-3.54985800	0.60317100	0.65309000
C	-4.19788400	-1.66001300	-0.82811300
H	-2.26446100	-1.42905200	-1.73821000
C	-4.77621100	-0.02348000	0.83889300
H	-3.31800600	1.50054500	1.21505300
C	-5.10503200	-1.15939600	0.10093700
H	-4.44594400	-2.54033300	-1.41036500
H	-5.48271900	0.38350400	1.55343400
H	-6.06397600	-1.64411200	0.24425300

C	2.10710400	-0.10468400	0.29484500
C	3.15783200	-0.60399200	-0.51355800
C	3.76229900	-1.84301300	-0.27357200
C	3.29463200	-2.58201100	0.79888300
C	2.24958900	-2.10540200	1.61797500
C	1.65357200	-0.87975600	1.37706100
C	1.73411400	1.18063100	-0.24541400
C	2.55283100	1.39243100	-1.32581500
H	4.56488900	-2.20509900	-0.90606800
H	3.73994000	-3.54663000	1.01452700
H	1.91084700	-2.71331800	2.44910700
H	0.85060400	-0.52165200	2.01223800
H	0.15769800	0.72153700	-1.70834000
H	2.59082800	2.23594500	-2.00030000
H	4.09707200	0.24232400	-2.22165100
N	3.40749800	0.32887900	-1.48841400

The direct hydrogen proton transfer reaction pathway

Transition State2 TS2(b)

Imaginary frequency -1471.97 cm^{-1}

Basis set superposition error correction = 0.002593445 Hartree

Electronic energy (in solution) = -2518.76755 Hartree

Entropic correction (in solution) = -2518.26434 Hartree

Sum of electronic and thermal Free Energies (in solution)= -2518.27407 Hartree

C	-3.03788300	-2.39220500	-0.72530300
C	-3.44704900	-1.18744500	-1.57390300
H	-4.44211900	-1.16903800	-2.00405300
C	-2.50721100	-0.22066500	-1.91603900
C	2.86779100	0.25371500	1.25732400
C	1.45817800	-1.10451300	3.27265700
C	2.87524100	-1.14277800	1.33860200
C	2.06740200	0.94385500	2.17031900
C	1.37822000	0.27734700	3.17577700
C	2.18953300	-1.82118900	2.33354100
H	0.76848700	0.85516000	3.86099800
H	2.22415700	-2.90431900	2.35152400
C	2.94246100	-2.32135300	-0.82158900
N	3.80865600	-3.09455100	-1.46991300
C	0.96937400	2.89141500	1.15921000
N	1.00642600	4.21198200	1.32020200
I	1.04578100	-1.74811100	-1.39735500
I	-0.16273200	1.76225600	-0.16126900
C	3.57533500	-3.71943700	-2.77407300
H	4.45513400	-4.30870500	-3.01884200
H	3.42701600	-2.94350500	-3.52401800

H	2.70026100	-4.36503700	-2.71386300
C	0.21774200	5.18047100	0.55512400
H	0.49369700	5.12027600	-0.49674100
H	0.44548200	6.17014300	0.94250700
H	-0.84220800	4.96687800	0.68480000
O	-1.28457700	-0.28872300	-1.54408400
H	0.92325700	-1.62564100	4.05660300
H	5.44236700	-2.29740000	1.24643300
H	3.15918400	3.15115100	3.53936600
C	4.79632400	-2.48162800	0.40424900
C	4.96678800	-3.20795000	-0.72579400
C	2.42733000	3.36242000	2.77769300
C	1.90486500	4.52609900	2.32070300
N	3.53248200	-1.92395900	0.32631500
N	1.83829900	2.35399600	2.03939000
H	5.80110300	-3.79389800	-1.07417200
H	2.08412700	5.54790900	2.61143300
H	-2.01030700	-2.68714300	-0.95352900
C	-3.95918300	-3.59056400	-0.89567700
H	-3.76260500	-4.35383600	-0.13968400
H	-5.00879200	-3.29942000	-0.83421200
H	-3.79786900	-4.03101200	-1.88251800
C	-2.92296900	0.99978100	-2.68351200
C	-1.95283400	1.67999500	-3.42640000
C	-4.23215300	1.49206100	-2.66589300
C	-2.28618100	2.82054300	-4.15038500
H	-0.93708300	1.30022100	-3.43918400
C	-4.56295400	2.63689100	-3.38326400
H	-4.99140300	0.99359900	-2.07405800
C	-3.59237700	3.30307300	-4.12929400
H	-1.52644400	3.33284900	-4.72993500
H	-5.57875100	3.01447500	-3.35358400
H	-3.85294700	4.19509100	-4.68760600
C	-4.07674000	-1.77487600	1.72735700
C	-3.49214100	-1.18474300	2.86350100
C	-4.18193900	-0.96402400	4.05232800
C	-5.50553500	-1.37184600	4.09382700
C	-6.11349600	-1.96673100	2.97636500
C	-5.41959000	-2.16408500	1.79069100
C	-3.05215100	-1.74547100	0.66683000
C	-1.88932800	-1.24487000	1.30413400
H	-3.69809600	-0.49630500	4.90157000
H	-6.08033800	-1.22799000	5.00100900
H	-7.15029700	-2.27558800	3.04081600

H	-5.91799600	-2.61169700	0.94144500
H	-3.40150300	-0.69922800	-0.06046700
H	-0.89762800	-1.12783700	0.89318700
H	-1.51500500	-0.43427800	3.18819000
N	-2.16850500	-0.88478400	2.55621000
C	3.71582100	0.93125300	0.19845200
F	3.79865700	2.25336500	0.35047600
F	3.24524400	0.70744500	-1.03743700
F	4.96904200	0.45809300	0.22868800

COM3(b)

Basis set superposition error correction = 0.001329101 Hartree
Electronic energy (in solution) = -2518.86213 Hartree
Entropic correction (in solution) = -2518.35527 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2518.36500 Hartree

C	3.51040500	-2.30148000	-0.95513700
C	2.88539100	-1.27959600	-1.94687100
H	3.59820200	-1.09793400	-2.75154600
C	2.50150500	-0.00395600	-1.24350900
C	-3.81777100	-0.06721100	-0.10725900
C	-4.15533400	-0.19251300	-2.89493100
C	-3.82276000	-1.28915000	-0.78612900
C	-3.89000400	1.09184100	-0.88500300
C	-4.06814800	1.03800300	-2.25969000
C	-4.00317500	-1.35950500	-2.15957700
H	-4.12145900	1.96486200	-2.81837400
H	-4.00237900	-2.33148300	-2.63856000
C	-2.31528300	-2.95951300	0.20953000
N	-2.44508600	-4.14566100	0.79897100
C	-2.52064200	2.94441600	-0.00656900
N	-2.74901100	4.16451200	0.47360800
I	-0.57566000	-1.93732300	-0.20856000
I	-0.69607600	2.03812400	-0.28946400
C	-1.34329700	-4.98097500	1.28423300
H	-1.77854000	-5.86700300	1.73875300
H	-0.77082200	-4.42807900	2.02746200
H	-0.70990400	-5.26655000	0.44545000
C	-1.72196700	5.11186000	0.91453900
H	-1.15166400	4.67157200	1.73116000
H	-2.22985300	6.00867100	1.25946200
H	-1.06964200	5.35292200	0.07645700
O	1.40322400	0.06786100	-0.69899900
H	-4.30116900	-0.24111700	-3.96630100
H	-5.53806600	-3.30435900	0.15969700
H	-5.75623300	3.05032000	-0.15466100

