

Development of RT-TDDFT for the Interaction with the Explicit Solvent and for Correct Description of Excitation Process

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Supplementary Information

Entry: 4a

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -1607.796254 hartrees

C	-0.56851900	-0.44888400	0.03372000
C	-1.46298500	0.76396400	0.03386700
C	0.84002200	-0.29897600	0.01265000
C	-1.07643300	2.02904100	-0.05765500
C	1.52937900	1.01017900	-0.14847900
C	1.98313500	1.77196100	0.96282600
C	1.80355000	1.55086500	-1.41331600
C	2.46840600	2.75239900	-1.60255300
C	2.91002600	3.50922900	-0.49007400
C	2.64797800	2.98465300	0.79781900
C	-2.94732800	0.62165400	0.20999300
C	-3.80450200	0.32451500	-0.87585400
C	-3.53757200	0.77213700	1.46553500
C	-5.17695300	0.17255600	-0.68370100
C	-5.76172700	0.31329800	0.59691800
C	-4.90102000	0.62214400	1.67631200
O	-1.13455400	-1.57327400	0.05206900
O	-0.89689100	3.17881200	-0.12935300
H	2.93824500	3.52082600	1.68461800
H	2.65420100	3.08743700	-2.61405600
H	1.48274400	0.99211100	-2.28787100
H	-2.89958500	1.00089000	2.31365900
H	-5.28169100	0.72671900	2.68307000
H	-5.78077900	-0.03740400	-1.54911200
N	3.57033900	4.70946400	-0.64703000
N	1.68707500	1.24364000	2.23613900
N	-7.12182000	0.15567400	0.77575000
N	-3.20410900	0.20374300	-2.14696800
C	-3.75473700	-0.08298200	-3.36593600
C	-2.76291700	-0.13623000	-4.51336200
H	-1.73500300	0.08886100	-4.22555200
H	-3.07653300	0.57273500	-5.28253700
H	-2.79305600	-1.13378400	-4.95759800
O	-4.95044900	-0.28800200	-3.55460000
C	3.72383400	5.33822300	-1.95867800
C	4.12142400	5.44695300	0.49057400
C	4.97841500	4.89753100	-2.71999600
H	4.97232900	3.82295000	-2.91728300
H	5.88375500	5.12883500	-2.15199200
H	5.04298800	5.41818300	-3.68031800
H	3.75561300	6.41954400	-1.80078600
H	2.82853400	5.15591600	-2.55768000

C	3.12648000	6.40241000	1.15755800
H	2.76280600	7.15038800	0.44751300
H	3.60642800	6.93206800	1.98596000
H	2.26105300	5.86746400	1.55475100
H	4.98224400	6.01304200	0.12430500
H	4.52275000	4.74156100	1.22132800
C	-8.00185600	-0.27754500	-0.30948500
C	-7.76404000	0.41932700	2.06242800
C	-7.79162900	-0.78720000	3.00695800
H	-6.78325800	-1.12921500	3.25126100
H	-8.32974700	-1.62591500	2.55661700
H	-8.29774200	-0.52733500	3.94180900
H	-8.78776300	0.74340800	1.85637600
H	-7.27898200	1.27142600	2.54454200
C	-8.54176700	0.86753100	-1.17284100
H	-9.11247400	1.57924100	-0.56962900
H	-9.20660500	0.47686000	-1.94915800
H	-7.73428500	1.41472300	-1.66431000
H	-8.83765100	-0.81673500	0.14479500
H	-7.48162400	-1.01074800	-0.92983300
C	2.03055800	1.68068800	3.48475000
H	1.13200200	0.39715200	2.17384400
C	1.49798000	0.83160300	4.62410300
H	2.33995600	0.47026900	5.21887300
H	0.90115600	-0.02254700	4.30137400
H	0.88648500	1.46059700	5.27487300
O	2.71542600	2.67647100	3.70508900
P	1.70862800	-1.84158600	-0.11770200
C	3.50324400	-1.42315000	-0.06877300
C	4.52450600	-2.42767700	-0.61737300
H	3.72468200	-1.18500900	0.97718100
H	3.59066600	-0.48051400	-0.61462800
C	5.95675300	-1.88603000	-0.51243300
H	4.30430500	-2.64868300	-1.66629600
H	4.46462700	-3.37825800	-0.08083600
C	7.00191100	-2.85861800	-1.06290700
H	6.82471100	-3.07787600	-2.12062500
H	6.98611600	-3.80993200	-0.52161600
H	8.01121000	-2.44676900	-0.97618900
H	6.18221700	-1.65966800	0.53662600
H	6.02272000	-0.93238200	-1.04965000
C	1.32284200	-2.96514500	1.30140100
C	2.31460200	-4.08084400	1.65647000
H	0.32817800	-3.36527200	1.09927400
H	1.20524300	-2.29193200	2.15587300
C	1.82223100	-4.91169400	2.84954200

H	3.29175600	-3.65247100	1.90290300
H	2.47303300	-4.74683000	0.80314400
C	2.79615000	-6.02439200	3.24307300
H	2.95526800	-6.72563300	2.41774100
H	2.41999700	-6.59787200	4.09486500
H	3.77312700	-5.61844000	3.52430600
H	0.84492800	-5.34601700	2.60805400
H	1.65625300	-4.24831700	3.70688300
C	1.26242100	-2.67560500	-1.71986900
C	1.12862700	-4.20775400	-1.82473000
H	1.95607600	-2.28930400	-2.47397400
H	0.29107100	-2.22808700	-1.93418400
C	2.40896900	-4.98351400	-2.14940300
H	0.40407200	-4.40328800	-2.62387500
H	0.66539100	-4.61023500	-0.91789400
C	2.15224300	-6.48077600	-2.33625000
H	1.73770200	-6.93067000	-1.42837100
H	3.07488400	-7.01579600	-2.57796000
H	1.44105200	-6.66430300	-3.14786700
H	3.15514700	-4.84180000	-1.36235000
H	2.85462400	-4.57263300	-3.06345500
H	-2.20382100	0.34750700	-2.13126500

Entry: PBu3

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -815.044237 hartrees

P	-0.34027100	0.16429100	1.16036200
C	-1.77715600	-0.56904200	0.20903600
C	-3.00481200	0.35015800	0.15563700
H	-2.04253600	-1.50404200	0.71672300
H	-1.46680600	-0.83924500	-0.80647900
C	-4.19375000	-0.27613000	-0.58376200
H	-2.74271600	1.29707900	-0.33249100
H	-3.31012500	0.61113600	1.17636300
C	-5.42069400	0.63758900	-0.63302400
H	-5.19544300	1.57931200	-1.14415300
H	-5.77248900	0.88616800	0.37350900
H	-6.25121200	0.16438200	-1.16505800
H	-4.46129600	-1.22306000	-0.09846800
H	-3.88915000	-0.53534100	-1.60532700
C	0.40149100	1.27781800	-0.14936300
C	1.70582000	1.95875500	0.28297400
H	-0.35422000	2.04267300	-0.36144100
H	0.55100600	0.72360000	-1.08287500
C	2.24587900	2.94442100	-0.76096300
H	2.47262000	1.20102900	0.48612100

H	1.54640700	2.48840700	1.23061700
C	3.54980100	3.62125800	-0.33165900
H	3.41766000	4.18735900	0.59610700
H	3.90918800	4.31798800	-1.09464100
H	4.34182800	2.88558100	-0.15763000
H	1.48501000	3.70882800	-0.96178800
H	2.40243800	2.41673500	-1.70996600
C	0.85393900	-1.28040400	1.20369200
C	1.26108300	-1.97213000	-0.10267300
H	0.39665200	-2.00915000	1.88423900
H	1.74656600	-0.91959100	1.72788100
C	2.23558900	-3.13636800	0.12276200
H	1.72622200	-1.24857400	-0.78209100
H	0.37206800	-2.34924000	-0.62066000
C	2.65032500	-3.83412000	-1.17488600
H	1.78288100	-4.24856700	-1.69888800
H	3.34363000	-4.65823000	-0.98248200
H	3.14661800	-3.13888100	-1.85985400
H	1.77550200	-3.86655200	0.80008900
H	3.12867800	-2.76499700	0.64060000

Entry: INT 1 a

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2422.840429 hartrees

C	0.51287300	-0.30766800	1.11119200
C	1.51177700	-0.33211700	0.10009500
C	-0.62158000	0.14684400	0.11662400
C	0.58264400	0.08398000	-0.89301000
C	-1.78516800	-0.79449600	-0.16798600
C	-2.58657800	-1.41145000	0.82218900
C	-2.10386800	-1.09190200	-1.50127800
C	-3.14332900	-1.93130800	-1.86497800
C	-3.94495400	-2.55582400	-0.88243500
C	-3.64127700	-2.25541100	0.46183800
C	2.92254300	-0.71736600	0.15602000
C	3.87293600	-0.52869500	-0.88481100
C	3.39956900	-1.31377300	1.33343800
C	5.19459500	-0.94353500	-0.72146600
C	5.65560900	-1.55303000	0.46412000
C	4.71731200	-1.71490900	1.50413100
O	0.44661300	-0.54087600	2.32506600
O	0.61265500	0.33874000	-2.10483300
H	-4.22388100	-2.67250500	1.26374000
H	-3.31427900	-2.09750400	-2.91945400
H	-1.51033100	-0.64180300	-2.28725700
H	2.70488900	-1.45371300	2.15331700

