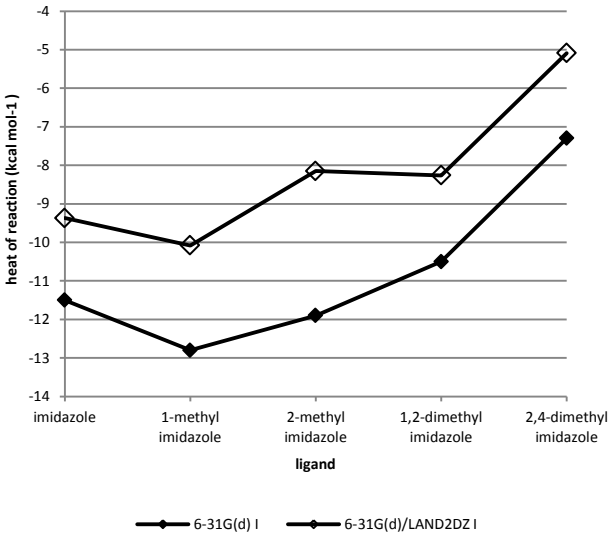


Figure S1. Energy of reaction I

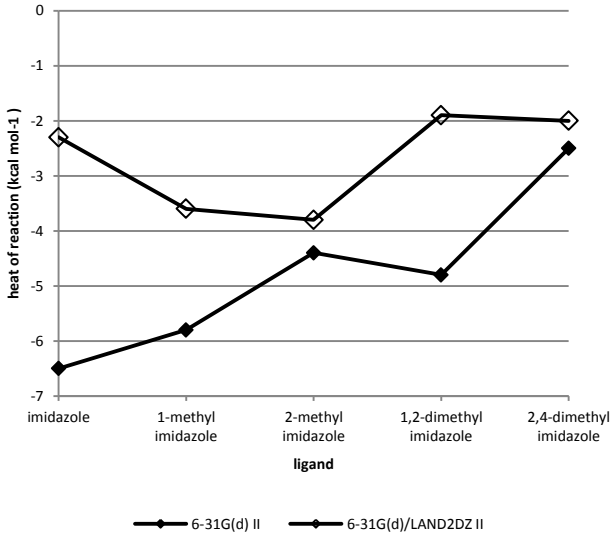
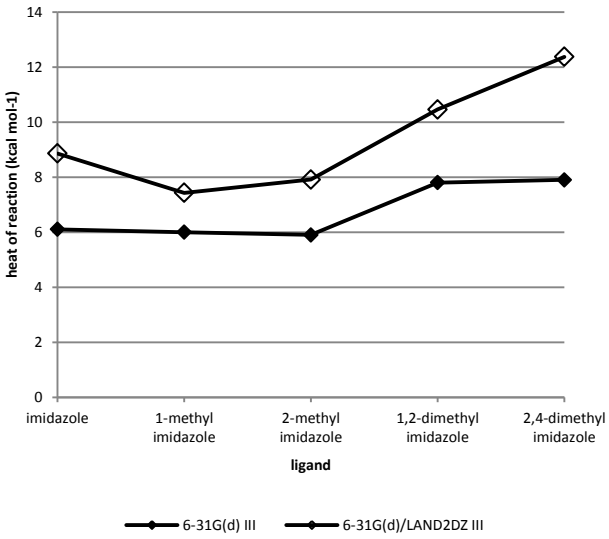
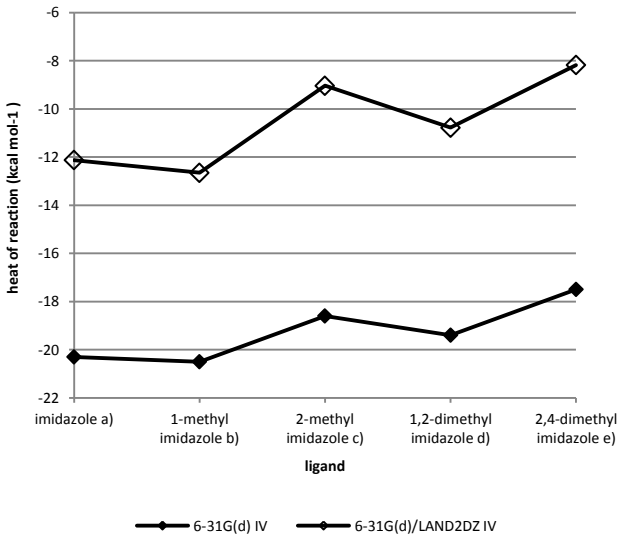


Figure S2. Energy of reaction II


14
12
10
8
6
4
2
0
heat of reaction (kcal mol-1)
imidazole
1-methyl imidazole
2-methyl imidazole
1,2-dimethyl imidazole
2,4-dimethyl imidazole
ligand
6-31G(d) III
6-31G(d)/LAND2DZ III



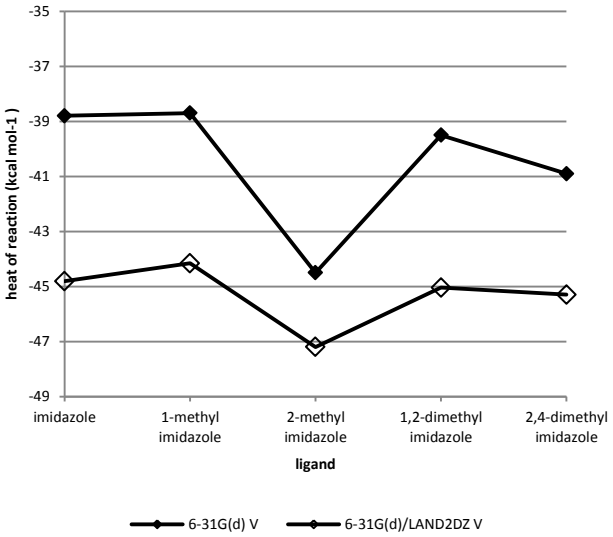


Figure S5. Energy of reaction V

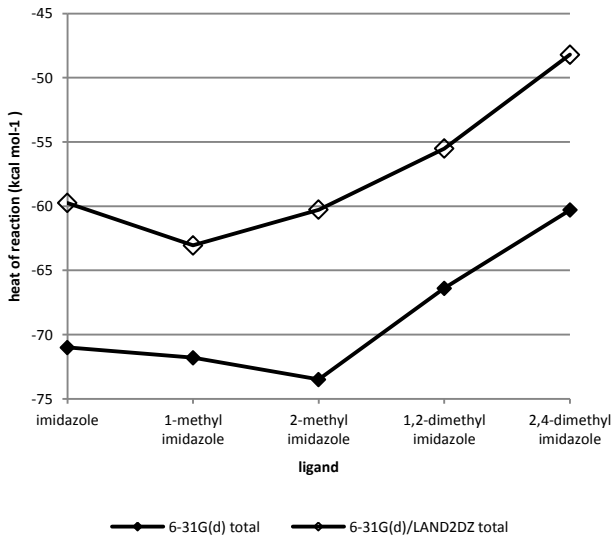


Figure S6. Total energy of reaction

Cobalt-salen (**1**) 6-31G(d)