C	-4.48173800	-3.45949500	0.30455400
C	-3.78385400	-4.47519900	0.86682500
C	-4.71775300	3.29330800	-0.00188300
C	-4.10841800	4.40156900	0.48336100
N	-3.55271500	-2.51687500	-0.09203400
N	-3.71469300	2.38850800	-0.29378200
H	-4.11005200	-5.40039700	1.31223700
H	-4.51091800	5.33559900	0.83839400
H	2.75128400	-2.53285700	-0.19886600
C	3.85430000	-3.58234000	-1.71263700
H	4.25579900	-4.33566500	-1.03149100
H	2.96578900	-3.99187200	-2.19948700
H	4.60226100	-3.38452700	-2.48557800
C	3.45790900	1.13275900	-1.12765300
C	3.24053400	2.07677200	-0.11537700
C	4.58793600	1.24819100	-1.94301700
C	4.13986500	3.11385100	0.08402600
H	2.38542500	1.96600000	0.54112300
C	5.48372000	2.29532800	-1.74786300
H	4.77721300	0.53357300	-2.73352000
C	5.26524200	3.22266000	-0.73327100
H	3.97388400	3.82914600	0.88113800
H	6.35542100	2.38172500	-2.38583500
H	5.97231000	4.02937800	-0.57622400
C	4.64925400	-0.94203100	0.97095000
C	5.94288500	-0.40261900	1.17762400
C	6.24027500	0.42451800	2.26678300
C	5.21396900	0.70266300	3.15357200
C	3.92010400	0.16931200	2.97083100
C	3.62950600	-0.64617100	1.89117700
C	4.69551400	-1.70121600	-0.25093300
C	5.98349600	-1.60912000	-0.71051900
H	7.23544100	0.83206900	2.40471600
H	5.40841000	1.34211300	4.00719600
H	3.14355600	0.40946100	3.68829500
H	2.62849800	-1.04286000	1.75072500
H	1.97566500	-1.70671400	-2.37703500
H	6.43293100	-2.02490200	-1.60036600
H	7.71584700	-0.62737300	0.02978600
N	6.73277300	-0.83180800	0.14191200
C	-3.73485100	-0.00265500	1.40611300
F	-4.30098100	-1.06748400	1.98161000
F	-4.36013000	1.07325900	1.89306000
F	-2.46675000	0.05049000	1.84028700

2.1.5 Cat4 ($(C_4H_5N_2I^+)_2C_3H_6$) catalyzed reaction

cat4 ($(C_4H_5N_2I^+)_2C_3H_6$)

Electronic energy (in solution) = -1242.67080 Hartree
Entropic correction (in solution) = -1242.43833 Hartree
Sum of electronic and thermal Free Energies (in solution) = -1242.44852 Hartree

C	0.00121000	1.67197600	-0.37273800
C	-1.25075200	1.69864400	-1.24135300
C	1.23039700	1.64262200	-1.27314900
C	-3.01582600	0.50535900	0.07163000
N	-4.09097900	0.84321300	0.78716800
C	3.01823600	0.49351400	0.05428900
N	4.11031000	0.85814700	0.73055800
I	-2.33336300	-1.40434900	-0.20560100
I	2.32317200	-1.42455200	-0.12045000
C	-4.98591000	-0.08352000	1.48319000
H	-4.42403400	-0.63816500	2.23364800
H	-5.43677900	-0.76412900	0.76202900
H	-5.75952800	0.50823000	1.96509200
C	5.01353000	-0.03889600	1.45478600
H	5.46490700	-0.74283100	0.75666400
H	4.45765700	-0.56844800	2.22738400
H	5.78633300	0.57325300	1.91213700
H	-2.94791700	3.70559200	-0.28333700
H	2.96280000	3.67318400	-0.45472500
C	-3.20969600	2.69908300	-0.00176300
C	-4.22785300	2.21248500	0.75278600
C	3.22476800	2.67987900	-0.12963400
C	4.25551800	2.22305700	0.62597500
N	-2.46505300	1.61970000	-0.42249700
N	2.46395900	1.58707000	-0.48106400
H	-5.03693900	2.70768300	1.26314000
H	5.07834200	2.73610300	1.09507400
H	-1.31769900	2.62549900	-1.80952300
H	-1.26722100	0.86604500	-1.94690400
H	1.21736300	0.77924700	-1.94078300
H	1.29446500	2.54279300	-1.88336200
H	-0.00965700	0.78871300	0.27321400
H	0.02861400	2.55686600	0.26769100

cat4 -Michael acceptor

Basis set superposition error correction = 0.001218012 Hartree
Electronic energy (in solution) = -1704.91802 Hartree
Entropic correction (in solution) = -1704.52942 Hartree
Sum of electronic and thermal Free Energies (in solution) = -1704.53927 Hartree

C	-2.06263200	-3.29315000	1.85003800

C	-2.95142800	-2.86760300	0.94474800
H	-3.79613900	-3.48616100	0.66180600
C	-2.82419300	-1.53505100	0.32749200
C	3.08825900	1.24979900	0.25522200
C	3.64832600	0.01557000	0.95868100
C	2.59205700	2.23549100	1.30941900
C	2.98442100	-1.92762700	-0.47532300
N	3.60387300	-2.78401000	-1.29218800
C	0.60307100	3.36845400	0.28678100
N	0.32717100	4.58174900	-0.20023500
I	0.96377600	-1.84676800	-0.09151600
I	-0.66645500	1.74863000	0.31600000
C	2.96553000	-3.87235100	-2.03386300
H	2.25208400	-3.45927800	-2.74601100
H	2.46457100	-4.54221300	-1.33634800
H	3.74625100	-4.41127800	-2.56448400
C	-0.95703100	5.01104800	-0.75621200
H	-1.73205000	4.91891900	0.00370100
H	-1.20087600	4.40128700	-1.62539600
H	-0.85467000	6.05164100	-1.05328200
O	-1.75073800	-0.93282000	0.31628100
H	6.02063100	-0.86612200	-0.23326500
H	3.43827400	4.83660200	0.74532500
C	5.13225900	-1.41334500	-0.50212000
C	4.94616900	-2.47830500	-1.32223300
C	2.41951000	4.61082400	0.47741400
C	1.44946600	5.37160800	-0.08953400
N	3.90094200	-1.08343400	0.01866400
N	1.87606700	3.36667900	0.70703300
H	5.63915700	-3.04907500	-1.91751900
H	1.44855100	6.39718900	-0.41870000
H	-1.25649200	-2.62123200	2.13996400
C	-2.10360700	-4.61992200	2.52191100
H	-2.17579500	-4.48990900	3.60585100
H	-2.94191500	-5.22469800	2.17508300
H	-1.16918300	-5.15826000	2.33408800
C	-4.02333200	-0.91861100	-0.30333100
C	-3.84127900	0.04245500	-1.30352900
C	-5.31601900	-1.26288000	0.10227200
C	-4.94034700	0.65069500	-1.89411400
H	-2.83706000	0.28718300	-1.63050000
C	-6.41455600	-0.63747700	-0.47790700
H	-5.46664400	-1.99892300	0.88344400
C	-6.22775900	0.31426900	-1.47689900

