

Supporting Information

A theoretical study about excited state intermolecular proton transfer mechanisms for 2-phenylimidazo[4,5-b]pyridine in methanol solvent

Dapeng Yang^{1,2,*†}, Jinfeng Zhao^{2,†}, Min Jia¹, Xiaoyan Song¹

1.College of Mathematics and Information Science, North China University of Water Resources and Electric Power, Zhengzhou 450046, China

2.State Key Laboratory of Molecular Reaction Dynamics, Theoretical and Computational Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China

Corresponding authors: Dapeng Yang, email: dpyang_ncwu@163.com.

†These authors contributed equally.

The optimized Cartesian Coordinates of PIP coupling with MeOH structures in different electronic states are provided below:

S₀-state PIP-MeOH (-742.96900164 a.u.):

	X	Y	Z
C	1.60971500	-0.28729000	-0.09256000
C	1.30043500	-1.66043600	0.02783900
C	2.36378400	-2.55663900	0.08209700
C	3.64308900	-2.01173100	0.01415900
C	3.82577600	-0.62827100	-0.10319100
C	-0.57477800	-0.60999200	-0.02415100
H	2.20476400	-3.62365600	0.17314900
H	4.51405000	-2.65216300	0.05136700
H	4.82585100	-0.21517700	-0.15476900
H	0.31540700	1.36801100	-0.18756200
N	2.81935400	0.25558600	-0.15858300
N	-0.06672000	-1.82732800	0.06807300
C	-2.00703900	-0.30264800	-0.01985500
C	-2.92734100	-1.33002900	0.22906600
C	-2.48542000	0.99168300	-0.26086000
C	-4.28979000	-1.06675600	0.23828200
H	-2.55932300	-2.32973900	0.41484900
C	-3.85088400	1.25055300	-0.25013800
H	-1.80268200	1.80581000	-0.46822900
C	-4.75744100	0.22428600	-0.00038100
H	-4.98963300	-1.86973900	0.43356200
H	-4.20592600	2.25570000	-0.43971900
N	0.39985000	0.35713400	-0.12512100
C	2.00046300	3.89621000	0.59175000
H	1.22161800	4.65428400	0.51812700
H	1.99140700	3.48438300	1.60596300
H	2.96845200	4.37469400	0.41456700
O	1.72205700	2.89774000	-0.39098400
H	2.38959300	2.18594800	-0.32380000
H	-5.82084500	0.42834600	0.00744900

S₁-state PIP-MeOH (-742.83680708 a.u.):

	X	Y	Z
C	1.60144500	-0.27175300	-0.09160900
C	1.26608600	-1.67437300	0.05061900
C	2.34887200	-2.59207900	0.11737400
C	3.61875700	-2.04145300	0.03965600

C	3.81490500	-0.65268200	-0.09847200
C	-0.60403400	-0.56865700	-0.01652700
H	2.18244300	-3.65531200	0.22286800
H	4.49416000	-2.67631100	0.08359500
H	4.82035500	-0.25428600	-0.15656500
H	0.35557900	1.39485300	-0.22195800
N	2.81390900	0.25894400	-0.16674700
N	-0.05321500	-1.83978200	0.09466900
C	-1.96928300	-0.28693800	-0.01281400
C	-2.91989900	-1.36414100	0.11593900
C	-2.48726800	1.05136700	-0.13403700
C	-4.26944000	-1.10664700	0.12059000
H	-2.54430500	-2.37339400	0.20806800
C	-3.84256400	1.27592100	-0.12627400
H	-1.81133300	1.89055600	-0.23386000
C	-4.75339600	0.20891600	0.00026100
H	-4.96988800	-1.92734400	0.21810100
H	-4.21601000	2.28848300	-0.21892800
N	0.41538800	0.38299400	-0.13109100
C	1.99882500	3.91058800	0.53788900
H	1.21558900	4.66249600	0.45030800
H	1.98371200	3.50734500	1.55535300
H	2.96515100	4.39328400	0.36412400
O	1.73562300	2.90123200	-0.43860600
H	2.40759000	2.19483400	-0.36033700
H	-5.81863700	0.40142800	0.00468500

S₀-state PIP-MeOH-PT (-742.96298024 a.u.):

