

XYZ coordinates of the optimized geometries

Chapter 2

B3LYP/6-31+G* level

68a

H	-2.858815000	0.887839000	-0.446740000
H	-2.858839000	-0.887749000	-0.446910000
H	-2.599337000	-0.000104000	1.080513000
C	-2.388863000	-0.000003000	-0.008695000
N	-0.965062000	0.000005000	-0.308312000
C	-0.299632000	-1.205899000	0.183915000
H	-0.379355000	-1.280715000	1.291644000
H	-0.807112000	-2.082559000	-0.239316000
C	-0.299630000	1.205901000	0.183932000
H	-0.807130000	2.082560000	-0.239273000
H	-0.379331000	1.280701000	1.291665000
H	1.686264000	2.082898000	0.206043000
C	1.181165000	1.208011000	-0.219940000
H	1.252610000	1.282179000	-1.313035000
H	1.252647000	-1.282217000	-1.313010000
H	1.686252000	-2.082895000	0.206101000
C	1.181173000	-1.208013000	-0.219922000
N	1.901062000	0.000005000	0.193879000
H	2.014872000	0.000011000	1.207605000

68a cation

N	1.636402000	0.047406000	-0.345258000
C	0.862312000	1.243044000	-0.313688000
C	-0.205762000	1.158843000	0.894575000
N	-0.948203000	-0.054961000	0.756457000
C	-0.152061000	-1.241316000	0.798272000
C	0.916207000	-1.180567000	-0.410038000
C	-2.183547000	-0.058840000	-0.018276000
H	-1.986326000	-0.221629000	-1.092247000
H	-2.826940000	-0.864314000	0.341018000
H	-2.690627000	0.898284000	0.104978000
H	0.414267000	-1.286141000	1.732102000
H	-0.769211000	-2.134944000	0.684567000
H	-0.860224000	2.031476000	0.854402000
H	0.362146000	1.150922000	1.828509000
H	1.496304000	2.120167000	-0.166511000
H	0.294373000	1.356807000	-1.243342000
H	0.352386000	-1.244937000	-1.347074000
H	1.589470000	-2.037099000	-0.333130000
H	2.494163000	0.044959000	0.197916000

68a anion

H	-2.873206000	0.891147000	-0.434498000
H	-2.873206000	-0.891147000	-0.434498000
H	-2.587167000	0.000000000	1.082725000
C	-2.390124000	0.000000000	-0.008169000
N	-0.972035000	0.000000000	-0.323207000
C	-0.300947000	-1.198319000	0.184485000
H	-0.388976000	-1.268910000	1.288679000
H	-0.808216000	-2.088656000	-0.223030000
C	-0.300948000	1.198319000	0.184485000
H	-0.808216000	2.088656000	-0.223030000
H	-0.388976000	1.268910000	1.288679000
H	1.678062000	2.075589000	0.248877000
C	1.179591000	1.208798000	-0.210579000
H	1.260322000	1.323988000	-1.300985000
H	1.260322000	-1.323988000	-1.300985000
H	1.678062000	-2.075589000	0.248877000
C	1.179592000	-1.208798000	-0.210579000
N	1.915122000	0.000000000	0.171147000
H	2.046604000	0.000000000	1.185755000

68b

C	-0.778496000	1.030686000	-0.056647000
C	-1.164956000	-0.446672000	0.170680000
N	-0.000911000	-1.171705000	-0.350714000
C	1.164121000	-0.448556000	0.171019000
C	0.780279000	1.029303000	-0.057091000
H	-1.327529000	-0.630106000	1.250578000
H	-2.075525000	-0.741402000	-0.362291000
H	-0.001753000	-2.154754000	-0.086979000
H	2.074455000	-0.745061000	-0.361373000
H	1.325772000	-0.631831000	1.251078000
H	1.163500000	1.378106000	-1.021457000
H	1.200967000	1.677939000	0.718469000
H	-1.161681000	1.381014000	-1.020481000
H	-1.197514000	1.679467000	0.719688000

68b cation

C	0.743728000	1.021421000	-0.208390000
C	1.209760000	-0.409998000	0.113129000
N	-0.000005000	-1.195816000	0.000007000
C	-1.209769000	-0.409995000	-0.113087000
C	-0.743716000	1.021439000	0.208362000
H	1.994966000	-0.836456000	-0.525336000
H	1.566802000	-0.516203000	1.156600000
H	0.000015000	-2.219000000	-0.000205000
H	-1.994911000	-0.836421000	0.525457000
H	-1.566896000	-0.516244000	-1.156531000
H	-0.853104000	1.211835000	1.281465000
H	-1.333206000	1.767121000	-0.328610000
H	1.333231000	1.767131000	0.328532000
H	0.853115000	1.211747000	-1.281505000

68b anion

C	-0.771817000	1.034387000	-0.055210000
C	-1.157097000	-0.440542000	0.168040000
N	-0.006519000	-1.172610000	-0.364914000
C	1.152036000	-0.453389000	0.168198000
C	0.783376000	1.025661000	-0.055416000
H	-1.313228000	-0.634150000	1.246324000
H	-2.081065000	-0.738136000	-0.350068000
H	-0.011942000	-2.144551000	-0.021330000
H	2.072712000	-0.761435000	-0.349660000
H	1.305771000	-0.648506000	1.246556000
H	1.175347000	1.385990000	-1.015081000
H	1.210340000	1.669840000	0.729034000
H	-1.159986000	1.399452000	-1.014633000
H	-1.191299000	1.683055000	0.729579000

68c

C	1.210415000	0.722640000	-0.217967000
C	1.182779000	-0.749969000	0.199708000
O	-0.000019000	-1.395103000	-0.273797000
C	-1.182803000	-0.749937000	0.199704000
H	-1.210393000	0.722676000	-0.217962000
N	0.000022000	1.451022000	0.182473000
H	2.024171000	-1.305689000	-0.226234000
H	1.230785000	-0.832394000	1.300393000
H	-2.024201000	-1.305626000	-0.226265000
H	-1.230831000	-0.832390000	1.300387000
H	-2.087222000	1.224636000	0.207448000
H	-1.292468000	0.782845000	-1.311046000
H	1.292472000	0.782789000	-1.311051000
H	2.087273000	1.224572000	0.207422000
H	0.000026000	1.592475000	1.191122000

70c cation

C	1.223144000	0.755973000	-0.226146000
C	1.175454000	-0.784652000	0.217320000
O	0.000000000	-1.334708000	-0.299894000
C	-1.175455000	-0.784651000	0.217320000
C	-1.223144000	0.755973000	-0.226146000

N	0.00000000	1.346348000	0.206625000
H	2.022610000	-1.302335000	-0.236369000
H	1.214626000	-0.846092000	1.311628000
H	-2.022611000	-1.302335000	-0.236369000
H	-1.214626000	-0.846092000	1.311628000
H	-2.084647000	1.252034000	0.224906000
H	-1.289902000	0.771230000	-1.317939000
H	1.289902000	0.771230000	-1.317939000
H	2.084647000	1.252034000	0.224906000
H	0.000000000	1.847703000	1.094234000

70c anion

C	1.212067000	0.721133000	-0.200423000
C	1.175023000	-0.753128000	0.201448000
O	0.000000000	-1.409790000	-0.286091000
C	-1.175023000	-0.753128000	0.201449000
C	-1.212067000	0.721132000	-0.200423000
N	-0.000001000	1.466411000	0.134064000
H	2.031410000	-1.305236000	-0.213868000
H	1.218207000	-0.846587000	1.298321000
H	-2.031410000	-1.305238000	-0.213866000
H	-1.218206000	-0.846586000	1.298321000
H	-2.066226000	1.209726000	0.301640000
H	-1.381807000	0.798348000	-1.285255000
H	1.381807000	0.798349000	-1.285255000
H	2.066225000	1.209727000	0.301641000
H	-0.000001000	1.684887000	1.136300000

70d

N	-0.339664000	-1.240160000	0.106406000
C	1.093408000	-1.281313000	-0.208882000
C	1.883331000	-0.059197000	0.291297000
C	1.226966000	1.242068000	-0.195077000
C	-0.267953000	1.270991000	0.165236000
C	-0.995073000	0.003716000	-0.331622000
C	-2.466916000	-0.021104000	0.081720000
H	-0.382085000	1.337284000	1.259280000
H	-0.745090000	2.166715000	-0.257166000
H	2.926661000	-0.118523000	-0.049309000
H	1.907120000	-0.070060000	1.392044000
H	1.506483000	-2.209852000	0.203636000
H	1.186469000	-1.352339000	-1.302800000
H	-0.946097000	-0.002402000	-1.432536000
H	-0.471113000	-1.351550000	1.112813000
H	-2.995191000	0.863068000	-0.294271000
H	-2.961601000	-0.917077000	-0.308444000
H	-2.566610000	-0.026001000	1.176344000
H	1.739577000	2.116064000	0.227700000
H	1.336543000	1.314824000	-1.288169000

68d cation

N	0.277431000	-1.131235000	-0.141397000
C	-1.101322000	-1.307827000	0.222728000
C	-1.898500000	-0.049952000	-0.296895000
C	-1.223606000	1.229836000	0.197955000
C	0.256760000	1.283390000	-0.179366000
C	1.029771000	-0.005104000	0.345715000
C	2.492314000	-0.051053000	-0.082864000
H	0.393064000	1.344503000	-1.265748000
H	0.767991000	2.140467000	0.271997000
H	-2.922899000	-0.153720000	0.075864000
H	-1.935536000	-0.084507000	-1.391732000
H	-1.483374000	-2.234382000	-0.209637000
H	-1.174751000	-1.342548000	1.315900000
H	0.926913000	0.000326000	1.439597000
H	0.627941000	-1.615971000	-0.970803000
H	3.011580000	0.831211000	0.301532000
H	2.996187000	-0.936357000	0.318309000
H	2.592566000	-0.046301000	-1.174726000
H	-1.732267000	2.094951000	-0.249409000
H	-1.341937000	1.325229000	1.284998000

68d anion

N	-0.342811000	-1.252054000	0.099355000
C	1.099098000	-1.282238000	-0.198497000
C	1.874960000	-0.050092000	0.285750000
C	1.219851000	1.241623000	-0.206386000
C	-0.261850000	1.265374000	0.181703000
C	-0.992203000	0.006725000	-0.327476000
C	-2.466714000	-0.018449000	0.074785000
H	-0.367818000	1.331913000	1.275016000
H	-0.747449000	2.169906000	-0.226202000
H	2.924774000	-0.107704000	-0.059065000
H	1.917041000	-0.051618000	1.385767000
H	1.514657000	-2.204915000	0.236226000
H	1.206629000	-1.378140000	-1.288414000
H	-0.938975000	0.011493000	-1.426642000
H	-0.469921000	-1.349792000	1.107818000
H	-2.987684000	0.878416000	-0.286900000
H	-2.967794000	-0.903574000	-0.337999000
H	-2.579357000	-0.042015000	1.168640000
H	1.742163000	2.125829000	0.196627000
H	1.314554000	1.306915000	-1.299630000

68e

C	-1.996734000	-0.589693000	-0.255156000
C	-1.070847000	0.263399000	0.615831000
N	-0.030960000	0.938804000	-0.169646000
H	0.351971000	1.715384000	0.365353000
C	1.066373000	0.106399000	-0.672636000
C	1.986109000	-0.534093000	0.381483000
H	0.634744000	-0.675789000	-1.308697000
H	1.667817000	0.739330000	-1.337900000
H	-0.662720000	-0.360795000	1.432190000
H	-1.664073000	1.051413000	1.095534000
H	-2.803510000	-1.016434000	0.353450000
H	-2.441064000	0.018956000	-1.050581000
H	-1.464469000	-1.425251000	-0.724548000
H	2.786947000	-1.105624000	-0.105483000
H	2.457875000	0.232783000	1.010160000
H	1.443799000	-1.221678000	1.040920000

68e cation

C	-2.471295000	-0.330025000	0.150877000
C	-1.247239000	0.463168000	-0.314152000
N	0.000014000	-0.197693000	-0.000664000
H	0.000160000	-1.222863000	-0.001580000
C	1.247040000	0.462998000	0.314129000
C	2.471482000	-0.329868000	-0.150273000
H	1.201612000	1.477109000	-0.098362000
H	1.260848000	0.574069000	1.417131000
H	-1.201543000	1.477063000	0.098791000
H	-1.262015000	0.574648000	-1.417090000
H	-3.372153000	0.205327000	-0.162168000
H	-2.504421000	-1.327638000	-0.300694000
H	-2.490483000	-0.424927000	1.240634000
H	3.372072000	0.205510000	0.163492000
H	2.504462000	-1.327598000	0.301056000
H	2.491436000	-0.424486000	-1.240045000

68e anion

C	-1.873494000	-0.645047000	-0.338801000
C	-1.069291000	0.253571000	0.600228000
N	-0.039004000	1.032960000	-0.081196000
H	0.309468000	1.732802000	0.584294000
C	1.115143000	0.295125000	-0.600699000
C	1.817235000	-0.713294000	0.328118000
H	0.813359000	-0.219285000	-1.525210000
H	1.852842000	1.055361000	-0.904082000
H	-0.666962000	-0.359725000	1.426919000
H	-1.747137000	0.976746000	1.078409000
H	-2.687331000	-1.134565000	0.220830000
H	-2.317382000	-0.061090000	-1.156348000