H	-4.79728200	1.38335900	-2.67966000
H	-7.41546900	-0.89459200	-0.15209500
H	-7.08618500	0.79262500	-1.93456500
H	4.59872700	0.23355600	1.44474400
H	2.95607300	-0.35185700	1.71856800
H	1.91479100	1.74996600	2.01460000
H	3.42091400	2.66017500	1.87497100
H	2.26201200	0.96048800	-0.39956100
H	3.85794500	1.71424700	-0.36508100

COM1

Basis set superposition error correction = 0.003795948 Hartree
Electronic energy (in solution) = -2068.70816 Hartree
Entropic correction (in solution) = -2068.19624 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2068.20604 Hartree

C	-2.67277000	-2.57249800	-1.27749200
C	-3.10649700	-1.30989700	-1.37276400
H	-4.16091900	-1.08123100	-1.26247200
C	-2.17880400	-0.20445400	-1.65210000
C	3.27489900	0.23736300	1.41512800
C	3.07464200	-1.22605900	1.79789600
C	2.42580900	1.11826100	2.32466300
C	3.16290800	-2.46614100	-0.37320500
N	4.02780600	-3.27545200	-0.99113700
C	1.77771900	3.08116200	0.90839300
N	2.12075400	4.36979200	0.82552900
I	1.35689200	-1.80063800	-1.10573700
I	0.43028100	2.12786000	-0.31787300
C	3.83872000	-3.88299100	-2.30920100
H	3.74392500	-3.10067100	-3.06150800
H	2.94820900	-4.50996100	-2.29668000
H	4.71456200	-4.49099900	-2.51997800
C	1.58152900	5.34202100	-0.12721700
H	0.50237800	5.41680200	0.00052500
H	1.82545900	5.03125000	-1.14252900
H	2.04487900	6.30195000	0.08580900
O	-0.96706400	-0.36471500	-1.79016600
H	5.51671600	-2.59073000	1.82975600
H	3.94245900	3.25350700	3.29063600
C	4.91698200	-2.72748500	0.94518100
C	5.12953100	-3.45039200	-0.18356200
C	3.29033500	3.48337200	2.46440900
C	3.06557300	4.63929200	1.78963800
N	3.68670400	-2.12354800	0.81180800
N	2.47755600	2.52321200	1.90463800

H	5.95381400	-4.07425100	-0.48653700
H	3.48170400	5.62600200	1.90647500
H	-1.61105400	-2.76742100	-1.41236100
C	-3.54204600	-3.75170100	-1.01921800
H	-3.15415300	-4.32641400	-0.17320000
H	-4.57261400	-3.45860700	-0.81300000
H	-3.52577400	-4.42013200	-1.88677100
C	-2.73472800	1.17573600	-1.79338000
C	-2.08694200	2.07107400	-2.65174400
C	-3.84269200	1.60050900	-1.05513700
C	-2.54235400	3.37828300	-2.76918600
H	-1.23711800	1.72997400	-3.23348400
C	-4.27819000	2.91797300	-1.15401400
H	-4.35031200	0.91500300	-0.38606100
C	-3.63207700	3.80490000	-2.01218200
H	-2.04813200	4.06475000	-3.44675500
H	-5.12480400	3.25072600	-0.56491400
H	-3.98168000	4.82760100	-2.09562000
C	-3.10002500	-2.21906000	2.09656700
C	-3.52076600	-0.88092200	1.89853600
C	-4.86049700	-0.49233100	2.00890900
C	-5.78442900	-1.47670500	2.31550800
C	-5.38946200	-2.81645100	2.51412300
C	-4.06221100	-3.19406400	2.41026700
C	-1.67662600	-2.24067700	1.89880300
C	-1.30128300	-0.95780500	1.60521800
H	-5.15930200	0.53957300	1.86146000
H	-6.83183700	-1.21297500	2.40811100
H	-6.14232700	-3.55868500	2.75376800
H	-3.76696300	-4.22651500	2.56449700
H	-1.01928600	-3.09503800	1.96377300
H	-0.32105400	-0.55576500	1.39866500
H	-2.39543700	0.85815100	1.43090500
N	-2.40361600	-0.13929700	1.59591000
H	3.53865100	-1.45347900	2.75696800
H	2.01392400	-1.47745600	1.86600000
H	1.38029500	0.80529700	2.31948000
H	2.78181500	1.08890100	3.35371600
H	2.97914300	0.39236900	0.37383600
H	4.32924200	0.50861500	1.50590800

Transition State1 (TS1)

Imaginary frequency -430.34 cm^{-1}

Basis set superposition error correction = 0.004402507 Hartree

Electronic energy (in solution) = -2068.67629 Hartree

Entropic correction (in solution) = -2068.16019 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2068.16994 Hartree