H	4.99995600	-2.14023400	2.45680600
H	5.86210200	-0.78057500	-1.54892900
N	-4.95674500	-3.45061800	-1.21526500
N	-2.28826400	-1.20321600	2.19357900
N	6.97671200	-2.00279800	0.57235700
N	3.45006500	0.07255000	-2.09621000
C	4.20319300	0.60896200	-3.10366100
C	3.39429000	1.15890300	-4.26533500
H	3.63225200	0.58138400	-5.16236600
H	3.70212600	2.18979600	-4.45270900
H	2.31653000	1.12926800	-4.10440500
O	5.43215100	0.66120600	-3.11620800
C	-5.79844800	-3.98283700	-0.13199700
C	-5.51497300	-3.42829600	-2.57072500
C	-6.70928000	-5.14073200	-0.53028200
H	-6.14842700	-5.95526800	-0.99637300
H	-7.51435400	-4.84372800	-1.20553300
H	-7.17763300	-5.53648900	0.37445500
H	-6.40234600	-3.18194300	0.32071200
H	-5.13230200	-4.34756000	0.65218600
C	-6.45929400	-2.25369300	-2.85038700
H	-7.32380600	-2.27019200	-2.18084000
H	-6.83176500	-2.30293600	-3.87800800
H	-5.95289400	-1.29385000	-2.72142200
H	-6.03875100	-4.36896800	-2.73274800
H	-4.69602600	-3.43523600	-3.29078000
C	7.37671500	-2.63746600	1.83471300
C	8.02627000	-1.30427800	-0.18073800
C	8.41080200	0.06613600	0.38868900
H	8.79446600	-0.01604200	1.40967700
H	7.55359700	0.74393400	0.40293300
H	9.19194900	0.52504900	-0.22474300
H	7.71147500	-1.20090600	-1.21856700
H	8.90167200	-1.95215000	-0.21351100
C	8.70555700	-3.38782600	1.77753000
H	8.73007500	-4.09617000	0.94491700
H	8.82565100	-3.95663400	2.70330300
H	9.57008600	-2.72621800	1.69280000
H	6.60136600	-3.36104500	2.09298000
H	7.40642500	-1.90621000	2.65844300
C	-3.12510200	-1.30343100	3.27172600
H	-1.31534300	-0.97566900	2.40690800
C	-2.44603000	-1.09820400	4.61346200
H	-2.52417900	-2.02407100	5.18901900
H	-2.98216200	-0.32562800	5.16854800
H	-1.39377800	-0.82250000	4.53742100

O	-4.32964200	-1.53571800	3.20275100
P	-1.16411600	1.92110900	0.38509900
C	0.28583900	2.94408500	0.87017300
C	1.23566600	3.40959300	-0.24477700
H	0.82766500	2.37017400	1.62782100
H	-0.13129000	3.81521800	1.38386800
C	2.36477200	4.28392100	0.31659800
H	0.68037400	3.98056700	-0.99585800
H	1.66781700	2.55050900	-0.76198600
C	3.32350100	4.77743500	-0.76882600
H	2.80086100	5.37966700	-1.51876300
H	3.80097300	3.94155600	-1.28882400
H	4.11678200	5.39724400	-0.34216400
H	2.92267200	3.71402500	1.06860100
H	1.93120800	5.14292000	0.84301600
C	-1.88242800	2.62846400	-1.15272400
C	-3.34480800	2.27279600	-1.46680100
H	-1.22149000	2.31171300	-1.96434100
H	-1.77211300	3.71425200	-1.06355200
C	-3.80745700	2.92906800	-2.77425000
H	-3.99666800	2.60276900	-0.65178800
H	-3.46353000	1.18967200	-1.54151600
C	-5.26953000	2.62113000	-3.10360900
H	-5.43609400	1.54480100	-3.20947600
H	-5.57180800	3.09623600	-4.04087800
H	-5.94007300	2.98358100	-2.31808800
H	-3.16528200	2.58964200	-3.59535500
H	-3.66717300	4.01467900	-2.70595200
C	-2.38865400	2.04856900	1.74521700
C	-2.91587800	3.46395500	2.03655900
H	-1.90586100	1.63193000	2.63260700
H	-3.21076100	1.37505600	1.49116100
C	-4.00243200	3.44623700	3.12035100
H	-3.32389900	3.91819700	1.12799900
H	-2.09692500	4.11128300	2.36527400
C	-4.53367400	4.84371100	3.44497300
H	-3.73673000	5.49921100	3.80987400
H	-5.30605600	4.80178300	4.21758800
H	-4.97469400	5.31815300	2.56266800
H	-3.59847700	2.98549900	4.02918200
H	-4.82829300	2.80412100	2.79357600
H	2.44133300	0.14374700	-2.23449000

Entry: TS1 a

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2422.800060 hartrees

Single negative frequency: -177.98 cm-1

C	0.50927800	0.84062400	0.30722700
C	1.49306800	0.26123800	-0.58939500
C	-0.85094300	0.48462500	-0.17879700
C	0.83622800	0.06637500	-1.75675100
C	-1.33271200	-0.89918000	0.17454400
C	-1.99141700	-1.75382700	-0.74085500
C	-1.11708700	-1.42653900	1.45615000
C	-1.52682700	-2.69533300	1.83927000
C	-2.21681400	-3.53173800	0.93464700
C	-2.41793200	-3.03210500	-0.36911600
C	2.93890400	-0.04602000	-0.43559200
C	3.89548900	0.86899900	0.06492800
C	3.41889400	-1.29395100	-0.84614400
C	5.24469100	0.52612700	0.12707100
C	5.72638400	-0.72086600	-0.32832700
C	4.76340300	-1.63884400	-0.80320600
O	0.76287600	1.61669900	1.25097300
O	0.62293500	-0.12386300	-2.89548000
H	-2.89361300	-3.62987500	-1.12597400
H	-1.31850900	-3.01392600	2.85162400
H	-0.60667100	-0.81047000	2.18999400
H	2.70876400	-2.03116300	-1.20860700
H	5.04271000	-2.63163600	-1.12521900
H	5.91915500	1.26739600	0.51990400
N	-2.70359000	-4.78524600	1.31613200
N	-2.16111200	-1.27737900	-2.06119600
N	7.08989600	-1.01597700	-0.32169600
N	3.44446300	2.12893300	0.53093700
C	4.12678100	3.31058300	0.56653800
C	3.33965600	4.47442700	1.14203100
H	2.31374300	4.22090000	1.41180300
H	3.32681900	5.28716000	0.41252500
H	3.85649600	4.84405100	2.03107400
O	5.28248300	3.46366200	0.17555900
C	-3.38142700	-5.59940200	0.29724300
C	-2.02765600	-5.50267400	2.40344900
C	-4.14864000	-6.79999000	0.84594600
H	-4.83796700	-6.50663500	1.64247500
H	-3.49785000	-7.59012400	1.22618900
H	-4.74082700	-7.23362800	0.03601200
H	-2.67329700	-5.94045700	-0.47421100
H	-4.10038900	-4.95316000	-0.20917500
C	-0.67224600	-6.10798800	2.02060300
H	-0.77419900	-6.83752400	1.21228300
H	-0.23039200	-6.62226200	2.87938400