H	-1.262191000	-1.441321000	-0.782820000
H	2.727041000	-1.102097000	-0.159225000
H	2.125481000	-0.243364000	1.270921000
H	1.188284000	-1.576309000	0.581610000

4

O	0.000007000	-0.972535000	0.000820000
C	-1.131994000	-0.158315000	0.000198000
C	-0.668721000	1.258909000	0.000324000
C	0.668506000	1.258942000	-0.000397000
C	1.132209000	-0.158056000	-0.000018000
O	-2.246561000	-0.600584000	-0.000710000
O	2.246652000	-0.600502000	-0.000320000
H	1.362066000	2.090261000	-0.000464000
H	-1.362851000	2.089819000	0.001493000

4 cation

C	-1.172157000	-0.121013000	-0.000129000
O	0.055350000	-0.985098000	-0.000053000
C	1.073984000	-0.158112000	-0.000091000
C	0.672619000	1.280610000	-0.000069000
C	-0.662467000	1.281896000	0.000066000
O	2.228603000	-0.612793000	0.000119000
O	-2.222945000	-0.641775000	0.000078000
H	-1.348471000	2.123515000	0.000269000
H	1.388528000	2.093532000	-0.000078000

4 anion

O	-0.000009000	-0.937520000	-0.000252000
C	-1.151773000	-0.118128000	0.000111000
C	-0.700876000	1.237215000	-0.000239000
C	0.700877000	1.237217000	0.000160000
C	1.151787000	-0.118115000	0.000300000
O	-2.278671000	-0.631178000	-0.000352000
O	2.278669000	-0.631188000	-0.000207000
H	1.375658000	2.084978000	-0.000283000
H	-1.375658000	2.084973000	-0.001216000

Acrolein

C	1.336423000	0.789195000	0.000000000
C	0.000000000	0.894870000	0.000000000
C	-0.888221000	-0.294778000	0.000000000
H	-1.976478000	-0.074998000	0.000000000
O	-0.501780000	-1.450561000	0.000000000
H	-0.490798000	1.867034000	0.000000000
H	1.979428000	1.664852000	0.000000000
H	1.812877000	-0.188124000	0.000000000

Acrolein cation

C	1.351966000	0.787880000	0.000000000
C	0.000000000	0.892302000	0.000000000
C	-0.858098000	-0.271822000	0.000000000
H	-1.965016000	-0.129930000	0.000000000
O	-0.538845000	-1.461297000	0.000000000
H	-0.524225000	1.842742000	0.000000000
H	1.958398000	1.691118000	0.000000000
H	1.878389000	-0.163711000	0.000000000

Acrolein anion

C	1.397478000	0.825468000	0.000000000
C	0.000000000	0.855485000	0.000000000
C	-0.880917000	-0.262495000	0.000000000
H	-1.967134000	0.007009000	0.000000000
O	-0.569189000	-1.496430000	0.000000000
H	-0.497571000	1.831189000	0.000000000
H	1.984772000	1.742249000	0.000000000
H	1.934081000	-0.119756000	0.000000000

C=O Addition product 69a

O	1.804222000	0.366842000	-0.824927000
C	1.145279000	0.595812000	0.446723000
O	1.390560000	1.957061000	0.730320000
H	0.775445000	2.210578000	1.439483000
N	-0.267176000	0.350073000	0.400864000
C	-0.979546000	1.104885000	-0.651352000
C	-2.484703000	1.007393000	-0.419501000
N	-2.916611000	-0.388315000	-0.420491000
C	-2.196578000	-1.149188000	0.595404000
C	-0.685698000	-1.059771000	0.380398000
C	2.867902000	-0.487708000	-0.666114000
C	2.927264000	-0.882128000	0.767253000
C	1.913840000	-0.300342000	1.406946000
C	-4.359887000	-0.519566000	-0.284381000
O	3.578432000	-0.824620000	-1.580063000
H	-0.420467000	-1.540056000	-0.575994000
H	-0.179277000	-1.601626000	1.184574000
H	-2.504574000	-2.199592000	0.531328000
H	-2.436636000	-0.788784000	1.617566000
H	-3.005640000	1.535386000	-1.226972000
H	-2.744938000	1.510781000	0.535032000
H	-0.734786000	0.703443000	-1.646204000
H	-0.659861000	2.148749000	-0.618425000
H	-4.856883000	0.019484000	-1.098317000
H	-4.642531000	-1.575893000	-0.352646000
H	-4.739932000	-0.120845000	0.677866000
H	3.702610000	-1.530682000	1.154742000
H	1.661028000	-0.353833000	2.460467000

Maleimic acid derivative 70a

C	1.712846000	0.579322000	1.330244000
C	0.716978000	1.211465000	0.388925000
O	2.315833000	-0.433315000	-1.279251000
C	3.203371000	-0.680688000	-0.280466000
C	2.793897000	-0.163017000	1.041920000
O	0.912570000	2.389688000	0.087101000
N	-0.384337000	0.505608000	0.012988000
C	-1.354080000	1.111755000	-0.900449000
C	-2.778185000	0.816094000	-0.432024000
N	-2.985431000	-0.622687000	-0.265730000
C	-2.040548000	-1.168017000	0.705585000
C	-0.598167000	-0.918799000	0.259297000
C	-4.365190000	-0.939228000	0.079342000
O	4.243657000	-1.282316000	-0.472546000
H	-0.396848000	-1.479635000	-0.664338000
H	0.095915000	-1.264681000	1.027623000
H	-2.205112000	-2.248802000	0.788803000
H	-2.194368000	-0.726112000	1.712425000
H	-3.485280000	1.187496000	-1.182815000
H	-2.974299000	1.362931000	0.513192000
H	-1.202086000	0.698695000	-1.908335000
H	-1.164078000	2.185544000	-0.931964000
H	-5.034916000	-0.561750000	-0.700886000
H	-4.490162000	-2.025851000	0.140176000
H	-4.677939000	-0.499087000	1.047144000
H	3.498050000	-0.417272000	1.828535000
H	1.587485000	0.909530000	2.361346000
H	2.710004000	-0.787232000	-2.098385000

Chapter 3

B3LYP/6-31+G* level

6a

H	-2.858815000	0.887839000	-0.446740000
H	-2.858839000	-0.887749000	-0.446910000
H	-2.599337000	-0.000104000	1.080513000
C	-2.388863000	-0.000030000	-0.008695000
N	-0.965062000	0.000005000	-0.308312000
C	-0.299632000	-1.205899000	0.183915000
H	-0.379355000	-1.280715000	1.291644000
H	-0.807112000	-2.082559000	-0.239316000
C	-0.299630000	1.205901000	0.183932000
H	-0.807130000	2.082560000	-0.239273000
H	-0.379331000	1.280701000	1.291665000
H	1.686264000	2.082898000	0.206043000
C	1.181165000	1.208011000	-0.219940000
H	1.252610000	1.282179000	-1.313035000
H	1.252647000	-1.282217000	-1.313010000
H	1.686252000	-2.082895000	0.206101000
C	1.181173000	-1.208013000	-0.219922000
N	1.901062000	0.000005000	0.193879000
H	2.014872000	0.000011000	1.207605000

6b

C	1.210415000	0.722640000	-0.217967000
C	1.182779000	-0.749969000	0.199708000
O	-0.000019000	-1.395103000	-0.273797000
C	-1.182803000	-0.749937000	0.199704000
C	-1.210393000	0.722676000	-0.217962000
N	0.000022000	1.451022000	0.182473000
H	2.024171000	-1.305689000	-0.226234000
H	1.230785000	-0.832394000	1.300393000
H	-2.024201000	-1.305626000	-0.226265000
H	-1.230831000	-0.832390000	1.300387000
H	-2.087222000	1.224636000	0.207448000
H	-1.292468000	0.782845000	-1.311046000
H	1.292472000	0.782789000	-1.311051000
H	2.087273000	1.224572000	0.207422000
H	0.000026000	1.592475000	1.191122000

6c

C	-0.778496000	1.030686000	-0.056647000
C	-1.164956000	-0.446672000	0.170680000
N	-0.000911000	-1.171705000	-0.350714000
C	1.164121000	-0.448556000	0.171019000
C	0.780279000	1.029303000	-0.057091000
H	-1.327529000	-0.630106000	1.250578000
H	-2.075525000	-0.741402000	-0.362291000
H	-0.001753000	-2.154754000	-0.086979000
H	2.074455000	-0.745061000	-0.361373000
H	1.325772000	-0.631831000	1.251078000
H	1.163500000	1.378106000	-1.021457000
H	1.200967000	1.677939000	0.718469000
H	-1.161681000	1.381014000	-1.020481000
H	-1.197514000	1.679467000	0.719688000

6d

C	-1.996734000	-0.589693000	-0.255156000
C	-1.070847000	0.263399000	0.615831000
N	-0.030960000	0.938804000	-0.169646000
H	0.351971000	1.715384000	0.365353000
C	1.066373000	0.106399000	-0.672636000
C	1.986109000	-0.534093000	0.381483000
H	0.634744000	-0.675789000	-1.308697000
H	1.667817000	0.739330000	-1.337900000
H	-0.662720000	-0.360795000	1.432190000
H	-1.664073000	1.051413000	1.095534000
H	-2.803510000	-1.016434000	0.353450000

H	-2.441064000	0.018956000	-1.050581000
H	-1.464469000	-1.425251000	-0.724548000
H	2.786947000	-1.105624000	-0.105483000
H	2.457875000	0.232783000	1.010160000
H	1.443799000	-1.221678000	1.040920000

6e

C	2.315640000	0.000157000	0.227089000
C	1.625780000	1.208246000	0.088441000
C	0.254807000	1.204701000	-0.182497000
C	-0.451706000	-0.000120000	-0.316193000
C	0.255024000	-1.204841000	-0.182323000
C	1.625951000	-1.208106000	0.088589000
C	-1.952957000	-0.000270000	-0.553786000
N	-2.792822000	0.000149000	0.657464000
H	-2.235274000	-0.880212000	-1.143797000
H	2.156140000	2.152676000	0.184415000
H	3.382751000	0.000214000	0.434306000
H	2.156539000	-2.152395000	0.184689000
H	-0.272492000	-2.150573000	-0.297738000
H	-0.272799000	2.150367000	-0.298043000
H	-2.235307000	0.879231000	-1.144452000
H	-2.582255000	-0.815187000	1.231655000
H	-2.582781000	0.816224000	1.230799000

React._{comp. 1a}

C	-4.115958000	-2.129622000	-0.258252000
C	-4.371221000	-0.713761000	-0.130047000
C	-3.284794000	0.066308000	-0.008980000
C	-3.644576000	1.462934000	0.114572000
C	-3.883447000	2.642728000	0.221634000
O	-2.139154000	-0.344578000	-0.003869000
H	-3.519740000	-2.325253000	-1.152975000
H	-3.585576000	-2.497997000	0.623327000
H	-5.101301000	-2.587623000	-0.339369000
H	-4.097871000	3.685052000	0.317116000
H	0.033781000	0.139096000	0.357961000
N	1.044000000	0.155820000	0.482467000
C	1.655693000	1.162210000	-0.383544000
C	3.162906000	1.200080000	-0.129885000
H	1.485741000	0.956951000	-1.458447000
H	1.220433000	2.141512000	-0.151993000
N	3.755796000	-0.119416000	-0.357997000
H	3.637607000	1.914981000	-0.813590000
H	3.346219000	1.547599000	0.907538000
C	3.115164000	-1.135132000	0.480267000
C	5.199482000	-0.103205000	-0.183836000
C	1.608350000	-1.168106000	0.225673000
H	3.555383000	-2.110627000	0.238481000
H	3.294951000	-0.937859000	1.557064000
H	1.434031000	-1.508158000	-0.813602000
H	1.137395000	-1.890614000	0.902358000
H	5.611901000	-1.091210000	-0.419150000
H	5.647156000	0.625535000	-0.869510000
H	5.507389000	0.161330000	0.848939000

TS_{comp 1a} (NImag = 1)

C	3.317436000	-2.393196000	-0.447202000
C	3.291577000	-1.184285000	0.489199000
N	1.974204000	-0.516597000	0.495839000
C	0.860037000	-1.464502000	0.729539000
C	0.940753000	-2.671882000	-0.205065000
N	2.245748000	-3.326413000	-0.111549000
C	1.920583000	0.916748000	1.718914000
C	1.718442000	2.092956000	1.306955000
C	1.396725000	2.921050000	0.204350000
O	2.482851000	3.585877000	-0.294344000
C	2.210339000	4.513426000	-1.354999000
C	2.307662000	-4.540853000	-0.914975000
O	0.264474000	3.088531000	-0.261685000
H	2.085569000	0.357109000	2.626751000