C	2.70385200	-2.42147600	-0.23577000
C	3.00608600	-1.42451900	0.74180900
H	3.98111600	-1.43025200	1.21526300
C	2.09811300	-0.41450000	1.03438400
C	-3.98917500	0.28939400	-1.01322200
C	-3.94348000	-1.12777800	-1.58241300
C	-3.44911400	1.26707700	-2.05468500
C	-3.25368000	-2.59531600	0.32422200
N	-3.84611400	-3.49776600	1.11202000
C	-2.20646100	3.01317700	-0.75920200
N	-2.40087500	4.29553700	-0.43665000
I	-1.30787800	-1.90621900	0.46132700
I	-0.64508600	1.79583300	-0.15305100
C	-3.19964400	-4.23355100	2.19913100
H	-2.81110400	-3.52978600	2.93433900
H	-2.39359600	-4.84589800	1.79692400
H	-3.95095100	-4.86944700	2.66066500
C	-1.49982700	5.11666700	0.37233300
H	-0.50860700	5.12359000	-0.07885800
H	-1.45298100	4.71771600	1.38531900
H	-1.90194100	6.12631600	0.39171900
O	0.93721000	-0.34316700	0.49928700
H	-6.24606400	-2.56172500	-0.88911100
H	-5.04273200	3.56108100	-2.20279300
C	-5.36883300	-2.77277800	-0.30017400
C	-5.16565700	-3.62394500	0.73672900
C	-4.13081700	3.66209500	-1.63805600
C	-3.59569600	4.71853800	-0.97586500
N	-4.16927700	-2.14140200	-0.54505500
N	-3.25366300	2.60981400	-1.49487000
H	-5.83008300	-4.30753900	1.23848300
H	-3.94658500	5.72833600	-0.84303600
H	1.64306400	-2.58102300	-0.41063200
C	3.50481500	-3.70201600	-0.18295800
H	3.35701800	-4.32226700	-1.06803500
H	4.57020200	-3.49757500	-0.06076900
H	3.17244600	-4.27132500	0.69045700
C	2.46308600	0.65117900	2.02456000
C	1.45916500	1.19644700	2.83105500
C	3.77130600	1.12849900	2.15173800
C	1.75780200	2.19023700	3.75731200
H	0.44553300	0.82150000	2.73736500

C	4.06767000	2.13199200	3.06976400
H	4.55631500	0.72806100	1.51888800
C	3.06331300	2.66299900	3.87614400
H	0.97374200	2.59559200	4.38708700
H	5.08302400	2.50313500	3.15229500
H	3.29648800	3.44261300	4.59246500
C	4.46737700	-1.30110700	-1.93408900
C	4.39074600	0.07151900	-1.66004700
C	5.50255700	0.86356800	-1.40250300
C	6.73823700	0.22843500	-1.43241000
C	6.84412100	-1.14211600	-1.71163200
C	5.71655700	-1.91912500	-1.95753500
C	3.08728000	-1.78958600	-2.02117100
C	2.28752700	-0.61386100	-2.03136500
H	5.40648000	1.92177800	-1.18969300
H	7.63646000	0.80411800	-1.24219400
H	7.82509100	-1.60208100	-1.73777400
H	5.80815200	-2.97820500	-2.16958900
H	2.79076300	-2.67355700	-2.56906500
H	1.21950100	-0.52212400	-2.16312700
H	2.69169500	1.37684700	-1.58700500
N	3.03743900	0.43246000	-1.72331400
H	-4.71235800	-1.27782100	-2.33928200
H	-2.97378000	-1.33526700	-2.03903300
H	-2.48778900	0.92790700	-2.44491900
H	-4.13596400	1.37531400	-2.89359800
H	-3.37678100	0.34175200	-0.10938700
H	-5.01223000	0.55464400	-0.73770400

COM2

Basis set superposition error correction = 0.002082718 Hartree

Electronic energy (in solution) = -2068.68307 Hartree

Entropic correction (in solution) = -2068.16499 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2068.17473 Hartree

C	2.80361500	-2.43028000	-0.58607300
C	2.91919500	-1.61250300	0.66285200
H	3.77535900	-1.77513100	1.30843300
C	2.00255200	-0.65720700	0.96845200
C	-3.97094100	0.44073900	-0.90121000
C	-4.01476900	-0.91418300	-1.60697500
C	-3.48550600	1.49624900	-1.89304800
C	-3.20624800	-2.58322200	0.07491800
N	-3.75395100	-3.56709800	0.79536800
C	-2.08645600	3.09782000	-0.56987200
N	-2.20766700	4.35988200	-0.14695600

I	-1.24355100	-1.89505600	0.15825400
I	-0.53654500	1.77669200	-0.15791400
C	-3.04133700	-4.42085300	1.74572500
H	-2.65376100	-3.81314400	2.56289900
H	-2.22703000	-4.93374800	1.23597600
H	-3.75021100	-5.14892300	2.13234900
C	-1.21252100	5.08965400	0.63825600
H	-0.27369700	5.13225500	0.08783000
H	-1.06750300	4.59193600	1.59665700
H	-1.59121600	6.09585800	0.79845400
O	0.94603200	-0.42213300	0.22368100
H	-6.28100400	-2.39990400	-0.90392800
H	-5.00067800	3.84442100	-1.74937100
C	-5.36661300	-2.67810900	-0.40662800
C	-5.09973000	-3.64282300	0.50904200
C	-4.04612600	3.87329700	-1.25079000
C	-3.42202900	4.86147700	-0.56161500
N	-4.17938100	-2.02849600	-0.66552500
N	-3.20244200	2.78377100	-1.24680000
H	-5.73432500	-4.37620400	0.97798100
H	-3.72169300	5.87054500	-0.33261500
H	1.75332400	-2.67473700	-0.77311200
C	3.60714500	-3.72466000	-0.50511600
H	3.57443100	-4.27731800	-1.44709700
H	4.65123800	-3.52771300	-0.25186500
H	3.19175300	-4.35866000	0.28189800
C	2.15435400	0.17594900	2.20491300
C	1.01480400	0.53749500	2.93128100
C	3.40427600	0.61799900	2.65101900
C	1.12178400	1.30500700	4.08690600
H	0.04213900	0.19950200	2.58932600
C	3.51207800	1.39202500	3.80330000
H	4.29456400	0.36731200	2.08363400
C	2.37205100	1.73649600	4.52610400
H	0.23005300	1.56701800	4.64572600
H	4.48700700	1.73433100	4.13228500
H	2.45647300	2.34037400	5.42247600
C	4.58768200	-0.93955300	-1.74460000
C	4.38446400	0.43896000	-1.71384700
C	5.38837200	1.37199700	-1.53879600
C	6.67902800	0.86536100	-1.39476200
C	6.91976700	-0.50886800	-1.43889100
C	5.88011000	-1.42559200	-1.61321700
C	3.24396900	-1.60625700	-1.87304300

C	2.34157200	-0.44019300	-2.04873600
H	5.18047100	2.43481300	-1.51995300
H	7.50648100	1.55075900	-1.25613200
H	7.93565300	-0.87253200	-1.33903600
H	6.08830500	-2.48746000	-1.65487000
H	3.15661000	-2.27902600	-2.73205500
H	1.28351400	-0.45783700	-2.26516300
H	2.58313200	1.59656700	-1.99005200
N	2.99692200	0.66828200	-1.92029700
H	-4.84931300	-0.96994400	-2.30506400
H	-3.09353500	-1.08995000	-2.16547100
H	-2.57051900	1.16925600	-2.39071000
H	-4.23418000	1.69132900	-2.65995500
H	-3.28658900	0.39110100	-0.05104100
H	-4.96001900	0.70350600	-0.51972000

The indirect hydrogen proton transfer reaction pathway

Transition State2 TS2(a)