H	0.02970000	-5.33738000	1.69210200
H	-2.69779600	-6.28666900	2.75399200
H	-1.91175800	-4.83068900	3.25378000
C	7.49974500	-2.36985200	-0.72066000
C	7.97958200	-0.27452900	0.57858600
C	7.86421100	-0.66960500	2.05534900
H	8.11359300	-1.72375500	2.20672200
H	6.85292000	-0.50529400	2.43543700
H	8.55269000	-0.07360300	2.66191100
H	7.79645400	0.79326700	0.45713600
H	9.00208300	-0.42421300	0.23518300
C	8.99726600	-2.54638800	-0.95853100
H	9.38344800	-1.80591100	-1.66414700
H	9.16454700	-3.53624400	-1.39100800
H	9.58845700	-2.49200700	-0.04212600
H	6.99139300	-2.60156500	-1.65852400
H	7.15678300	-3.11713400	0.01228300
C	-2.88385800	-1.79018400	-3.10283400
H	-1.60845700	-0.45395200	-2.25681300
C	-2.73930200	-1.03338000	-4.41009900
H	-3.73130900	-0.74659800	-4.76526600
H	-2.30825600	-1.70531200	-5.15615700
H	-2.11261500	-0.14335200	-4.34326500
O	-3.60466300	-2.78203200	-3.02437800
P	-2.01556900	1.83396300	0.08343400
C	-1.23175200	3.37631000	-0.56406200
C	-2.15102400	4.45676100	-1.15258600
H	-0.51647200	3.04569900	-1.32228000
H	-0.64092300	3.78025200	0.26174600
C	-1.35895400	5.70232100	-1.57168700
H	-2.91901700	4.75008800	-0.42942300
H	-2.68097600	4.06191800	-2.02546000
C	-2.24404500	6.78915500	-2.18527200
H	-3.01019200	7.12539800	-1.47943500
H	-2.75691600	6.42689200	-3.08184200
H	-1.65448400	7.66377100	-2.47347600
H	-0.58216500	5.41181200	-2.28887300
H	-0.83184300	6.10605100	-0.69917500
C	-3.61056200	1.58593300	-0.80099300
C	-4.60644100	0.59616800	-0.17467400
H	-3.36865800	1.29963600	-1.82725400
H	-4.07435700	2.57437300	-0.86253500
C	-5.88766300	0.48074500	-1.01064900
H	-4.87037100	0.92621100	0.83542500
H	-4.15248600	-0.39136200	-0.06778200
C	-6.91033400	-0.47667800	-0.39516600

H	-6.50169500	-1.48716400	-0.29947000
H	-7.81181200	-0.54180700	-1.01068400
H	-7.21500300	-0.14666200	0.60315200
H	-5.63103100	0.14243700	-2.02130000
H	-6.33722900	1.47471100	-1.12613800
C	-2.42897100	2.10186000	1.86156000
C	-3.35201000	3.28168700	2.19903900
H	-1.46081200	2.20846600	2.35666100
H	-2.85718200	1.16002100	2.21894900
C	-3.64915400	3.36099900	3.70271200
H	-4.29828200	3.20085000	1.65264200
H	-2.88866800	4.22090000	1.87878900
C	-4.55445200	4.53896400	4.06886800
H	-4.09875200	5.49416600	3.78932600
H	-4.74969500	4.56923500	5.14438500
H	-5.52125600	4.47256800	3.55974700
H	-2.70389300	3.43796100	4.25274500
H	-4.11524700	2.42329100	4.02786200
H	2.48229100	2.13558300	0.87603800

Entry: INT 2 a

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2422.821612 hartrees

C	0.59731600	-0.58379500	0.01909800
C	1.23754300	0.77617800	0.12776700
C	-0.81585000	-0.71288900	0.05834800
C	0.62595000	1.91546100	0.42047300
C	-1.74794000	0.43123900	0.25862700
C	-2.21466200	1.22281900	-0.82506800
C	-2.24252300	0.77911700	1.52412800
C	-3.11767100	1.83169700	1.73943000
C	-3.55510800	2.63641900	0.66023300
C	-3.09476200	2.28756500	-0.62992700
C	2.70275100	0.95617600	-0.15017000
C	3.68992700	0.73462000	0.83948000
C	3.14441500	1.33652100	-1.41574800
C	5.04339100	0.88214000	0.54270600
C	5.48162600	1.27628400	-0.74276300
C	4.49042500	1.48865700	-1.72706900
O	1.37224300	-1.56636100	-0.10536600
O	0.23453800	2.98214900	0.67815700
H	-3.41353700	2.82989800	-1.50189700
H	-3.44336100	2.02632300	2.75184100
H	-1.91481300	0.19729200	2.38014500
H	2.40616900	1.50570300	-2.19346000
H	4.75137900	1.75930800	-2.73984000

H	5.74437200	0.69579200	1.33676800
N	-4.37995300	3.73883000	0.85468100
N	-1.73510700	0.87211900	-2.10351400
N	6.83598100	1.47233200	-1.00706600
N	3.23677200	0.36267400	2.12275400
C	3.93577000	0.10816400	3.27100700
C	3.07788600	-0.25468500	4.46867900
H	2.00813400	-0.28634700	4.25751000
H	3.25791000	0.47333100	5.26294400
H	3.39230600	-1.23099600	4.84361300
O	5.15886000	0.16225900	3.36304100
C	-4.85042800	4.47582800	-0.32870500
C	-5.17500100	3.83464100	2.08255700
C	-5.50871000	5.82068400	-0.03312100
H	-4.86359500	6.46249200	0.57284000
H	-6.47431600	5.72763600	0.46827200
H	-5.68698600	6.33211400	-0.98243900
H	-5.53760600	3.85672800	-0.92532700
H	-3.98183200	4.66879100	-0.96064700
C	-6.40133100	2.91549700	2.11789800
H	-7.09474600	3.14607700	1.30424900
H	-6.94114200	3.03929600	3.06157400
H	-6.11568700	1.86442000	2.02851700
H	-5.48771700	4.87096900	2.19949300
H	-4.52970800	3.63763500	2.93910200
C	7.22473800	1.81356300	-2.38308500
C	7.83648500	0.80839200	-0.16343800
C	7.98420000	-0.69557900	-0.41969900
H	8.29366100	-0.89624100	-1.44941600
H	7.04507400	-1.22467300	-0.24052900
H	8.74197600	-1.12029000	0.24546300
H	7.59551400	0.99071000	0.88379900
H	8.79152000	1.30669300	-0.32292700
C	8.66680900	2.28629900	-2.54783400
H	8.90098000	3.11125600	-1.86965900
H	8.79662700	2.65001300	-3.57043100
H	9.40057900	1.49263100	-2.39338100
H	6.57534900	2.62641800	-2.71350500
H	7.03826100	0.96894900	-3.06476100
C	-1.98801400	1.41495800	-3.33295100
H	-1.08961000	0.09119900	-2.06608900
C	-1.24455500	0.75803700	-4.48108600
H	-0.60782600	1.50533500	-4.96032000
H	-1.96991500	0.42341300	-5.22579500
H	-0.62603600	-0.08990100	-4.18389300
O	-2.74832200	2.35918300	-3.53002700

P	-1.37446800	-2.38888900	0.04438500
C	-0.70412800	-3.43137400	1.41160600
C	-0.89200400	-2.85263200	2.81869300
H	0.35625900	-3.57248900	1.19346800
H	-1.18886900	-4.40964300	1.33216600
C	-0.31438600	-3.77091500	3.90335400
H	-1.95633800	-2.68608800	3.02228800
H	-0.40785000	-1.87226500	2.87679700
C	-0.49692500	-3.21182500	5.31597600
H	-1.55601200	-3.07307200	5.55595400
H	-0.00372900	-2.24105600	5.42733300
H	-0.07405400	-3.88452800	6.06741700
H	0.75187100	-3.93417200	3.70653600
H	-0.79042000	-4.75666900	3.83541800
C	-3.20312500	-2.45049500	0.23254900
C	-4.03460500	-2.04781800	-0.99439000
H	-3.45344900	-1.81251300	1.08413600
H	-3.44654300	-3.47527800	0.53080800
C	-5.54026000	-2.09070400	-0.70381500
H	-3.81433000	-2.71921300	-1.83127600
H	-3.75970300	-1.04157400	-1.32223400
C	-6.38995700	-1.71183700	-1.91865700
H	-6.16140500	-0.69886800	-2.26410700
H	-7.45729200	-1.74772600	-1.68314800
H	-6.21390300	-2.39397600	-2.75657000
H	-5.76619300	-1.41356800	0.12838800
H	-5.81536400	-3.09609800	-0.36202600
C	-0.94927000	-3.27380400	-1.51702800
C	-1.29325200	-4.76864100	-1.58596000
H	0.12238400	-3.11200800	-1.65102600
H	-1.45396600	-2.72749700	-2.31990700
C	-0.96638200	-5.36805800	-2.96030400
H	-2.35620600	-4.92930800	-1.37037700
H	-0.73618500	-5.31597900	-0.81862000
C	-1.28324900	-6.86237100	-3.04935200
H	-0.71016300	-7.43573100	-2.31380400
H	-1.04196200	-7.26107400	-4.03867400
H	-2.34473600	-7.05673500	-2.86510700
H	0.09481300	-5.20304700	-3.18122200
H	-1.52579800	-4.82700100	-3.73291600
H	2.23160300	0.27781400	2.18365600