H	1.822437000	-0.014349000	-0.380134000
H	0.933975000	-1.794574000	1.772614000
H	-0.077754000	-0.915789000	0.586128000
H	0.162997000	-3.391874000	0.074561000
H	0.726038000	-2.347409000	-1.245424000
H	4.281119000	-2.906470000	-0.345321000
H	3.240177000	-2.046800000	-1.500670000
H	3.494471000	-1.506737000	1.517139000
H	4.046816000	-0.445486000	0.204461000
H	3.176997000	4.954058000	-1.605070000
H	1.786993000	4.002195000	-2.225183000
H	1.511949000	5.286819000	-1.022422000
H	3.278099000	-5.028380000	-0.772184000
H	1.525469000	-5.235525000	-0.590936000
H	2.172177000	-4.346931000	-1.997405000
H	-1.128857000	1.574496000	-0.069189000
N	-1.782710000	0.787591000	-0.047877000
C	-2.593340000	0.788136000	-1.268315000
C	-3.570671000	-0.386644000	-1.237773000
H	-3.170699000	1.723993000	-1.384169000
H	-1.929605000	0.693981000	-2.136062000
N	-4.421776000	-0.317623000	-0.050010000
H	-4.213378000	-0.360561000	-2.126530000
H	-2.997838000	-1.338293000	-1.264339000
C	-3.619995000	-0.274250000	1.173006000
C	-5.405610000	-1.387476000	-0.020081000
C	-2.641050000	0.898797000	1.134997000
H	-4.298125000	-0.166477000	2.028570000
H	-3.052468000	-1.219521000	1.310936000
H	-3.219131000	1.841205000	1.141547000
H	-2.010627000	0.886286000	2.031729000
H	-6.061924000	-1.263440000	0.848901000
H	-6.024358000	-1.347821000	-0.923933000
H	-4.944697000	-2.395822000	0.037727000

TS_{a1a} (NImag = 1)

C	-1.471768000	-1.169726000	0.519685000
N	-0.751493000	0.062706000	0.139169000
C	-1.589365000	1.269355000	0.300813000
C	-2.945867000	1.118951000	-0.389145000
N	-3.633693000	-0.081888000	0.080859000
C	-2.830879000	-1.275797000	-0.174316000
C	0.887935000	0.223050000	0.994445000
C	1.889760000	0.224752000	0.234671000
C	3.268622000	0.362487000	-0.052980000
O	3.853507000	1.417850000	-0.277506000
O	3.904663000	-0.854615000	-0.103864000
C	5.300450000	-0.799829000	-0.426454000
H	0.526302000	0.287076000	2.012713000
H	-0.397025000	-0.005259000	-0.816910000
H	-1.731692000	1.421673000	1.376927000
H	-1.030185000	2.120517000	-0.098633000
H	-3.565346000	1.993871000	-0.159678000
H	-2.800491000	1.098915000	-1.490299000
C	-4.977600000	-0.195546000	-0.472826000
H	-3.365507000	-2.151185000	0.212778000
H	-2.679068000	-1.438446000	-1.262853000
H	-1.609045000	-1.140789000	1.606859000
H	-0.830958000	-2.021636000	0.273686000
H	5.635279000	-1.838992000	-0.431342000
H	5.456353000	-0.343554000	-1.408915000
H	5.853010000	-0.224974000	0.323067000
H	-5.476030000	-1.074198000	-0.049946000
H	-5.561705000	0.690820000	-0.203746000
H	-4.980676000	-0.291626000	-1.576297000

TS_{a1b} (NImag = 1)

C	-1.948220000	-1.230298000	0.372149000
N	-1.213898000	0.009760000	0.039836000
C	-2.055679000	1.215444000	0.206665000
C	-3.399123000	1.059391000	-0.506918000

O	-4.070408000	-0.123396000	-0.084585000
C	-3.298157000	-1.290178000	-0.345751000
C	0.404211000	0.151167000	0.936784000
C	1.416393000	0.201744000	0.191167000
C	2.809210000	0.375504000	-0.011953000
O	3.383391000	1.450121000	-0.152966000
O	3.468397000	-0.826242000	-0.086631000
C	4.878516000	-0.734721000	-0.331864000
H	0.021234000	0.163352000	1.949077000
H	-0.830646000	-0.036005000	-0.906611000
H	-2.216300000	1.351880000	1.282601000
H	-1.493446000	2.075331000	-0.171017000
H	-4.063481000	1.894583000	-0.267784000
H	-3.250536000	1.034458000	-1.599980000
H	-3.888699000	-2.138908000	0.010892000
H	-3.148051000	-1.403423000	-1.433169000
H	-2.102042000	-1.234921000	1.457784000
H	-1.312993000	-2.082145000	0.108890000
H	5.231102000	-1.767205000	-0.369357000
H	5.076651000	-0.228196000	-1.281423000
H	5.380554000	-0.189294000	0.473022000

TS_{a1c} (NImag = 1)

H	5.049749000	-0.172529000	0.481155000
H	4.962136000	-1.613262000	-0.585586000
H	4.739483000	0.035857000	-1.259790000
C	4.566217000	-0.613543000	-0.395988000
O	3.163403000	-0.800121000	-0.168873000
C	2.454992000	0.350768000	0.086666000
O	2.988441000	1.457099000	0.106832000
C	1.079596000	0.093702000	0.270483000
C	0.003137000	-0.099145000	0.889177000
H	-0.454574000	-0.260637000	1.858757000
N	-1.531069000	-0.115962000	-0.124509000
H	-1.108836000	-0.161681000	-1.051908000
C	-2.332845000	1.124766000	0.023943000
C	-3.713681000	0.756450000	-0.529031000
C	-3.903646000	-0.705015000	-0.058438000
C	-2.461396000	-1.257314000	0.115386000
H	-2.382146000	1.355242000	1.096218000
H	-1.827785000	1.951358000	-0.480127000
H	-3.704413000	0.813682000	-1.624730000
H	-4.503545000	1.424179000	-0.169496000
H	-4.484909000	-1.296154000	-0.772610000
H	-4.437426000	-0.734860000	0.897799000
H	-2.213521000	-2.070538000	-0.570418000
H	-2.285721000	-1.618763000	1.135440000

TS_{a1d} (NImag = 1)

H	-4.795053000	1.294286000	0.375829000
H	-4.490113000	0.290930000	-1.081725000
C	-4.330816000	0.381440000	-0.002758000
H	-4.756915000	-0.496255000	0.493000000
O	-2.935546000	0.513802000	0.298739000
C	-2.146718000	-0.535531000	-0.110375000
O	-2.608480000	-1.509771000	-0.696468000
C	-0.776418000	-0.310959000	0.178363000
C	0.192682000	-0.492140000	0.965473000
N	1.852360000	0.057488000	0.390308000
H	0.488204000	-0.919931000	1.915618000
H	2.292242000	0.464802000	1.217985000
H	0.806567000	0.783095000	-1.228576000
H	2.566444000	1.068969000	-1.327625000
C	1.697731000	1.086460000	-0.661310000
C	2.593682000	-1.161850000	-0.019349000
H	2.130976000	-1.505508000	-0.949675000
H	2.388975000	-1.927236000	0.737974000
C	1.492892000	2.473506000	-0.061358000
C	4.103368000	-0.970000000	-0.173773000
H	4.567212000	-1.923202000	-0.452898000
H	4.355198000	-0.240182000	-0.950307000

H	4.562367000	-0.642000000	0.767451000
H	1.328830000	3.202866000	-0.861823000
H	0.613877000	2.486603000	0.590565000
H	2.368459000	2.802543000	0.514402000

TS_a1e (NImag = 1)

C	-5.491764000	1.162863000	-0.556314000
O	-4.141381000	0.688806000	-0.647271000
C	-3.742703000	-0.137742000	0.374398000
C	-2.387343000	-0.531170000	0.235181000
C	-1.515027000	-1.361089000	-0.131878000
N	0.218473000	-0.914072000	0.336422000
O	-4.485676000	-0.440823000	1.301822000
C	1.071028000	-0.494758000	-0.807484000
C	2.465200000	-0.069794000	-0.402525000
H	-5.630933000	1.803096000	-1.429556000
H	-6.200896000	0.329707000	-0.577612000
H	-5.643020000	1.734038000	0.364773000
H	-1.313868000	-2.290775000	-0.645762000
H	0.660719000	-1.664245000	0.874415000
H	0.530541000	0.317001000	-1.303579000
H	1.106646000	-1.342095000	-1.500631000
C	3.522014000	-0.991962000	-0.399158000
C	4.801463000	-0.608549000	0.011003000
H	3.346188000	-2.014788000	-0.728339000
C	5.040206000	0.706434000	0.419763000
H	5.611209000	-1.333555000	0.004351000
C	3.995760000	1.636172000	0.411524000
H	6.035494000	1.007153000	0.735967000
C	2.718043000	1.250089000	0.001113000
H	4.177149000	2.662950000	0.718238000
H	1.911876000	1.981439000	-0.012518000
H	0.034791000	-0.138249000	0.975146000

Int.a

C	-1.343188000	-1.219251000	0.353079000
N	-0.643002000	0.052191000	-0.025857000
C	-1.467137000	1.251895000	0.340982000
C	-2.880792000	1.140449000	-0.220469000
N	-3.525596000	-0.090052000	0.229440000
C	-2.762153000	-1.255063000	-0.207539000
C	0.792712000	0.132304000	0.478720000
C	1.719036000	0.205108000	-0.454337000
C	3.122301000	0.364673000	-0.165912000
O	3.715608000	1.432731000	-0.048747000
O	3.787908000	-0.838888000	-0.127672000
C	5.210638000	-0.749845000	0.015416000
H	0.802446000	0.136730000	1.572122000
H	-0.478841000	0.057086000	-1.044256000
H	-1.481960000	1.302253000	1.433172000
H	-0.938796000	2.125119000	-0.049086000
H	-3.463093000	1.998882000	0.132370000
H	-2.848007000	1.202796000	-1.328794000
C	-4.922643000	-0.161452000	-0.186482000
H	-3.255722000	-2.163169000	0.156063000
H	-2.723389000	-1.326730000	-1.315181000
H	-1.353002000	-1.260498000	1.445754000
H	-0.731651000	-2.040167000	-0.029256000
H	5.568491000	-1.781626000	0.006736000
H	5.650733000	-0.186864000	-0.813750000
H	5.481748000	-0.260881000	0.956504000
H	-5.379643000	-1.069838000	0.219232000
H	-5.467582000	0.700939000	0.210831000
H	-5.042316000	-0.172664000	-1.286932000

Int.b

C	-1.794085000	-1.257818000	0.290403000
N	-1.096021000	0.022807000	-0.066148000
C	-1.939919000	1.213142000	0.291898000
C	-3.346518000	1.067338000	-0.282073000
O	-3.957438000	-0.144680000	0.142995000

C	-3.210157000	-1.276982000	-0.281715000
C	0.331199000	0.112838000	0.465617000
C	1.268436000	0.203574000	-0.454557000
C	2.666816000	0.378069000	-0.147661000
O	3.242636000	1.453311000	-0.014352000
O	3.346107000	-0.816393000	-0.110353000
C	4.766140000	-0.711348000	0.052803000
H	0.321294000	0.108406000	1.558800000
H	-0.906852000	0.036433000	-1.080651000
H	-1.965539000	1.266367000	1.384028000
H	-1.423939000	2.095923000	-0.095217000
H	-3.982534000	1.881900000	0.073845000
H	-3.318979000	1.107519000	-1.384117000
H	-3.745977000	-2.160078000	0.075809000
H	-3.179156000	-1.314856000	-1.383831000
H	-1.812170000	-1.315646000	1.382493000
H	-1.180138000	-2.074589000	-0.098941000
H	5.136464000	-1.738540000	0.039265000
H	5.209748000	-0.135100000	-0.765147000
H	5.018002000	-0.228178000	1.002089000

Int.c

H	4.655852000	-0.271889000	1.051329000
H	4.805280000	-1.730777000	0.016239000
H	4.891519000	-0.088132000	-0.703217000
C	4.429555000	-0.706865000	0.072588000
O	3.015238000	-0.808248000	-0.131615000
C	2.331415000	0.385849000	-0.128011000
O	2.901654000	1.453610000	0.075556000
C	0.944177000	0.223441000	-0.484235000
C	-0.018547000	0.078595000	0.404294000
H	-0.045477000	0.013352000	1.496560000
N	-1.424596000	0.010513000	-0.150747000
H	-1.231009000	0.077606000	-1.160814000
C	-2.349948000	1.128174000	0.243708000
C	-3.721668000	0.647224000	-0.231872000
C	-3.689305000	-0.891627000	-0.014037000
C	-2.194136000	-1.256374000	0.137706000
H	-2.291592000	1.216227000	1.333294000
H	-1.987573000	2.054758000	-0.205314000
H	-3.852741000	0.884017000	-1.294247000
H	-4.536433000	1.133316000	0.312506000
H	-4.151624000	-1.421520000	-0.851840000
H	-4.238808000	-1.174343000	0.889115000
H	-1.833002000	-2.032220000	-0.539752000
H	-1.936616000	-1.547385000	1.158998000