Co	-0.00017900	0.25191400	0.00004500
N	-1.27248500	1.60483000	0.00015900
N	1.27247500	1.60495900	-0.00014100
C	-0.76851600	2.99027000	0.00055600
C	0.76859200	2.99026000	-0.00051800
H	-1.15154300	3.51664200	-0.88209800
H	-1.15032500	3.51563100	0.88434200
H	1.15150000	3.51679500	0.88212400
H	1.15028900	3.51582200	-0.88426500
O	-1.24884800	-1.09355700	0.00008200
O	1.24906800	-1.09361000	0.00005600
C	-2.57475400	1.45843700	0.00013700
H	-3.18800100	2.36497300	0.00021500
C	2.57481000	1.45831900	-0.00020100
H	3.18810600	2.36484700	-0.00031200
C	-3.26767400	0.22006100	0.00002200
C	-4.68358500	-2.19565300	-0.00015800
C	-2.54598400	-1.01977700	0.00002100
C	-4.68833000	0.21070500	-0.00004800
C	-5.39370100	-0.97099900	-0.00016000
C	-3.30551200	-2.22442300	-0.00008900
H	-5.21332100	1.16429500	-0.00001000
H	-6.47936500	-0.96780900	-0.00021300
H	-2.75514900	-3.15998700	-0.00010300
H	-5.23653000	-3.13212000	-0.00022700
C	2.54587100	-1.01983700	0.00004100
C	5.39379900	-0.97082300	0.00001600
C	3.30570100	-2.22452300	0.00011700
C	3.26766000	0.22009000	-0.00013300
C	4.68842600	0.21075000	-0.00006200
C	4.68364500	-2.19561800	0.00010500
H	2.75532800	-3.16009000	0.00018500
H	5.21327400	1.16442500	-0.00013300
H	5.23673900	-3.13200100	0.00016400
H	6.47945900	-0.96772600	0.00000700

Cobalt-salen (1) 6-31G(d)/LANL2DZ

Co	0.00528000	0.22542900	0.05674600
N	-1.26442300	1.59941900	-0.15674100
N	1.27592200	1.60212900	0.20254400
C	-0.64813600	2.91944400	-0.34408200
C	0.65811200	2.90644400	0.45152200
H	-0.41947800	3.05088800	-1.40683000
H	-1.30718600	3.73295800	-0.02055200
H	0.43974200	2.98493400	1.52071800
H	1.30912400	3.73868100	0.15972200
O	-1.26100600	-1.11711000	-0.05718400
O	1.26419400	-1.11400900	0.22737600
C	-2.56515600	1.47550600	-0.18091200
H	-3.16340500	2.38407900	-0.28166600
C	2.57093200	1.48185500	0.08746100
H	3.17295100	2.39345400	0.07589300
C	-3.26376300	0.23947500	-0.09005300
C	-4.71994700	-2.15648100	0.05797600
C	-2.56500200	-1.00820500	-0.03429600
C	-4.68980600	0.24749700	-0.06684300
C	-5.41202600	-0.92184300	0.00704300
C	-3.34027400	-2.20041400	0.03586000
H	-5.20865800	1.20221100	-0.10701300
H	-6.49792300	-0.90116200	0.02387400
H	-2.80881900	-3.14541100	0.07294900
H	-5.28724100	-3.08166400	0.11399400
C	2.56516700	-1.00791900	0.08965300
C	5.39415300	-0.93145000	-0.22659600
C	3.33551900	-2.20242200	0.04541700
C	3.26003100	0.23881500	-0.00640200
C	4.67552500	0.24201400	-0.17186400
C	4.70776300	-2.16403000	-0.11162500
H	2.80831900	-3.14615900	0.13334500
H	5.19143000	1.19580400	-0.25303300
H	5.27146200	-3.09230100	-0.14615600
H	6.47258300	-0.91450900	-0.35310500

Imidazole adduct (2b) 6-31G(d)

Co	-0.04719500	-0.17564200	0.27763100
N	1.22638000	-0.03645100	1.70417400
N	-1.33526100	0.36185300	1.58729100
C	0.57831400	0.10131500	3.00979400
C	-0.71000300	0.89617000	2.79327600
H	0.32617300	-0.90131000	3.37829000
H	1.23804700	0.58635600	3.74085700
H	-0.46618300	1.95476100	2.62962600
H	-1.37736700	0.82661800	3.66174400
O	1.26735700	-0.68482000	-0.99170100
O	-1.35799000	-0.35561200	-1.07656000
C	2.50823700	-0.21076700	1.62291100
H	3.09715100	-0.13095900	2.54360200
C	-2.61978700	0.20787100	1.50246600
H	-3.22727400	0.46390700	2.37760500
C	3.22748600	-0.51767400	0.42634800
C	4.73250700	-1.21335100	-1.83113400
C	2.54445900	-0.77054100	-0.81925400
C	4.64173700	-0.62448500	0.49453900
C	5.39617400	-0.95999400	-0.60754000
C	3.36162400	-1.12393800	-1.93783800
H	5.12584500	-0.43826500	1.45218100
H	6.47659500	-1.04010900	-0.53906500
H	2.85045900	-1.32520400	-2.87402400
H	5.31617900	-1.48839300	-2.70706700
C	-2.63102100	-0.50823300	-0.89523000
C	-5.46689700	-0.82232700	-0.66380100
C	-3.43373900	-0.91544300	-2.00269700
C	-3.31844500	-0.25236300	0.34533200
C	-4.72533900	-0.41822700	0.42424000
C	-4.79864100	-1.06947800	-1.88517400
H	-2.91886000	-1.11051100	-2.93803700
H	-5.21531500	-0.21788300	1.37592200
H	-5.37285900	-1.39122800	-2.75135500
H	-6.54214100	-0.95071600	-0.58767400
O	-0.33722600	-1.96036200	0.86667800
O	-0.28697300	-2.87865000	-0.02669500
C	1.35051700	2.38291200	-0.60210000
C	-0.79762400	2.64128000	-0.69954300
H	2.33728100	1.97134100	-0.45292500
C	-0.25170500	3.78971200	-1.20301300
H	-1.83612700	2.36892600	-0.59730900
H	-0.69436200	4.68905300	-1.60151600
N	0.21020700	1.77665700	-0.32552900
N	1.11659700	3.60926900	-1.13195700
H	1.82310000	4.25756200	-1.44802000

Imidazole adduct (2b) 6-31G(d)/LANL2DZ

Co	0.03925400	-0.25825600	-0.25053600
N	-1.23872600	-0.35544100	-1.69161900
N	1.33525500	0.02819500	-1.64146300
C	-0.59256900	-0.43957500	-3.00273600
C	0.71167100	0.35559400	-2.92115500
H	-0.36159400	-1.49310400	-3.21095300
H	-1.24508900	-0.06549500	-3.80291600
H	0.48547900	1.43073000	-2.93969000
H	1.37351200	0.12753100	-3.76714900
O	-1.29221200	-0.56845700	1.08451500
O	1.36465700	-0.27204100	1.12166300
C	-2.52521800	-0.46435100	-1.58107700
H	-3.11868700	-0.51648200	-2.50158500
C	2.62367000	-0.06261000	-1.52336900
H	3.23254300	0.06088200	-2.42667000
C	-3.24937700	-0.54156000	-0.34910700
C	-4.77617800	-0.79760200	1.98730100
C	-2.57317800	-0.61887300	0.92403400
C	-4.66667200	-0.59767300	-0.40246200
C	-5.43201200	-0.71727300	0.73690100
C	-3.40180300	-0.75262200	2.08194000
H	-5.14647400	-0.54775400	-1.37901800
H	-6.51516400	-0.75936800	0.67792500
H	-2.89610200	-0.82019700	3.04035700
H	-5.36774400	-0.89997500	2.89464400
C	2.64410500	-0.37544900	0.96531000
C	5.49488500	-0.59550000	0.78656000
C	3.45923800	-0.56509300	2.12354500
C	3.32883800	-0.29293700	-0.30221900
C	4.74284100	-0.40607900	-0.35156300
C	4.83008200	-0.67304100	2.03249700
H	2.94667100	-0.62910700	3.07844600
H	5.23048400	-0.33925300	-1.32315300
H	5.41212600	-0.82305600	2.93935200
H	6.57547200	-0.68362400	0.73144600
O	0.31927100	-2.27327500	-0.50830900
O	0.25057000	-3.00174900	0.50563900
C	-1.31268200	2.50777500	0.32180200
C	0.82765500	2.78249700	0.18911300
H	-2.30288900	2.07723500	0.32194800
C	0.31180400	3.99436900	0.56097900
H	1.85839100	2.50075400	0.03678800
H	0.77386700	4.94461900	0.77900700
N	-0.19382400	1.86748800	0.03942400
N	-1.05457800	3.80286900	0.63885300
H	-1.74041300	4.49100200	0.91351200

Imidazole complex (2a) 6-31G(d)