Imaginary frequency -257.09 cm^{-1}

Basis set superposition error correction = 0.002401873 Hartree

Electronic energy (in solution) = -2068.67488 Hartree

Entropic correction (in solution) = -2068.16354 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2068.17334 Hartree

C	-2.69230200	-2.85687000	-1.87743400
C	-2.00264700	-3.36913500	-0.63697100
H	-2.37587400	-4.28937600	-0.20304900
C	-1.00233800	-2.69672300	-0.01580500
C	2.58251100	2.68114600	-0.32133300
C	1.41347500	3.51675700	-0.83702500
C	3.32097500	2.07222000	-1.51184300
C	-0.42822500	3.21400000	0.83504100
N	-1.00465200	3.95924100	1.78270900
C	3.97806400	-0.22385900	-0.77584100
N	5.11581100	-0.84183400	-0.44253100
I	-0.86601500	1.24660200	0.40254400
I	2.05359300	-1.00971200	-0.69647500
C	-2.09170100	3.52801100	2.66256000
H	-1.74621800	2.71013300	3.29426700
H	-2.94229800	3.20948200	2.06055600
H	-2.37369400	4.37777500	3.27916000
C	5.23063800	-2.23697200	-0.01861600
H	4.87899400	-2.89169300	-0.81482300
H	4.64387200	-2.39262400	0.88619700
H	6.27991100	-2.43514400	0.18448400
O	-0.53467600	-1.53081100	-0.44970200

H	1.24990800	5.95231100	0.52477500
H	6.10324900	2.17828800	-1.17798000
C	0.55691300	5.19233200	0.84546900
C	-0.40299500	5.19782900	1.80455900
C	5.63983900	1.22982400	-0.96225900
C	6.16316100	0.04668800	-0.55372200
N	0.52775200	3.95046800	0.25039800
N	4.28089100	1.04387600	-1.09570900
H	-0.71745900	5.96311300	2.49424200
H	7.17665400	-0.24785500	-0.33818900
H	-2.07975900	-3.07353000	-2.76292900
C	-4.06625800	-3.49661100	-2.07027300
H	-4.55102800	-3.11630100	-2.97322100
H	-3.96836900	-4.58130100	-2.16121700
H	-4.71330800	-3.28491900	-1.21447400
C	-0.39982800	-3.21459000	1.25359400
C	0.12069100	-2.31324000	2.18818100
C	-0.32458000	-4.58417200	1.53507300
C	0.67478500	-2.76299700	3.38329900
H	0.08633900	-1.25137100	1.97439700
C	0.23449400	-5.03531400	2.72611900
H	-0.68901300	-5.30362900	0.81043400
C	0.73351200	-4.12674600	3.65777800
H	1.06390900	-2.04737300	4.09920200
H	0.29033900	-6.10017600	2.92301000
H	1.17125800	-4.47995400	4.58448700
C	-3.66158200	-0.59593300	-0.85201700
C	-4.10446200	0.57168400	-1.48269700
C	-4.83885200	1.56245800	-0.84676200
C	-5.15088800	1.33778800	0.48865100
C	-4.73373800	0.17035900	1.14304100
C	-3.98157900	-0.80070300	0.48936700
C	-2.79151600	-1.31945100	-1.81623800
C	-2.91303200	-0.53711400	-3.02154400
H	-5.14722400	2.46140000	-1.36677600
H	-5.72673500	2.07761700	1.03205800
H	-4.99809500	0.02617600	2.18428800
H	-3.64710400	-1.69015200	1.01014300
H	-1.69194000	-1.09832200	-1.42666800
H	-2.46555100	-0.73089900	-3.98817200
H	-3.77907900	1.27686800	-3.49125500
N	-3.62185500	0.54257400	-2.80490700
H	1.76003600	4.42130500	-1.33579700
H	0.81077700	2.94842600	-1.54803700

H	2.62089700	1.60482100	-2.20627300
H	3.88516400	2.82796800	-2.05726400
H	2.20632300	1.88513500	0.32642400
H	3.26003300	3.30089200	0.27011200

COM3(a)

Basis set superposition error correction = 0.002047154 Hartree
Electronic energy (in solution) = -2068.71694 Hartree
Entropic correction (in solution) = -2068.19975 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2068.20954 Hartree

C	-3.26888100	-2.87621100	-1.63074600
C	-2.52550400	-3.26889000	-0.37008900
H	-2.94391100	-4.08545400	0.20827000
C	-1.40405000	-2.71496400	0.10059200
C	2.73568900	2.47715900	-0.34062700
C	1.63603800	3.40538200	-0.84613300
C	3.44414600	1.84763100	-1.53673600
C	-0.21341100	3.24189200	0.83421400
N	-0.72097700	4.01819800	1.79545000
C	4.03283300	-0.46481600	-0.78406000
N	5.14564800	-1.11839400	-0.43901300
I	-0.86077500	1.35041000	0.36980000
I	2.11899600	-1.21731200	-0.74074500
C	-1.84189800	3.66947400	2.67015900
H	-1.55759400	2.83575200	3.31163400
H	-2.70638300	3.40418500	2.06225200
H	-2.07158300	4.54185500	3.27616900
C	5.22051300	-2.51424800	-0.00503300
H	4.87403100	-3.16545000	-0.80638400
H	4.61206300	-2.65078700	0.88827500
H	6.26107200	-2.73104300	0.22178800
O	-0.77255100	-1.65045200	-0.51039700
H	1.69595700	5.82398200	0.55518500
H	6.22450000	1.86378900	-1.20350500
C	0.94017600	5.12303100	0.86839600
C	-0.01146200	5.19782500	1.83327900
C	5.73210100	0.93168700	-0.98058400
C	6.21774000	-0.26258200	-0.55680500
N	0.79888200	3.89885700	0.25317200
N	4.36949400	0.78819800	-1.11838900
H	-0.25521200	5.97719600	2.53562000
H	7.22092500	-0.58566000	-0.33393400
H	-2.73271500	-3.29455000	-2.49247100
C	-4.67570600	-3.49157800	-1.60968900
H	-5.20512800	-3.26492700	-2.53706200