Int.d

H	-4.718591000	1.333005000	0.262673000
H	-4.590495000	-0.054230000	-0.869719000
C	-4.258213000	0.358020000	0.088336000
H	-4.532688000	-0.339895000	0.885811000
O	-2.846367000	0.599640000	0.077748000
C	-2.060211000	-0.507661000	-0.157064000
O	-2.551614000	-1.622912000	-0.310577000
C	-0.670469000	-0.171991000	-0.291062000
C	0.186480000	-0.204477000	0.699204000
N	1.694293000	0.038891000	0.386121000
H	0.107027000	-0.454635000	1.761520000
H	2.137513000	0.317512000	1.267130000
H	1.186823000	0.948507000	-1.405146000
H	2.921908000	1.088860000	-0.981897000
C	1.899281000	1.158243000	-0.603314000
C	2.328856000	-1.262344000	-0.046406000
H	1.915848000	-1.471187000	-1.036279000
H	1.935224000	-2.021355000	0.634803000
C	1.635318000	2.518161000	0.029936000
C	3.855023000	-1.256120000	-0.025220000
H	4.213764000	-2.261887000	-0.270504000
H	4.292391000	-0.567003000	-0.754019000
H	4.246095000	-1.004367000	0.968897000
H	1.784503000	3.299478000	-0.723068000

H	0.605869000	2.584927000	0.391570000
H	2.322204000	2.725222000	0.861547000

Int.e

C	5.536552000	0.734001000	0.725256000
O	4.109697000	0.658792000	0.615068000
C	3.638570000	-0.089444000	-0.438421000
C	2.205590000	-0.001068000	-0.570881000
C	1.370330000	-0.875286000	-0.051505000
N	-0.101717000	-0.637176000	-0.362603000
O	4.396702000	-0.677144000	-1.203049000
C	-0.948521000	-0.193542000	0.810460000
C	-2.391062000	0.009493000	0.421163000
H	5.727553000	1.378106000	1.586173000
H	5.971400000	-0.257324000	0.887555000
H	5.973992000	1.167121000	-0.179718000
H	1.479558000	-1.766061000	0.572865000
H	-0.536265000	-1.456644000	-0.804436000
H	-0.473920000	0.721818000	1.171695000
H	-0.835157000	-0.965343000	1.576373000
C	-3.319934000	-1.033347000	0.554612000
C	-4.649527000	-0.854266000	0.165244000
H	-3.005854000	-1.986300000	0.976976000
C	-5.064683000	0.372629000	-0.359937000
H	-5.360282000	-1.668430000	0.278560000
C	-4.147925000	1.420258000	-0.490316000
H	-6.099402000	0.514170000	-0.660157000
C	-2.819302000	1.239866000	-0.100445000
H	-4.467778000	2.378960000	-0.889475000
H	-2.112416000	2.062044000	-0.194260000
H	-0.061133000	0.109169000	-1.071456000

Int.compa

C	4.069141000	-1.509509000	-0.405171000
C	3.636686000	-0.148828000	0.133994000
N	2.154605000	0.031567000	0.002532000
C	1.407287000	-1.119247000	0.622313000
C	1.909271000	-2.446388000	0.066383000
N	3.351133000	-2.589737000	0.263375000
C	1.637065000	1.372276000	0.487344000
C	1.014759000	2.106393000	-0.411045000
C	0.263773000	3.286228000	-0.094739000
O	0.937369000	4.456673000	-0.309844000
C	0.168245000	5.656093000	-0.148323000
C	3.833415000	-3.903275000	-0.149422000
O	-0.922590000	3.275332000	0.250663000
H	1.804714000	1.471739000	1.563105000
H	1.907209000	0.081041000	-0.996652000
H	1.585814000	-1.059059000	1.699957000
H	0.342011000	-0.947626000	0.425714000
H	1.395110000	-3.258137000	0.592436000
H	1.635358000	-2.531091000	-1.006562000
H	5.143686000	-1.628732000	-0.226345000
H	3.918153000	-1.537512000	-1.505686000
H	3.874156000	-0.055340000	1.197361000
H	4.107317000	0.673592000	-0.410775000
H	0.855537000	6.472986000	-0.377255000
H	-0.681741000	5.668056000	-0.837519000
H	-0.204934000	5.748218000	0.876321000
H	4.902793000	-3.987899000	0.070505000
H	3.306774000	-4.680234000	0.414096000
H	3.683535000	-4.095148000	-1.229620000
H	-1.530002000	1.107146000	0.216967000
N	-1.926211000	0.164512000	0.175974000
C	-2.507176000	-0.056702000	-1.151088000
C	-3.101786000	-1.462764000	-1.222151000
H	-3.301630000	0.675457000	-1.384765000
H	-1.718228000	0.054917000	-1.904057000
N	-4.108289000	-1.651676000	-0.177393000
I	-3.581023000	-1.617246000	-2.196913000
H	-2.284899000	-2.210801000	-1.126667000
C	-3.551498000	-1.383782000	1.148948000

C	-4.734873000	-2.960727000	-0.252505000
C	-2.953748000	0.021494000	1.210553000
H	-4.356530000	-1.480091000	1.888078000
H	-2.766121000	-2.126143000	1.408475000
H	-3.768579000	0.758921000	1.092000000
H	-2.493961000	0.184573000	2.192453000
H	-5.523682000	-3.038781000	0.504537000
H	-5.193492000	-3.096588000	-1.238743000
H	-4.017617000	-3.792493000	-0.088961000

TS2a (NImag = 1)

H	5.537922000	-0.239370000	0.524249000
H	5.424864000	-1.830121000	-0.301247000
C	5.090069000	-0.791523000	-0.307243000
O	3.661529000	-0.851877000	-0.168159000
C	3.017620000	0.350916000	-0.168930000
O	3.611978000	1.414190000	-0.266664000
C	1.567526000	0.196208000	-0.136848000
C	0.746859000	0.234443000	0.910127000
N	-0.614553000	0.098145000	0.325116000
C	-1.334764000	-1.152274000	0.668173000
C	-2.620824000	-1.272123000	-0.145950000
N	-3.472751000	-0.102091000	0.053841000
C	-2.768333000	1.111357000	-0.354254000
C	-1.485165000	1.292946000	0.453307000
C	-4.758000000	-0.240392000	-0.620467000
H	0.852492000	0.340860000	1.988425000
H	0.158177000	0.056976000	-0.697421000
H	-1.723402000	1.452436000	1.513159000
H	-0.912089000	2.150749000	0.088673000
H	-3.419937000	1.975318000	-0.181563000
H	-2.521549000	1.092504000	-1.435752000
H	-3.163606000	-2.166800000	0.179552000
H	-2.365751000	-1.409906000	-1.216993000
H	-1.565212000	-1.152087000	1.741718000
H	-0.657609000	-1.984532000	0.453574000
H	5.364818000	-0.304557000	-1.247527000
H	-5.274487000	-1.131384000	-0.247858000
H	-5.382883000	0.632235000	-0.402564000
H	-4.658601000	-0.330563000	-1.720021000

TS2b (NImag = 1)

C	-1.959024000	1.224115000	0.341863000
N	-1.063196000	0.046384000	0.209932000
C	-1.781852000	-1.225704000	0.474971000
C	-3.039028000	-1.306516000	-0.388747000
O	-3.882675000	-0.179364000	-0.182755000
C	-3.209075000	1.029606000	-0.514609000
C	0.270400000	0.180569000	0.859186000
C	1.135617000	0.193183000	-0.151814000
C	2.582920000	0.373666000	-0.112655000
O	3.158803000	1.450670000	-0.148158000
O	3.248541000	-0.816349000	-0.120869000
C	4.681007000	-0.726437000	-0.191149000
H	5.079104000	-0.195680000	0.678613000
H	5.034554000	-1.758645000	-0.204565000
H	0.324586000	0.249654000	1.944199000
H	-0.252871000	0.053414000	-0.776824000
H	-2.235939000	1.350504000	1.396919000
H	-1.392902000	2.103953000	0.019272000
H	-3.919596000	1.841739000	-0.339678000
H	-2.937600000	1.024482000	-1.582969000
H	-3.626427000	-2.189549000	-0.123551000
H	-2.761686000	-1.376018000	-1.453415000
H	-2.048124000	-1.275329000	1.539150000
H	-1.092978000	-2.045255000	0.245941000
H	4.989104000	-0.202496000	-1.100626000

TS2c (NImag = 1)

H	4.740847000	-0.219507000	0.759449000
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H	4.710652000	-0.126591000	-1.019195000
C	4.376563000	-0.703270000	-0.151650000
H	4.740032000	-1.730484000	-0.211055000
O	2.943903000	-0.807337000	-0.135397000
C	2.267494000	0.376187000	-0.080387000
O	2.836821000	1.456461000	-0.032559000
C	0.824108000	0.189557000	-0.181684000
C	-0.080465000	0.101606000	0.792538000
H	-0.059509000	0.091549000	1.881468000
H	-0.529612000	0.095161000	-0.865626000
N	-1.379912000	0.012579000	0.092138000
C	-2.343574000	1.135183000	0.225476000
C	-3.563408000	0.624188000	-0.543678000
C	-3.611867000	-0.885357000	-0.194462000
C	-2.164719000	-1.252576000	0.217535000
H	-2.572119000	1.302030000	1.287577000
H	-1.888552000	2.042795000	-0.180650000
H	-3.404446000	0.765932000	-1.618921000
H	-4.482179000	1.151802000	-0.270437000
H	-3.962564000	-1.486366000	-1.038731000
H	-4.298624000	-1.066759000	0.639111000
H	-1.693915000	-2.006889000	-0.419762000
H	-2.111217000	-1.606831000	1.253335000

TS2d (NImag = 1)

N	-1.565095000	-0.094775000	0.132378000
H	-0.709307000	-0.111298000	-0.831276000
C	0.645041000	0.083631000	-0.168584000
C	-0.255540000	0.117498000	0.810399000
H	-0.232140000	0.249688000	1.891248000
O	2.655725000	1.362367000	-0.125321000
C	4.199538000	-0.796064000	-0.080693000
C	-2.520103000	1.047395000	0.220684000
C	-3.198537000	-1.872835000	-0.617909000
H	-4.105289000	-1.259802000	-0.632577000
C	2.087665000	0.280437000	-0.087619000
O	2.767284000	-0.902320000	-0.054261000
C	-2.185203000	-1.417645000	0.432253000
C	-1.954899000	2.348232000	-0.344896000
H	4.563815000	-0.243497000	0.790433000
H	4.531003000	-0.286110000	-0.989998000
H	4.565838000	-1.823838000	-0.062352000
H	-2.643632000	-1.379273000	1.430903000
H	-1.354657000	-2.127833000	0.477156000
H	-2.806423000	1.173307000	1.275218000
H	-3.421495000	0.764907000	-0.329700000
H	-2.754365000	-1.860218000	-1.619614000
H	-1.071891000	2.684717000	0.204215000
H	-1.670932000	2.232289000	-1.396340000
H	-2.722292000	3.128041000	-0.280771000
H	-3.504407000	-2.901931000	-0.398341000

TS2e (NImag = 1)

C	-5.424217000	0.791539000	-0.738772000
O	-4.010497000	0.534636000	-0.719895000
C	-3.524229000	0.001747000	0.437225000
C	-2.070675000	-0.128002000	0.412312000
C	-1.333029000	-1.188774000	0.092807000
N	0.068010000	-0.753709000	0.340886000
O	-4.237562000	-0.254682000	1.395016000
C	0.983966000	-0.655968000	-0.832326000
C	2.355674000	-0.170654000	-0.424967000
H	-5.625355000	1.227086000	-1.718805000
H	-5.988263000	-0.136686000	-0.608370000
H	-5.698724000	1.490486000	0.056637000
H	-1.523879000	-2.198130000	-0.266125000
H	0.522217000	-1.244055000	1.118174000
H	0.498725000	0.034771000	-1.530250000
H	1.048756000	-1.635217000	-1.320989000
C	3.435679000	-1.060736000	-0.350870000
C	4.700718000	-0.615808000	0.044448000
H	3.289452000	-2.107207000	-0.611876000

C	4.897718000	0.728126000	0.370549000
H	5.529597000	-1.317177000	0.093408000
C	3.826565000	1.624833000	0.297900000
H	5.880722000	1.076892000	0.676001000
C	2.564869000	1.178010000	-0.098633000
H	3.975022000	2.672604000	0.545693000
H	1.736031000	1.880307000	-0.157631000
H	-0.614148000	0.266771000	0.678916000