Co	0.04926300	-0.43924900	0.05377000
N	-1.19790800	-1.58677000	-0.81012800
N	1.34876100	-1.27748100	-1.03446600
C	-0.56134600	-2.57471800	-1.68847400
C	0.74474100	-1.95525700	-2.18107200
H	-0.33752800	-3.47986500	-1.10662700
H	-1.21590000	-2.86015000	-2.52248100
H	0.52475000	-1.20752500	-2.95495600
H	1.41427100	-2.71124900	-2.61227000
O	-1.25254200	0.20384300	1.26875900
O	1.36001500	0.35075800	1.16782000
C	-2.48702500	-1.62466100	-0.64158400
H	-3.06682300	-2.34795400	-1.22583800
C	2.64096700	-1.28697500	-0.87878200
H	3.24426100	-1.85556500	-1.59493700
C	-3.21680700	-0.80761300	0.27873600
C	-4.72970700	0.63969900	2.14239000
C	-2.53612300	0.04833900	1.21964300
C	-4.63140100	-0.90607100	0.30657500
C	-5.39011800	-0.19444800	1.21158600
C	-3.35533900	0.75505400	2.15286500
H	-5.11545300	-1.56869300	-0.40979400
H	-6.47252300	-0.27954900	1.21784500
H	-2.84568600	1.39100400	2.87045600
H	-5.31643900	1.19992900	2.86746700
C	2.64295900	0.18062400	1.14687900
C	5.49205800	-0.09838600	1.20559800
C	3.43978900	0.80710700	2.15295900
C	3.34349500	-0.60560200	0.16144100
C	4.75586800	-0.72219300	0.22171800
C	4.81167000	0.67142700	2.17720100
H	2.91543500	1.39665800	2.89891400
H	5.25616000	-1.32381200	-0.53602500
H	5.38181800	1.16701800	2.96023800
H	6.57288900	-0.19654500	1.23781000
C	-1.28274900	1.97034700	-1.44412000
C	0.85830300	2.07943700	-1.69949500
H	-2.27810600	1.65334200	-1.16918000
C	0.35486000	3.23424000	-2.23511400
H	1.88703200	1.76182900	-1.61594800
H	0.82464500	4.08731000	-2.69955100
N	-0.17031100	1.29940300	-1.21412400
N	-1.01394400	3.14866500	-2.06629600
H	-1.69345800	3.84790500	-2.32812900

Imidazole complex (2a) 6-31G(d)/LANL2DZ

Co	0.04926300	-0.43924900	0.05377000
N	-1.19790800	-1.58677000	-0.81012800
N	1.34876100	-1.27748100	-1.03446600
C	-0.56134600	-2.57471800	-1.68847400
C	0.74474100	-1.95525700	-2.18107200
H	-0.33752800	-3.47986500	-1.10662700
H	-1.21590000	-2.86015000	-2.52248100
H	0.52475000	-1.20752500	-2.95495600
H	1.41427100	-2.71124900	-2.61227000
O	-1.25254200	0.20384300	1.26875900
O	1.36001500	0.35075800	1.16782000
C	-2.48702500	-1.62466100	-0.64158400
H	-3.06682300	-2.34795400	-1.22583800
C	2.64096700	-1.28697500	-0.87878200
H	3.24426100	-1.85556500	-1.59493700
C	-3.21680700	-0.80761300	0.27873600
C	-4.72970700	0.63969900	2.14239000
C	-2.53612300	0.04833900	1.21964300
C	-4.63140100	-0.90607100	0.30657500
C	-5.39011800	-0.19444800	1.21158600
C	-3.35533900	0.75505400	2.15286500
H	-5.11545300	-1.56869300	-0.40979400
H	-6.47252300	-0.27954900	1.21784500
H	-2.84568600	1.39100400	2.87045600
H	-5.31643900	1.19992900	2.86746700
C	2.64295900	0.18062400	1.14687900
C	5.49205800	-0.09838600	1.20559800
C	3.43978900	0.80710700	2.15295900
C	3.34349500	-0.60560200	0.16144100
C	4.75586800	-0.72219300	0.22171800
C	4.81167000	0.67142700	2.17720100
H	2.91543500	1.39665800	2.89891400
H	5.25616000	-1.32381200	-0.53602500
H	5.38181800	1.16701800	2.96023800
H	6.57288900	-0.19654500	1.23781000
C	-1.28274900	1.97034700	-1.44412000
C	0.85830300	2.07943700	-1.69949500
H	-2.27810600	1.65334200	-1.16918000
C	0.35486000	3.23424000	-2.23511400
H	1.88703200	1.76182900	-1.61594800
H	0.82464500	4.08731000	-2.69955100
N	-0.17031100	1.29940300	-1.21412400
N	-1.01394400	3.14866500	-2.06629600
H	-1.69345800	3.84790500	-2.32812900

1-methylimidazole adduct (3b) 6-31G(d)

Co	-0.16494100	-0.40158800	0.24198100
N	1.07705100	-0.72384500	1.66696200
N	-1.44044000	-0.09352900	1.63483500
C	0.40684500	-0.85402300	2.96207900
C	-0.80663700	0.07624600	2.93846400
H	0.06462400	-1.89110300	3.07121800
H	1.08326300	-0.61983200	3.79426500
H	-0.47388600	1.11829400	3.03975500
H	-1.50025800	-0.14591600	3.75941700
O	1.13935700	-0.69353100	-1.10500300
O	-1.44891000	-0.13864600	-1.12414800
C	2.34329200	-0.97603900	1.55431600
H	2.91223400	-1.17181000	2.47026600
C	-2.73035700	-0.11055100	1.50650400
H	-3.33856700	-0.02408600	2.41376300
C	3.06807800	-1.03907500	0.32363600
C	4.57312600	-1.28787000	-2.02568000
C	2.40024800	-0.92481200	-0.95037500
C	4.46739500	-1.27433400	0.37268400
C	5.22234200	-1.39301500	-0.77299200
C	3.21658800	-1.06354700	-2.11612100
H	4.93934600	-1.36704800	1.34988700
H	6.29101000	-1.57602400	-0.71895200
H	2.71581900	-0.99012600	-3.07639400
H	5.15615800	-1.39015200	-2.93849800
C	-2.73458200	-0.21704900	-0.99367200
C	-5.59230300	-0.32800000	-0.86483900
C	-3.53771700	-0.26911300	-2.17240000
C	-3.43251100	-0.21233700	0.26729200
C	-4.84993000	-0.26862100	0.29379700
C	-4.91335100	-0.32673700	-2.10522600
H	-3.01505900	-0.27419200	-3.12363100
H	-5.34772100	-0.26476300	1.26238000
H	-5.48813100	-0.37520300	-3.02762700
H	-6.67621000	-0.37628400	-0.82936900
O	-0.61518100	-2.24375400	0.37433800
O	-0.59387300	-2.92352000	-0.71344600
C	1.45354500	2.16678400	0.02317800
C	-0.65903000	2.61908300	-0.01769800
H	2.40019300	1.64938600	0.07369000
C	-0.00256900	3.80121100	-0.22672700
H	-1.71960100	2.42437000	0.01126500
H	-0.35898300	4.80545900	-0.39881200
N	0.26165000	1.60683000	0.14118000
N	1.34711000	3.50041600	-0.19939200
C	2.44722800	4.43020100	-0.40496500
H	2.38219600	4.88458900	-1.39806400
H	2.43013500	5.21826400	0.35401600
H	3.38990800	3.88513800	-0.32862800