	X	Y	Z
C	1.54715200	-0.23372200	-0.08064400
C	1.33499100	-1.64196000	0.05395100
C	2.42995500	-2.48639700	0.11535800
C	3.70896100	-1.91113100	0.04185700
C	3.87153500	-0.54559200	-0.08824500
C	-0.52734700	-0.60972100	-0.01365200
H	2.31295300	-3.55810900	0.21637500
H	4.59159400	-2.53256500	0.08598100
H	4.83806700	-0.06920700	-0.14801200
H	0.96455100	2.26942900	-0.34184100
N	2.79656100	0.27447400	-0.14863700
N	-0.01540000	-1.84467800	0.09395100
C	-1.97241700	-0.35095000	-0.01362000
C	-2.88228200	-1.41011100	0.11242400

C	-2.46913500	0.95322800	-0.13916100
C	-4.24999400	-1.16912600	0.11249300
H	-2.50348600	-2.41848200	0.21001500
C	-3.83845100	1.19084900	-0.13878400
H	-1.77541900	1.77693700	-0.23705200
C	-4.73437100	0.13178800	-0.01316500
H	-4.94113400	-1.99740300	0.21079100
H	-4.20727300	2.20459000	-0.23676700
N	0.38345000	0.41561100	-0.12352700
C	1.60678900	3.92841100	0.53365600
H	0.71002500	4.53224500	0.36749000
H	1.58263200	3.53327300	1.55398800
H	2.48082200	4.56989700	0.42893000
O	1.71978300	2.88599200	-0.43755600
H	2.88512600	1.29219300	-0.24372700
H	-5.80132400	0.31802800	-0.01304900

S₁-state PIP-MeOH-PT (-742.83857944 a.u.):

	X	Y	Z
C	1.53747800	-0.22249600	-0.09163800
C	1.31841100	-1.63886500	0.05854200
C	2.43543300	-2.52492200	0.12905500
C	3.69635900	-1.93535100	0.04586300
C	3.87281400	-0.56050900	-0.09891900
C	-0.55012900	-0.57206700	-0.01728400
H	2.30828900	-3.59253500	0.24017900
H	4.58858500	-2.54510300	0.09254100
H	4.85078000	-0.10704000	-0.16263600
H	0.96653800	2.29851000	-0.35743900
N	2.80844500	0.29617700	-0.16930500
N	0.00509600	-1.84876500	0.10492900
C	-1.93970000	-0.34269100	-0.01566000
C	-2.85939800	-1.43490900	0.11814800
C	-2.48004100	0.97731200	-0.14804400
C	-4.21716800	-1.20914500	0.11729400
H	-2.46112900	-2.43453300	0.21911100
C	-3.84050300	1.17826000	-0.14651600
H	-1.79978200	1.81115900	-0.24996700
C	-4.72526900	0.09294400	-0.01465700
H	-4.90075900	-2.04306500	0.21907800
H	-4.23609800	2.18135700	-0.24786400
N	0.39568900	0.43570700	-0.13881000
C	1.56787700	3.93945800	0.57030100

H	0.64447800	4.51491800	0.45544100
H	1.58725500	3.50066800	1.57294400
H	2.41340300	4.61924200	0.47211200
O	1.69488300	2.94558400	-0.44814800
H	2.91245600	1.30595000	-0.27020900
H	-5.79466800	0.26184700	-0.01470300

S₀-state PIP-2MeOH (-858.76169881 a.u.):

	X	Y	Z
C	1.22050900	-0.97378700	-0.07108200
C	0.67559400	-2.27443700	0.05168100
C	1.55849200	-3.34733900	0.11593400
C	2.91564200	-3.04539200	0.05382600
C	3.34349000	-1.71944700	-0.06942500
C	-0.98266300	-0.91494200	-0.02191600
H	1.20654000	-4.36696000	0.20915200
H	3.65654000	-3.83219900	0.09818000
H	4.40145500	-1.49252100	-0.12049800
H	0.19371600	0.90153600	-0.15154000
N	2.51295600	-0.66808300	-0.13390000
N	-0.69866700	-2.20241000	0.07999900
C	-2.34064900	-0.36403900	-0.04352000
C	-3.42033100	-1.18348400	0.31266000
C	-2.58953700	0.96137900	-0.42342300
C	-4.71627400	-0.68692900	0.29222400
H	-3.22880000	-2.20673800	0.60573500
C	-3.88970400	1.45318600	-0.44194500
H	-1.77533200	1.61128600	-0.71821300
C	-4.95632100	0.63327100	-0.08444400
H	-5.54153400	-1.32973800	0.57250000
H	-4.06914300	2.47837400	-0.74085500
N	0.14302600	-0.12772600	-0.11682900
C	0.29992400	3.56619400	0.80300700
H	-0.78090000	3.60589000	0.93219900
H	0.75248200	3.22693200	1.73967500
H	0.66077500	4.57400400	0.57977000
O	0.57715500	2.66914300	-0.27532700
H	1.55348400	2.60082900	-0.39432200
C	4.26084700	2.50054600	0.26820500
H	5.20903800	2.01310600	0.02428400
H	4.36820100	3.57114300	0.09800500
H	4.04018200	2.33434200	1.32707000
O	3.20741000	2.02926500	-0.57455500

H	3.06937500	1.06288900	-0.41775200
H	-5.96791100	1.01942600	-0.09990400

S₁-state PIP-2MeOH (-858.62936938 a.u.):

	X	Y	Z
C	1.17202500	-0.97305700	-0.05525200
C	0.56934800	-2.28499600	0.09333100
C	1.44381300	-3.40188700	0.17773400
C	2.79879600	-3.12052500	0.10632700
C	3.26862100	-1.80209300	-0.04348400
C	-1.04486500	-0.83893200	0.00109200
H	1.06364600	-4.40786400	0.29054400
H	3.52901400	-3.91737400	0.16249700
H	4.33366600	-1.61386200	-0.10112300
H	0.23487400	0.92756200	-0.14823300
N	2.47218900	-0.70707900	-0.12671900
N	-0.75601100	-2.19090900	0.13068300
C	-2.33155600	-0.30185500	-0.04194100
C	-3.47313600	-1.16903500	0.11442500
C	-2.57892600	1.10246800	-0.24390200
C	-4.74765600	-0.65676000	0.08101200
H	-3.30061500	-2.22566700	0.26266400
C	-3.86596500	1.58294800	-0.27423500
H	-1.74953500	1.78257600	-0.38792800
C	-4.96687800	0.71964200	-0.11103100
H	-5.59453400	-1.32118900	0.20361100
H	-4.03657500	2.64125500	-0.43030100
N	0.13875300	-0.09958900	-0.10891500
C	0.51505800	3.53946900	0.89043300
H	-0.55320000	3.63246400	1.08174400
H	0.99783500	3.13667500	1.78580500
H	0.91953200	4.53449100	0.68621800
O	0.68315900	2.67476700	-0.23673900
H	1.64720000	2.56808000	-0.41584100
C	4.37593100	2.38642600	0.10225300
H	5.28922200	1.84774500	-0.16570800
H	4.52377400	3.44483600	-0.10884900
H	4.19514600	2.26463300	1.17460500
O	3.26556500	1.93782700	-0.67767700
H	3.09347200	0.98344100	-0.48478700
H	-5.97490300	1.11359600	-0.13550600

S₀-state PIP-2MeOH-PT (-858.75553252 a.u.):

	X	Y	Z
C	1.13353500	-0.93284400	-0.11436900
C	0.62767500	-2.25613500	0.08861700
C	1.51269000	-3.31507700	0.19723400
C	2.88310300	-3.03510000	0.10165600
C	3.32943900	-1.74223200	-0.09498800
C	-0.98138800	-0.86809300	-0.04078700
H	1.16373400	-4.32851700	0.35091200
H	3.61301700	-3.82781200	0.18001700
H	4.37603900	-1.48949100	-0.17472900
H	0.38894700	1.72839400	-0.13449900
N	2.46236800	-0.70949400	-0.20102000
N	-0.73491900	-2.17285400	0.13163700
C	-2.34625500	-0.32580900	-0.07573900
C	-3.42827400	-1.12228000	0.32505100
C	-2.59832100	0.98060400	-0.51493100
C	-4.72383400	-0.62347600	0.29204200
H	-3.23849000	-2.13194800	0.66303600
C	-3.89673600	1.47619600	-0.54844500
H	-1.77736900	1.60382800	-0.84217900
C	-4.96402300	0.67823700	-0.14417500
H	-5.54879600	-1.25011900	0.60842700
H	-4.07568200	2.48703100	-0.89400300
N	0.12265100	-0.06059000	-0.19385900
C	0.30984600	3.30269000	1.08498300
H	-0.77869000	3.35237100	1.17805200
H	0.71449400	2.77995900	1.95710000
H	0.70322500	4.31854400	1.07324100
O	0.69569000	2.67181800	-0.13764900
H	2.39405500	2.36801600	-0.44988700
C	4.29413800	2.56870200	0.11815100
H	5.22799700	2.05263000	-0.10057200
H	4.39673500	3.61569500	-0.17895600
H	4.10961900	2.52153500	1.19547800
O	3.25712100	1.92379300	-0.62648800
H	2.82319700	0.25682800	-0.35127000
H	-5.97479400	1.06643900	-0.17018500