H	-4.61759700	-4.57708800	-1.49695900
H	-5.25531400	-3.09029500	-0.77383100
C	-0.70812700	-3.14997200	1.33365700
C	-0.00960200	-2.22379600	2.11472300
C	-0.73384400	-4.48988500	1.73790100
C	0.63364000	-2.62284100	3.28228500
H	0.02413500	-1.18291800	1.81723000
C	-0.09246400	-4.88641400	2.90545400
H	-1.24213900	-5.22732900	1.12744900
C	0.59336600	-3.95497700	3.68269100
H	1.16452200	-1.88976400	3.87899700
H	-0.11751100	-5.92866900	3.20219600
H	1.09739300	-4.26755500	4.58994600
C	-3.85022600	-0.38634000	-0.92919500
C	-3.85427800	0.84893200	-1.62368900
C	-4.28204800	2.04101400	-1.03027200
C	-4.69902200	1.98085800	0.28759600
C	-4.69099500	0.76605100	1.00492100
C	-4.27461400	-0.41349900	0.41226900
C	-3.35395200	-1.38413500	-1.84865200
C	-3.07073700	-0.71921300	-3.01558500
H	-4.27909500	2.97293600	-1.58433100
H	-5.03865900	2.88509300	0.78012900
H	-5.02179500	0.75998700	2.03729300
H	-4.27856000	-1.34399500	0.96950800
H	-1.29419600	-1.37779100	-1.28600700
H	-2.68579000	-1.10832400	-3.94715100
H	-3.24828500	1.31119800	-3.60756500
N	-3.36817800	0.61455600	-2.88540300
H	2.05149200	4.28340600	-1.33942400
H	0.98473100	2.89296600	-1.55666500
H	2.72702400	1.40674900	-2.23176800
H	4.03563100	2.58333900	-2.08044800
H	2.29674700	1.69563400	0.28563900
H	3.44936600	3.03362600	0.27104400

P(a)

Electronic energy (in solution) = -826.02516 Hartree

Entropic correction (in solution) = -825.75400 Hartree

Sum of electronic and thermal Free Energies (in solution) = -825.76429 Hartree

C	0.68286700	2.12567600	0.28722200
C	-0.66510200	1.45540200	0.47252200
H	-1.14547200	1.56240400	1.43855200
C	-1.30001400	0.73405600	-0.46127200
O	-0.78164900	0.48299300	-1.69880900

H	0.57490800	2.92820000	-0.45446800
C	1.13886600	2.76049600	1.60726200
H	2.08332500	3.29129600	1.47195500
H	0.39008600	3.46887700	1.97108800
H	1.28220400	1.99183500	2.37177100
C	-2.62490600	0.09665800	-0.26801900
C	-2.96797400	-1.03544800	-1.01506300
C	-3.54990200	0.60327500	0.65295600
C	-4.19775100	-1.66012800	-0.82799100
H	-2.26429000	-1.42918200	-1.73803600
C	-4.77622800	-0.02340400	0.83878000
H	-3.31808800	1.50072700	1.21481200
C	-5.10496000	-1.15943700	0.10095000
H	-4.44574200	-2.54053600	-1.41014100
H	-5.48279500	0.38362800	1.55323600
H	-6.06388800	-1.64417900	0.24428700
C	2.10706200	-0.10468400	0.29483700
C	3.15781300	-0.60399300	-0.51354300
C	3.76227200	-1.84301100	-0.27353000
C	3.29457600	-2.58200400	0.79891500
C	2.24950200	-2.10540100	1.61797000
C	1.65348500	-0.87976300	1.37702900
C	1.73412600	1.18064600	-0.24538200
C	2.55281700	1.39242600	-1.32581600
H	4.56487200	-2.20510500	-0.90601000
H	3.73987100	-3.54663100	1.01455500
H	1.91073800	-2.71331100	2.44909800
H	0.85049700	-0.52165600	2.01217900
H	0.15775000	0.72138600	-1.70832300
H	2.59078000	2.23592900	-2.00031700
H	4.09709400	0.24231500	-2.22160800
N	3.40743600	0.32884100	-1.48844600

The direct hydrogen proton transfer reaction pathway

Transition State2 TS2(b)

Imaginary frequency -1480.82 cm^{-1}

Basis set superposition error correction = 0.001812631 Hartree

Electronic energy (in solution) = -2068.63780 Hartree

Entropic correction (in solution) = -2068.12857 Hartree

Sum of electronic and thermal Free Energies (in solution) = -2068.13829 Hartree

C	3.02904800	-2.06940400	0.53203700
C	3.03900300	-0.96665200	1.59120900
H	3.83630700	-0.95304000	2.32597300
C	1.94456400	-0.11611800	1.72193500
C	-3.66383300	0.03308200	-1.45733800

C	-3.43580400	-1.40679900	-1.91273900
C	-3.01706600	0.98269800	-2.46336000
C	-3.05522700	-2.72311200	0.18256100
N	-3.73890200	-3.62345900	0.89502600
C	-2.10734400	2.87646400	-1.10333000
N	-2.42003500	4.16026300	-0.90390400
I	-1.21204400	-1.90909200	0.64697800
I	-0.60955900	1.80217100	-0.16157100
C	-3.28047000	-4.25962000	2.13046100
H	-3.12436600	-3.50012100	2.89572500
H	-2.35611900	-4.80333800	1.94009000
H	-4.05517300	-4.95120300	2.45135400
C	-1.70431600	5.08232700	-0.02172000
H	-0.67953500	5.20139500	-0.37130000
H	-1.71532500	4.69392600	0.99606500
H	-2.21925200	6.03898500	-0.05584300
O	0.91621700	-0.20151600	0.96749300
H	-5.74656600	-2.95245000	-1.58643400
H	-4.68050000	3.16312600	-3.03335400
C	-4.99242900	-3.07322000	-0.82644900
C	-4.95008000	-3.85567400	0.28126600
C	-3.88387900	3.35309900	-2.33332500
C	-3.52468200	4.47712600	-1.66352100
N	-3.80532300	-2.37605500	-0.87419400
N	-2.99145600	2.36660300	-1.97417000
H	-5.66061300	-4.55610400	0.68743300
H	-3.94484200	5.46894300	-1.65816600
H	2.02316200	-2.48283100	0.41631800
C	4.00935700	-3.19268900	0.83336900
H	4.12032000	-3.86387600	-0.02107000
H	4.99269600	-2.80339100	1.10248900
H	3.64139800	-3.77259300	1.68323000
C	1.97122400	0.98664700	2.73748600
C	0.75834400	1.42200800	3.28003300
C	3.15905200	1.59674300	3.15270100
C	0.73211000	2.44071800	4.22735700
H	-0.16268200	0.94454400	2.96329500
C	3.13145800	2.62181200	4.09289100
H	4.10577900	1.28438500	2.72643400
C	1.91914600	3.04559800	4.63382600
H	-0.21386300	2.76240800	4.64833400
H	4.05734300	3.09581700	4.39855900
H	1.90033600	3.84443900	5.36651900
C	4.60891600	-1.07934400	-1.47242800