Entry: 6a

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2422.830280 hartrees

C	0.39584300	-1.20120900	0.44211700
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C	1.48362700	-0.32735900	0.70134200
C	-0.95995500	-0.91418000	0.39298800
C	1.48761300	0.70673500	1.69031100
C	-1.50097800	0.47234900	0.28832800
C	-1.40335000	1.22550500	-0.90736000
C	-2.17071700	1.08850100	1.35010300
C	-2.72825600	2.35486500	1.26737700
C	-2.61121700	3.11619700	0.08312300
C	-1.94867900	2.50898600	-1.00511000
C	2.82026600	-0.42660100	0.13672400
C	3.63275900	0.56872000	0.73344900
C	3.38653000	-1.21557400	-0.86443900
C	4.95008200	0.77095500	0.35323600
C	5.52613100	-0.05284800	-0.64028900
C	4.72503100	-1.04087700	-1.23409200
O	0.72425000	-2.51342900	0.14719400
O	0.63092100	1.06100300	2.49629500
H	-1.85542200	3.01009800	-1.95159400
H	-3.22237500	2.75171900	2.14351900
H	-2.23549500	0.56029600	2.29445200
H	2.80115100	-1.97289400	-1.37589300
H	5.13390300	-1.69551200	-1.99309900
H	5.51890600	1.56822300	0.80167200
N	-3.09465800	4.42295500	-0.00232400
N	-0.74362400	0.62153100	-2.00190100
N	6.87078600	0.18404700	-1.03081500
N	2.84072300	1.28058500	1.67246200
C	3.29975000	2.33193100	2.46258800
H	1.61403700	-2.70163700	0.47618200
C	2.32072500	3.05638700	3.35575300
H	1.44662700	3.40330200	2.80514100
H	2.85002900	3.90079700	3.79581600
H	1.94854000	2.40147000	4.14417600
O	4.47611700	2.67275700	2.42519600
C	-2.98319200	5.11884600	-1.29243700
C	-4.16900700	4.84432000	0.90191800
C	-3.26022600	6.61920500	-1.23956500
H	-2.64981400	7.11525700	-0.48007100
H	-4.30892000	6.85815600	-1.05044900
H	-3.00138900	7.05305800	-2.20882600
H	-3.63477900	4.65392900	-2.04878600
H	-1.95929400	4.98751400	-1.64642500
C	-5.55426000	4.29163600	0.54677300
H	-5.87048000	4.61743100	-0.44820300
H	-6.29981000	4.64483100	1.26566800
H	-5.56307700	3.19881500	0.56165800

H	-4.19623200	5.93311700	0.90538100
H	-3.90358700	4.56683100	1.92224600
C	7.31727200	-0.45395300	-2.27164500
C	7.86619600	0.22645400	0.05443700
C	8.24355100	-1.13846700	0.64459300
H	8.71017800	-1.79271700	-0.09693200
H	7.36495500	-1.65290100	1.04374300
H	8.95714000	-1.00854200	1.46393300
H	7.48057700	0.86762200	0.84659100
H	8.75923500	0.72894000	-0.32229000
C	8.60531300	0.14224500	-2.83798300
H	8.53149000	1.22974300	-2.92522600
H	8.78221800	-0.26580200	-3.83695000
H	9.48463900	-0.09299300	-2.23416100
H	6.52202700	-0.31200300	-3.00707100
H	7.44341300	-1.54391400	-2.15961600
C	-0.54385100	1.06480200	-3.28078400
H	-0.35038600	-0.28182700	-1.77953600
C	0.24980000	0.11786600	-4.16243900
H	1.16020500	0.62496100	-4.49016800
H	-0.33704900	-0.10771500	-5.05537100
H	0.52832000	-0.81793700	-3.67588800
O	-0.95555800	2.13587400	-3.71812000
P	-2.09549500	-2.30497500	0.36251900
C	-1.81228300	-3.47672000	1.75391800
C	-1.81546900	-2.83630900	3.14856700
H	-0.85752900	-3.96848500	1.55702200
H	-2.58975400	-4.24346100	1.68102200
C	-1.53816100	-3.86525300	4.25204100
H	-2.78212500	-2.35723700	3.34103300
H	-1.06218000	-2.04361000	3.19133100
C	-1.53485800	-3.24592300	5.65117400
H	-2.50072900	-2.78782200	5.88658400
H	-0.77021100	-2.46814700	5.74026000
H	-1.33133000	-3.99913300	6.41738400
H	-0.57148200	-4.34649500	4.06100500
H	-2.29019100	-4.66216400	4.20438900
C	-3.83363000	-1.73167400	0.52078700
C	-4.45945500	-1.06909300	-0.71584200
H	-3.87334200	-1.05341200	1.37552700
H	-4.40783100	-2.62043000	0.80311200
C	-5.91228000	-0.64948600	-0.45737300
H	-4.43486100	-1.75981100	-1.56520500
H	-3.87417200	-0.19287600	-1.00685600
C	-6.56758900	-0.00442000	-1.68026900
H	-6.02788800	0.89448300	-1.99338800

H	-7.60023900	0.28654900	-1.46877200
H	-6.58625800	-0.69206100	-2.53179500
H	-5.94117000	0.04911400	0.38692500
H	-6.49431600	-1.52640100	-0.14832200
C	-1.99221700	-3.28401200	-1.19670600
C	-2.90983200	-4.51216900	-1.29511600
H	-0.94394300	-3.57192100	-1.29473600
H	-2.19989300	-2.58055700	-2.00908100
C	-2.78011000	-5.21043600	-2.65566400
H	-3.95563600	-4.22497700	-1.13966600
H	-2.66386900	-5.22743400	-0.50339300
C	-3.67161400	-6.44815700	-2.77515500
H	-3.42165500	-7.19459600	-2.01461500
H	-3.55942100	-6.92366500	-3.75337200
H	-4.72866500	-6.19194200	-2.65204600
H	-1.73328500	-5.49380200	-2.81669400
H	-3.02933000	-4.49898900	-3.45181600

Entry: 6a*

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2422.835390 hartrees

C	0.53867500	-1.20268900	0.06310300
C	1.62555900	-0.32873600	0.36428800
C	-0.80235800	-0.90137400	-0.02741300
C	1.60734300	0.65514400	1.38716600
C	-1.31444500	0.46933100	-0.32594400
C	-2.03286800	1.26631900	0.58271700
C	-1.14482600	0.99996700	-1.61561600
C	-1.69172000	2.20974400	-2.01019500
C	-2.47267200	2.97883300	-1.11522900
C	-2.59690400	2.48417100	0.19752100
C	2.97532800	-0.41401500	-0.16520100
C	3.77655600	0.54256600	0.50431100
C	3.56271900	-1.16186500	-1.18498100
C	5.10648200	0.75078400	0.17404400
C	5.70380300	-0.03077200	-0.84048700
C	4.91307800	-0.98257900	-1.50455800
O	0.87298900	-2.52062800	-0.18588600
O	0.71424600	0.99824700	2.17661500
H	-3.10806700	3.05401200	0.95711600
H	-1.52707400	2.53623500	-3.02827400
H	-0.57930700	0.42397100	-2.34153900
H	2.98362400	-1.88898100	-1.74537900
H	5.34050900	-1.60348500	-2.28150000
H	5.66974700	1.51930800	0.67649700
N	-3.10055700	4.16057500	-1.51970000

N	-2.07243700	0.86516100	1.94567600
N	7.06204400	0.21199000	-1.17964000
N	2.95759900	1.21171200	1.45361800
C	3.39916200	2.21956000	2.31034900
H	1.75347300	-2.70126400	0.17154500
C	2.40121100	2.90419400	3.21364500
H	1.55642100	3.30529500	2.65404100
H	2.92929300	3.70724800	3.72640000
H	1.98600200	2.20806900	3.94278500
O	4.57768500	2.55194800	2.32182500
C	-3.90966800	4.88034400	-0.52658300
C	-2.47158700	4.96707800	-2.57379500
C	-4.83224800	5.94701200	-1.11217300
H	-5.44731000	5.54422700	-1.92155100
H	-4.29606400	6.82074200	-1.48831000
H	-5.50456700	6.29729300	-0.32475700
H	-3.27644800	5.33369600	0.25236000
H	-4.53576600	4.14097100	-0.02414800
C	-1.22717300	5.74092700	-2.12413600
H	-1.46146700	6.44717000	-1.32278200
H	-0.81400000	6.31254900	-2.96056400
H	-0.44831600	5.06556200	-1.76098000
H	-3.22120400	5.65848900	-2.95717300
H	-2.22592200	4.32134300	-3.41647800
C	7.53768500	-0.36403800	-2.43986200
C	8.02540000	0.18107800	-0.06538800
C	8.37089800	-1.21923100	0.45770000
H	8.85175600	-1.83674500	-0.30589700
H	7.47570000	-1.74441900	0.80225800
H	9.06183400	-1.14404100	1.30290500
H	7.62310200	0.78145600	0.75019000
H	8.93453400	0.69297300	-0.38708900
C	8.84662800	0.24804400	-2.93715400
H	8.78467600	1.33932200	-2.96892400
H	9.04903900	-0.10884200	-3.95076500
H	9.70595300	-0.02737900	-2.32161900
H	6.76481900	-0.17510500	-3.18847000
H	7.65116000	-1.45961100	-2.38278600
C	-3.11447100	0.98293000	2.81135900
H	-1.14744500	0.62411200	2.30081000
C	-2.78531900	0.66734700	4.25805400
H	-3.51603700	-0.04476800	4.64596200
H	-2.88047300	1.58414200	4.84607100
H	-1.78110700	0.26668700	4.40101100
O	-4.25348700	1.30977100	2.47464700
P	-1.95634700	-2.27297500	-0.15158500