1-methylimidazole adduct (3b) 6-31G(d)/LANL2DZ

Co	-0.09687000	-0.51019100	0.09603400
N	1.17331600	-1.28309000	1.30549900
N	-1.38351400	-0.87474400	1.48281700
C	0.53348200	-1.98284900	2.41929800
C	-0.75108600	-1.22023500	2.75276400
H	0.27942700	-3.00029400	2.09446900
H	1.19839100	-2.05442600	3.29066000
H	-0.50198700	-0.29224200	3.28582200
H	-1.41802300	-1.81378100	3.39156300
O	1.18656600	-0.17888200	-1.26659600
O	-1.42994100	0.20280800	-1.08599600
C	2.45358700	-1.35790500	1.11466300
H	3.05513600	-1.86264800	1.87957000
C	-2.66924100	-0.89806100	1.34029800
H	-3.27484100	-1.21800700	2.19605100
C	3.15784100	-0.85018300	-0.01818200
C	4.65573900	0.01119400	-2.22352000
C	2.46888300	-0.30784000	-1.16291800
C	4.57378200	-0.94272800	-0.02344000
C	5.32562600	-0.51747900	-1.09630800
C	3.28164700	0.11085100	-2.26099800
H	5.06400100	-1.36767300	0.85133700
H	6.40835200	-0.59491000	-1.08346200
H	2.76581900	0.50752900	-3.13023400
H	5.23568400	0.34243900	-3.08247100
C	-2.71052300	0.00607200	-0.99953500
C	-5.55371000	-0.31634000	-0.94306600
C	-3.53011100	0.37009800	-2.10823100
C	-3.38201800	-0.53052300	0.15480800
C	-4.79171600	-0.67487000	0.14893200
C	-4.90078900	0.21149700	-2.07793900
H	-3.02589300	0.76472900	-2.98539700
H	-5.27119500	-1.08221900	1.03776500
H	-5.48754500	0.49462500	-2.94924000
H	-6.63232600	-0.43813500	-0.93292500
O	-0.51139600	-2.25519200	-0.64362300
O	0.46275300	-3.03445000	-0.89904700
C	-0.12247200	2.48328500	0.05743800
C	1.01340300	1.96297300	1.81928600
H	-0.71418500	2.40717500	-0.84219800
C	1.06423000	3.32725800	1.71304500
H	1.47479000	1.32370600	2.55653900
H	1.54296300	4.08300300	2.31732700
N	0.26642600	1.44852700	0.78248000
N	0.33534000	3.64694600	0.58251800
C	0.11074200	4.97992500	0.04393100
H	-0.42227400	5.60242400	0.76905300
H	1.06335600	5.45514300	-0.20858400
H	-0.49277600	4.89612300	-0.86160400

1-methylimidazole complex (3a) 6-31G(d)

Co	0.07759900	-0.64429200	-0.01032900
N	-1.17017200	-1.70868300	-0.96808300
N	1.36738100	-1.35779600	-1.19368300
C	-0.54360300	-2.59722600	-1.95309200
C	0.75598800	-1.92620300	-2.39438400
H	-0.31034900	-3.55868600	-1.47430900
H	-1.20808200	-2.79575000	-2.80451800
H	0.52971600	-1.10824400	-3.09208200
H	1.42516200	-2.63312600	-2.90259300
O	-1.19008300	-0.17326100	1.30989900
O	1.40171000	0.08997000	1.14074900
C	-2.45493600	-1.78081600	-0.77210300
H	-3.04144300	-2.44372000	-1.41818800
C	2.65932600	-1.37620700	-1.05256300
H	3.25786800	-1.87220700	-1.82444800
C	-3.16783700	-1.08184200	0.24929100
C	-4.65085200	0.12695900	2.29680000
C	-2.47446400	-0.32897700	1.26488900
C	-4.58016700	-1.19818700	0.29553400
C	-5.32470500	-0.60287700	1.29134100
C	-3.27765600	0.25477600	2.29103200
H	-5.07472400	-1.77909400	-0.48188900
H	-6.40610000	-0.69860600	1.30997200
H	-2.75821100	0.80895000	3.06722400
H	-5.22591200	0.59429200	3.09361900
C	2.68678000	-0.08933400	1.09488100
C	5.53290700	-0.39178900	1.10794900
C	3.49518000	0.44508800	2.14160600
C	3.37178100	-0.79505700	0.04293900
C	4.78221800	-0.92525400	0.08103700
C	4.86753200	0.29834000	2.14479500
H	2.98182800	0.96937900	2.94245500
H	5.27183700	-1.46311600	-0.72964000
H	5.44646800	0.72113900	2.96328500
H	6.61308200	-0.50069900	1.12148100
C	0.09585700	2.34066500	-0.36499700
C	-0.89421100	1.68316800	-2.16113500
H	0.61664900	2.34301300	0.58152600
C	-0.92777800	3.05276900	-2.18246900
H	-1.29983600	0.98702100	-2.88129000
H	-1.33771100	3.75928600	-2.88863100
N	-0.25035400	1.24979500	-1.02391600
N	-0.28947100	3.46302800	-1.02651600
C	-0.08321300	4.83451100	-0.58988600
H	0.51136800	5.38709800	-1.32408600
H	-1.04267200	5.34181500	-0.44894900
H	0.45228100	4.82403100	0.36133400

1-methylimidazole complex (3a) 6-31G(d)/LANL2DZ

Co	-0.08847400	-0.69046600	-0.04829800
N	1.13458400	-1.79738900	0.93399100
N	-1.42189000	-1.42720800	1.10361900
C	0.46364900	-2.72731000	1.84754600
C	-0.84663300	-2.07247200	2.28371600
H	0.24053600	-3.65766500	1.30606600
H	1.09524700	-2.97927100	2.71001700
H	-0.63212600	-1.30506700	3.04067600
H	-1.53391500	-2.80555200	2.72730600
O	1.25983400	-0.13599200	-1.28781500
O	-1.37713500	0.06842300	-1.23238800
C	2.42296900	-1.85504200	0.78689100
H	2.98656000	-2.54135300	1.42988800
C	-2.71101400	-1.37628500	0.94404100
H	-3.34163000	-1.87162000	1.69151500
C	3.18009200	-1.11638300	-0.17652100
C	4.76645800	0.16283100	-2.10150500
C	2.54019200	-0.31649900	-1.19019000
C	4.59182400	-1.24229600	-0.16358500
C	5.38734500	-0.61292600	-1.09793600
C	3.39462500	0.30269400	-2.15213200
H	5.04582200	-1.85921300	0.61077700
H	6.46753400	-0.71835100	-1.07037600
H	2.91511100	0.88907100	-2.93092900
H	5.37992400	0.65615200	-2.85267500
C	-2.66513300	-0.03674100	-1.17548800
C	-5.52630000	-0.18389800	-1.18056200
C	-3.44952200	0.56044100	-2.20994900
C	-3.38621100	-0.72571400	-0.13278600
C	-4.80343400	-0.77760000	-0.16884500
C	-4.82626400	0.48902500	-2.20813700
H	-2.91014000	1.07311400	-3.00097300
H	-5.31939800	-1.30482100	0.63259500
H	-5.38460800	0.95929100	-3.01502100
H	-6.61086200	-0.23226300	-1.19186000
C	0.58285900	2.27856300	0.36489800
C	-0.20030300	1.75510500	2.29936300
H	0.93036300	2.22001300	-0.65610800
C	0.01627900	3.10795700	2.32644800
H	-0.59609500	1.12327900	3.08178100
H	-0.13543600	3.85361400	3.09260600
N	0.15885200	1.24642800	1.07130300
N	0.51907000	3.43268100	1.08009100
C	0.90067100	4.75662700	0.61631000
H	0.04216200	5.43511100	0.63949500
H	1.70081300	5.16750800	1.23996500
H	1.26014000	4.67913100	-0.41156800

2-methylimidazole adduct (4b) 6-31G(d)