8a

H	-5.595645000	0.249942000	-0.691052000
H	-5.894543000	-1.388878000	-0.020039000
C	-5.320738000	-0.467019000	0.088237000
O	-3.946492000	-0.855570000	-0.043073000
C	-3.032739000	0.154739000	0.061794000
O	-3.367712000	1.316906000	0.255453000
C	-1.673911000	-0.351153000	-0.092484000
C	-0.637020000	0.529232000	-0.031497000
N	0.699415000	0.274695000	-0.087300000
C	1.211546000	-1.062825000	-0.370203000
C	2.606336000	-1.245555000	0.230158000
N	3.512982000	-0.187209000	-0.207314000
C	2.995982000	1.116944000	0.200704000
C	1.622262000	1.361358000	-0.419445000
C	4.874778000	-0.407666000	0.262419000
H	-0.885860000	1.580459000	0.101871000
H	-1.552507000	-1.414898000	-0.256482000
H	1.729904000	1.443702000	-1.513292000
H	1.202366000	2.300316000	-0.045712000
H	3.686596000	1.895051000	-0.144606000
H	2.922437000	1.195415000	1.304954000
H	3.007560000	-2.211690000	-0.097054000
H	2.525174000	-1.272834000	1.336372000
H	1.245992000	-1.232314000	-1.458759000
H	0.534900000	-1.799627000	0.069161000
H	-5.502324000	-0.014646000	1.067688000
H	5.240425000	-1.371300000	-0.108443000
H	5.530012000	0.378870000	-0.127230000
H	4.953398000	-0.408991000	1.367791000

8b

C	-1.632981000	-1.152567000	-0.264568000
N	-1.156670000	0.205422000	-0.010997000
C	-2.114669000	1.257086000	-0.363005000
C	-3.476640000	0.959921000	0.259575000
O	-3.933306000	-0.336220000	-0.112108000
C	-3.028331000	-1.339814000	0.333174000
C	0.175083000	0.498341000	0.002600000
C	1.231387000	-0.356269000	-0.063521000
C	2.581690000	0.188086000	0.039675000
O	2.889479000	1.363543000	0.190506000
O	3.516716000	-0.801396000	-0.060077000
C	4.884429000	-0.375972000	0.022242000
H	5.079497000	0.111644000	0.981869000
H	5.477567000	-1.286894000	-0.072432000
H	0.397690000	1.559060000	0.103218000
H	1.133260000	-1.427018000	-0.194720000
H	-1.654270000	-1.352569000	-1.348742000
H	-0.946138000	-1.865110000	0.200434000
H	-3.449625000	-2.298746000	0.019198000
H	-2.967541000	-1.321413000	1.433582000
H	-4.226266000	1.669251000	-0.101921000
H	-3.415245000	1.032628000	1.357782000
H	-2.222528000	1.321776000	-1.458482000
H	-1.733235000	2.217222000	-0.000016000
H	5.120598000	0.321931000	-0.786397000

8c

H	4.740753000	0.239707000	0.924740000
H	4.772787000	0.167821000	-0.854252000
C	4.533912000	-0.391510000	0.055303000

H	5.118815000	-1.311695000	0.102938000
O	3.163188000	-0.810754000	0.047510000
C	2.236361000	0.193901000	-0.006128000
O	2.561986000	1.375048000	-0.044969000
C	0.883287000	-0.340593000	-0.009211000
C	-0.171923000	0.523994000	-0.058597000
H	0.044539000	1.590022000	-0.096882000
H	0.761435000	-1.416773000	0.031031000
N	-1.483111000	0.203994000	-0.060346000
C	-1.981366000	-1.172266000	-0.002680000
C	-3.503417000	-1.023522000	-0.174590000
C	-3.792281000	0.396039000	0.349278000
C	-2.567074000	1.192680000	-0.118690000
H	-1.523596000	-1.782558000	-0.791968000
H	-1.715232000	-1.625993000	0.963986000
H	-4.059473000	-1.799712000	0.359936000
H	-3.769900000	-1.093977000	-1.236406000
H	-3.840028000	0.394100000	1.445285000
H	-4.731280000	0.811286000	-0.029714000
H	-2.339426000	2.051272000	0.522321000
H	-2.704003000	1.561840000	-1.147033000

8d

N	-1.603465000	-0.157249000	-0.399404000
H	0.745920000	1.385226000	-0.313115000
C	0.791724000	0.309975000	-0.191913000
C	-0.305019000	-0.501774000	-0.208251000
H	-0.132898000	-1.565128000	-0.055894000
O	2.352142000	-1.479656000	0.169738000
C	4.422425000	0.174125000	0.173598000
C	-2.645641000	-1.184935000	-0.441489000
C	-2.050620000	2.123396000	0.579820000
H	-2.823227000	1.777567000	1.274414000
C	2.102549000	-0.290942000	0.004445000
O	3.086267000	0.659273000	-0.012292000
C	-1.980662000	1.231552000	-0.667593000
C	-3.627944000	-1.136325000	0.733776000
H	4.690176000	-0.534753000	-0.615624000
H	4.522985000	-0.320681000	1.144274000
H	5.061267000	1.057735000	0.126932000
H	-2.954712000	1.215515000	-1.169601000
H	-1.261536000	1.647923000	-1.385631000
H	-2.146559000	-2.158509000	-0.465289000
H	-3.195574000	-1.086908000	-1.389016000
H	-1.095645000	2.134175000	1.113893000
H	-3.102261000	-1.248339000	1.688568000
H	-4.185018000	-0.193155000	0.757300000
H	-4.357246000	-1.950603000	0.642971000
H	-2.289561000	3.153305000	0.287715000

8e

C	5.212919000	-0.124285000	1.267116000
O	3.862119000	-0.164625000	0.786369000
C	3.681959000	0.251823000	-0.506220000
C	2.297401000	0.183799000	-0.951574000
C	1.275577000	-0.252405000	-0.168606000
N	-0.042932000	-0.278708000	-0.511703000
O	4.614672000	0.635436000	-1.197628000
C	-1.043583000	-1.047051000	0.220910000
C	-2.420607000	-0.412644000	0.155226000
H	5.164937000	-0.482452000	2.296962000
H	5.857073000	-0.772320000	0.665629000
H	5.604614000	0.896537000	1.234303000
H	1.484566000	-0.592829000	0.842654000
H	-0.279617000	-0.039312000	-1.468433000
H	-0.702161000	-1.102690000	1.262471000
H	-1.099967000	-2.082521000	-0.148641000
C	-3.539103000	-1.183351000	-0.184192000
C	-4.816893000	-0.614807000	-0.211957000
H	-3.412083000	-2.236209000	-0.428700000
C	-4.986580000	0.736847000	0.094587000
H	-5.674791000	-1.226891000	-0.478360000

C	-3.873448000	1.516329000	0.428532000
H	-5.977711000	1.182428000	0.070889000
C	-2.600014000	0.945555000	0.458503000
H	-3.998334000	2.569546000	0.667132000
H	-1.736516000	1.554931000	0.714000000
H	2.130419000	0.517387000	-1.971858000

Int.Comp.a

N	-2.651334000	-2.532301000	-0.219839000
C	-2.256858000	-1.882584000	1.028139000
C	-0.739538000	-1.891273000	1.186901000
N	-0.060356000	-1.240908000	0.018738000
C	-0.539794000	-1.836897000	-1.270541000
C	-2.062980000	-1.831664000	-1.359010000
C	1.450307000	-1.308972000	0.140113000
C	2.145300000	-0.187944000	0.200174000
C	3.577081000	-0.190874000	0.383753000
O	4.257705000	-0.129445000	-0.811454000
C	5.678703000	0.019506000	-0.703931000
C	-4.099695000	-2.653720000	-0.340288000
O	4.166811000	-0.157579000	1.459749000
N	-0.258472000	1.689835000	0.088832000
C	-0.611163000	2.409634000	1.323337000
C	-2.091301000	2.790390000	1.296216000
N	-2.353659000	3.603347000	0.106346000
C	-2.019017000	2.891379000	-1.128836000
C	-0.538373000	2.510475000	-1.099550000
H	1.758720000	-2.359563000	0.173729000
H	-0.302460000	-0.212206000	0.024777000
H	-0.363147000	-2.916976000	1.248032000
H	-0.422494000	-1.346695000	2.079656000
H	-2.695383000	-2.431156000	1.869464000
H	-2.632334000	-0.840873000	1.081176000
H	-2.356633000	-2.344141000	-2.282248000
H	-2.430948000	-0.788150000	-1.430360000
H	-0.153669000	-2.859930000	-1.314310000
H	-0.085098000	-1.254710000	-2.075755000
H	6.044531000	0.067980000	-1.731850000
H	5.934232000	0.937458000	-0.165025000
H	6.125531000	-0.831774000	-0.180715000
H	-4.347253000	-3.190889000	-1.261844000
H	-4.490876000	-3.229388000	0.505107000
H	-4.613404000	-1.672847000	-0.360413000
H	0.743302000	1.426846000	0.114746000
H	0.063725000	3.434817000	-1.101678000
H	-0.274489000	1.934896000	-1.994817000
H	-2.218615000	3.551379000	-1.980884000
H	-2.623099000	1.971165000	-1.261360000
C	-3.721722000	4.052234000	0.083889000
H	-2.342819000	3.378201000	2.186814000
H	-2.700286000	1.864105000	1.315200000
H	-0.011563000	3.328372000	1.437320000
H	-0.396801000	1.761060000	2.180789000
H	-3.946608000	4.577709000	1.010832000
H	-3.869241000	4.724922000	-0.759704000
H	-4.383916000	3.193541000	-0.016444000

Int.Comp.d

C	-2.643303000	0.118153000	-0.562415000
C	-1.261435000	-0.178321000	-0.277533000
C	-0.807178000	-1.418315000	-0.266131000
N	0.675412000	-1.671548000	-0.063976000
H	1.101277000	-0.723921000	0.132084000
N	1.524426000	1.132601000	0.184605000
C	1.884756000	1.719051000	1.482577000
C	1.602173000	3.215384000	1.689070000
O	-3.408985000	0.199924000	0.581125000
C	-4.760265000	0.634355000	0.387079000
O	-3.116466000	0.370256000	-1.667337000
C	0.939518000	-2.590343000	1.096762000
C	0.431838000	-2.034844000	2.422701000
C	1.285179000	-2.171830000	-1.349441000

C	2.805445000	-2.317389000	-1.320120000
C	2.200676000	1.687461000	-1.002948000
C	1.457877000	2.821079000	-1.725105000
H	-4.788639000	1.630082000	-0.066994000
H	-5.204254000	0.659120000	1.384706000
H	-5.309066000	-0.060860000	-0.256163000
H	-1.314054000	-2.377833000	-0.422095000
H	2.017160000	-2.766103000	1.144289000
H	3.157714000	-2.514902000	-2.338676000
H	3.144150000	-3.147473000	-0.692381000
H	3.288366000	-1.396807000	-0.973763000
H	0.450570000	-3.541251000	0.855648000
H	0.793572000	-3.121767000	-1.585452000
H	0.977756000	-1.445779000	-2.105579000
H	0.638109000	-2.764358000	3.214052000
H	0.940517000	-1.101056000	2.683484000
H	-0.642969000	-1.841196000	2.393277000
H	0.500202000	1.149804000	0.052002000
H	2.952540000	1.522893000	1.656904000
H	1.333967000	1.153863000	2.245344000
H	2.353853000	0.872029000	-1.725393000
H	3.204301000	2.015895000	-0.700573000
H	2.008782000	3.121867000	-2.625980000
H	0.460885000	2.488153000	-2.035677000
H	1.835958000	3.500909000	2.723141000
H	0.546180000	3.445314000	1.504859000
H	1.335734000	3.704757000	-1.091267000
H	2.210449000	3.843156000	1.028526000

TS3a(NImag = 1)

N	-2.657995000	-2.459113000	-0.054537000
C	-2.272849000	-1.738976000	1.154143000
C	-0.753285000	-1.676592000	1.288163000
C	-0.112861000	-1.057314000	0.097372000
C	-0.567031000	-1.751511000	-1.136759000
C	-2.089625000	-1.812073000	-1.232000000
C	1.377200000	-1.141065000	0.215103000
C	2.141212000	-0.056140000	0.194905000
C	3.574272000	-0.143877000	0.364483000
O	4.243416000	-0.189323000	-0.843503000
C	5.672745000	-0.150516000	-0.760917000
C	-4.099357000	-2.631525000	-0.159579000
O	4.187239000	-0.097049000	1.432058000
N	-0.156237000	1.535996000	0.008019000
C	-0.569134000	2.301680000	1.205614000
C	-2.053009000	2.655134000	1.134137000
N	-2.309940000	3.387422000	-0.106461000
C	-1.983784000	2.585656000	-1.285962000
C	-0.498212000	2.231497000	-1.252262000
H	1.693495000	-2.187216000	0.320130000
H	-0.356087000	0.253222000	0.040635000
H	-0.354895000	-2.692279000	1.415428000
H	-0.462762000	-1.090494000	2.164670000
H	-2.680038000	-2.264122000	2.025322000
H	-2.697341000	-0.713732000	1.163278000
H	-2.362367000	-2.391055000	-2.121387000
H	-2.502071000	-0.790779000	-1.368019000
H	-0.158335000	-2.771084000	-1.139192000
H	-0.143263000	-1.218024000	-1.992224000
H	6.026690000	-0.178555000	-1.793322000
H	6.009869000	0.766449000	-0.268264000
H	6.057438000	-1.010290000	-0.204424000
H	-4.335970000	-3.225161000	-1.048393000
H	-4.471146000	-3.169796000	0.718148000
H	-4.643577000	-1.668960000	-0.231280000
H	0.886582000	1.350563000	0.050192000
H	0.095931000	3.150820000	-1.332246000
H	-0.228801000	1.577880000	-2.087831000
H	-2.197904000	3.172066000	-2.185504000
H	-2.580573000	1.655121000	-1.340550000
C	-3.674585000	3.844141000	-0.158915000
H	-2.316688000	3.292395000	1.984497000