C	-1.70790300	-3.55088400	1.14929700
C	-1.65463700	-3.02580900	2.58966500
H	-0.78587500	-4.07719800	0.89735600
H	-2.52890500	-4.26526200	1.03275400
C	-1.43316100	-4.15952700	3.59922900
H	-2.58471800	-2.50176100	2.83506100
H	-0.84996400	-2.29039700	2.68341300
C	-1.36520800	-3.66341400	5.04501300
H	-2.29214600	-3.16071500	5.33819800
H	-0.54534300	-2.95187300	5.18380800
H	-1.20485000	-4.49185400	5.74057800
H	-0.50565800	-4.68844700	3.34885000
H	-2.23968900	-4.89629100	3.50142700
C	-3.69263200	-1.69355300	0.02260700
C	-4.34014400	-1.03069200	-1.20354300
H	-3.72283000	-1.01921400	0.88065000
H	-4.26384400	-2.58296500	0.30904700
C	-5.80100900	-0.64988700	-0.92999500
H	-4.30500600	-1.70996000	-2.06176800
H	-3.77793000	-0.13804600	-1.48840900
C	-6.47414200	0.00922400	-2.13577000
H	-5.95628700	0.92819300	-2.42725500
H	-7.51261600	0.27125800	-1.91485700
H	-6.47954800	-0.65717400	-3.00444900
H	-5.84211600	0.02645200	-0.06923600
H	-6.36217400	-1.54731100	-0.64156800
C	-1.81560100	-3.13355700	-1.77454300
C	-2.72186900	-4.35640000	-1.98275700
H	-0.76279700	-3.40875100	-1.86801100
H	-2.00691200	-2.37312800	-2.53796900
C	-2.56362100	-4.94927500	-3.38942400
H	-3.77225300	-4.08851300	-1.82381500
H	-2.48431700	-5.12772400	-1.24270800
C	-3.44240700	-6.18096200	-3.61683700
H	-3.19831700	-6.98090300	-2.91069100
H	-3.31051700	-6.58044700	-4.62613100
H	-4.50343600	-5.94255600	-3.49222800
H	-1.51187300	-5.21213900	-3.55340700
H	-2.80555700	-4.18169000	-4.13400300

Entry: 6a*

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2422.835390 hartrees

C	0.53867500	-1.20268900	0.06310300
C	1.62555900	-0.32873600	0.36428800
C	-0.80235800	-0.90137400	-0.02741300

C	1.60734300	0.65514400	1.38716600
C	-1.31444500	0.46933100	-0.32594400
C	-2.03286800	1.26631900	0.58271700
C	-1.14482600	0.99996700	-1.61561600
C	-1.69172000	2.20974400	-2.01019500
C	-2.47267200	2.97883300	-1.11522900
C	-2.59690400	2.48417100	0.19752100
C	2.97532800	-0.41401500	-0.16520100
C	3.77655600	0.54256600	0.50431100
C	3.56271900	-1.16186500	-1.18498100
C	5.10648200	0.75078400	0.17404400
C	5.70380300	-0.03077200	-0.84048700
C	4.91307800	-0.98257900	-1.50455800
O	0.87298900	-2.52062800	-0.18588600
O	0.71424600	0.99824700	2.17661500
H	-3.10806700	3.05401200	0.95711600
H	-1.52707400	2.53623500	-3.02827400
H	-0.57930700	0.42397100	-2.34153900
H	2.98362400	-1.88898100	-1.74537900
H	5.34050900	-1.60348500	-2.28150000
H	5.66974700	1.51930800	0.67649700
N	-3.10055700	4.16057500	-1.51970000
N	-2.07243700	0.86516100	1.94567600
N	7.06204400	0.21199000	-1.17964000
N	2.95759900	1.21171200	1.45361800
C	3.39916200	2.21956000	2.31034900
H	1.75347300	-2.70126400	0.17154500
C	2.40121100	2.90419400	3.21364500
H	1.55642100	3.30529500	2.65404100
H	2.92929300	3.70724800	3.72640000
H	1.98600200	2.20806900	3.94278500
O	4.57768500	2.55194800	2.32182500
C	-3.90966800	4.88034400	-0.52658300
C	-2.47158700	4.96707800	-2.57379500
C	-4.83224800	5.94701200	-1.11217300
H	-5.44731000	5.54422700	-1.92155100
H	-4.29606400	6.82074200	-1.48831000
H	-5.50456700	6.29729300	-0.32475700
H	-3.27644800	5.33369600	0.25236000
H	-4.53576600	4.14097100	-0.02414800
C	-1.22717300	5.74092700	-2.12413600
H	-1.46146700	6.44717000	-1.32278200
H	-0.81400000	6.31254900	-2.96056400
H	-0.44831600	5.06556200	-1.76098000
H	-3.22120400	5.65848900	-2.95717300
H	-2.22592200	4.32134300	-3.41647800

C	7.53768500	-0.36403800	-2.43986200
C	8.02540000	0.18107800	-0.06538800
C	8.37089800	-1.21923100	0.45770000
H	8.85175600	-1.83674500	-0.30589700
H	7.47570000	-1.74441900	0.80225800
H	9.06183400	-1.14404100	1.30290500
H	7.62310200	0.78145600	0.75019000
H	8.93453400	0.69297300	-0.38708900
C	8.84662800	0.24804400	-2.93715400
H	8.78467600	1.33932200	-2.96892400
H	9.04903900	-0.10884200	-3.95076500
H	9.70595300	-0.02737900	-2.32161900
H	6.76481900	-0.17510500	-3.18847000
H	7.65116000	-1.45961100	-2.38278600
C	-3.11447100	0.98293000	2.81135900
H	-1.14744500	0.62411200	2.30081000
C	-2.78531900	0.66734700	4.25805400
H	-3.51603700	-0.04476800	4.64596200
H	-2.88047300	1.58414200	4.84607100
H	-1.78110700	0.26668700	4.40101100
O	-4.25348700	1.30977100	2.47464700
P	-1.95634700	-2.27297500	-0.15158500
C	-1.70790300	-3.55088400	1.14929700
C	-1.65463700	-3.02580900	2.58966500
H	-0.78587500	-4.07719800	0.89735600
H	-2.52890500	-4.26526200	1.03275400
C	-1.43316100	-4.15952700	3.59922900
H	-2.58471800	-2.50176100	2.83506100
H	-0.84996400	-2.29039700	2.68341300
C	-1.36520800	-3.66341400	5.04501300
H	-2.29214600	-3.16071500	5.33819800
H	-0.54534300	-2.95187300	5.18380800
H	-1.20485000	-4.49185400	5.74057800
H	-0.50565800	-4.68844700	3.34885000
H	-2.23968900	-4.89629100	3.50142700
C	-3.69263200	-1.69355300	0.02260700
C	-4.34014400	-1.03069200	-1.20354300
H	-3.72283000	-1.01921400	0.88065000
H	-4.26384400	-2.58296500	0.30904700
C	-5.80100900	-0.64988700	-0.92999500
H	-4.30500600	-1.70996000	-2.06176800
H	-3.77793000	-0.13804600	-1.48840900
C	-6.47414200	0.00922400	-2.13577000
H	-5.95628700	0.92819300	-2.42725500
H	-7.51261600	0.27125800	-1.91485700
H	-6.47954800	-0.65717400	-3.00444900

H	-5.84211600	0.02645200	-0.06923600
H	-6.36217400	-1.54731100	-0.64156800
C	-1.81560100	-3.13355700	-1.77454300
C	-2.72186900	-4.35640000	-1.98275700
H	-0.76279700	-3.40875100	-1.86801100
H	-2.00691200	-2.37312800	-2.53796900
C	-2.56362100	-4.94927500	-3.38942400
H	-3.77225300	-4.08851300	-1.82381500
H	-2.48431700	-5.12772400	-1.24270800
C	-3.44240700	-6.18096200	-3.61683700
H	-3.19831700	-6.98090300	-2.91069100
H	-3.31051700	-6.58044700	-4.62613100
H	-4.50343600	-5.94255600	-3.49222800
H	-1.51187300	-5.21213900	-3.55340700
H	-2.80555700	-4.18169000	-4.13400300