Co	0.00713100	-0.16935800	0.26603100
N	1.29120700	0.22955400	1.62737200
N	-1.26926400	-0.16512800	1.70012300
C	0.65998600	0.72227800	2.84619800
C	-0.63523900	-0.07360600	3.01865400
H	1.31785200	0.61567500	3.71835000
H	0.42356300	1.78643500	2.71693600
H	-1.30132300	0.39297100	3.75589700
H	-0.39123900	-1.08702800	3.36325500
O	1.34579500	-0.27240500	-1.07517700
O	-1.29220100	-0.57037300	-1.04892800
C	2.55406700	-0.05622600	1.57834600
H	3.15092200	0.08093800	2.48702700
C	-2.53046300	-0.45819100	1.60866600
H	-3.11491600	-0.50290800	2.53454700
C	3.24223700	-0.52084400	0.41419100
C	4.71021600	-1.34263900	-1.82254100
C	2.58222400	-0.60282300	-0.86417300
C	4.61477100	-0.85804100	0.52660200
C	5.34971400	-1.26803900	-0.56485500
C	3.37781700	-1.01748200	-1.97236200
H	5.08481100	-0.78752600	1.50639500
H	6.39802000	-1.53068800	-0.46250600
H	2.88344800	-1.08372400	-2.93654300
H	5.27840000	-1.66735700	-2.69156500
C	-2.55271800	-0.79056700	-0.87491600
C	-5.36744200	-1.27796000	-0.65760500
C	-3.35394000	-1.09861500	-2.01750500
C	-3.23202200	-0.73498900	0.39688600
C	-4.62844500	-0.98569100	0.46615800
C	-4.70685500	-1.33278600	-1.90806800
H	-2.84483500	-1.14695000	-2.97487500
H	-5.11018000	-0.94536100	1.44202600
H	-5.27895100	-1.56853900	-2.80289100
H	-6.43360600	-1.47013100	-0.58834700
O	0.28199900	-2.00451400	0.70783800
O	0.20682500	-2.85254700	-0.24921700
C	0.49909800	2.78322100	-0.66399000
C	-1.58600400	2.41094400	-0.16121500
C	-1.54159400	3.68549000	-0.64582600
H	-2.44316500	1.85152900	0.17638500
H	-2.30489900	4.43228900	-0.79782200
N	-0.31843100	1.85737000	-0.17125000
N	-0.21437400	3.90615300	-0.95575400
H	0.17372500	4.74730300	-1.35722800
C	1.96501200	2.69296600	-0.92888200
H	2.49154900	2.24083600	-0.08657700
H	2.16067800	2.06868500	-1.80469800
H	2.38178400	3.69091100	-1.10274400

2-methylimidazole adduct (4b) 6-31G(d)/LANL2DZ

Co	0.08757100	-0.49117500	-0.06233900
N	1.37422700	-1.28950900	1.13638000
N	-1.19207300	-1.56075200	0.88418000
C	0.76631900	-2.09586700	2.19595000
C	-0.56415000	-2.62975700	1.66116700
H	1.42569600	-2.91708100	2.50508700
H	0.59025300	-1.46267200	3.07619800
H	-1.21528600	-2.97689100	2.47493700
H	-0.37457000	-3.47679300	0.98970900
O	1.42167800	0.47081500	-1.03350100
O	-1.21358200	0.23245200	-1.25796300
C	2.66367100	-1.20669900	1.03526900
H	3.26980500	-1.77191100	1.75250400
C	-2.47917600	-1.50531900	0.74879700
H	-3.08729000	-2.19645500	1.34376100
C	3.38128200	-0.43983100	0.06684900
C	4.90886900	1.01703000	-1.77426400
C	2.70645700	0.35731600	-0.92428100
C	4.79852100	-0.47765500	0.09935800
C	5.56476000	0.23486700	-0.79758700
C	3.53248900	1.07800200	-1.83966100
H	5.27920700	-1.09158700	0.85961200
H	6.64881200	0.19403700	-0.75927100
H	3.02845000	1.66769900	-2.59954200
H	5.50007600	1.57921700	-2.49404200
C	-2.50034300	0.16659600	-1.11922200
C	-5.35964300	0.13000700	-0.94935100
C	-3.31815600	0.92774400	-2.00828800
C	-3.18522300	-0.63417500	-0.13704900
C	-4.60239200	-0.63177800	-0.08590000
C	-4.69443600	0.91146800	-1.92007300
H	-2.80855500	1.51763400	-2.76439200
H	-5.09040100	-1.25763300	0.65986600
H	-5.27819800	1.50858600	-2.61749500
H	-6.44376300	0.12199500	-0.89460500
O	0.44778000	-1.97787800	-1.31349800
O	-0.52764600	-2.68796800	-1.69570600
C	-0.22026400	2.49881100	0.82144300
C	-0.56866800	1.21414000	2.54245300
C	-0.73832400	2.49145100	2.99439200
H	-0.68246300	0.29043700	3.08667700
H	-0.99974500	2.89400100	3.96053800
N	-0.24516100	1.22385600	1.19957100
N	-0.51294300	3.29082300	1.89194900
H	-0.56615000	4.29879200	1.86431800
C	0.07373600	3.06004600	-0.52989900
H	1.15159500	3.18247000	-0.67995400
H	-0.28871600	2.37208000	-1.29407900
H	-0.40933700	4.03711400	-0.64650900

2-methylimidazole complex (4a) 6-31G(d)

Co	-0.10897000	0.48555600	-0.25663400
N	-1.39419100	1.69380800	0.42888300
N	1.13699500	1.89469100	0.02090100
C	-0.78914800	2.82812600	1.12861200
C	0.50500400	3.16597000	0.39038000
H	-1.46521400	3.69226000	1.16979100
H	-0.56245100	2.52902500	2.16080300
H	1.17065500	3.79118400	1.00046300
H	0.26278900	3.72380000	-0.52510000
O	-1.43439800	-0.68851300	-0.92723500
O	1.15907700	-0.57249100	-1.19378500
C	-2.68999400	1.62273500	0.32919900
H	-3.28566000	2.44011900	0.74975400
C	2.42111500	1.85950500	-0.18402000
H	3.00533100	2.76204400	0.02794300
C	-3.40900900	0.55979400	-0.29738900
C	-4.91119000	-1.44600500	-1.55011900
C	-2.72274100	-0.54685000	-0.91182600
C	-4.82470900	0.62123300	-0.33119900
C	-5.57808200	-0.36020900	-0.93998300
C	-3.53451100	-1.53759300	-1.54132300
H	-5.31515500	1.47146900	0.14077800
H	-6.66201400	-0.29968400	-0.95486700
H	-3.02062900	-2.36728400	-2.01777700
H	-5.49356100	-2.22420400	-2.03905700
C	2.44618500	-0.41947900	-1.21700900
C	5.29815500	-0.20183400	-1.35020300
C	3.25247500	-1.43757400	-1.80886500
C	3.13676400	0.73772900	-0.70622800
C	4.54964000	0.81272200	-0.79164000
C	4.62710500	-1.33356700	-1.86426600
H	2.73616100	-2.30286600	-2.21419100
H	5.04219800	1.70336800	-0.40380700
H	5.20400400	-2.13705100	-2.31759700
H	6.38022300	-0.13011700	-1.40332000
C	0.32321600	-1.94206100	1.71031000
C	0.78598600	-0.12229200	2.79773000
C	1.01622800	-1.14400200	3.67565900
H	0.92477400	0.93710600	2.95355200
H	1.36302500	-1.16621700	4.69710400
N	0.35672000	-0.62125800	1.58441400
N	0.71601700	-2.29227700	2.96955700
H	0.78534800	-3.23925300	3.31289800
C	-0.08110500	-2.94238600	0.67863700
H	-1.16945500	-3.06459700	0.65088600
H	0.23423800	-2.59235700	-0.30540700
H	0.37307000	-3.91725100	0.88940000