C	4.28333600	-0.36140800	-2.63857000
C	5.22884800	0.04686200	-3.57548900
C	6.54722200	-0.30099800	-3.32850400
C	6.90030800	-1.02121300	-2.17577800
C	5.95003100	-1.40580400	-1.24020500
C	3.35394000	-1.23487000	-0.71419100
C	2.35177200	-0.69800200	-1.56036900
H	4.93831400	0.60834800	-4.45555900
H	7.31713300	-0.01157200	-4.03388200
H	7.94006900	-1.27912800	-2.01160400
H	6.25221500	-1.94691200	-0.35386100
H	3.40613200	-0.28367600	0.20711900
H	1.28505000	-0.68162800	-1.39687400
H	2.40109600	0.34853400	-3.36329300
N	2.90707700	-0.15860900	-2.64528000
H	-4.03456900	-1.64515700	-2.79119400
H	-2.38655100	-1.57493500	-2.16256500
H	-1.98671500	0.68801300	-2.67048300
H	-3.56161900	0.99353100	-3.40668200
H	-3.21575700	0.18166200	-0.47160500
H	-4.73293300	0.24008600	-1.37290500

COM3(b)

Basis set superposition error correction = 0.001234776957 Hartree
Electronic energy (in solution) = -2068.73462 Hartree
Entropic correction (in solution) = -2068.21811 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2068.22867 Hartree

C	-2.97141400	2.35285600	-0.80035300
C	-2.42560000	1.39427200	-1.89648000
H	-3.18322100	1.28832200	-2.67333200
C	-2.03576700	0.06289000	-1.30677600
C	4.35827400	0.06520300	-0.04672000
C	4.40834400	1.33665900	-0.88958200
C	4.48613800	-1.14655700	-0.96567300
C	2.83340600	2.93086300	0.22485900
N	2.93704900	4.04607600	0.95270400
C	3.02356700	-2.90766300	0.05222700
N	3.20732500	-4.05367200	0.71398500
I	1.09417700	1.94475600	-0.27002700
I	1.21447000	-2.02061900	-0.36534100
C	1.81893500	4.80916700	1.51032500
H	2.23415400	5.66649800	2.03404700
H	1.26389500	4.18365300	2.20868300
H	1.17084300	5.14763300	0.70287000
C	2.15176900	-4.93194100	1.22033200

H	1.56701700	-4.40448600	1.97292500
H	2.63303000	-5.79784100	1.66773700
H	1.51567100	-5.24927400	0.39513700
O	-0.91349000	-0.06792800	-0.82822200
H	6.03917100	3.28218900	0.29136300
H	6.24577700	-3.03333100	0.10833700
C	4.97918600	3.41101300	0.43560700
C	4.26995000	4.36229500	1.09430100
C	5.19782700	-3.24562100	0.24155400
C	4.55897500	-4.28126300	0.84207100
N	4.06925300	2.52733600	-0.10081800
N	4.22736100	-2.40019500	-0.24728800
H	4.58449100	5.23350700	1.64438300
H	4.93517100	-5.15817900	1.34203800
H	-2.16789100	2.51167600	-0.07185100
C	-3.32462600	3.69336500	-1.44128000
H	-3.66794700	4.40257400	-0.68507900
H	-2.45479100	4.11903300	-1.94771700
H	-4.11999700	3.56957500	-2.18162400
C	-3.01427700	-1.05880200	-1.22188900
C	-2.76852900	-2.08346700	-0.29872200
C	-4.18974600	-1.08555200	-1.97838100
C	-3.68297100	-3.11282600	-0.12954300
H	-1.87698000	-2.04381100	0.31582300
C	-5.10153300	-2.12419700	-1.81463500
H	-4.40357300	-0.30743700	-2.69939300
C	-4.85350700	-3.13278900	-0.88842900
H	-3.49277600	-3.89187300	0.59951200
H	-6.00836400	-2.14074500	-2.40773200
H	-5.57195300	-3.93361000	-0.75445800
C	-4.03308200	0.87583800	1.08226200
C	-5.32516800	0.34626700	1.32154000
C	-5.58062500	-0.55507900	2.36137500
C	-4.51272700	-0.92036900	3.16342500
C	-3.21869700	-0.40015600	2.94633900
C	-2.97034100	0.49064300	1.91688700
C	-4.12976000	1.72537900	-0.07565900
C	-5.44272900	1.69127600	-0.46722200
H	-6.57564200	-0.95331800	2.52518100
H	-4.67346400	-1.61983000	3.97602900
H	-2.40887600	-0.71036100	3.59711300
H	-1.96965200	0.87747700	1.74846900
H	-1.52943500	1.83224700	-2.34374500
H	-5.93085300	2.17978600	-1.29776500

H	-7.15277500	0.68721200	0.29428000
N	-6.16105900	0.86625100	0.36670700
H	5.16444200	0.06798500	0.69028200
H	3.77907000	-1.08806800	-1.79535300
H	5.49027000	-1.22748800	-1.38048600
H	5.40565900	1.50360000	-1.29470900
H	3.70718000	1.28391500	-1.72472600
H	3.41085400	0.01615100	0.49647600

2.1.6 Cat2 ($(C_4H_5N_2I^+)_2C_6H_4$) catalyzed reaction—a water-bridge mechanism

H_2O

Electronic energy (in solution) = -76.40817 Hartree
Entropic correction (in solution) = -76.41322 Hartree
Sum of electronic and thermal Free Energies (in solution) = -76.42582 Hartree

O	0.00000000	0.00000000	0.11788000
H	0.00000000	0.76093400	-0.47151900
H	0.00000000	-0.76093400	-0.47151900

TS3(c)

Imaginary frequency -415.24 cm^{-1}
Basis set superposition error correction = 0.004723446 Hartree
Electronic energy (in solution) = -2257.59218 Hartree
Entropic correction (in solution) = -2257.66382 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2257.67351 Hartree

C	3.19659800	-1.40344700	0.10257600
C	3.09980100	-0.20756800	1.02647400
H	3.96109900	0.01537700	1.64638300
C	1.94679500	0.49003900	1.23665300
H	-3.80380300	-0.11109900	0.38520200
C	-3.84153700	-0.47497500	-0.63516700
C	-4.05004300	-1.42222300	-3.26136000
C	-3.78810200	-1.83510200	-0.91523500
C	-3.96341800	0.40028200	-1.70732600
C	-4.07201200	-0.05440900	-3.01573000
C	-3.89455200	-2.32081000	-2.21227100
H	-4.16614800	0.65849200	-3.82663200
H	-3.84891100	-3.38870000	-2.39197400
C	-2.55148500	-2.89469400	0.96139400
N	-2.78660200	-3.90807500	1.79590600
C	-2.98842900	2.56738600	-0.97399100
N	-3.40383700	3.83473200	-0.96336900
I	-0.86852900	-1.67581000	0.88189900
I	-1.16183700	1.83799200	-0.31446600
C	-1.87660800	-4.37043900	2.84494000
H	-1.69206500	-3.55931300	3.54810300