Entry: 4e

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -1381.016360 hartrees

C	0.03714300	-0.99643500	-0.20762800
C	-1.04362400	-0.00708700	-0.11633500
C	1.05061300	0.06391000	-0.10906400
C	-0.03085000	1.05295300	-0.01742400
C	2.45655100	0.03451800	-0.11252900
C	3.30684200	1.20210800	-0.00336000
C	3.10670400	-1.22820100	-0.22356600
C	4.46654600	-1.37542900	-0.23974300
C	5.31918800	-0.22694000	-0.15321600
C	4.70205400	1.03356500	-0.02191200
C	-2.45069300	0.02378200	-0.11603100
C	-3.30306000	-1.14358200	-0.22075500
C	-3.09817700	1.28480300	0.00367100
C	-4.69588300	-0.97328300	-0.20474000
C	-5.31348400	0.29173500	-0.10994100
C	-4.45974000	1.43497700	0.01120500
O	0.08234100	-2.23064500	-0.32168300
O	-0.07523600	2.28719400	0.09838400
H	5.31016000	1.91621100	0.08669200
H	4.87629300	-2.37113900	-0.32223800
H	2.47719200	-2.10708900	-0.29781800
H	-2.46810200	2.16137500	0.09812800
H	-4.86786300	2.42776500	0.12512300
H	-5.30463100	-1.86024500	-0.26933500
N	6.68714000	-0.35197100	-0.21074100
N	2.76677000	2.43979200	0.12363400
N	-6.68073700	0.43313900	-0.14045000

N	-2.76200300	-2.38408600	-0.32891900
C	-3.53620300	-3.60244700	-0.44245200
C	7.51725700	0.85807500	-0.06569500
C	7.32363100	-1.66426200	-0.03805000
C	8.99614200	0.68689400	-0.39742800
H	9.14691400	0.30063400	-1.40858100
H	9.52357200	0.03929800	0.30562000
H	9.46964900	1.67056500	-0.34730200
H	7.41688900	1.25948100	0.95235300
H	7.11330600	1.61479400	-0.74128900
C	7.41325800	-2.12458200	1.42000000
H	7.99877600	-1.42485700	2.02256500
H	7.89891400	-3.10313200	1.47632100
H	6.42275300	-2.21206700	1.87275300
H	8.31968500	-1.61240400	-0.47230600
H	6.79010600	-2.39940400	-0.63954600
C	-7.27044600	1.77187100	0.06508200
C	-7.55193900	-0.74111600	-0.02170800
C	-7.72802900	-1.24292900	1.41527300
H	-8.18513400	-0.47749400	2.04819700
H	-6.77153300	-1.52232500	1.86262700
H	-8.37884800	-2.12199700	1.42978400
H	-7.16384000	-1.53417400	-0.66131900
H	-8.52106800	-0.48542500	-0.44470800
C	-8.75589100	1.89133000	-0.26047700
H	-8.97616500	1.58642800	-1.28661500
H	-9.03922800	2.94220800	-0.16187300
H	-9.39365800	1.32096800	0.41759500
H	-6.73804400	2.47118100	-0.58065900
H	-7.09813000	2.10079400	1.09873300
C	3.54054000	3.65957200	0.22893500
H	1.75137400	2.53575800	0.13401800
H	2.84856100	4.49755100	0.30388700
H	4.17616700	3.81996100	-0.64944900
H	4.18018400	3.66636600	1.11893000
H	-4.17205900	-3.77017900	0.43444200
H	-2.84479900	-4.44042900	-0.52324900
H	-4.17610200	-3.60222900	-1.33254700
H	-1.74702300	-2.48005600	-0.33987600

Entry: INT 1 e

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2196.050376 hartrees

C	0.64585200	-0.13949900	1.08668500
C	1.56799600	-0.26176000	0.01084500
C	-0.57237900	0.16639000	0.13531100

C	0.56052800	0.03178100	-0.95141400
C	-1.72152500	-0.82760800	0.02634900
C	-2.40647200	-1.38299500	1.14479000
C	-2.14479100	-1.23671600	-1.24371900
C	-3.18272600	-2.13218600	-1.45763700
C	-3.87323500	-2.69382700	-0.36065200
C	-3.46779500	-2.28258500	0.92410700
C	2.98795000	-0.61835800	0.00114300
C	3.85719400	-0.42991100	-1.11860800
C	3.55004200	-1.16970300	1.15792700
C	5.19848300	-0.82765800	-1.01807000
C	5.74692500	-1.38194800	0.15538300
C	4.88932700	-1.54018500	1.25818900
O	0.68451200	-0.21003700	2.32218500
O	0.49066400	0.16934700	-2.18026700
H	-3.97866500	-2.66719700	1.79174600
H	-3.42975000	-2.39439800	-2.47688600
H	-1.63145100	-0.83494300	-2.10907100
H	2.90984400	-1.30277400	2.02295800
H	5.24746300	-1.93368200	2.19959700
H	5.82673900	-0.72183800	-1.89063700
N	-4.88151000	-3.64655300	-0.53913100
N	-2.07081400	-1.02025400	2.43822900
N	7.09488600	-1.79845500	0.18066500
N	3.38983400	0.17039100	-2.27655300
C	-5.57204100	-4.15688400	0.65235900
C	-5.63015700	-3.65608300	-1.80050200
C	-6.44098200	-5.38944400	0.41240600
H	-5.88070400	-6.18562100	-0.08525700
H	-7.33638600	-5.17793000	-0.17569300
H	-6.77501400	-5.77282200	1.38006400
H	-6.18007300	-3.37008700	1.12697400
H	-4.80590600	-4.43484300	1.37850700
C	-6.65620000	-2.52564300	-1.93956300
H	-7.41616400	-2.57596800	-1.15453000
H	-7.16890000	-2.59382200	-2.90386100
H	-6.17626700	-1.54547500	-1.88148500
H	-6.12879700	-4.62072600	-1.88792000
H	-4.92548900	-3.62699700	-2.63108100
C	7.54440400	-2.53677700	1.36571400
C	8.09483400	-0.91681100	-0.43980800
C	8.44008700	0.33457200	0.37727200
H	8.87086100	0.08013600	1.34960300
H	7.55261300	0.94877900	0.55176200
H	9.17276300	0.94558700	-0.15885600
H	7.73956300	-0.62092900	-1.42578800

H	8.99675600	-1.50292200	-0.62199200
C	8.86507400	-3.28030600	1.17137300
H	8.84191300	-3.90160500	0.27169600
H	9.03277600	-3.93722800	2.02914400
H	9.72710700	-2.61291500	1.10493200
H	6.77337400	-3.27483900	1.59390600
H	7.62175000	-1.88510400	2.25132600
H	-1.11834300	-0.69097600	2.56617400
P	-1.15752800	1.93948300	0.27688800
C	0.28176000	3.05976300	0.52551700
C	1.12406600	3.42399500	-0.70697700
H	0.90273500	2.59326200	1.29634500
H	-0.13009100	3.97084100	0.96994500
C	2.25800400	4.39052900	-0.34051400
H	0.49034500	3.88874200	-1.46948100
H	1.54894500	2.52530400	-1.15840300
C	3.10951500	4.78509000	-1.54900500
H	2.50743000	5.28402600	-2.31515000
H	3.57306400	3.90832900	-2.01107200
H	3.91126800	5.47068500	-1.26084500
H	2.89485800	3.92680500	0.42180100
H	1.83463500	5.29105200	0.12109600
C	-2.03377100	2.47353100	-1.24986200
C	-3.50725200	2.05953700	-1.39089900
H	-1.43953600	2.08764500	-2.08299600
H	-1.94699600	3.56458000	-1.28134100
C	-4.10455500	2.56876400	-2.70923200
H	-4.09207500	2.45955300	-0.55644200
H	-3.59974800	0.97227900	-1.34404700
C	-5.58174900	2.20361600	-2.86908300
H	-5.72839500	1.11940100	-2.85000900
H	-5.98061200	2.57447700	-3.81731500
H	-6.18783100	2.63327700	-2.06514300
H	-3.53065100	2.15752000	-3.54793900
H	-3.98781300	3.65797300	-2.76508600
C	-2.25809200	2.16683300	1.72806900
C	-2.81004100	3.58627700	1.93904200
H	-1.68102600	1.84506300	2.59850000
H	-3.06823100	1.44204700	1.62035600
C	-3.78849800	3.63869700	3.12036200
H	-3.31906500	3.94197300	1.03723100
H	-1.99041900	4.28671600	2.12748600
C	-4.33762900	5.04447800	3.37138100
H	-3.53413300	5.75202800	3.59890100
H	-5.03256100	5.05214700	4.21551100
H	-4.87568700	5.42488100	2.49733100