H	-2.653929000	1.728673000	1.208115000
H	0.021897000	3.224338000	1.266821000
H	-0.347354000	1.696879000	2.090183000
H	-3.893170000	4.437371000	0.727775000
H	-3.819034000	4.454831000	-1.048923000
H	-4.343564000	2.985615000	-0.195266000

TS3d(NImag = 1)

C	-2.595324000	-0.114378000	-0.607476000
C	-1.183196000	-0.194537000	-0.318408000
C	-0.547592000	-1.358192000	-0.250414000
N	0.935989000	-1.428296000	-0.049808000
H	1.275048000	-0.168833000	0.162137000
N	1.236142000	1.148196000	0.193000000
C	1.412854000	1.711954000	1.548210000
C	1.032313000	3.186292000	1.706078000
O	-3.365687000	-0.099951000	0.537097000
C	-4.766555000	0.118617000	0.334453000
O	-3.104183000	0.024087000	-1.716444000
C	1.281739000	-2.354079000	1.068400000
C	0.693879000	-1.949702000	2.417831000
C	1.565732000	-1.880772000	-1.331021000
C	3.094993000	-1.939374000	-1.320530000
C	2.009445000	1.789039000	-0.901645000
C	1.211917000	2.809309000	-1.719698000
H	-4.944854000	1.080761000	-0.156783000
H	-5.209922000	0.114217000	1.332794000
H	-5.204501000	-0.675021000	-0.279207000
H	-0.967041000	-2.367691000	-0.368977000
H	2.372127000	-2.404330000	1.141797000
H	3.450937000	-2.103403000	-2.344173000
H	3.485074000	-2.757626000	-0.707121000
H	3.537427000	-1.002316000	-0.961785000
H	0.925561000	-3.359101000	0.792969000
H	1.150690000	-2.866176000	-1.589411000
H	1.215310000	-1.182633000	-2.096225000
H	0.931812000	-2.723128000	3.157381000
H	1.118131000	-1.006201000	2.776787000
H	-0.392531000	-1.839156000	2.367489000
H	0.199149000	1.093693000	-0.044970000
H	2.457360000	1.555368000	1.850340000
H	0.785535000	1.108158000	2.212124000
H	2.360921000	0.996548000	-1.572861000
H	2.906291000	2.248282000	-0.462728000
H	1.832159000	3.201008000	-2.535168000
H	0.324852000	2.341865000	-2.160345000
H	1.127035000	3.479494000	2.758591000
H	-0.005182000	3.357599000	1.398858000
H	0.879862000	3.654847000	-1.109811000
H	1.681573000	3.846313000	1.120596000

Pr.Comp.a

N	-4.895372000	-1.675361000	0.163692000
C	-5.226736000	-0.310138000	-0.236059000
C	-4.276290000	0.684286000	0.427694000
N	-2.883296000	0.348073000	0.133324000
C	-2.523422000	-1.039238000	0.418624000
C	-3.524547000	-1.997439000	-0.227524000
C	-1.948555000	1.336866000	0.085267000
C	-0.592873000	1.207128000	0.152183000
C	0.313421000	2.333212000	0.013022000
O	-0.304318000	3.537868000	-0.170445000
C	0.563448000	4.672487000	-0.302963000
C	-5.851723000	-2.643962000	-0.356627000
O	1.538906000	2.243879000	0.055860000
N	2.292543000	-0.814357000	0.254215000
C	3.137535000	-1.224977000	1.378049000
C	4.631787000	-0.956378000	1.149752000
N	5.080504000	-1.574114000	-0.099801000
C	4.294943000	-1.083826000	-1.234183000
C	2.800555000	-1.353176000	-1.009451000
H	-2.370282000	2.330452000	-0.045131000

H	2.252649000	0.206787000	0.203767000
H	-4.445175000	0.672516000	1.516895000
H	-4.476175000	1.696091000	0.061264000
H	-6.252772000	-0.088243000	0.080054000
H	-5.178445000	-0.187197000	-1.337834000
H	-3.295506000	-3.018439000	0.098371000
H	-3.403038000	-1.961803000	-1.329644000
H	-2.496941000	-1.202774000	1.507820000
H	-1.526421000	-1.239126000	0.021160000
H	-0.099426000	5.529198000	-0.436216000
H	1.175946000	4.797879000	0.594562000
H	1.220223000	4.557954000	-1.170128000
H	-5.597191000	-3.644730000	0.008528000
H	-6.857537000	-2.396222000	-0.000415000
H	-5.873070000	-2.673959000	-1.464251000
H	-0.094582000	0.256473000	0.306744000
H	2.632884000	-2.439496000	-1.012348000
H	2.218350000	-0.923052000	-1.833213000
H	4.637997000	-1.596892000	-2.142588000
H	4.452464000	0.005563000	-1.386907000
C	6.508591000	-1.394531000	-0.310913000
H	5.220479000	-1.376645000	1.976136000
H	4.810146000	0.140480000	1.137830000
H	2.992485000	-2.301997000	1.542304000
H	2.799819000	-0.701344000	2.280242000
H	7.063988000	-1.823654000	0.531117000
H	6.816026000	-1.915397000	-1.225161000
H	6.798949000	-0.327980000	-0.407507000

Pr.Comp.d

C	0.240961000	2.025722000	-0.072090000
C	0.741419000	0.676803000	0.105484000
C	2.070411000	0.394939000	0.254485000
N	2.639051000	-0.821577000	0.448438000
H	-2.323587000	0.717651000	-0.048360000
N	-2.861806000	-0.144691000	0.029911000
C	-3.658712000	-0.083039000	1.256834000
C	-4.156251000	-1.446504000	1.745759000
O	1.210282000	2.990034000	-0.097218000
C	0.748341000	4.336544000	-0.273000000
O	-0.948127000	2.315885000	-0.194132000
C	4.082587000	-0.940667000	0.661425000
C	4.828769000	-1.673187000	-0.459134000
C	1.816801000	-2.030665000	0.556396000
C	1.342974000	-2.596957000	-0.788594000
C	-3.612224000	-0.360952000	-1.213246000
C	-3.578792000	-1.811821000	-1.710872000
H	0.220913000	4.443600000	-1.225312000
H	1.648107000	4.954279000	-0.263257000
H	0.076841000	4.624955000	0.540821000
H	2.778046000	1.218861000	0.223904000
H	4.254241000	-1.455140000	1.618487000
H	0.713186000	-3.477958000	-0.617200000
H	2.189622000	-2.896119000	-1.415377000
H	0.750173000	-1.862539000	-1.341545000
H	4.484397000	0.071551000	0.771112000
H	2.411606000	-2.780674000	1.089837000
H	0.950944000	-1.801603000	1.190606000
H	5.902877000	-1.694059000	-0.237834000
H	4.490962000	-2.710370000	-0.560594000
H	4.683567000	-1.169572000	-1.421336000
H	-0.028125000	-0.086406000	0.111434000
H	-4.530621000	0.592462000	1.142655000
H	-3.018525000	0.359550000	2.030128000
H	-3.172008000	0.280891000	-1.987349000
H	-4.663442000	-0.034700000	-1.101999000
H	-4.128726000	-1.908036000	-2.656972000
H	-2.543970000	-2.132664000	-1.878252000
H	-4.658991000	-1.342124000	2.715971000
H	-3.318775000	-2.145058000	1.859766000
H	-4.027574000	-2.500595000	-0.987317000
H	-4.876795000	-1.890954000	1.049663000

Pr.5e.Comp1

C	-1.293042000	2.731804000	0.794355000
C	-0.837381000	2.148189000	2.115024000
H	0.209869000	2.412925000	2.300262000
H	-1.433075000	2.584766000	2.931315000
N	-0.912415000	0.667725000	2.093129000
H	-1.880919000	0.371204000	1.967921000
H	-0.609853000	0.291144000	2.992098000
H	0.094795000	-0.351347000	0.654256000
N	0.546035000	-0.871645000	-0.110770000
C	1.885315000	-0.750627000	-0.266972000
C	2.735891000	-0.104027000	0.583422000
C	4.172684000	-0.038191000	0.394388000
O	4.951172000	0.534278000	1.147342000
C	-0.335109000	-1.360113000	-1.161500000
C	-1.452488000	-2.240405000	-0.626982000
C	-1.168993000	-3.331698000	0.208265000
C	-2.194640000	-4.156927000	0.672495000
C	-3.522351000	-3.901777000	0.310000000
C	-3.814910000	-2.815663000	-0.517444000
C	-2.784076000	-1.989922000	-0.979665000
O	4.611063000	-0.684661000	-0.735511000
C	6.024855000	-0.639228000	-0.963394000
H	6.188175000	-1.195290000	-1.888585000
H	6.367718000	0.394071000	-1.072851000
H	6.567067000	-1.106638000	-0.135955000
H	2.293363000	-1.238169000	-1.150189000
H	0.280544000	-1.927485000	-1.871512000
H	-0.774070000	-0.521547000	-1.723393000
H	-3.018481000	-1.141987000	-1.620242000
H	-4.843299000	-2.606373000	-0.801504000
H	-4.320673000	-4.544877000	0.671753000
H	-1.958857000	-5.000984000	1.316085000
H	-0.139533000	-3.527742000	0.498412000
I	2.370252000	0.395020000	1.475497000
C	-2.571932000	3.289258000	0.663559000
C	-3.007527000	3.805411000	-0.561456000
C	-2.161630000	3.773444000	-1.672395000
C	-0.880281000	3.224025000	-1.551637000
C	-0.450191000	2.707756000	-0.327693000
H	-3.231689000	3.327351000	1.528785000
H	-4.002084000	4.236765000	-0.643987000
H	-2.494104000	4.179726000	-2.624350000
H	-0.212137000	3.206262000	-2.409194000
H	0.548608000	2.285863000	-0.239994000

TS_A(NImag = 1)

C	0.763961000	-2.853384000	-0.588185000
N	1.236650000	-1.552602000	-1.055896000
N	0.470560000	1.207975000	-0.839332000
C	-0.143679000	1.657160000	0.446269000
C	-1.569085000	2.127859000	0.276486000
C	-1.850285000	3.495914000	0.149259000
C	-3.162797000	3.938034000	-0.037959000
C	-4.208571000	3.013235000	-0.097026000
C	-3.937068000	1.647593000	0.034437000
C	-2.625757000	1.206220000	0.222432000
C	-0.689689000	-2.807540000	-0.151631000
C	-1.721278000	-2.798969000	-1.103209000
C	-3.061308000	-2.757185000	-0.709217000
C	-3.392837000	-2.725246000	0.649913000
C	-2.375031000	-2.729892000	1.608033000
C	-1.035221000	-2.768963000	1.206784000
C	2.360101000	-1.115585000	-0.566719000
C	2.962488000	0.124259000	-0.988375000
C	4.134120000	0.683284000	-0.349033000
O	4.843066000	1.579658000	-0.799347000
O	4.378965000	0.148114000	0.900667000
C	5.519832000	0.675768000	1.585167000
H	0.144250000	0.271080000	-1.138986000
H	5.569436000	0.133057000	2.531696000

H	6.433793000	0.514232000	1.005395000
H	5.405014000	1.749118000	1.767208000
H	2.853136000	-1.665551000	0.249562000
H	1.383586000	-3.235683000	0.241516000
H	0.858296000	-3.574171000	-1.413944000
H	-1.467778000	-2.834333000	-2.160628000
H	-3.846659000	-2.761673000	-1.461520000
H	-4.435047000	-2.706840000	0.959343000
H	-2.622693000	-2.712589000	2.666784000
H	-0.247906000	-2.784217000	1.958180000
H	2.909140000	0.354768000	-2.053129000
H	-0.074488000	0.806685000	1.129612000
H	0.490369000	2.457529000	0.839575000
H	-2.426924000	0.142414000	0.331704000
H	-4.746861000	0.923844000	-0.002901000
H	-5.230600000	3.354754000	-0.238827000
H	-3.367094000	5.001483000	-0.130433000
H	-1.040292000	4.220965000	0.206274000
H	0.314444000	1.879455000	-1.592983000
H	1.610787000	0.980521000	-0.762025000