H	-0.94247100	-4.70471100	2.39567000
H	-2.35904200	-5.19907200	3.35671900
C	-2.62077700	4.97875500	-0.49305200
H	-1.70111400	5.05170000	-1.07169000
H	-2.39449000	4.85431100	0.56520500
H	-3.22117400	5.87275700	-0.64092000
O	0.84131600	0.29105000	0.55014400
H	-4.13370900	-1.78859500	-4.27663300
H	-5.49107300	-3.83754700	-0.02948600
H	-5.96888600	2.24504500	-2.20553600
C	-4.55186200	-3.75180100	0.49097000
C	-4.02211300	-4.45599000	1.51915100
C	-5.05725700	2.64132800	-1.79063300
C	-4.68609100	3.90287900	-1.46780100
N	-3.62865800	-2.77643400	0.15868700
N	-3.99288600	1.81761500	-1.47106100
H	-4.40695200	-5.28887400	2.08362800
H	-5.21087700	4.84048100	-1.54388500
H	2.19663000	-1.59981800	-0.29786000
C	3.65253900	-2.64207100	0.89262000
H	3.69902600	-3.52019500	0.24369400
H	4.64479300	-2.47871100	1.32203500
H	2.95518300	-2.84554200	1.70908200
C	1.89428700	1.57013800	2.27870000
C	0.68720800	1.80232400	2.94502400
C	3.00313700	2.36025400	2.59913700
C	0.59396300	2.78658400	3.92463300
H	-0.17724300	1.19618700	2.69666900
C	2.90812800	3.35074300	3.57201700
H	3.94058200	2.21275300	2.07367600
C	1.70449400	3.56565600	4.24033000
H	-0.34639800	2.94664200	4.44036800
H	3.77365300	3.96169700	3.80282300
H	1.63168300	4.33852200	4.99705000
C	5.50036100	-0.78368200	-1.08314100
C	5.94675000	-0.82585200	-2.42544600
C	7.25268700	-0.48075400	-2.79343400
C	8.11560500	-0.10225300	-1.78233800
C	7.69780800	-0.06527900	-0.43500800
C	6.40496100	-0.39956300	-0.07650400
C	4.11059200	-1.18903300	-1.08731200
C	3.79986800	-1.45703800	-2.40533600
H	7.56874400	-0.51619300	-3.82952200
H	9.13623000	0.16808600	-2.02783200

H	8.40710500	0.22961500	0.32951800
H	6.09896700	-0.37294000	0.96274300
H	3.18860900	0.36189000	-1.78215800
H	2.87179300	-1.81905500	-2.82610300
H	4.91015200	-1.34137200	-4.20882500
N	4.89442500	-1.23986000	-3.20306700
O	2.65107800	1.20224700	-1.55649500
H	2.46242600	1.10460600	-0.57784400
H	3.20308400	1.99940000	-1.70566100

COM3(c)

Basis set superposition error correction = -0.024714515 Hartree
Electronic energy (in solution) = -2257.66068 Hartree
Entropic correction (in solution) = -2257.73270 Hartree
Sum of electronic and thermal Free Energies (in solution) = -2257.74239 Hartree

C	3.04513400	-0.51142700	0.13703000
C	3.01891400	1.02001000	0.16680900
H	3.84598100	1.42082100	0.76075700
C	1.72576000	1.60593900	0.67213600
H	-3.87472000	-0.91670700	0.58593300
C	-3.81299200	-1.24127700	-0.44691800
C	-3.76524500	-2.12485900	-3.10564400
C	-3.37948900	-2.51914300	-0.77529100
C	-4.19366000	-0.40757100	-1.49035100
C	-4.17845300	-0.83050600	-2.81357000
C	-3.35289700	-2.97532800	-2.08656100
H	-4.48359700	-0.14905100	-3.59908700
H	-3.00883400	-3.98075300	-2.29913700
C	-1.87250500	-3.27369200	1.04783600
N	-1.81634600	-4.32671200	1.86300300
C	-3.90751400	1.92008700	-0.66535800
N	-4.67274800	3.01030100	-0.61298700
I	-0.52812000	-1.72254400	0.97284600
I	-1.95325400	1.78160900	-0.04405600
C	-0.77801100	-4.57271900	2.86658400
H	-0.73722300	-3.73235600	3.55826100
H	0.18238100	-4.70594400	2.36988500
H	-1.04623400	-5.47882300	3.40318900
C	-4.25881700	4.32187700	-0.10852400
H	-3.45493400	4.71262500	-0.73129800
H	-3.92961000	4.22622300	0.92514800
H	-5.12166900	4.98052500	-0.16139300
O	0.71484400	0.92606000	0.79606400
H	-3.74849200	-2.46618700	-4.13273300
H	-4.49905300	-4.90324100	0.09370500

H	-6.65069500	0.78448800	-1.95044100
C	-3.59811000	-4.59396500	0.59707000
C	-2.88112700	-5.16153500	1.59696300
C	-5.89680700	1.41524900	-1.50948600
C	-5.91443200	2.71702800	-1.13514500
N	-2.96054500	-3.41232000	0.26898300
N	-4.63947700	0.92785000	-1.20488800
H	-3.02846600	-6.07530200	2.14814400
H	-6.69213000	3.46096800	-1.18511000
H	2.13381800	-0.84886300	-0.36683400
C	3.07369900	-1.08602300	1.55953800
H	2.98970500	-2.17530800	1.53847900
H	4.01191800	-0.82750600	2.05710000
H	2.25646300	-0.68957300	2.16772000
C	1.68031100	3.06043000	0.99982200
C	0.68169400	3.52374100	1.86308900
C	2.60428000	3.96059200	0.46101300
C	0.60164700	4.87391400	2.17725000
H	-0.01104300	2.81714600	2.30634000
C	2.51078000	5.31448600	0.76438700
H	3.38570600	3.61429400	-0.20541700
C	1.51233900	5.77090500	1.62132500
H	-0.16477700	5.22718200	2.85708500
H	3.21894800	6.01266800	0.33410300
H	1.44752300	6.82594400	1.86194200
C	5.61659000	-0.82269500	-0.43643200
C	6.30868200	-1.48708400	-1.48165800
C	7.70430600	-1.47605800	-1.58612100
C	8.40987400	-0.78279400	-0.61925000
C	7.74650900	-0.11288500	0.43044100
C	6.36652600	-0.12596300	0.53068500
C	4.20491500	-1.01282400	-0.68046700
C	4.11440700	-1.76058900	-1.82607700
H	8.20630000	-1.98704300	-2.39983000
H	9.49227000	-0.75108800	-0.66936700
H	8.33205700	0.42217500	1.16927300
H	5.87312000	0.39826100	1.34140800
H	4.84216500	0.70447700	-2.57025000
H	3.23421700	-2.11822700	-2.34052900
H	5.56608700	-2.58049200	-3.14378200
N	5.36941700	-2.04866900	-2.30750800
O	5.50653300	1.35537000	-2.82878800
H	3.14933400	1.42293100	-0.84622200
H	6.24534900	1.16874500	-2.23810400