H	-3.28427700	3.27372500	4.02271800
H	-4.61798600	2.94689400	2.93305600
H	2.38390000	0.15320600	-2.41527900
C	-2.62196900	-1.69366300	3.59916100
H	-2.13326200	-1.29534400	4.48888900
H	-3.69570500	-1.50759600	3.70089100
H	-2.46691200	-2.78172100	3.58246100
C	4.16524700	0.19032400	-3.50121400
H	5.06781600	0.80078400	-3.39581200
H	4.47348200	-0.81107200	-3.83547500
H	3.55507600	0.63726100	-4.28689800

Entry: TS 1 e

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2196.009924 hartrees

Single negative frequency: -183.27 cm-1

C	-0.48880500	-0.86130700	0.49901800
C	-1.46446500	-0.37657300	-0.46670700
C	0.87493800	-0.66637300	-0.08929200
C	-0.83457900	-0.33315200	-1.66205800
C	1.45251400	0.72245300	0.01117600
C	2.12992900	1.34647800	-1.07043000
C	1.30833200	1.47997100	1.18007200
C	1.78992600	2.77727200	1.31910700
C	2.47230000	3.39695000	0.25372900
C	2.61484800	2.65867200	-0.93645200
C	-2.89790500	-0.03277300	-0.27201800
C	-3.93117300	-0.98791400	-0.47923700
C	-3.27232400	1.24250500	0.14334000
C	-5.26754500	-0.61615600	-0.27731800
C	-5.63600500	0.68196300	0.13723900
C	-4.59751300	1.61236700	0.35878400
O	-0.75405000	-1.43607500	1.56333300
O	-0.66657400	-0.26875800	-2.82559100
H	3.08616900	3.11454500	-1.79397900
H	1.65513400	3.28213000	2.26708100
H	0.79772100	1.02977200	2.02649300
H	-2.49190000	1.97810800	0.31631100
H	-4.80084100	2.61340200	0.71041600
H	-6.03211200	-1.35630300	-0.45966600
N	3.01815700	4.68851600	0.39549300
N	2.32345700	0.63575400	-2.25199500
N	-6.98546300	1.03209000	0.28399200
N	-3.60258700	-2.27900300	-0.85316400
C	3.84047800	5.20421400	-0.70378100
C	2.22576100	5.68603200	1.12946200

C	4.68665000	6.42140500	-0.33355800
H	5.26814700	6.23990800	0.57461100
H	4.09416700	7.32686800	-0.18630200
H	5.38862400	6.62556500	-1.14648700
H	3.23428500	5.44155700	-1.59333400
H	4.52003700	4.40246100	-0.99957600
C	1.03307800	6.25353500	0.35020500
H	1.35070800	6.77160600	-0.55897900
H	0.48648800	6.97348100	0.96691800
H	0.33728600	5.46118900	0.06170700
H	2.89368500	6.49444000	1.42949500
H	1.87646000	5.24127100	2.05994400
C	-7.29039100	2.40522500	0.70738600
C	-7.94767600	-0.00567000	0.67382500
C	-7.85089600	-0.44493100	2.13958800
H	-8.03650000	0.38995500	2.82127100
H	-6.86277300	-0.85260200	2.36719700
H	-8.59322200	-1.21997100	2.35346700
H	-7.82936200	-0.86741300	0.01739100
H	-8.94865200	0.37058100	0.46506300
C	-8.75068500	2.81711600	0.53199900
H	-9.10419800	2.61733100	-0.48334500
H	-8.83369500	3.89280000	0.70839100
H	-9.42522600	2.32415300	1.23515500
H	-6.68488600	3.07403700	0.09367000
H	-6.98571000	2.57979400	1.75166500
H	1.64522300	-0.10669100	-2.35368200
P	1.97721400	-2.01607200	0.32752100
C	1.20678000	-3.61185600	-0.16122900
C	1.01905200	-3.81760100	-1.67129900
H	0.24665200	-3.66010300	0.35989600
H	1.83030600	-4.40944500	0.25352800
C	0.32076200	-5.14616500	-1.98784100
H	1.99172200	-3.79635400	-2.17548200
H	0.43625600	-2.99172300	-2.08963700
C	0.13217800	-5.37484100	-3.48904200
H	1.09327200	-5.39520500	-4.01276900
H	-0.47207700	-4.58155000	-3.94020500
H	-0.37067000	-6.32585000	-3.68595000
H	-0.65428400	-5.16948500	-1.48649300
H	0.90154900	-5.97274900	-1.56066200
C	3.59603200	-1.93971100	-0.54555500
C	4.63848300	-0.95868800	0.01196900
H	3.38485500	-1.70624200	-1.59029600
H	3.99250200	-2.96086300	-0.51996200
C	5.94468400	-1.00632900	-0.79085000

H	4.85629300	-1.19329500	1.05912400
H	4.23990300	0.05836300	-0.00299400
C	7.00820600	-0.04778300	-0.25064600
H	6.65755900	0.98872900	-0.27246100
H	7.92654500	-0.09888700	-0.84245600
H	7.26964900	-0.28545400	0.78548900
H	5.73205000	-0.76651100	-1.83937000
H	6.33769400	-2.03068300	-0.78625100
C	2.35154500	-2.14558200	2.13317600
C	3.25441800	-3.30242800	2.58582700
H	1.37302500	-2.19425900	2.61623800
H	2.78602800	-1.18180700	2.41814000
C	3.53976000	-3.24836700	4.09303600
H	4.20583100	-3.28687000	2.04260100
H	2.78122100	-4.26154300	2.34971400
C	4.42039900	-4.40342700	4.57448000
H	3.94887100	-5.37207300	4.38023600
H	4.60784500	-4.33799600	5.64993500
H	5.39178000	-4.40198300	4.06956300
H	2.58950100	-3.25723300	4.63975400
H	4.02093200	-2.29316700	4.33490500
H	-2.65432800	-2.39462400	-1.17604800
C	2.64567200	1.30962400	-3.49910200
H	2.60944400	0.57811000	-4.30692900
H	1.95090100	2.12640600	-3.74137000
H	3.65806900	1.72156700	-3.47464900
C	-4.57205600	-3.22012400	-1.37889900
H	-5.29135600	-3.52167600	-0.61147200
H	-5.13476000	-2.82080900	-2.23402700
H	-4.04423500	-4.11664900	-1.70418600

Entry: INT 2 e

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2196.029726 hartrees

C	0.42735200	-1.22051800	0.48198900
C	1.48725800	-0.22574900	0.80974900
C	-0.91348000	-0.81248000	0.28070200
C	1.35669600	0.76521900	1.75546500
C	-1.36509000	0.58205300	-0.00147700
C	-2.18695000	1.31934600	0.89031500
C	-0.99444500	1.22780000	-1.18664200
C	-1.40382600	2.51373500	-1.52291600
C	-2.24442600	3.23640700	-0.65263500
C	-2.61000700	2.61809300	0.55629800
C	2.83377200	-0.27753100	0.25867800
C	3.65020900	0.73252300	0.78744900

C	3.41677000	-1.10339000	-0.70635900
C	4.95294100	0.96791400	0.40653200
C	5.54273200	0.12579000	-0.56219600
C	4.74619000	-0.90431300	-1.09330300
O	0.77955100	-2.43889900	0.38837700
O	0.57641700	1.23545100	2.56092000
H	-3.20531600	3.16182800	1.27464600
H	-1.10006500	2.92673000	-2.47686200
H	-0.36664800	0.68418800	-1.88727200
H	2.84582300	-1.91616900	-1.13780600
H	5.16625600	-1.58348400	-1.82492500
H	5.50813000	1.80087200	0.82294600
N	-2.72388200	4.51613400	-1.00967400
N	-2.57525300	0.72669900	2.08922500
N	6.87444800	0.37891200	-0.98464700
N	2.89078600	1.49931800	1.76750900
C	3.44360500	1.54001200	3.14451300
C	-3.73342800	5.12761900	-0.14010500
C	-1.76909500	5.44494100	-1.63243900
C	-4.46956800	6.30701700	-0.77439800
H	-4.86660400	6.04430500	-1.75891400
H	-3.84260700	7.19461200	-0.88361200
H	-5.31210100	6.58556600	-0.13567000
H	-3.30789000	5.44467900	0.82625500
H	-4.47019200	4.35472700	0.08771500
C	-0.75872400	6.07114700	-0.66303700
H	-1.25089600	6.66911400	0.10899100
H	-0.07382100	6.73068900	-1.20480500
H	-0.16221600	5.30208600	-0.16494100
H	-2.33709500	6.22879000	-2.13577200
H	-1.23667500	4.91993200	-2.42399000
C	7.29700600	-0.26303300	-2.23335600
C	7.89135000	0.42084200	0.08198500
C	8.28817700	-0.94308300	0.66084300
H	8.74948000	-1.58985600	-0.09010400
H	7.42049900	-1.46741500	1.07065200
H	9.01313600	-0.81020200	1.46959100
H	7.51666200	1.05767800	0.88409600
H	8.77366800	0.93069200	-0.30994100
C	8.55425400	0.35679100	-2.84140000
H	8.45186200	1.44111900	-2.93868300
H	8.71434900	-0.05882900	-3.83996200
H	9.45474900	0.14938500	-2.25885900
H	6.47603800	-0.14578200	-2.94442600
H	7.45080500	-1.34801400	-2.11458000
C	-3.09051400	1.52363200	3.18945800