Int.8e.Comp1

C	-1.776343000	2.657207000	0.505779000
N	-2.161413000	1.608576000	-0.437027000
N	0.302801000	-2.024752000	-0.772221000
C	1.099500000	-2.015573000	0.472010000
C	2.605417000	-2.075425000	0.283329000
C	3.278182000	-3.306048000	0.257843000
C	4.655926000	-3.366705000	0.030823000
C	5.384233000	-2.190723000	-0.170861000
C	4.726927000	-0.956888000	-0.139939000
C	3.349481000	-0.901644000	0.087789000
C	-0.346554000	3.115113000	0.273472000
C	0.075911000	3.521881000	-1.001536000
C	1.385243000	3.958469000	-1.210240000
C	2.294365000	3.997118000	-0.146539000
C	1.883771000	3.592300000	1.125300000
C	0.571301000	3.151382000	1.330246000
C	-2.518700000	0.485429000	0.038548000
C	-2.872305000	-0.668044000	-0.862245000
C	-4.165973000	-1.384569000	-0.532063000
O	-4.924258000	-1.852940000	-1.355421000
O	-4.371498000	-1.482396000	0.803576000
C	-5.560676000	-2.187569000	1.207987000
H	0.573004000	-1.234529000	-1.358498000
H	-5.560072000	-2.152811000	2.297895000
H	-6.449943000	-1.695879000	0.805059000
H	-5.528094000	-3.221330000	0.853737000
H	-2.554243000	0.294440000	1.121835000
H	-1.897761000	2.340348000	1.555553000
H	-2.457639000	3.503337000	0.338699000
H	-0.625937000	3.483852000	-1.830306000
H	1.697242000	4.271675000	-2.203744000
H	3.312734000	4.341280000	-0.309495000
H	2.581379000	3.617401000	1.959050000
H	0.259248000	2.835151000	2.323807000
H	-2.920173000	-0.335022000	-1.901311000
H	0.829593000	-1.106262000	1.021263000
H	0.765454000	-2.865517000	1.078552000
H	2.847529000	0.064137000	0.118525000
H	5.287422000	-0.036839000	-0.286838000
H	6.456459000	-2.234914000	-0.344377000
H	5.160689000	-4.329720000	0.017850000
H	2.719251000	-4.226007000	0.422924000
H	0.518059000	-2.861759000	-1.314065000
H	-2.056113000	-1.409364000	-0.784835000

Int.8e.Comp2

C	-2.956726000	-0.826972000	-1.482634000
N	-2.564242000	0.585788000	-1.494736000
7	1.451275000	-1.213800000	-0.240208000
C	2.631585000	-1.299835000	-1.116781000

C	3.982923000	-1.173846000	-0.429430000
C	4.391602000	0.049747000	0.126347000
C	5.619850000	0.163355000	0.779940000
C	6.464588000	-0.947347000	0.889671000
C	6.070417000	-2.169369000	0.340548000
C	4.838521000	-2.277659000	-0.314177000
C	-3.983720000	-1.100797000	-0.399050000
C	-5.243395000	-0.484294000	-0.435574000
C	-6.188461000	-0.738091000	0.559628000
C	-5.888124000	-1.615430000	1.607959000
C	-4.636204000	-2.232301000	1.654000000
C	-3.690219000	-1.972595000	0.656278000
C	-1.330286000	0.849811000	-1.345077000
C	-0.851753000	2.284528000	-1.365757000
C	0.030534000	2.614488000	-0.176195000
O	0.938940000	1.913726000	0.234899000
O	-0.293970000	3.797666000	0.374069000
C	0.498854000	4.216201000	1.504394000
H	1.538222000	-1.882990000	0.523994000
H	0.083018000	5.178007000	1.804352000
H	0.415277000	3.487442000	2.314436000
H	1.547516000	4.319930000	1.214048000
H	-0.566295000	0.072429000	-1.200120000
H	-2.091298000	-1.495893000	-1.356822000
H	-3.401380000	-1.038362000	-2.464751000
H	-5.476037000	0.203507000	-1.244872000
H	-7.161016000	-0.253494000	0.517486000
H	-6.625457000	-1.815412000	2.381523000
H	-4.392765000	-2.914505000	2.464978000
H	-2.714604000	-2.452613000	0.698409000
H	-0.231116000	2.439258000	-2.262103000
H	2.586044000	-2.255785000	-1.652603000
H	2.525675000	-0.511103000	-1.872095000
H	4.539951000	-3.232343000	-0.744173000
H	6.720206000	-3.037886000	0.418436000
H	7.421813000	-0.858442000	1.397413000
H	5.921610000	1.119451000	1.201415000
H	3.738220000	0.916955000	0.048990000
H	1.397267000	-0.285584000	0.180293000
H	-1.703756000	2.964813000	-1.419910000

TS_c(NImag = 1)

H	-1.502464000	1.281619000	-0.357590000
N	-1.775546000	0.153780000	-0.579449000
H	-0.795261000	-0.199967000	-0.609440000
N	0.992395000	0.666473000	-0.552299000
C	0.632592000	1.914959000	-0.582350000
C	-0.502580000	2.421888000	0.153204000
C	-0.923262000	3.785418000	-0.098556000
O	-1.752290000	4.257682000	0.895168000
C	-2.250724000	5.586205000	0.704557000
C	2.156272000	0.272825000	-1.330649000
C	3.248652000	-0.387648000	-0.500067000
C	4.134689000	-1.291730000	-1.104025000
C	5.174807000	-1.874494000	-0.375891000
C	5.340999000	-1.565151000	0.977651000
C	4.459264000	-0.670679000	1.590465000
C	3.421308000	-0.087288000	0.857160000
C	-2.576142000	-0.469982000	0.510119000
C	-2.762314000	-1.957740000	0.317841000
C	-3.983834000	-2.471365000	-0.138227000
C	-4.147923000	-3.845422000	-0.337776000
C	-3.088807000	-4.719566000	-0.082316000
C	-1.867000000	-4.216250000	0.377117000
C	-1.705741000	-2.844504000	0.578771000
O	-0.647796000	4.473033000	-1.078260000
H	-2.891332000	5.784107000	1.566488000
H	-1.430219000	6.309490000	0.667393000
H	-2.826076000	5.659667000	-0.223881000
H	1.148665000	2.625664000	-1.246652000
H	2.588378000	1.137803000	-1.866880000
H	1.839863000	-0.445193000	-2.103059000

H	4.009488000	-1.542438000	-2.156476000
H	5.851104000	-2.572844000	-0.863440000
H	6.147391000	-2.018979000	1.548506000
H	4.578050000	-0.425110000	2.643352000
H	2.732805000	0.600851000	1.338645000
H	-2.040844000	-0.251003000	1.439109000
H	-3.538941000	0.048227000	0.550581000
H	-0.754345000	-2.460803000	0.942614000
H	-1.041668000	-4.892146000	0.584455000
H	-3.214900000	-5.788180000	-0.234842000
H	-5.102207000	-4.230389000	-0.687598000
H	-4.815311000	-1.795765000	-0.330565000
H	-2.205643000	0.034684000	-1.498088000
H	-0.615324000	2.076364000	1.182185000

Pr.8e'.Comp2

C	-2.586180000	1.166550000	-1.132174000
N	-1.354012000	0.633266000	-1.036718000
H	-1.222191000	-0.293793000	-0.629410000
N	-0.101869000	-2.130511000	-0.237971000
C	0.844993000	-2.533884000	0.820373000
C	2.277013000	-2.252156000	0.414059000
C	3.137354000	-3.296844000	0.052297000
C	4.453705000	-3.039323000	-0.346307000
C	4.926904000	-1.726057000	-0.384206000
C	4.077855000	-0.674170000	-0.021123000
C	2.764971000	-0.936646000	0.373997000
C	-0.157683000	1.336645000	-1.464732000
C	0.395844000	2.357807000	-0.474396000
C	1.333159000	3.301821000	-0.919880000
C	1.892426000	4.226903000	-0.036172000
C	1.517783000	4.223805000	1.311662000
C	0.581649000	3.290644000	1.762531000
C	0.024594000	2.363237000	0.875105000
C	-3.786912000	0.633578000	-0.733815000
C	-3.915071000	-0.650513000	-0.092772000
O	-5.210192000	-0.949700000	0.210723000
C	-5.432723000	-2.210444000	0.854838000
O	-2.994109000	-1.429051000	0.176849000
H	-6.510150000	-2.265336000	1.018454000
H	-5.100980000	-3.035614000	0.217269000
H	-4.898449000	-2.258513000	1.808494000
H	-2.604530000	2.153186000	-1.594622000
H	-0.353282000	1.834113000	-2.424326000
H	0.601876000	0.570080000	-1.657053000
H	1.626979000	3.314146000	-1.968530000
H	2.614969000	4.953466000	-0.400087000
H	1.948350000	4.945825000	2.000814000
H	0.279776000	3.282560000	2.807071000
H	-0.708435000	1.644770000	1.231043000
H	-4.688968000	1.207403000	-0.906872000
H	0.590786000	-1.954013000	1.716029000
H	0.753415000	-3.598409000	1.091499000
H	2.110840000	-0.115065000	0.656719000
H	4.440710000	0.350669000	-0.039922000
H	5.950276000	-1.521931000	-0.689322000
H	5.106797000	-3.863827000	-0.622003000
H	2.776022000	-4.323222000	0.087165000
H	0.075829000	-2.672748000	-1.083319000
H	-1.062162000	-2.328725000	0.047445000

Pr.8e'

C	3.030759000	2.204843000	-0.651236000
O	2.474863000	0.914321000	-0.348683000
C	3.359327000	-0.004149000	0.184234000
C	2.750236000	-1.290340000	0.470600000
C	1.450417000	-1.663816000	0.266641000
N	0.420382000	-0.924305000	-0.209304000
O	4.530284000	0.284109000	0.377099000
C	-0.871609000	-1.479933000	-0.582453000
C	-2.031076000	-0.570803000	-0.212046000

H	2.202235000	2.793748000	-1.048552000
H	3.433348000	2.669395000	0.252809000
H	3.828749000	2.114234000	-1.393199000
H	1.172438000	-2.683256000	0.531600000
H	0.643648000	0.018401000	-0.512255000
H	-0.971013000	-2.445150000	-0.068694000
H	-0.909582000	-1.693824000	-1.661417000
C	-3.060167000	-0.331644000	-1.130967000
C	-4.151085000	0.473746000	-0.788719000
H	-3.008712000	-0.775921000	-2.123183000
C	-4.219773000	1.055191000	0.479195000
H	-4.940418000	0.651158000	-1.514809000
C	-3.192697000	0.826951000	1.401417000
H	-5.064123000	1.685255000	0.746737000
C	-2.106439000	0.019953000	1.057955000
H	-3.237802000	1.278386000	2.389357000
H	-1.306510000	-0.148586000	1.774693000
H	3.426542000	-2.021139000	0.896980000

The starting geometry of the for exploring the transition structure in **route 3**

C	4.130472000	-3.717673000	-0.576638000
N	3.578473000	-2.803876000	0.427642000
C	3.992199000	-3.213317000	1.772178000
C	3.500104000	-4.633030000	2.052306000
N	4.012380000	-5.563415000	1.046383000
C	3.640757000	-5.139464000	-0.303678000
C	3.613186000	-6.934815000	1.317157000
O	4.471711000	0.120810000	0.004161000
C	3.741827000	0.876154000	-0.646959000
O	3.738428000	2.227442000	-0.436313000
C	4.663509000	2.704494000	0.551737000
C	2.876253000	0.481735000	-1.695860000
C	1.770631000	-0.040188000	-2.010871000
N	1.386534000	-0.422417000	-3.816318000
C	1.184281000	-1.868088000	-4.040929000
C	0.800089000	-2.175562000	-5.488975000
N	-0.373966000	-1.402748000	-5.884485000
C	-0.120417000	0.031471000	-5.747023000
C	0.250652000	0.391473000	-4.308110000
C	-0.831677000	-1.751676000	-7.223493000
H	0.853005000	-0.402139000	-1.573219000
H	2.252552000	-0.108849000	-4.257115000
H	-0.597934000	0.191814000	-3.642932000
H	0.538215000	1.445845000	-4.226183000
H	-1.026686000	0.579611000	-6.029341000
H	0.688907000	0.365200000	-6.430655000
H	0.570437000	-3.243879000	-5.581038000
H	1.666631000	-1.967979000	-6.153632000
H	0.380991000	-2.189402000	-3.367666000
H	2.102801000	-2.389357000	-3.754770000
H	4.533138000	3.787968000	0.566158000
H	4.441364000	2.279899000	1.535693000
H	5.690259000	2.446375000	0.276690000
H	-1.063677000	-2.821310000	-7.266822000
H	-1.745324000	-1.194322000	-7.455872000
H	-0.080280000	-1.527140000	-8.006182000
H	3.908501000	-1.853382000	0.240987000
H	5.090864000	-3.190521000	1.894685000
H	3.558757000	-2.521047000	2.503810000
H	3.850632000	-4.961657000	3.038601000
H	2.389202000	-4.636772000	2.071366000
H	4.093229000	-5.834112000	-1.022147000
H	2.539364000	-5.180035000	-0.444871000
H	5.236070000	-3.718677000	-0.574181000
H	3.797994000	-3.394064000	-1.569841000
H	4.068256000	-7.605916000	0.579732000
H	3.962674000	-7.233303000	2.312212000
H	2.512970000	-7.078921000	1.281053000