2-methylimidazole complex (4a) 6-31G(d)/LANL2DZ

Co	-0.05447600	0.39831700	-0.23385700
N	1.19962800	0.74589800	-1.65249900
N	-1.37225300	0.44656100	-1.61751500
C	0.56034200	0.94276000	-2.96082500
C	-0.78137000	0.21155800	-2.93280200
H	0.38502100	2.01705800	-3.11467000
H	1.19618700	0.58246200	-3.78038500
H	-0.61383800	-0.86760800	-3.04981000
H	-1.43840400	0.54955100	-3.74582300
O	1.27959600	0.57477500	1.11603700
O	-1.37359400	0.50940900	1.14553700
C	2.47139200	0.98801900	-1.52895600
H	3.04001000	1.23345500	-2.43388500
C	-2.65148400	0.63554800	-1.48797100
H	-3.26179500	0.67149100	-2.39790800
C	3.20162800	0.98844000	-0.30026300
C	4.72443100	1.10642200	2.05109700
C	2.54332000	0.80593200	0.97069600
C	4.60059100	1.22249100	-0.34417300
C	5.36406000	1.27708600	0.80175900
C	3.36642600	0.88326500	2.13703600
H	5.06828400	1.36291900	-1.31785700
H	6.43354100	1.45637800	0.74955600
H	2.87179000	0.75808000	3.09577800
H	5.31425600	1.15550800	2.96407400
C	-2.64206700	0.72424400	1.01747900
C	-5.46739300	1.18581200	0.88789700
C	-3.43263500	0.90097800	2.19536900
C	-3.33862100	0.79413900	-0.24532000
C	-4.73900100	1.02316100	-0.26996300
C	-4.79135400	1.12246600	2.12867400
H	-2.91179500	0.85284100	3.14697000
H	-5.23589400	1.06971600	-1.23823200
H	-5.35500800	1.25111300	3.05040100
H	-6.53826100	1.36083000	0.85153700
C	0.84296500	-2.77041600	0.12154800
C	-1.30031000	-2.53476900	-0.10995200
C	-1.10581900	-3.84709000	0.21840900
H	-2.22916800	-2.01548300	-0.29139400
H	-1.78603100	-4.67250100	0.36083700
N	-0.08824900	-1.87510800	-0.17228800
N	0.26247000	-3.98247300	0.36036800
H	0.75476900	-4.82568000	0.61725600
C	2.31316500	-2.54129000	0.23764200
H	2.64409500	-1.80984200	-0.50187400
H	2.57431800	-2.14307200	1.22440400
H	2.86999000	-3.47194500	0.08183900

1,2-dimethylimidazole adduct (5b) 6-31G(d)

Co	-0.12476900	-0.33996000	0.26804900
N	1.12332400	-0.58023900	1.71325900
N	-1.42765600	-0.13268600	1.64911000
C	0.47228700	-0.62066600	3.02946200
C	-0.81595300	0.19609800	2.93079700
H	0.22113300	-1.66292200	3.26571500
H	1.13244800	-0.23727500	3.81829000
H	-0.57749300	1.26783700	2.94100800
H	-1.49055900	-0.01581200	3.77036300
O	1.21165100	-0.52160200	-1.06254400
O	-1.42923900	-0.26038900	-1.10474600
C	2.33927300	-1.02035500	1.59623000
H	2.88479900	-1.26907100	2.51375200
C	-2.70293700	-0.33088700	1.53050800
H	-3.31841400	-0.28386700	2.43578300
C	3.03831000	-1.22137800	0.36753200
C	4.51192400	-1.64664200	-1.97561600
C	2.41414900	-0.96849900	-0.90773700
C	4.37869300	-1.68579400	0.42095300
C	5.11657900	-1.89908600	-0.72206500
C	3.21281000	-1.19583700	-2.06996000
H	4.81878800	-1.87567400	1.39881800
H	6.13885800	-2.25985300	-0.66560100
H	2.74423100	-1.01238000	-3.03182400
H	5.08215400	-1.81739300	-2.88630800
C	-2.68928900	-0.52486400	-0.96586900
C	-5.50053100	-1.04887900	-0.81940000
C	-3.47673800	-0.73228800	-2.13803900
C	-3.38112300	-0.58097000	0.29821400
C	-4.77525900	-0.84179100	0.33299900
C	-4.82895800	-0.98938500	-2.06233100
H	-2.95938500	-0.69145200	-3.09130000
H	-5.26844800	-0.87788800	1.30327300
H	-5.39032400	-1.15227800	-2.97987200
H	-6.56561500	-1.25449800	-0.77719600
O	-0.40129200	-2.22239700	0.42328700
O	-0.29473200	-2.91820400	-0.64663300
C	1.03482400	2.58796400	-0.10515100
C	-1.13641400	2.49963100	-0.04016700
C	-0.81659200	3.78880700	-0.34693300
H	-2.11264800	2.05509500	0.06125300
H	-1.42420200	4.65867400	-0.54431100
N	0.01788500	1.75726700	0.11151300
N	0.56476700	3.83895600	-0.39005800
C	2.49164300	2.26968800	-0.08647900
H	2.68374500	1.41271500	0.55620400
H	2.85797600	2.01501100	-1.08805500
H	3.07664800	3.11796600	0.28472300
C	1.36468700	5.01347500	-0.70374200
H	2.00995800	4.82485700	-1.56669500
H	0.69159800	5.83778900	-0.94505700
H	1.98585900	5.30694000	0.14879800

1,2-dimethylimidazole adduct (5b) 6-31G(d)/LANL2DZ

Co	-0.11123500	-0.41164200	0.26933300
N	1.12887800	-0.82797300	1.68521700
N	-1.42421000	-0.36407800	1.66200400
C	0.47636500	-1.00713500	2.98841300
C	-0.81265300	-0.18561300	2.97626500
H	0.22760600	-2.06987100	3.11804900
H	1.13431400	-0.70879600	3.81543000
H	-0.57148200	0.87792400	3.10553400
H	-1.48809400	-0.48864100	3.78780600
O	1.21863300	-0.58139700	-1.08823800
O	-1.43397100	-0.30226400	-1.10871400
C	2.37860900	-1.15447400	1.54834800
H	2.93568500	-1.44840800	2.44602300
C	-2.71158500	-0.45762200	1.52828200
H	-3.32531100	-0.46261400	2.43668700
C	3.10194300	-1.18292100	0.31526400
C	4.61788200	-1.32569700	-2.03872400
C	2.46128700	-0.90728500	-0.94861500
C	4.48023700	-1.52043800	0.35018600
C	5.24001000	-1.59145400	-0.79683200
C	3.28135500	-0.99745000	-2.11634600
H	4.93397900	-1.72836200	1.31833700
H	6.29266500	-1.85310400	-0.75180400
H	2.80032100	-0.79912700	-3.06952400
H	5.20466200	-1.38477600	-2.95308100
C	-2.71206000	-0.45143800	-0.98078000
C	-5.55926500	-0.75261800	-0.85555200
C	-3.51622700	-0.51987300	-2.16047400
C	-3.40716500	-0.53952100	0.28165900
C	-4.81843400	-0.68699600	0.30399700
C	-4.88516300	-0.66676000	-2.09575800
H	-2.99689600	-0.45515500	-3.11183200
H	-5.31383900	-0.74902800	1.27209900
H	-5.45827300	-0.71794600	-3.01919500
H	-6.63820400	-0.86798100	-0.82079300
O	-0.42468300	-2.73925500	0.13723100
O	-0.41181000	-3.25802100	-0.97407200
C	1.01627300	2.70654700	0.05468700
C	-1.14483800	2.57721000	0.15158200
C	-0.85684000	3.87646600	-0.15426600
H	-2.11055300	2.10998800	0.26683500
H	-1.48308200	4.73662900	-0.33727300
N	0.02335400	1.85525000	0.28182300
N	0.52322900	3.95365400	-0.21777100
C	2.47695700	2.40243000	0.05864400
H	3.05099800	3.19440300	0.55396000
H	2.65783100	1.46486100	0.58257900
H	2.86919600	2.28868400	-0.95991100
C	1.30173500	5.14140100	-0.52982500
H	1.95122400	4.96411800	-1.39246500
H	0.61670700	5.95596500	-0.77145200
H	1.91926400	5.44455000	0.32252100

1,2-dimethylimidazole complex (5a) 6-31G(d)