H	-1.89678900	0.03171000	2.37553000
P	-1.99335700	-2.17426800	-0.06094300
C	-1.99855400	-3.49705300	1.22665800
C	-2.10783200	-3.00003700	2.67212200
H	-1.07485800	-4.06057700	1.08865400
H	-2.83323100	-4.16434600	0.98761000
C	-2.12465300	-4.15509600	3.68120300
H	-3.01501300	-2.39809500	2.80006700
H	-1.26214000	-2.34016700	2.88999600
C	-2.21520600	-3.67711400	5.13214100
H	-3.12770900	-3.09721300	5.30458000
H	-1.36506700	-3.03941900	5.39440300
H	-2.22330900	-4.51976900	5.82951300
H	-1.21968400	-4.76053600	3.55005300
H	-2.96951200	-4.81921800	3.46060800
C	-3.74286400	-1.60519200	-0.17677800
C	-4.16695300	-0.91280000	-1.48106300
H	-3.90076600	-0.94101200	0.67677400
H	-4.36445800	-2.49091700	-0.00820800
C	-5.63029300	-0.45461900	-1.43334600
H	-4.03712700	-1.59485500	-2.32865800
H	-3.52309400	-0.05040600	-1.67322300
C	-6.08266500	0.22639000	-2.72700200
H	-5.47811400	1.11309700	-2.94185000
H	-7.12711300	0.54541700	-2.66510200
H	-5.99433900	-0.44850500	-3.58459400
H	-5.76521700	0.23306200	-0.59002100
H	-6.27556900	-1.31801400	-1.22818200
C	-1.60252800	-3.03097400	-1.65030000
C	-2.43075900	-4.27724500	-1.99279400
H	-0.53990000	-3.27276400	-1.58203500
H	-1.70429000	-2.27250700	-2.43302500
C	-2.05948200	-4.85676400	-3.36439200
H	-3.50167200	-4.04231700	-1.98373700
H	-2.27866800	-5.04732200	-1.22897900
C	-2.86081500	-6.11099500	-3.71999800
H	-2.69709800	-6.90895200	-2.98863200
H	-2.57612700	-6.50019200	-4.70171900
H	-3.93546200	-5.90342500	-3.74636800
H	-0.98781600	-5.08853800	-3.37856400
H	-2.21482900	-4.09088100	-4.13387000
H	-3.19415600	0.88048700	4.06434100
H	-4.08224000	1.92082800	2.95598900
H	-2.43842500	2.36759600	3.45593400
H	3.64238000	0.51922300	3.46550700
H	2.69571800	1.99326200	3.79328400

H	4.36338200	2.12324800	3.16632000
H	2.72594700	2.45323500	1.44575100

Entry: 6e*

Free Energy(6-311+G(d),B3LYP,CPCM,solvent=chloroform): -2196.060885 hartrees

C	0.58051500	-1.04693400	0.10489600
C	1.64364200	-0.18122600	0.46539300
C	-0.78113600	-0.80125000	0.10065500
C	1.61436300	0.75462700	1.56154400
C	-1.37568800	0.56096500	-0.05764200
C	-2.10684000	1.22676600	0.95840100
C	-1.27813800	1.20746700	-1.29526900
C	-1.89325800	2.42128900	-1.57384300
C	-2.67162800	3.06168900	-0.58717300
C	-2.74401400	2.44653200	0.67718000
C	2.99812600	-0.18917800	-0.06233800
C	3.74435900	0.75912700	0.69189900
C	3.65491000	-0.82701200	-1.11528600
C	5.07152500	1.05564200	0.42437200
C	5.73406400	0.37981500	-0.62383000
C	5.00607000	-0.55598800	-1.37824200
O	0.94892900	-2.31819400	-0.31273600
O	0.71321600	1.04090700	2.37326500
H	-3.26479900	2.94429200	1.48060200
H	-1.79602800	2.83666300	-2.56852900
H	-0.71462100	0.71903500	-2.08520700
H	3.13522700	-1.53968600	-1.74892800
H	5.48637000	-1.09551900	-2.18490500
H	5.58840300	1.82031700	0.99303100
N	-3.36586200	4.25251100	-0.87194400
N	-2.17645400	0.63940500	2.22439100
N	7.09355700	0.70632800	-0.90003400
N	2.90879100	1.31139800	1.64997200
C	3.30506800	2.27419100	2.65178700
H	1.84413300	-2.50452200	0.00281200
C	-4.25717800	4.78561900	0.16403200
C	-2.69906000	5.24753900	-1.72452300
C	-5.24027000	5.84189100	-0.33816300
H	-5.78630500	5.49136900	-1.21842000
H	-4.76030200	6.79060500	-0.58731100
H	-5.97016500	6.04841400	0.44913600
H	-3.69291500	5.19295800	1.01859200
H	-4.83769600	3.94582200	0.55080900
C	-1.58304200	6.03686100	-1.02970700
H	-1.96075100	6.61021900	-0.17854500

H	-1.12826800	6.74455900	-1.72951800
H	-0.79625300	5.37095900	-0.66570100
H	-3.45945600	5.93143800	-2.10321300
H	-2.30011100	4.74602900	-2.60491700
C	7.61470500	0.28729000	-2.20344300
C	8.02773600	0.55467400	0.22946100
C	8.39250800	-0.89149600	0.59034500
H	8.91358600	-1.40057500	-0.22503800
H	7.50056800	-1.47417900	0.83675800
H	9.05418800	-0.90530400	1.46194500
H	7.58750600	1.04179200	1.09988100
H	8.93397600	1.11998300	0.00120500
C	8.90548900	1.00183800	-2.60254900
H	8.79647600	2.08693500	-2.52107300
H	9.14476200	0.76294100	-3.64257800
H	9.76334000	0.69901000	-1.99762800
H	6.84664700	0.52344100	-2.94342900
H	7.77457300	-0.80238600	-2.26233800
C	-2.73349500	1.38395000	3.34332300
H	-1.26286900	0.25555300	2.45113900
P	-1.87146100	-2.20868100	-0.07795000
C	-1.50744400	-3.56975200	1.10863600
C	-1.39763000	-3.14019200	2.57720900
H	-0.58105800	-4.04036400	0.77484400
H	-2.30680600	-4.30718800	0.98380700
C	-1.12205700	-4.33072700	3.50411000
H	-2.31960100	-2.64096500	2.89450600
H	-0.59693500	-2.40200500	2.68261800
C	-0.99660900	-3.92151500	4.97325400
H	-1.91506600	-3.44819800	5.33475400
H	-0.17898700	-3.20880800	5.11931000
H	-0.79837800	-4.78741300	5.61124600
H	-0.20129200	-4.83288400	3.18319700
H	-1.92515800	-5.07006600	3.39626900
C	-3.61672000	-1.72117400	0.23623500
C	-4.36667600	-1.01631600	-0.90473700
H	-3.59274200	-1.09367100	1.13027700
H	-4.13709100	-2.64552200	0.50857200
C	-5.80648000	-0.67089300	-0.50291700
H	-4.39142500	-1.65627100	-1.79342700
H	-3.84030100	-0.10248200	-1.19147800
C	-6.58402600	0.02302200	-1.62340600
H	-6.10280700	0.96008600	-1.91997800
H	-7.60493200	0.25993500	-1.31064200
H	-6.65056200	-0.61033100	-2.51392700
H	-5.78851600	-0.02765600	0.38466200

H	-6.33115100	-1.58714300	-0.20479900
C	-1.79805300	-2.95129600	-1.76487600
C	-2.65148700	-4.20607500	-2.00274800
H	-0.74158600	-3.15963200	-1.94646200
H	-2.08062300	-2.15164100	-2.45696700
C	-2.56754600	-4.68711800	-3.45761000
H	-3.70017200	-4.01224200	-1.75078300
H	-2.31957300	-5.01312200	-1.34109800
C	-3.39220500	-5.94990200	-3.71566000
H	-3.05262700	-6.78240600	-3.09126200
H	-3.31494100	-6.26757700	-4.75919800
H	-4.45241900	-5.78528300	-3.49848100
H	-1.51827700	-4.87386200	-3.71528500
H	-2.90599900	-3.88418900	-4.12323200
H	-2.61089700	0.78801200	4.24892900
H	-3.80417700	1.55562300	3.20426500
H	-2.24873200	2.35761700	3.50623400
H	4.11208600	1.88382100	3.28027300
H	2.43859400	2.48144200	3.27738600
H	3.64309700	3.20874300	2.19294500