Chapter 4**B3LYP/6-31+G* level****30**

C	-0.021361000	0.451327000	-0.226847000
C	0.497753000	0.590102000	1.229810000
H	0.856953000	0.525460000	-0.890202000
N	-0.686328000	-0.849788000	-0.359764000
C	-0.938272000	1.629509000	-0.549687000
H	0.872475000	1.613867000	1.367305000
H	-0.314154000	0.422302000	1.945908000
C	1.635784000	-0.360902000	1.517606000
O	1.633385000	-1.194905000	2.401291000
H	2.518415000	-0.263742000	0.847429000
C	-0.423950000	2.759117000	-1.199905000
C	-1.230626000	3.874734000	-1.444291000
C	-2.567339000	3.872442000	-1.036886000
C	-3.088303000	2.748890000	-0.386585000
C	-2.279725000	1.635658000	-0.145531000
H	0.615561000	2.764164000	-1.525416000
H	-0.817000000	4.740293000	-1.956176000
H	-3.198976000	4.736597000	-1.226831000
H	-4.128524000	2.738851000	-0.069495000
H	-2.685236000	0.753980000	0.342700000
C	-0.711178000	-1.520514000	-1.683627000
H	-0.313603000	-1.501913000	0.324809000
H	-1.088041000	-2.525577000	-1.455668000
C	-1.737265000	-0.879749000	-2.629060000
C	0.675730000	-1.709571000	-2.307515000
C	1.222496000	-0.814008000	-3.239897000
C	2.510705000	-1.003429000	-3.751060000
C	3.277475000	-2.097434000	-3.342629000
C	2.744704000	-3.002802000	-2.420180000
C	1.458494000	-2.806503000	-1.912390000
H	0.639082000	0.036246000	-3.582543000
H	2.912431000	-0.296744000	-4.473441000
H	4.276699000	-2.246941000	-3.743776000
H	3.326115000	-3.864330000	-2.100936000
H	1.052713000	-3.522712000	-1.199268000
H	-1.798856000	-1.456267000	-3.559119000
H	-2.720823000	-0.877885000	-2.149710000
H	-1.496909000	0.155082000	-2.886289000

31

C	1.452890000	-2.817355000	-1.929667000
C	0.674931000	-1.710973000	-2.306692000
C	1.224544000	-0.804288000	-3.227070000
C	2.510795000	-0.992280000	-3.743447000
C	3.272851000	-2.096065000	-3.352834000
C	2.737198000	-3.012268000	-2.442964000
C	-0.708777000	-1.522110000	-1.677953000
C	-1.739660000	-0.884342000	-2.619137000
N	-0.678048000	-0.849811000	-0.353533000
C	-0.015623000	0.452986000	-0.224861000
C	-0.934724000	1.628185000	-0.551984000
C	-0.418934000	2.760797000	-1.195934000
C	-1.227195000	3.874411000	-1.444167000
C	-2.566799000	3.867171000	-1.046694000
C	-3.088892000	2.740787000	-0.401961000
C	-2.278733000	1.629642000	-0.156943000
C	0.498966000	0.599647000	1.232459000
C	1.630229000	-0.355205000	1.535236000
H	0.863583000	0.526979000	-0.887137000
H	0.882174000	1.621658000	1.361470000
H	-0.316749000	0.446418000	1.947348000
H	0.622514000	2.768597000	-1.515015000
H	-0.811774000	4.742636000	-1.950077000
H	-4.131368000	2.726758000	-0.092602000
H	-2.684666000	0.746179000	0.327844000
H	-0.298823000	-1.501212000	0.328117000
H	-1.084358000	-2.526902000	-1.445853000

H	0.644853000	0.053746000	-3.555913000
H	2.914502000	-0.276729000	-4.455961000
H	4.270422000	-2.244968000	-3.758199000
H	4.270422000	-2.244968000	-3.758199000
H	3.314831000	-3.881511000	-2.138062000
H	1.044273000	-3.542384000	-1.227239000
H	-1.807084000	-1.465106000	-3.546254000
H	-2.720825000	-0.880940000	-2.134832000
H	-1.502884000	0.149448000	-2.884342000
O	-4.556819000	4.947871000	-0.936089000
O	-2.901384000	5.954460000	-1.865879000
H	3.390154000	-0.895901000	0.942792000

Chapter 5**B3LYP/lanl2dz level****7a**

C	5.805458000	-0.689252000	-1.847622000
C	4.474074000	-0.286000000	-1.177277000
N	4.696364000	0.157963000	0.214286000
C	5.428506000	-0.794362000	1.082779000
C	6.770975000	-1.201170000	0.443508000
C	4.123688000	1.264243000	0.772530000
O	4.259485000	1.600658000	1.984991000
C	3.367364000	2.248141000	-0.093100000
C	2.048747000	2.259980000	-0.409841000
C	1.073998000	1.196975000	-0.123147000
O	-0.163683000	1.358510000	-0.335985000
O	1.583719000	0.041214000	0.370701000
Br	-1.171933000	-1.726313000	0.632306000
Sn	-2.472060000	0.449086000	-0.191789000
C	-2.349126000	0.662921000	-2.297834000
C	-2.615132000	1.889067000	1.357578000
Br	-4.905414000	-0.563249000	-0.038556000
H	3.786149000	-1.145745000	-1.167182000
H	3.989852000	0.516945000	-1.740472000
H	5.591303000	-1.091667000	-2.847171000
H	6.430563000	0.205790000	-1.979297000
H	7.245552000	-1.967416000	1.071096000
H	7.441331000	-0.330169000	0.426771000
H	4.797696000	-1.685663000	1.231260000
H	5.570900000	-0.316932000	2.055081000
H	1.611696000	3.129494000	-0.892443000
H	3.949466000	3.136970000	-0.339183000
H	0.878132000	-0.642045000	0.566595000
H	7.533706000	-1.964538000	-1.457061000
H	5.990378000	-2.667012000	-0.961521000
H	-1.415056000	1.157046000	-2.574495000
H	-2.404444000	-0.329951000	-2.755704000
H	-3.207453000	1.250381000	-2.642671000
H	-3.502563000	2.507452000	1.182638000
H	-2.740357000	1.367306000	2.311844000
H	-1.717477000	2.511024000	1.383478000

7d

Sn	1.838692000	-0.215522000	-0.500035000
N	-4.881709000	-0.336745000	0.509421000
C	-6.196394000	0.145019000	0.022158000
O	-1.123529000	2.389425000	0.548448000
C	-1.214358000	1.653804000	-0.580736000
C	-2.512874000	1.841240000	-1.306975000
C	-3.651693000	1.182245000	-1.015861000
C	-3.675479000	0.149803000	0.070591000
O	-2.571620000	-0.257123000	0.554467000
C	0.471583000	-1.744051000	0.036298000
Br	1.973445000	1.612118000	1.430422000
Br	4.107647000	-1.471768000	0.040714000
C	2.412515000	0.609009000	-2.367585000
C	-4.849378000	-1.403957000	1.546467000
O	-0.257855000	0.997770000	-1.067706000
6C	-6.734073000	-0.626602000	-1.202214000

C	-4.558735000	-2.807675000	0.976516000
H	-0.244755000	2.280815000	1.015752000
H	-2.478459000	2.557210000	-2.125703000
H	-4.540189000	1.377746000	-1.607048000
H	-4.069135000	-1.142541000	2.269003000
H	-5.816213000	-1.391569000	2.062783000
H	-6.904929000	0.050121000	0.853370000
H	-6.132651000	1.215396000	-0.200646000
H	0.435910000	-2.480827000	-0.776015000
H	0.847728000	-2.234992000	0.938992000
H	-0.524965000	-1.330629000	0.209750000
H	2.730194000	-0.203749000	-3.030544000
H	1.575677000	1.155553000	-2.807577000
H	3.264860000	1.277257000	-2.208903000
H	-7.706621000	-0.218622000	-1.506933000
H	-6.047746000	-0.550784000	-2.054658000
H	-6.868399000	-1.689415000	-0.972291000
H	-4.532071000	-3.539702000	1.794087000
H	-5.327456000	-3.123116000	0.260862000
H	-3.584265000	-2.820699000	0.478103000

❖ **List of Papers Published**

1. Experimental and Theoretical Investigation of the Reaction of Amines with Methyl Propiolate, Manjinder Kour, Raakhi Gupta, and Raj K. Bansal *Chemistry Select* **2017**, 2, 8465 – 8470.
2. Experimental and Theoretical Investigation of the Reaction of Secondary Amines with Maleic Anhydride, Manjinder Kour, Raakhi Gupta, and Raj K. Bansal, *Aust. J. Chem.* **2017**, A-G, DOI 10.1071/CH17206.
3. Aromaticity of 1,4-Dehydrotropylium Ion and Its Mono- and Poly-phospha Analogues Aishvaryadeep Kaur, Manjinder Kour, Raakhi Gupta and Raj K. Bansal, *Phosphorus, Sulfur, and Silicon and the Related Elements* **2017**, 192, 674-682.
4. Analogy of Phosphaalkenes and Azaphospholes with their Respective Nonphosphorus Analogues, Raj K. Bansal, Raakhi Gupta, Pooja Maheshwari and Manjinder Kour, *Current Organic Chemistry*, **2016**, 20, 2099-2108.
5. Fluxional behaviour of Tricyclo[2.2.1.0^{2,6}]heptaphosphide Trisanion: A DFT Investigation, Meha Bhargava, Pooja Maheshwari, Manjinder Kour and Raj K. Bansal, *Z. Naturforsch.* **2015**, 70, 871–878.
6. Reinvestigation of the aromaticity of mono- and polyphosphacyclopentadienide ions at the DFT level, Raakhi Gupta, Pooja Maheshwari, Manjinder Kour, *Comp. Theo. Chem.* **2015**, 1060, 10–16.
7. Diels-Alder Reactions with the >C=P- Functionality of Annelated Azaphospholes, Raj K. Bansal, Raakhi Gupta, Manjinder Kour, *Synlett* **2015**, 26, 294-303.

❖ List of Papers presented in Conferences/Symposium/Workshops

1. *Synergy between experimental and theoretical results of Michael addition of amines to methyl propiolate*; National Conference On “New Vistas In Chemical Research”, Organized by The IIS University, Jaipur on 18-19 January, **2017**.
2. Aromaticity of 1,4-dehydrotropylium ion and its mono and poly-phospha analogues, National conference on new vistas in chemical research (NVCR), Organized by Department of chemistry, The IIS University, Jaipur, 18-19, January, **2017**.
3. Effect of the hydroxyl groups on the Cope rearrangement of cis-diethynylcyclopropane and its mono-hetero analogues: a DFT investigation, National conference on new vistas in chemical research (NVCR), Organized by Department of chemistry, The IIS University, Jaipur, 18-19, January, **2017**.
4. Theoretical and experimental investigation of the direct versus conjugate addition of secondary amines and related compound to maleic anhydride, “Anveshan: Student Research Convention”, Organized by Association of Indian Universities, 7-8, March **2017**.
5. *An experimental and theoretical investigation of the Michael addition of some amines to methyl propiolate*; National Conference On “New Frontiers In Chemistry –From Fundamentals To Applications”, Organized by Birla Institute of Technology and Science Pilani, K. K. Birla, Goa on 18 – 19 December, **2015**.
6. *Theoretical and experimental results of Stereoselective Michael addition of some secondary amines to methyl propiolate*; “XI J-NOST for Research Scholar”, Organized by NISER, Bhubaneswar on 14–17 December, **2015**.
7. *Stereoselective Michael addition of 1-methylpiperazine and morpholine with methyl propiolate*; National Conference on “Frontiers at the Chemistry-Allied Sciences Interface”, Organized by University of Rajasthan, Jaipur on 13-14 March, **2015**.
8. Stereoselective Michael addition of amines to methyl propiolate: Experimental and theoretical results, Biyani International Conference

- (BICON-2015), Organised by Biyani Group of Colleges, Jaipur, 21-27 September, **2015**.
9. Direct versus conjugate addition of secondary amines and related compound to maleic anhydride: Experimental and theoretical results, 17th National symposium in chemistry (CRSI-NSC-17), Organised by CRSI-NCL, Pune, 06-08 February, **2015**.
 10. Stereoselective Michael addition of 1-methylpiperazine and morpholine with methyl propiolate, National conference on Frontiers at the chemistry-allied sciences interface (FCASI-2015), Organised by Centre of advanced study, Department of chemistry, University of Rajasthan, Jaipur, 13-14 March, **2015**.
 11. "Direct versus conjugate addition of secondary amines and related compound to maleic anhydride: Experimental and theoretical results.", National Conference on "Emerging Areas in Chemical Education and Research and National Convention of Chemistry Teachers", Organised by ACT, Mumbai and The IIS University, Jaipur, 16-18 October, **2014**.
 12. "DFT investigation of the homoaromaticity and valence tautomerism in Aza- and Phospha-analogues of cyclohepta-1,3,5-triene.", National Conference on "Emerging Areas in Chemical Education and Research and National Convention of Chemistry Teachers", Organised by ACT, Mumbai and The IIS University, Jaipur, 16-18 October, **2014**.
 13. "Save our sky: Ozone friendly planet our target", Symposium on 'International Day for Preservation of Ozone Layer', Organised by The IIS University, Jaipur, 15 September, **2012**.

❖ **Fellowship/Recognitions**

Availed research fellowship (2014-2016).

Two months training from at Central Drugs Research Institute (CDRI),
Lucknow.