Co	-0.11231000	-0.54443000	0.23458200
N	1.10432700	-1.08463800	1.59860400
N	-1.42538900	-0.62622900	1.59357800
C	0.46162100	-1.32058100	2.90008900
C	-0.82693500	-0.50120700	2.92026600
H	0.21544000	-2.38757300	2.99374300
H	1.12417200	-1.05117500	3.73286400
H	-0.58910700	0.55608300	3.09609300
H	-1.50729100	-0.83848000	3.71360500
O	1.19006400	-0.71381700	-1.12345400
O	-1.42070700	-0.55847000	-1.14366500
C	2.35329600	-1.42696800	1.45519600
H	2.89419300	-1.79378400	2.33482200
C	-2.71159900	-0.77059800	1.46437100
H	-3.31872900	-0.83927600	2.37369600
C	3.08241000	-1.38603400	0.22715700
C	4.58043400	-1.42048800	-2.14189000
C	2.43544100	-1.04610600	-1.01625600
C	4.45817400	-1.73307900	0.23663800
C	5.20929700	-1.74924200	-0.91871700
C	3.24406000	-1.08498900	-2.19333000
H	4.91729500	-1.99200800	1.18982100
H	6.26141500	-2.01624800	-0.89394100
H	2.75744100	-0.83853000	-3.13229400
H	5.16137700	-1.43587200	-3.06174200
C	-2.69685000	-0.74411200	-1.03777700
C	-5.53415600	-1.12477800	-0.94441500
C	-3.48245900	-0.84799400	-2.22635400
C	-3.40335700	-0.84553200	0.21603100
C	-4.80923800	-1.03378300	0.22416700
C	-4.84822000	-1.03044500	-2.17728800
H	-2.95421700	-0.77535300	-3.17222000
H	-5.31376700	-1.10691100	1.18678700
H	-5.40919900	-1.10256500	-3.10679300
H	-6.61009800	-1.26858400	-0.92145900
C	0.91903300	2.54439800	0.14509600
C	-1.23953300	2.34899900	0.12909400
C	-0.97697000	3.67039000	-0.09284400
H	-2.19479700	1.84949800	0.17816000
H	-1.61912000	4.52180400	-0.26074900
N	-0.05702800	1.65509900	0.27883100
N	0.40165200	3.79066200	-0.08157300
C	2.38487500	2.27288600	0.20301800
H	2.55597300	1.27111000	0.59488700
H	2.84550600	2.32035500	-0.79181600
H	2.90503900	2.99290900	0.84664800
C	1.15863800	5.00875300	-0.31938600
H	1.72346500	4.94438900	-1.25539200
H	0.46335300	5.84739900	-0.38670100
H	1.85646700	5.19953000	0.50194900

1,2-dimethylimidazole complex (5a) 6-31G(d)/LANL2DZ

Co	-0.12481200	-0.61227900	0.20521400
N	1.10953500	-1.14663900	1.58129800
N	-1.44293300	-0.70512300	1.58606500
C	0.46052700	-1.41914400	2.87116600
C	-0.83807500	-0.61399700	2.91279200
H	0.22484300	-2.49106900	2.93382400
H	1.11572000	-1.16601700	3.71521400
H	-0.61036400	0.44062700	3.11796000
H	-1.51178600	-0.98184700	3.69878200
O	1.19440200	-0.74299600	-1.16219200
O	-1.44901000	-0.54574200	-1.17284400
C	2.36451100	-1.45283900	1.42868500
H	2.91815100	-1.81223700	2.30428700
C	-2.73028300	-0.81256400	1.44799100
H	-3.34146200	-0.88820000	2.35487700
C	3.09338000	-1.37975200	0.20149400
C	4.60997200	-1.34507900	-2.15664800
C	2.44587000	-1.04250000	-1.04376600
C	4.47858000	-1.68938400	0.21645500
C	5.23869300	-1.67156800	-0.93246200
C	3.26586700	-1.04528700	-2.21498100
H	4.93761800	-1.94725700	1.17002200
H	6.29736100	-1.91042700	-0.90273300
H	2.77944600	-0.79991000	-3.15442100
H	5.19791800	-1.33352400	-3.07211300
C	-2.72708700	-0.70412000	-1.05686700
C	-5.57265700	-1.02371500	-0.95175600
C	-3.52574800	-0.74700200	-2.24164000
C	-3.42598900	-0.83491300	0.19958800
C	-4.83641000	-0.99066300	0.21230300
C	-4.89446600	-0.90038300	-2.18664700
H	-3.00306500	-0.65248300	-3.18875400
H	-5.33508000	-1.08592500	1.17607300
H	-5.46425700	-0.92680100	-3.11321300
H	-6.65136800	-1.14362400	-0.92451400
C	0.94085600	2.54559800	0.19357800
C	-1.21798900	2.36698200	0.20931600
C	-0.94934900	3.68879700	-0.00656600
H	-2.17580300	1.87233100	0.26324900
H	-1.58794000	4.54611000	-0.15789900
N	-0.03904800	1.66233600	0.33493800
N	0.43012700	3.79765000	-0.01855600
C	2.40656000	2.26790400	0.23011500
H	2.93854200	2.98648400	0.86573400
H	2.58042000	1.26558000	0.61965500
H	2.85252600	2.31327800	-0.77176900
C	1.19422700	5.01729700	-0.22271200
H	1.89420600	4.90058000	-1.05568600
H	0.50416300	5.82910400	-0.45941000
H	1.75727700	5.28707500	0.67749400

2,4-dimethylimidazole adduct (6b) 6-31G(d)

Co	-0.02830900	-0.07107300	0.23477600
N	1.23081600	0.01862800	1.69432500
N	-1.33418600	0.24812100	1.58549900
C	0.60541300	0.27264500	3.00196800
C	-0.76274300	0.91221700	2.74814300
H	0.46726400	-0.68311100	3.52402100
H	1.23426700	0.91750600	3.62947300
H	-0.63703700	1.97654500	2.51247300
H	-1.41231300	0.82777900	3.62919000
O	1.31814400	-0.43158200	-1.04728600
O	-1.35337200	-0.34342500	-1.09166500
C	2.42726400	-0.48787200	1.66504300
H	2.97224900	-0.57324400	2.61226000
C	-2.54501300	-0.21398400	1.57418200
H	-3.14741600	-0.11163500	2.48375300
C	3.10668600	-0.95684800	0.50033600
C	4.55628800	-1.87283200	-1.71410600
C	2.49587900	-0.90964300	-0.80512700
C	4.42109400	-1.47120600	0.64849100
C	5.14636500	-1.92631600	-0.43042200
C	3.28176000	-1.38015800	-1.89986200
H	4.85239300	-1.50131500	1.64801700
H	6.14846500	-2.32271700	-0.30000700
H	2.82404800	-1.34846000	-2.88368800
H	5.11666800	-2.23313400	-2.57414500
C	-2.52690800	-0.84263700	-0.84793200
C	-5.15935000	-1.90123700	-0.47266300
C	-3.27276000	-1.39717900	-1.92867800
C	-3.17013200	-0.82329600	0.44237600
C	-4.47522800	-1.35546000	0.59211700
C	-4.53885300	-1.91281600	-1.74179000
H	-2.79350700	-1.41101300	-2.90247400
H	-4.93448200	-1.32563100	1.57908700
H	-5.06852700	-2.33958600	-2.59078500
H	-6.15537500	-2.31263800	-0.34172500
O	-0.15868000	-1.93201400	0.72284100
O	-0.05285300	-2.79625900	-0.20755200
C	1.17974800	2.75057900	-0.57241800
C	-1.00001400	2.90348200	-0.62906100
C	-0.51046600	4.09949100	-1.07762000
H	-1.01193700	4.99412800	-1.41287100
N	0.06916700	2.06059000	-0.31142400
N	0.86151800	3.98825200	-1.03376600
H	1.53107000	4.68862600	-1.31637800
C	2.60909200	2.34001000	-0.45307300
H	2.79069800	1.80464700	0.47804500
H	2.90072300	1.68101800	-1.27500100
H	3.25501200	3.22480400	-0.47237500
C	-2.45006700	2.56257300	-0.51126000
H	-2.71643600	1.72904300	-1.16307600
H	-2.72648200	2.28489000	0.50941800
H	-3.05043900	3.43250500	-0.79716900