S₁-state PIP-2MeOH-PT (-858.63014221 a.u.):

	X	Y	Z
C	1.07465300	-0.94855500	-0.10864100
C	0.52224200	-2.26165900	0.12712100

C	1.38895700	-3.38753700	0.25741900
C	2.75308600	-3.13016100	0.14249500
C	3.25024200	-1.84896700	-0.08862600
C	-1.04351600	-0.79165500	-0.01881500
H	1.00387800	-4.38185700	0.43456900
H	3.47241500	-3.93324200	0.23033700
H	4.30840900	-1.65196300	-0.17986500
H	0.46762000	1.74673500	-0.09901200
N	2.43077700	-0.76126100	-0.21513000
N	-0.80113200	-2.15141500	0.18800500
C	-2.34507900	-0.25684100	-0.07504200
C	-3.48341900	-1.09904400	0.15878900
C	-2.58562800	1.12454700	-0.37034700
C	-4.75861700	-0.58369300	0.10921300
H	-3.31377700	-2.14340700	0.37872000
C	-3.86946600	1.61597800	-0.41640300
H	-1.74701800	1.77603600	-0.57159300
C	-4.97031400	0.77441600	-0.17617700
H	-5.60717100	-1.23155200	0.29191300
H	-4.03558600	2.66170100	-0.64421100
N	0.11420600	-0.04463800	-0.19472300
C	0.53703300	3.25355200	1.20054700
H	-0.53818600	3.32904000	1.38540700
H	0.99407700	2.67457500	2.00872500
H	0.96070300	4.25706000	1.20646300
O	0.80332100	2.67737900	-0.08052600
H	2.48690000	2.33001100	-0.49976100
C	4.41573700	2.48357400	-0.03500800
H	5.32423500	1.94651100	-0.30463300
H	4.52823900	3.52931700	-0.33404800
H	4.28969900	2.43727500	1.05097600
O	3.32595100	1.86521600	-0.72324900
H	2.82532400	0.17784300	-0.39644200
H	-5.97637300	1.17262200	-0.21356200

T₁-state PIP-2MeOH-PT (-858.63150605 a.u.):

	X	Y	Z
C	1.12761600	-0.99131700	-0.10889500
C	0.64715500	-2.27677400	0.11560500
C	1.52024100	-3.36337200	0.24006100
C	2.91112900	-3.03118500	0.11241900
C	3.36473500	-1.75323300	-0.11051700
C	-1.03450000	-0.89186500	-0.02422300

H	1.19434200	-4.37632600	0.41799500
H	3.65181800	-3.81624100	0.19428400
H	4.40789900	-1.50024400	-0.20719000
H	0.39568100	1.79168700	-0.10026200
N	2.46570300	-0.70333400	-0.22368900
N	-0.75703800	-2.18649000	0.17513700
C	-2.37322800	-0.33514700	-0.07068900
C	-3.48387500	-1.13765700	0.25580300
C	-2.60640300	0.99946800	-0.45142700
C	-4.76972300	-0.62114000	0.20770700
H	-3.32029900	-2.16610600	0.54844100
C	-3.89794800	1.50858600	-0.49602800
H	-1.77569300	1.63428300	-0.72739400
C	-4.98793800	0.70572300	-0.16654900
H	-5.60959200	-1.25517100	0.46550100
H	-4.05415400	2.53814400	-0.79472000
N	0.11137200	-0.10829600	-0.19206200
C	0.34935500	3.36614500	1.11316300
H	-0.73706300	3.42090200	1.21975900
H	0.76717700	2.85225700	1.98341800
H	0.74786900	4.37880300	1.07790000
O	0.71592400	2.71859900	-0.10993900
H	2.42448200	2.40334800	-0.47130800
C	4.33334900	2.54523600	0.07291200
H	5.24974800	2.00808100	-0.16754800
H	4.46086900	3.59457100	-0.20568300
H	4.16088000	2.48220200	1.15140000
O	3.27028100	1.94206000	-0.67049100
H	2.79968800	0.26465400	-0.39056600
H	-5.99332900	1.10591000	-0.20233400