2,4-dimethylimidazole adduct (6b) 6-31G(d)/LANL2DZ

Co	-0.02237500	-0.07647200	0.25546200
N	1.22063100	-0.20959700	1.72457600
N	-1.33900400	0.10122300	1.62661200
C	0.59041900	-0.08311200	3.04852200
C	-0.75536500	0.61992700	2.85877300
H	0.42100100	-1.08640400	3.46403900
H	1.23202800	0.46895500	3.74779000
H	-0.59464400	1.69873700	2.73503000
H	-1.41237900	0.46318800	3.72527600
O	1.31132400	-0.49814500	-1.04048400
O	-1.34892900	-0.40002800	-1.08499600
C	2.44626300	-0.64175200	1.65896400
H	2.98928300	-0.79410200	2.59943400
C	-2.58537500	-0.25751100	1.56615800
H	-3.18750800	-0.18925700	2.47970000
C	3.15700100	-0.95814100	0.46048700
C	4.64766600	-1.63412700	-1.81596000
C	2.53092600	-0.87705800	-0.83710200
C	4.50757100	-1.38072500	0.56774000
C	5.25442100	-1.71341600	-0.54134600
C	3.33658500	-1.23291300	-1.96274900
H	4.95110100	-1.43853800	1.56090500
H	6.28626300	-2.03557700	-0.44085400
H	2.86648600	-1.17707800	-2.94011100
H	5.22496500	-1.89846600	-2.69947000
C	-2.57556500	-0.76677300	-0.88772400
C	-5.30838100	-1.57861700	-0.60720600
C	-3.34376600	-1.22448100	-2.00167900
C	-3.24666500	-0.72843800	0.38939200
C	-4.60101800	-1.13639200	0.48996000
C	-4.65847400	-1.61697600	-1.86173800
H	-2.84293600	-1.25348300	-2.96473700
H	-5.08078900	-1.09300100	1.46691300
H	-5.20563100	-1.96320700	-2.73608800
H	-6.34402900	-1.89024000	-0.51255500
O	-0.19260300	-2.83963900	0.54886000
O	-0.20690200	-3.51219400	-0.46437200
C	1.22615900	2.94203800	-0.44677700
C	-0.94253400	3.13488700	-0.47137500
C	-0.44339100	4.32892800	-0.91949500
H	-0.93071300	5.23761000	-1.23854100
N	0.11097300	2.27454100	-0.17692900
N	0.93040200	4.19329500	-0.89618500
H	1.60626100	4.88632400	-1.18203900
C	2.63579800	2.46272200	-0.34331500
H	2.77352100	1.85575400	0.55233100
H	2.90733700	1.84192800	-1.20306000
H	3.32896000	3.31019700	-0.29715500
C	-2.38295400	2.77054500	-0.31294500
H	-2.64311900	1.91083300	-0.93527200
H	-2.62317500	2.50915500	0.72316200
H	-3.01822200	3.61353100	-0.60424000

2,4-dimethylimidazole complex (6a) 6-31G(d)

Co	-0.03911400	-0.18454500	0.25597400
N	1.18152300	-0.38651800	1.71521300
N	-1.34369200	-0.01622700	1.61381700
C	0.56812600	-0.21485900	3.04348300
C	-0.75775700	0.51899900	2.83761700
H	0.37436300	-1.20077600	3.48818700
H	1.23022300	0.33818900	3.72222500
H	-0.57072600	1.59011300	2.69101700
H	-1.42231700	0.39820600	3.70354500
O	1.26580500	-0.67208600	-1.02273300
O	-1.35117100	-0.64063000	-1.04642400
C	2.38403400	-0.88899500	1.66334300
H	2.90361000	-1.08433100	2.60836100
C	-2.58003700	-0.41983800	1.58944500
H	-3.16574700	-0.35051000	2.51274500
C	3.08897000	-1.22673400	0.46868300
C	4.54851300	-1.95115700	-1.81185600
C	2.46886000	-1.10600000	-0.82755800
C	4.41671400	-1.71514900	0.57466500
C	5.14867500	-2.07151600	-0.53744600
C	3.25735800	-1.48800300	-1.95572900
H	4.85521900	-1.80294500	1.56784000
H	6.16423700	-2.44260800	-0.43905200
H	2.79212600	-1.40190200	-2.93311600
H	5.11454600	-2.23300000	-2.69725200
C	-2.56497700	-1.04124000	-0.83251400
C	-5.26994600	-1.92301500	-0.50721400
C	-3.31399700	-1.58795700	-1.91801000
C	-3.23910700	-0.95226300	0.43906500
C	-4.57903100	-1.39810000	0.56401300
C	-4.61620900	-2.01336700	-1.75702500
H	-2.81072800	-1.65667200	-2.87773000
H	-5.06065700	-1.31744400	1.53766400
H	-5.15047200	-2.42592400	-2.61032700
H	-6.29539500	-2.26168100	-0.39519100
C	1.23688900	2.70954100	-0.40079500
C	-0.92492600	2.86142300	-0.63495400
C	-0.40607400	4.06403000	-1.03385200
H	-0.87679100	4.96230100	-1.40286100
N	0.11215900	2.02183000	-0.23728500
N	0.96143400	3.95382700	-0.87814800
H	1.64886600	4.65928500	-1.09834600
C	2.63864000	2.25351000	-0.16565400
H	2.71130800	1.68196100	0.76062500
H	2.98467000	1.60561300	-0.97702100
H	3.31641100	3.11152600	-0.09721400
C	-2.36454500	2.46206100	-0.63330700
H	-2.54039000	1.62964500	-1.31933500
H	-2.69547000	2.14040900	0.35880600
H	-2.98886700	3.30637100	-0.94318200

2,4-dimethylimidazole complex (6a) 6-31G(d)/LANL2DZ

Co	-0.03429200	0.28070200	-0.25564500
N	1.20438200	0.43876800	-1.72656300
N	-1.35426900	0.13695600	-1.62753800
C	0.57299200	0.32372800	-3.05139800
C	-0.77601000	-0.37423400	-2.86533900
H	0.40826800	1.32999100	-3.46164700
H	1.21175700	-0.22763300	-3.75380700
H	-0.62056600	-1.45491600	-2.75154200
H	-1.43353300	-0.20645600	-3.72941800
O	1.29978400	0.71003700	1.03634000
O	-1.35429000	0.65220700	1.07945300
C	2.43077700	0.87114100	-1.66093600
H	2.96901900	1.03640700	-2.60195900
C	-2.59581700	0.51457000	-1.56763200
H	-3.19616300	0.46074800	-2.48328300
C	3.14651900	1.17167500	-0.46198400
C	4.64161700	1.82559000	1.81787500
C	2.52113100	1.08405600	0.83543200
C	4.49861400	1.58999000	-0.56769500
C	5.24773800	1.91109300	0.54318400
C	3.32890700	1.42940900	1.96298600
H	4.94133800	1.65359000	-1.56087100
H	6.28093200	2.22942500	0.44424600
H	2.85919000	1.36926800	2.94027600
H	5.22096300	2.08112400	2.70264300
C	-2.57693500	1.03238100	0.88338700
C	-5.30137300	1.87223000	0.60448100
C	-3.33600100	1.50924700	1.99572900
C	-3.25212800	0.99194200	-0.39139600
C	-4.60229300	1.41419200	-0.49136100
C	-4.64680200	1.91448900	1.85665700
H	-2.83164800	1.54112200	2.95686300
H	-5.08526200	1.36918000	-1.46668100
H	-5.18750200	2.27383800	2.72973800
H	-6.33398100	2.19406200	0.51065800
C	1.19230000	-2.72978500	0.43112300
C	-0.97826500	-2.90123300	0.47497600
C	-0.48682600	-4.10045200	0.91771200
H	-0.98000100	-5.00459100	1.24060900
N	0.08118400	-2.05151800	0.17177700
N	0.88817100	-3.97837500	0.88207400
H	1.55959000	-4.67836000	1.16137500
C	2.60475300	-2.26154800	0.31590500
H	2.73807800	-1.65223800	-0.57888000
H	2.88923600	-1.64581200	1.17517300
H	3.29097500	-3.11404900	0.26004600
C	-2.41555400	-2.51956700	0.32958600
H	-2.65689100	-1.65198500	0.94863400
H	-2.66348700	-2.26197900	-0.70572400
H	-3.05871700	-3.35195400	0.63364300

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics