

Supporting Information

Figure S1. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the lowest energy isomer of protonated imidacloprid

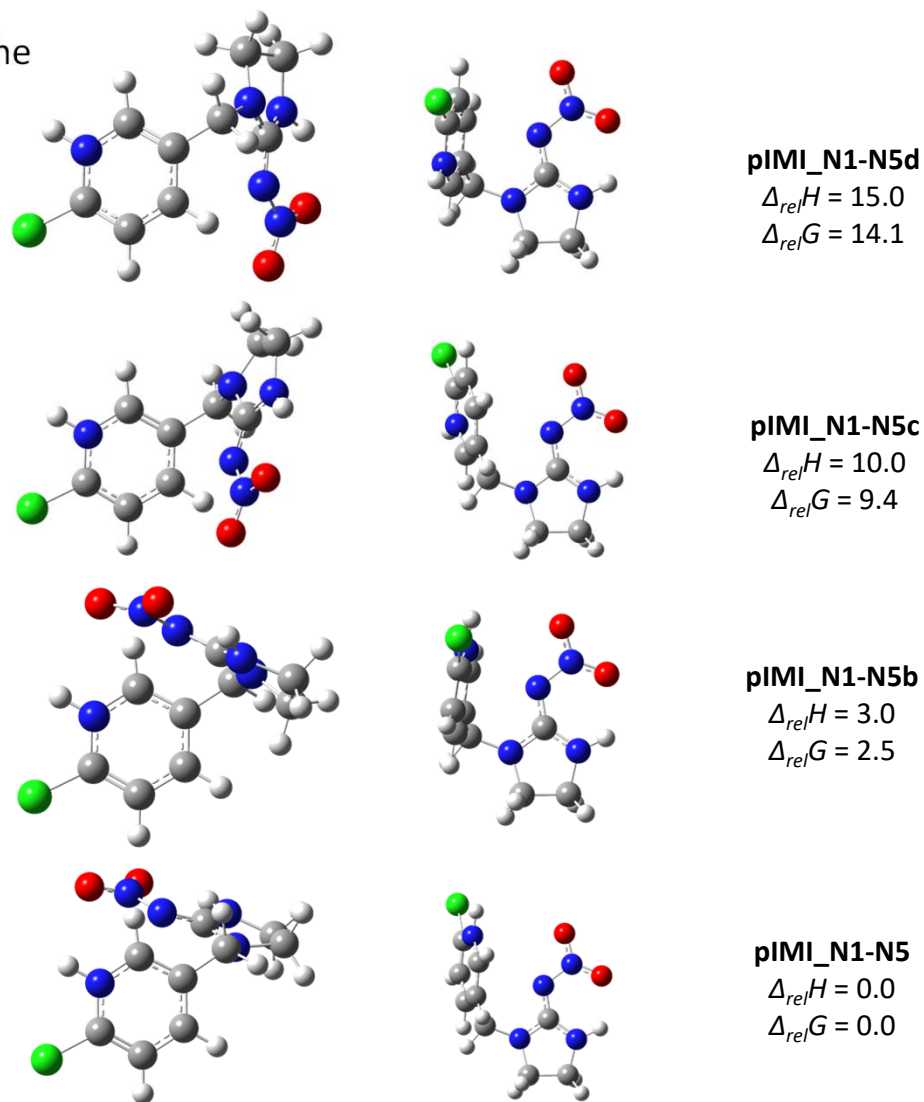
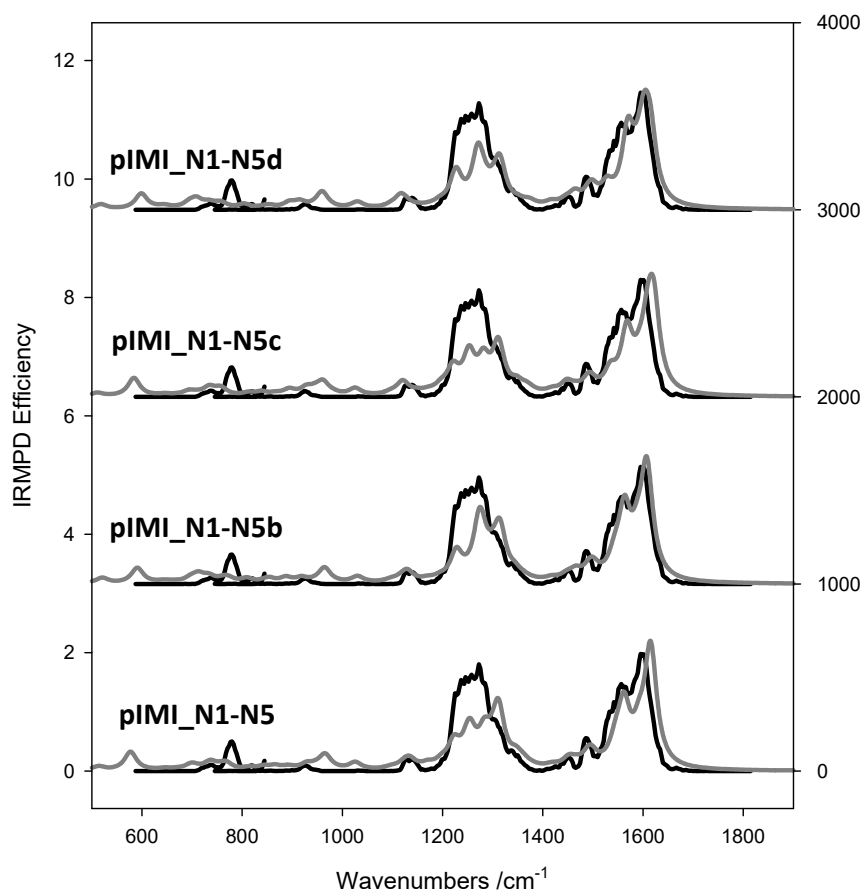
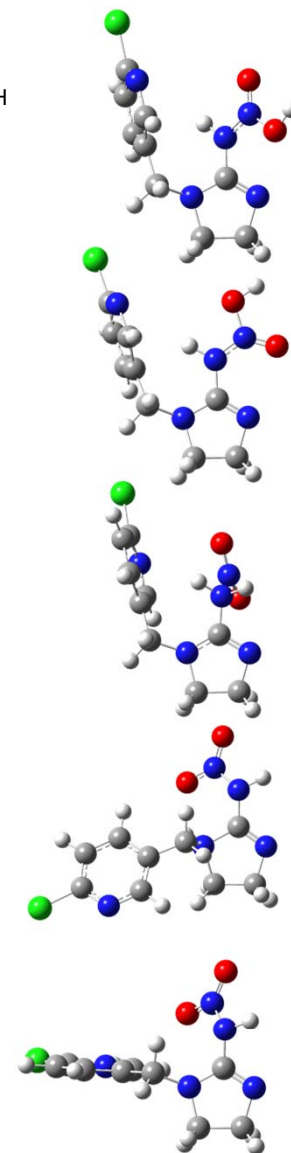
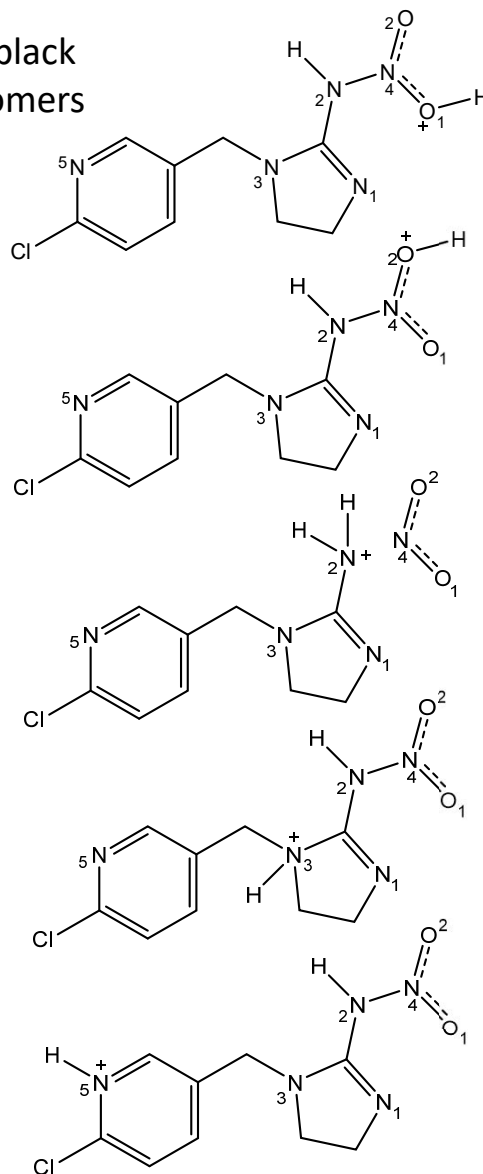
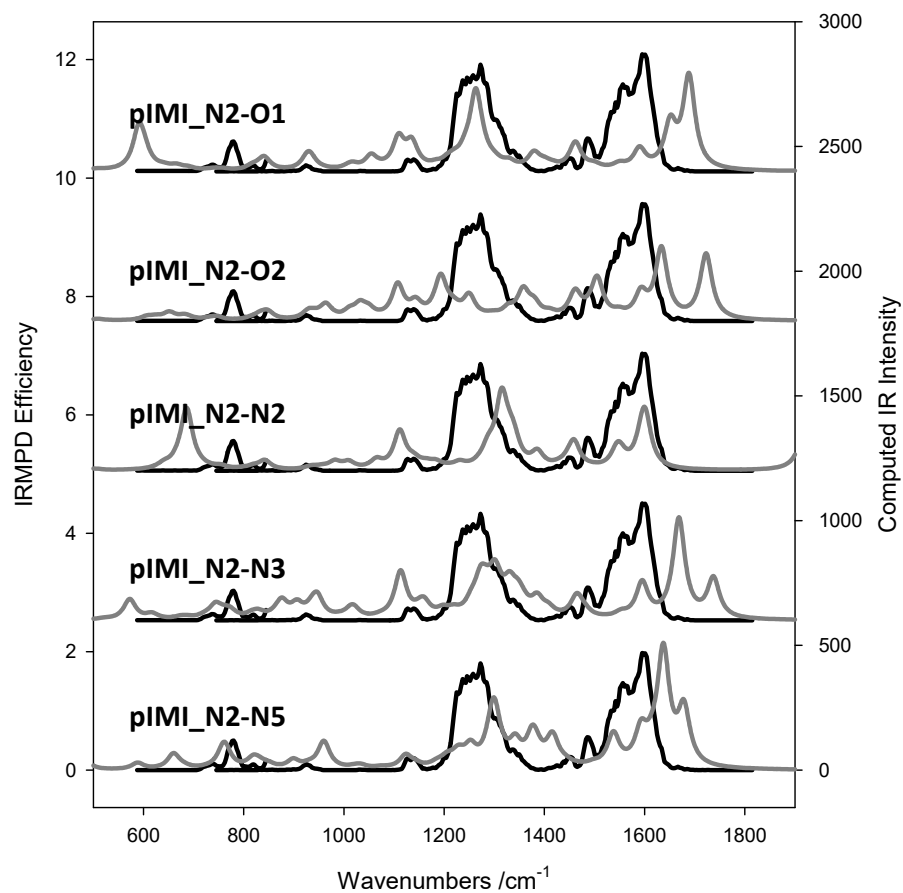


Figure S2. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for N2 tautomers of protonated imidacloprid



pIMI_N2-O1
 $\Delta_{rel}H = 211.0$
 $\Delta_{rel}G = 203.3$

pIMI_N2-O2
 $\Delta_{rel}H = 200.5$
 $\Delta_{rel}G = 196.6$

pIMI_N2-N2
 $\Delta_{rel}H = 188.1$
 $\Delta_{rel}G = 182.5$

pIMI_N2-N3
 $\Delta_{rel}H = 117.2$
 $\Delta_{rel}G = 115.6$

pIMI_N2-N5
 $\Delta_{rel}H = 64.5$
 $\Delta_{rel}G = 64.1$

Figure S3. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for tautomers of protonated imidacloprid

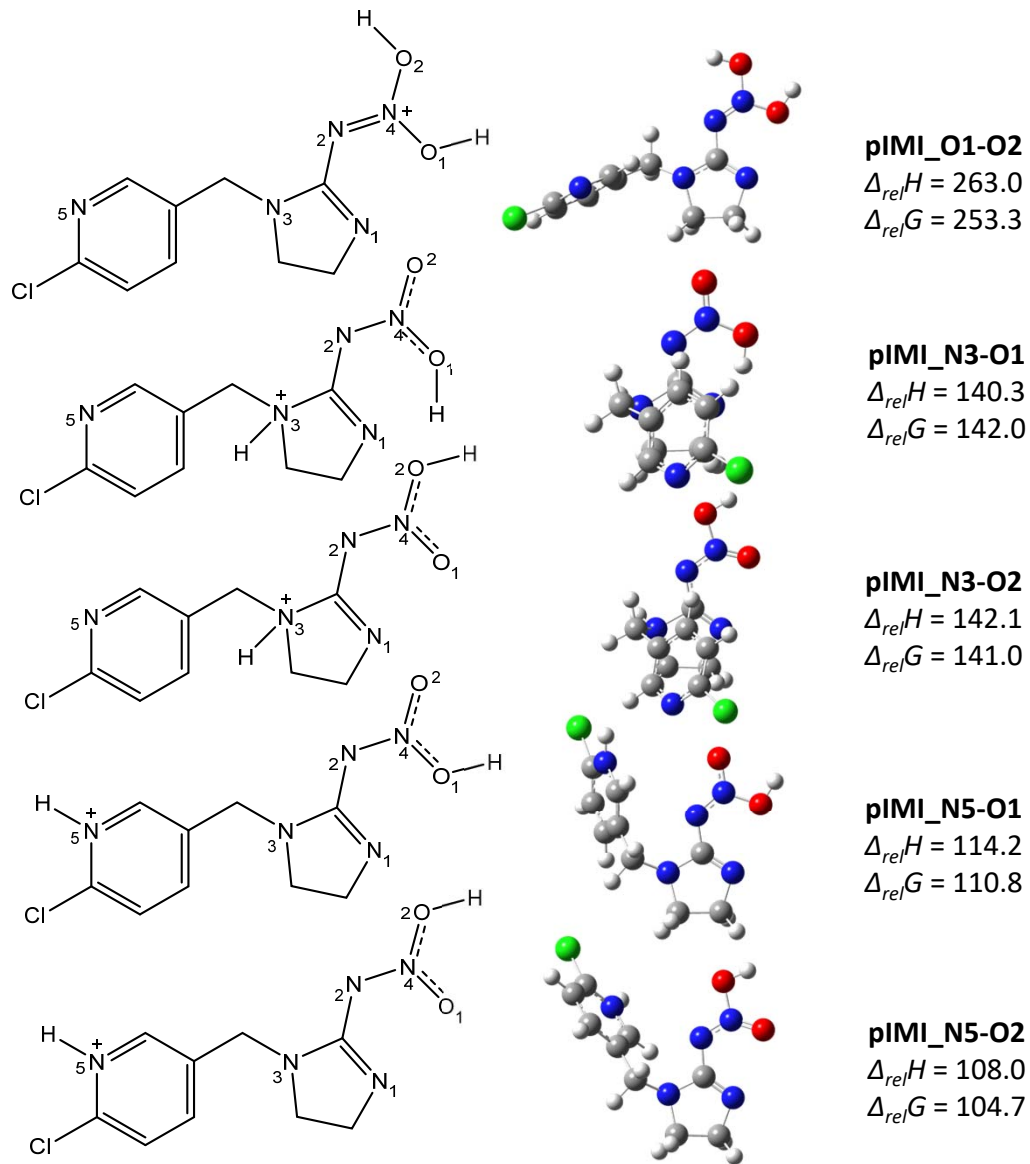
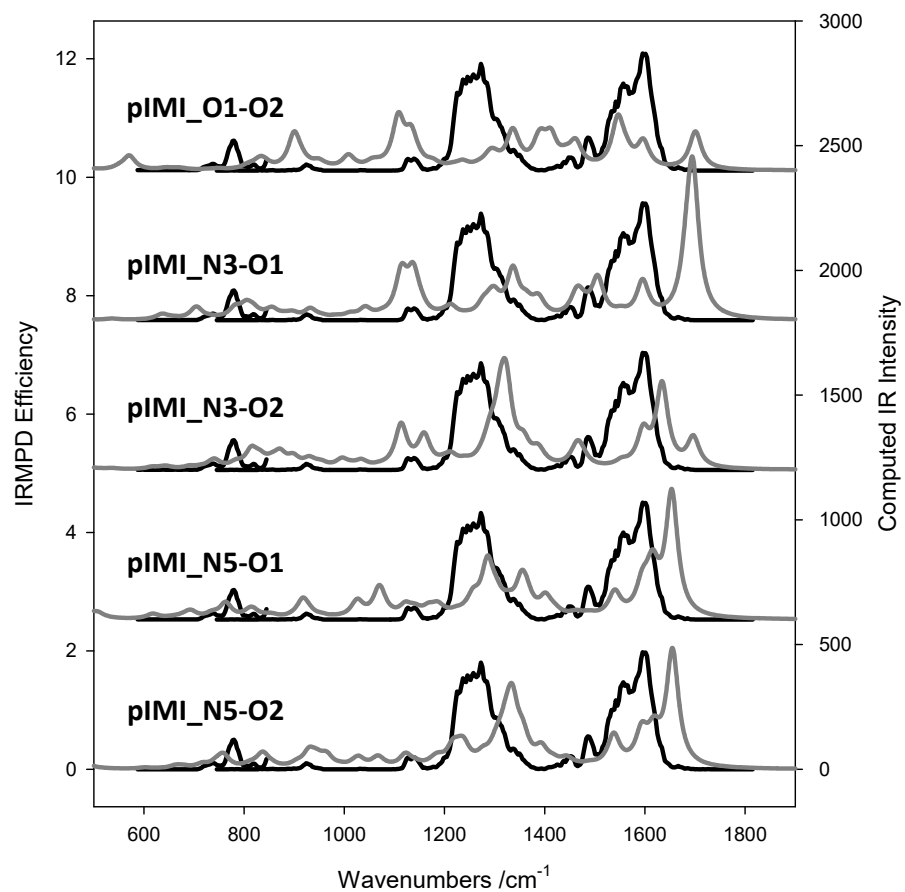


Figure S4. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for protonated desnitrosoimidacloprid – loss of NO radical

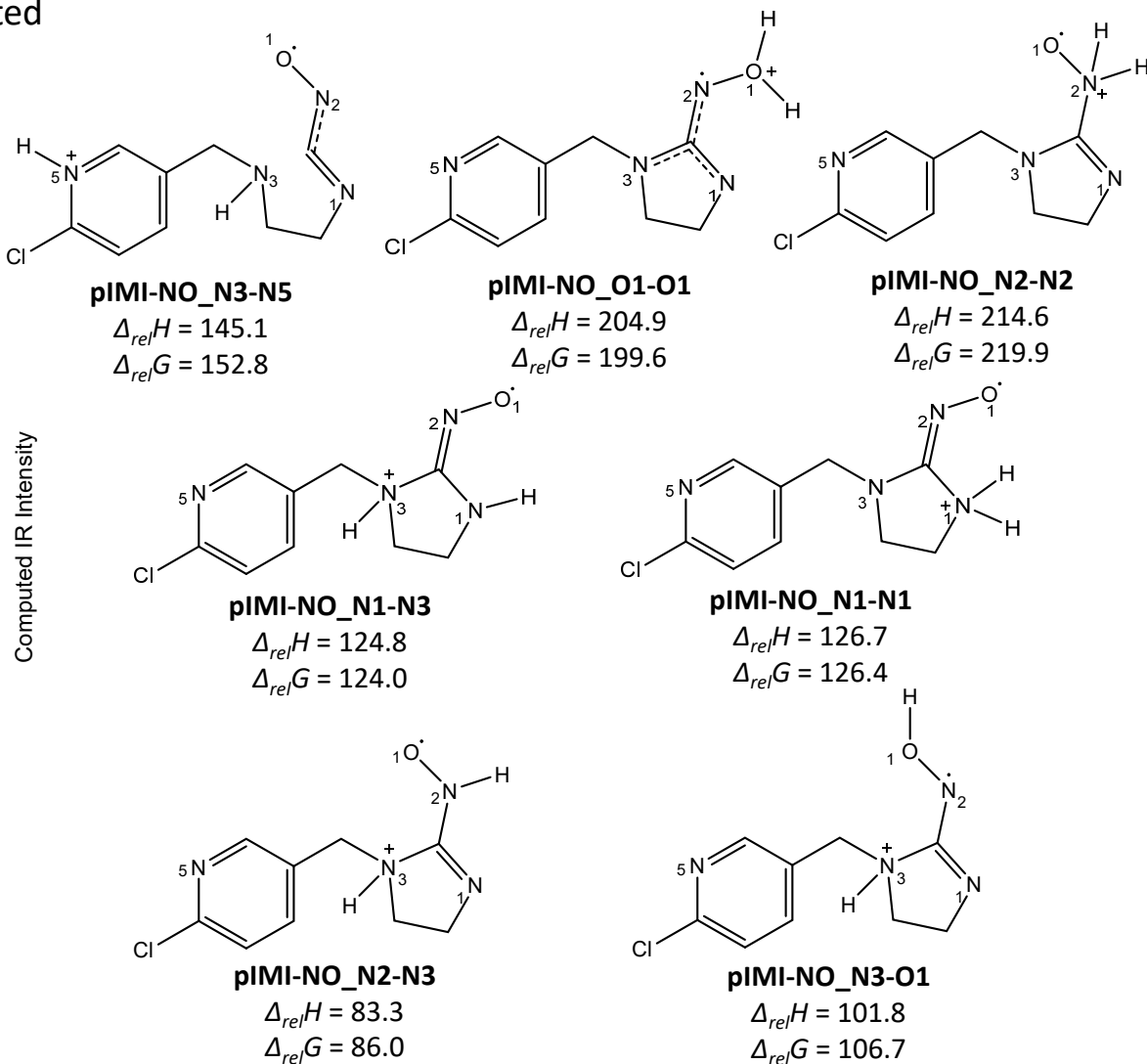
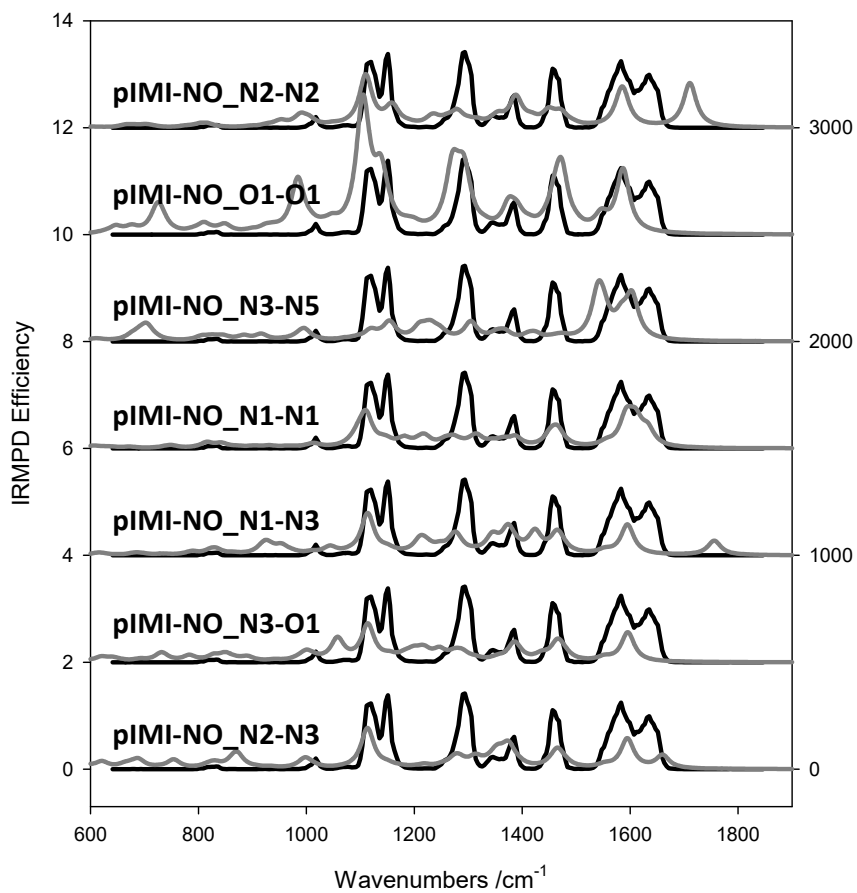


Figure S5. Gibbs Potential Energy Diagram Proton Transfer Following Loss of NO•

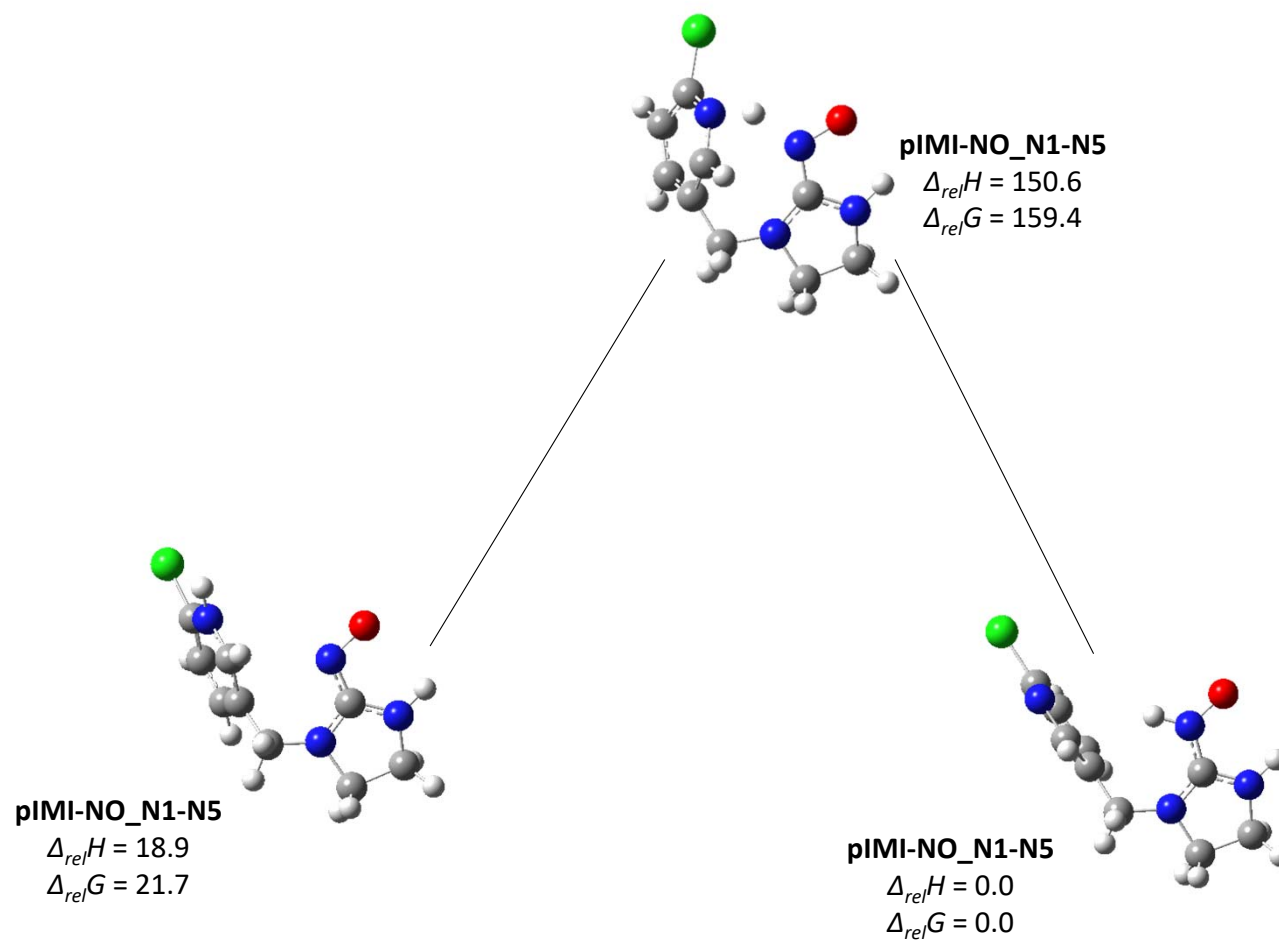


Figure S6. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the lowest energy isomer of protonated imidacloprid urea – loss of N_2O

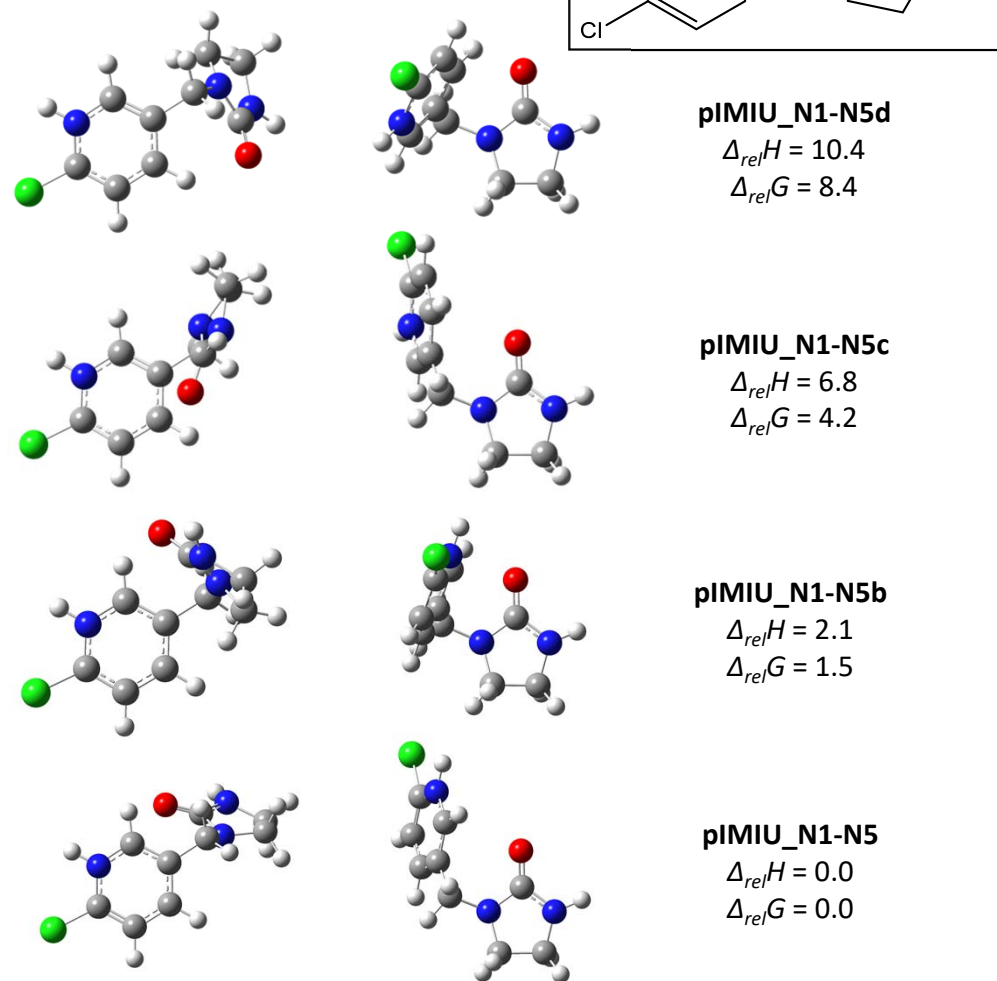
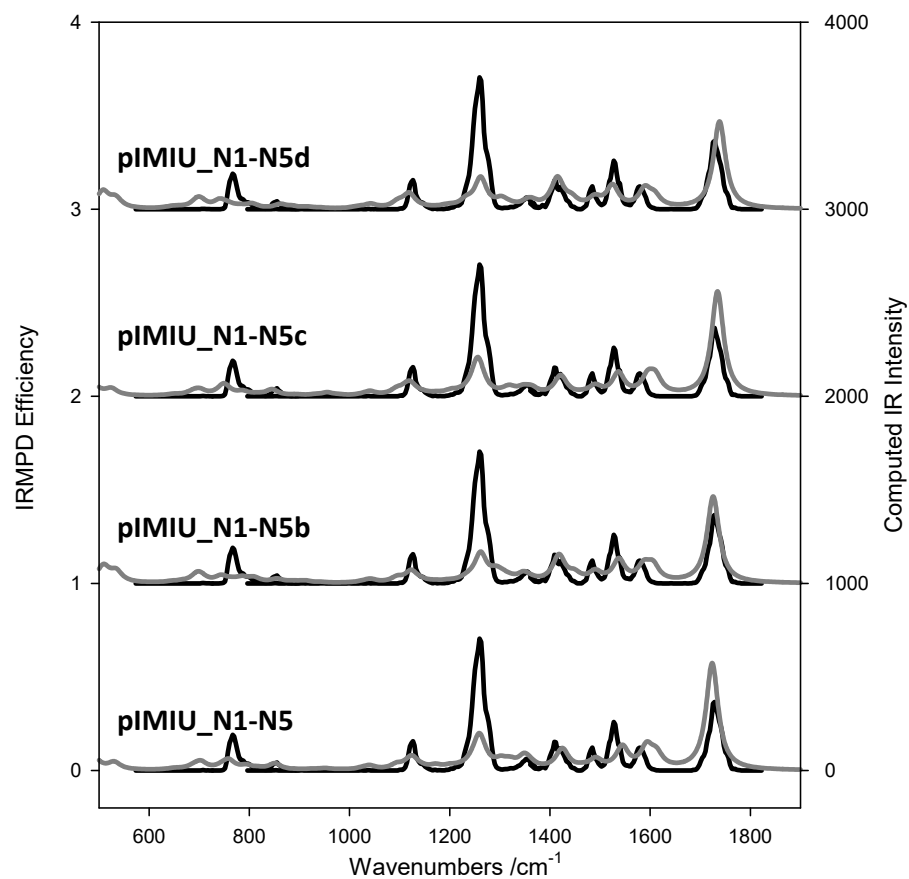


Figure S7. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for protonated imidacloprid urea – loss of N₂O

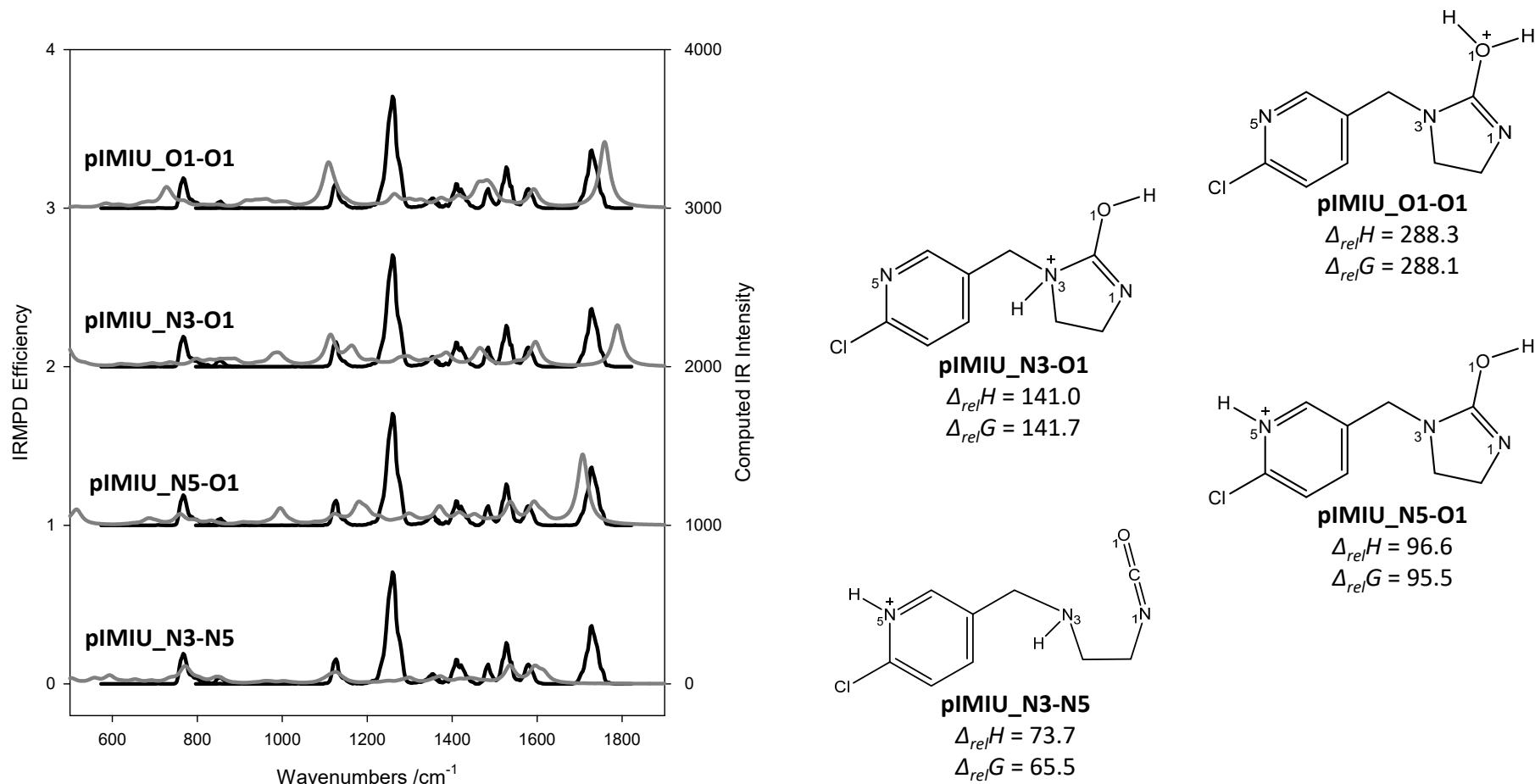


Figure S8. Gibbs Potential Energy Diagram Proton Transfer Preceding Loss of NO_2^\bullet

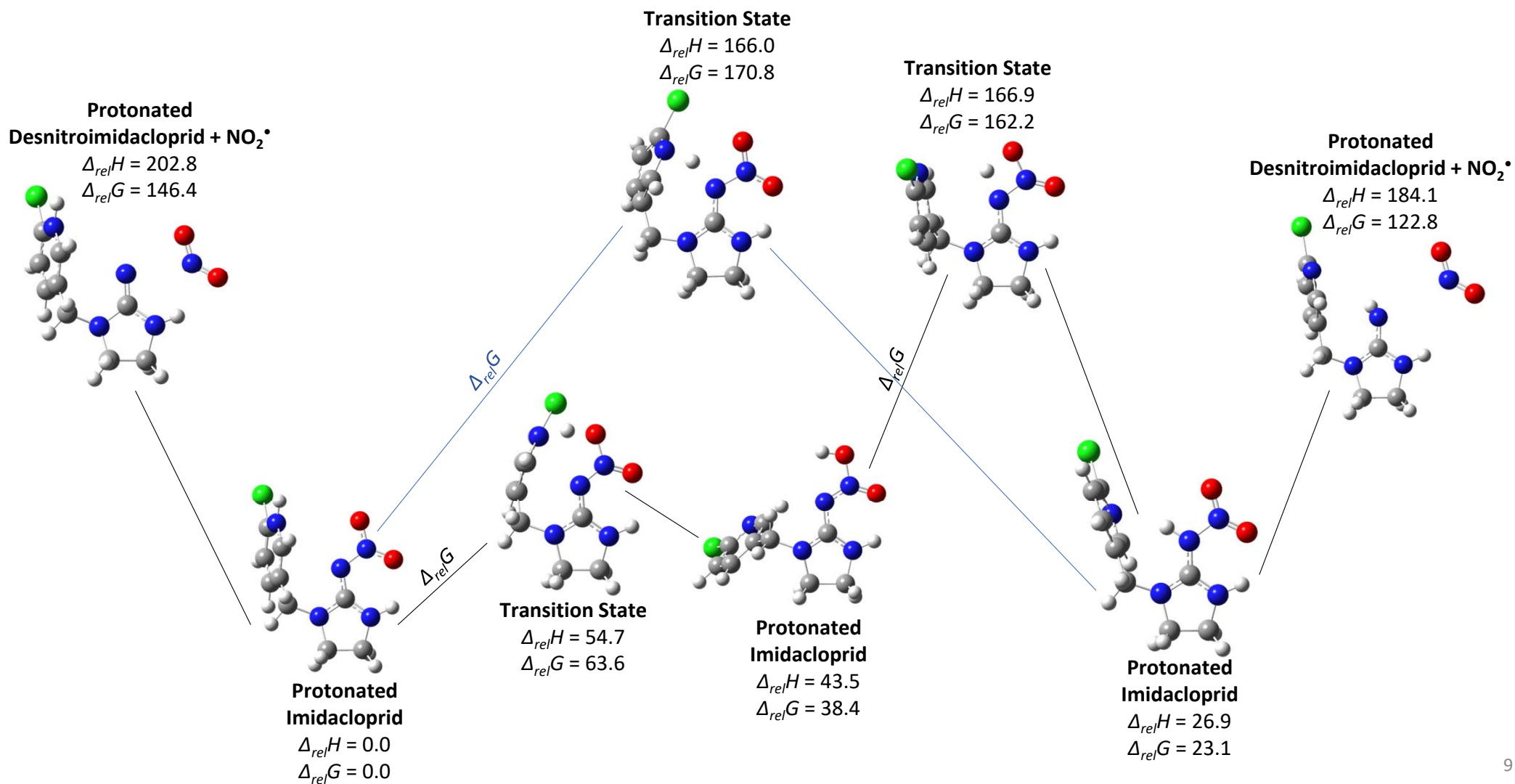


Figure S9. Gibbs Potential Energy Diagram Proton Transfer Following Loss of NO_2^\bullet

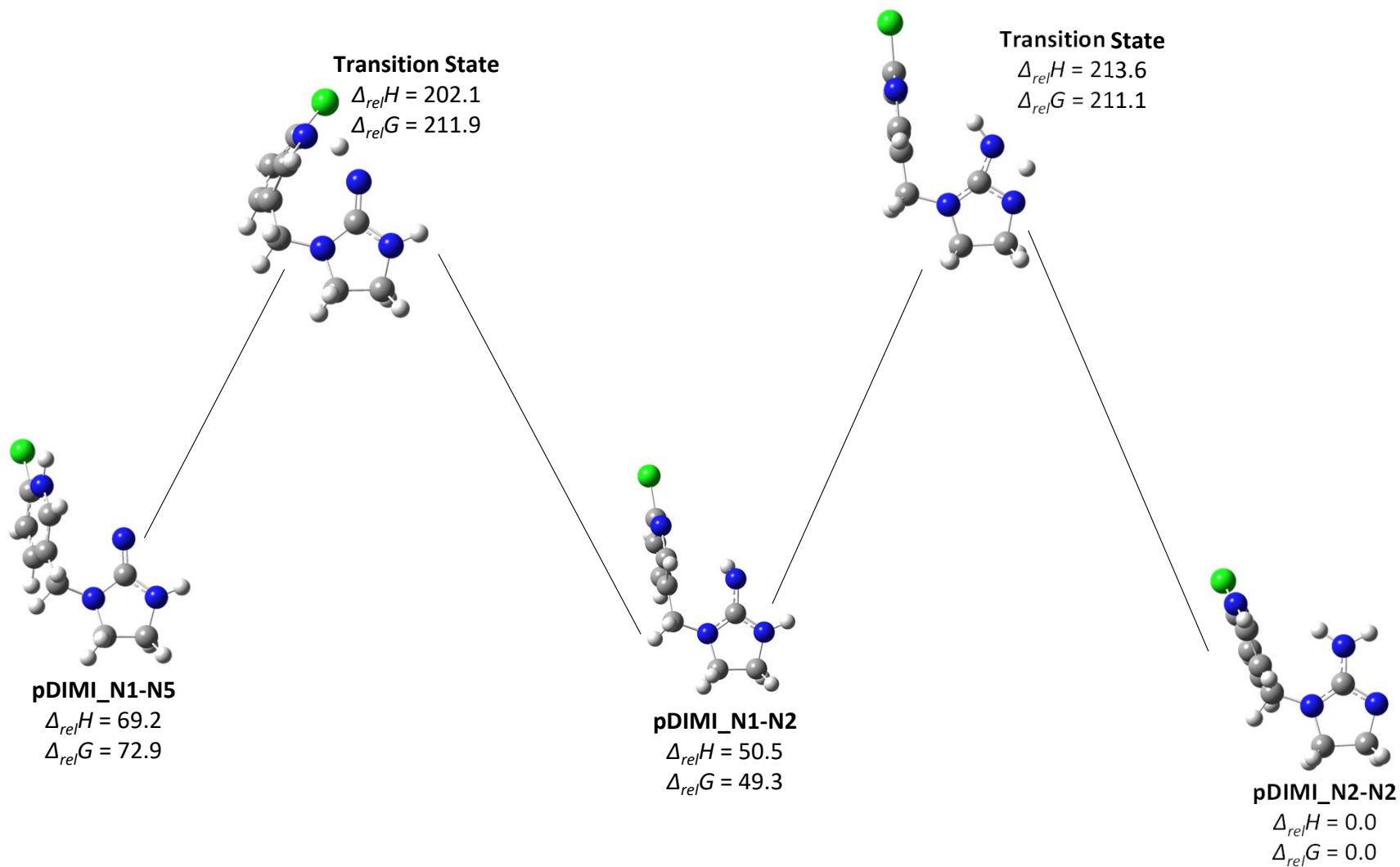


Figure S10. Gibbs Potential Energy Diagram Proton Transfer Following Loss of NO_2^\bullet

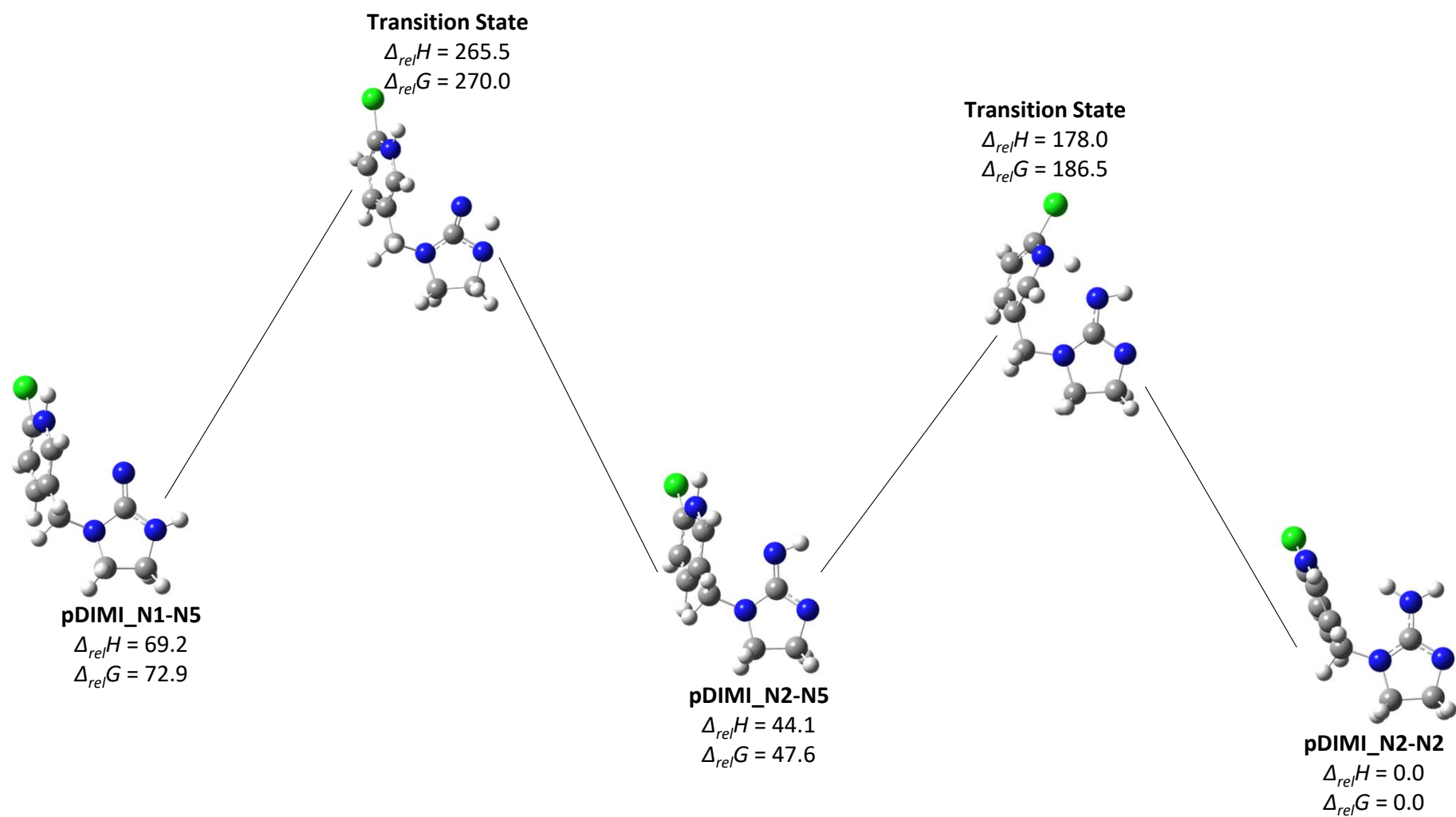


Figure S11. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for protonated desnitroimidacloprid – loss of NO₂ radical

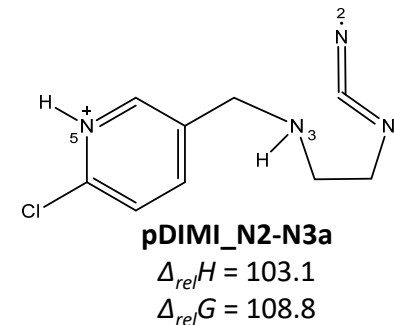
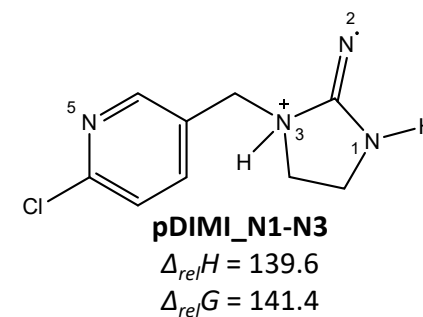
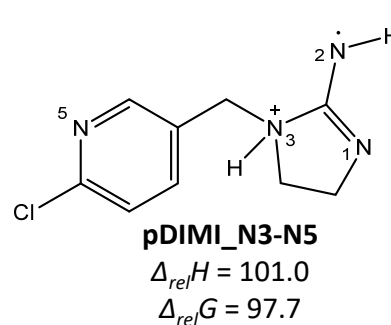
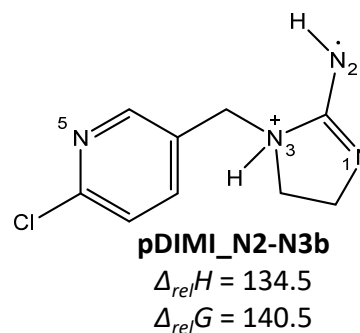
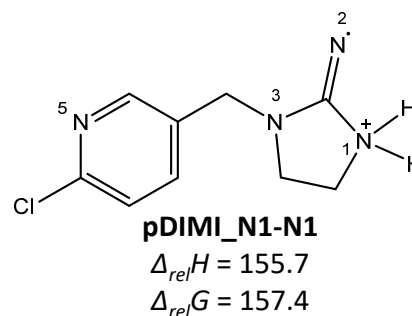
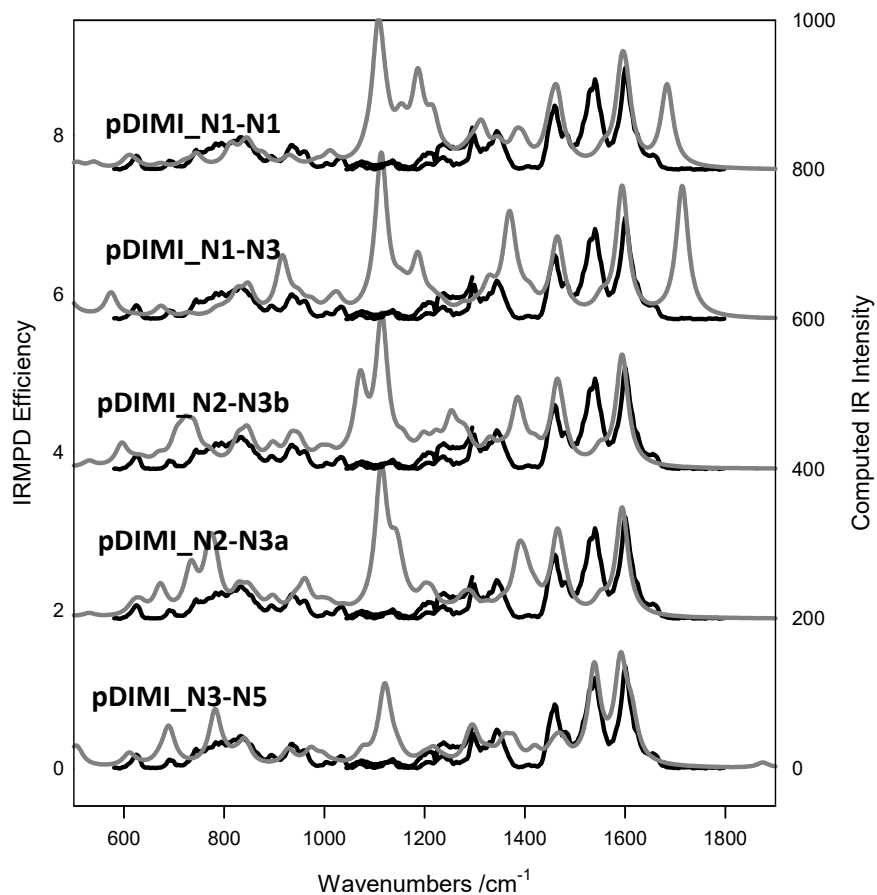


Figure S12. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the loss of NO[•] and [•]OH from protonated imidacloprid (*m/z* 209)

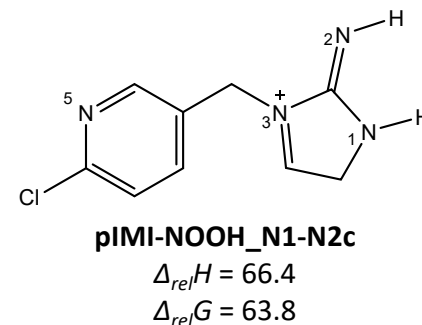
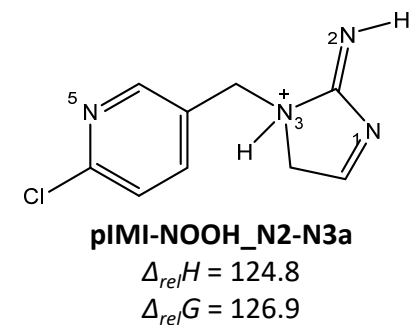
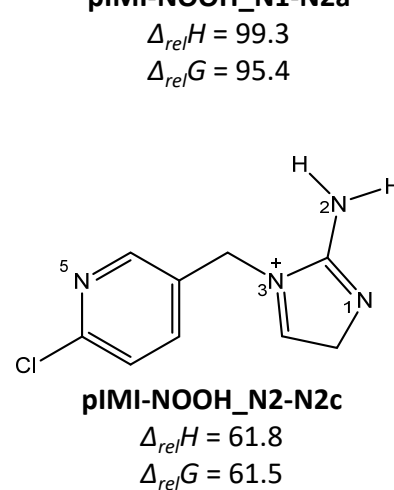
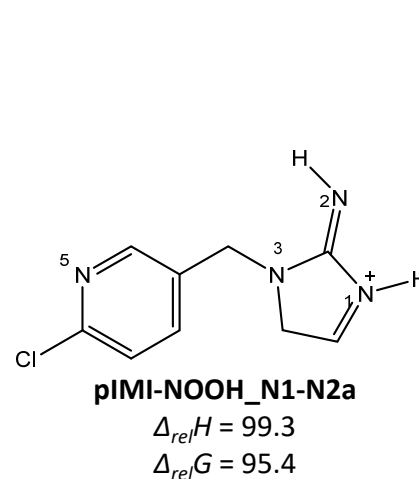
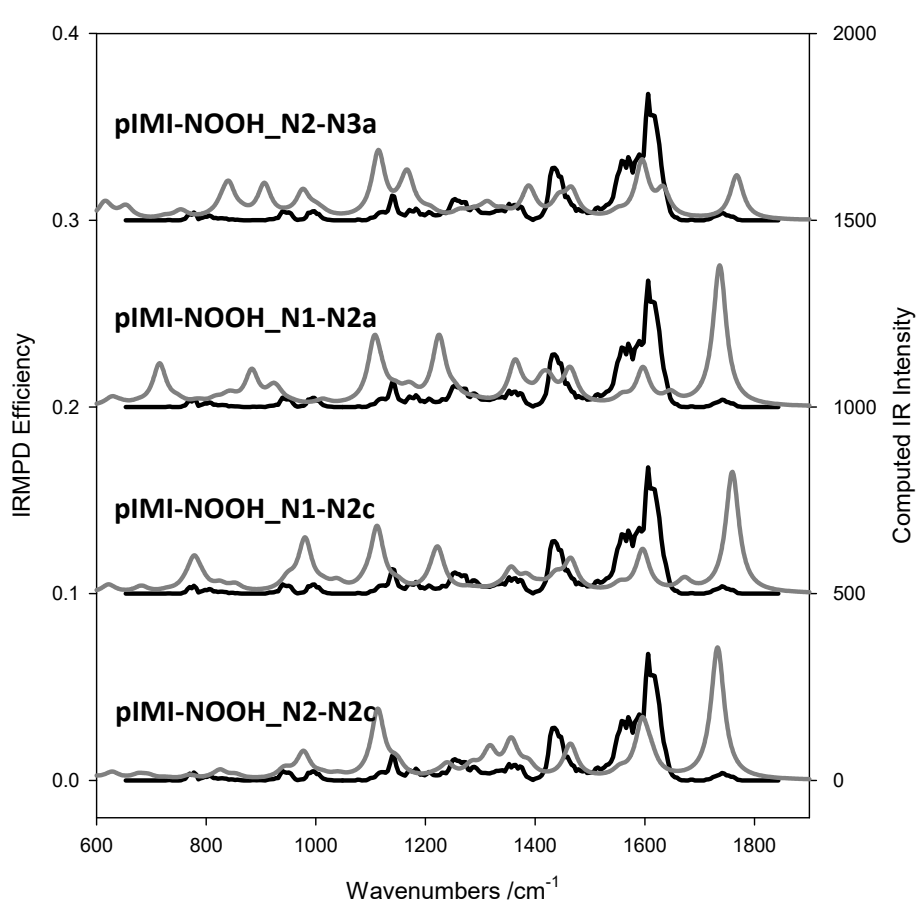


Figure S13. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the loss of NO_2^\bullet and H^\bullet from protonated imidacloprid (m/z 209)

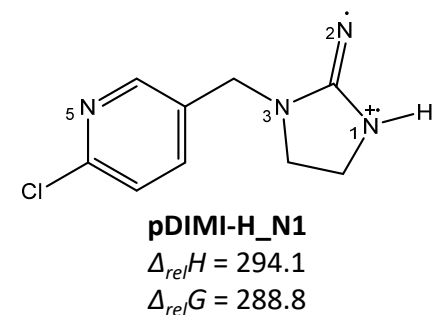
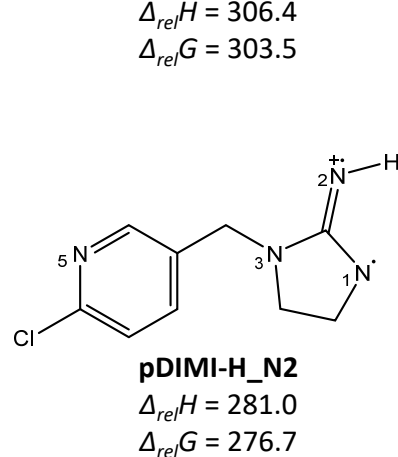
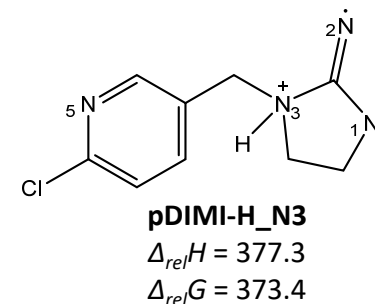
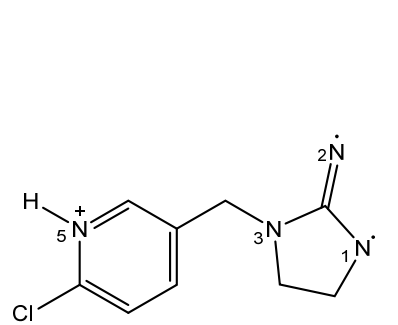
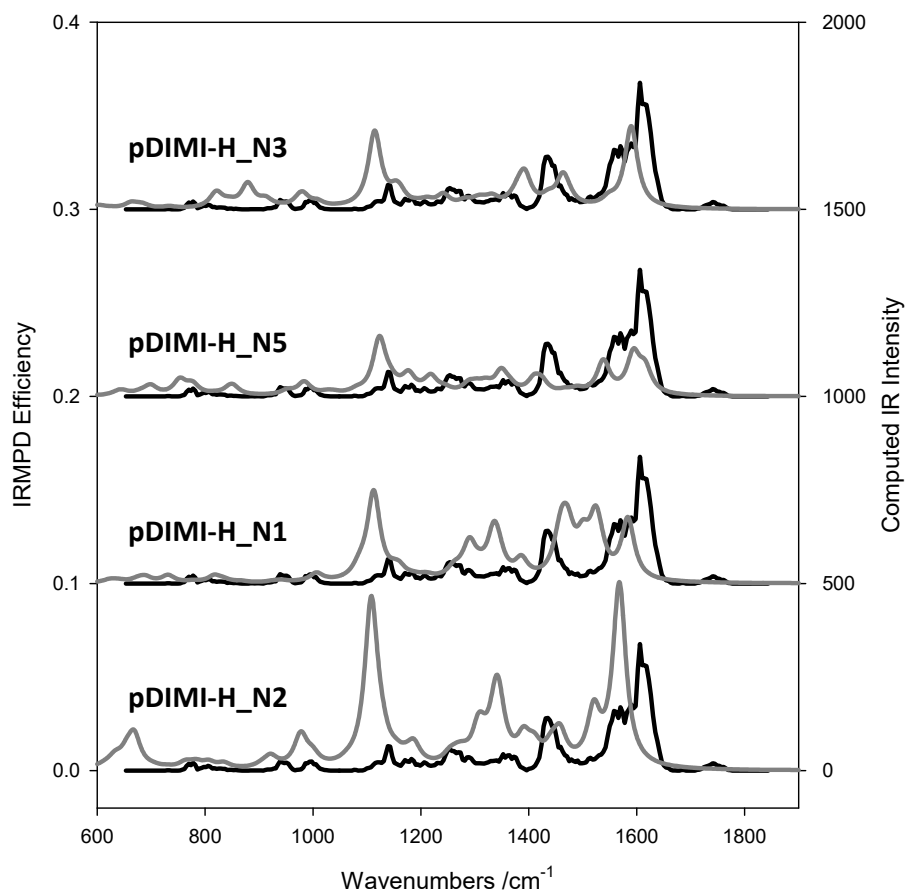
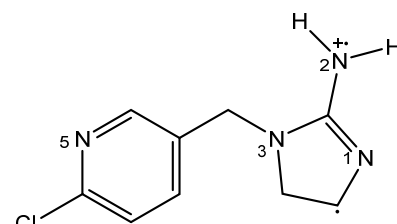
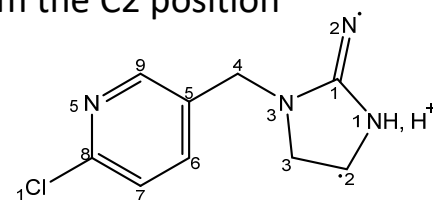
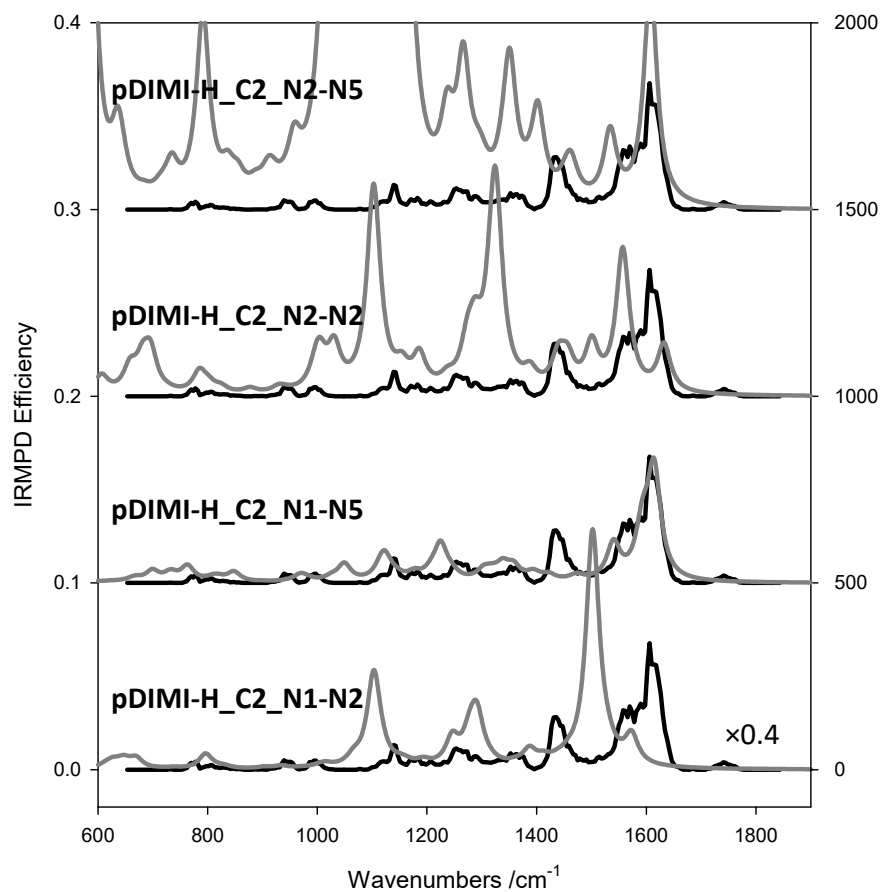


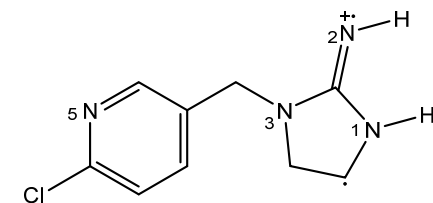
Figure S14. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the loss of NO_2^{\bullet} and $\bullet\text{H}$ from the C2 position of protonated imidacloprid (m/z 209)



pDIMI-H_C2_N2-N2

$$\Delta_{rel}H = 299.1$$

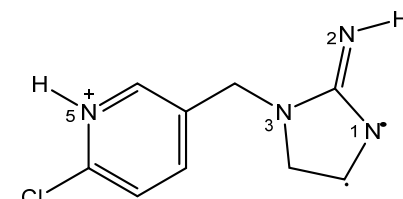
$$\Delta_{rel}G = 293.9$$



pDIMI-H_C2_N1-N2a

$$\Delta_{rel}H = 266.2$$

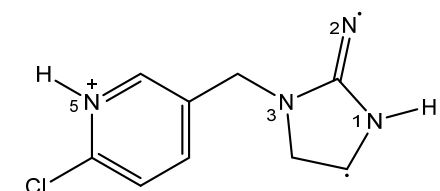
$$\Delta_{rel}G = 260.4$$



pDIMI-H_C2_N2-N5

$$\Delta_{rel}H = 298.8$$

$$\Delta_{rel}G = 295.7$$



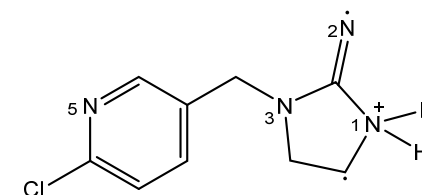
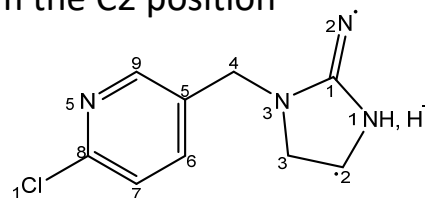
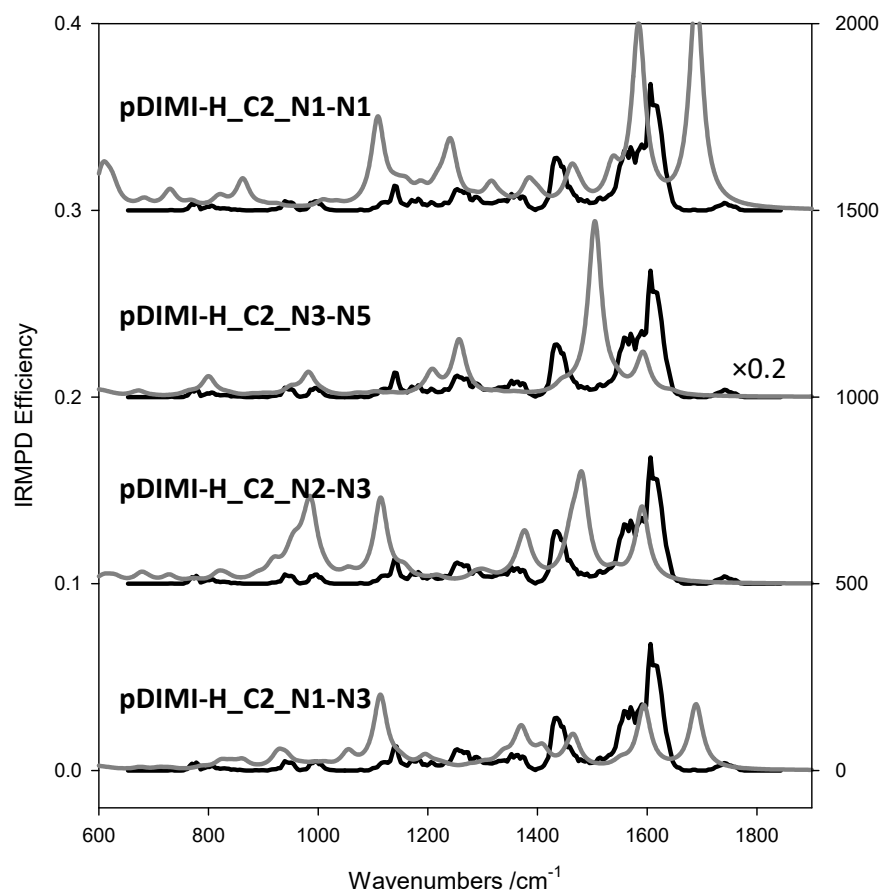
pDIMI-H_C2_N1-N5

$$\Delta_{rel}H = 298.7$$

$$\Delta_{rel}G = 293.2$$

Computed IR Intensity

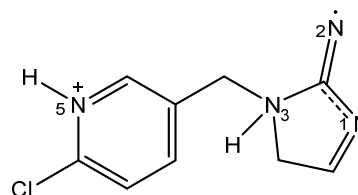
Figure S15. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the loss of NO_2^{\bullet} and H^{\bullet} from the C2 position of protonated imidacloprid (m/z 209)



pDIMI-H_C2_N1-N1

$$\Delta_{rel}H = 428.1$$

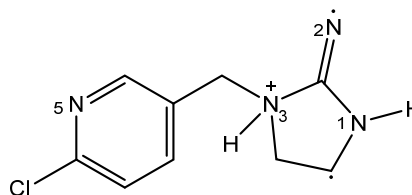
$$\Delta_{rel}G = 420.0$$



pDIMI-H_C2_N3-N5

$$\Delta_{rel}H = 394.5$$

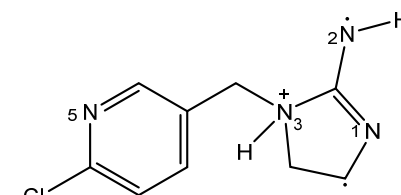
$$\Delta_{rel}G = 390.9$$



pDIMI-H_C2_N1-N3

$$\Delta_{rel}H = 372.1$$

$$\Delta_{rel}G = 367.9$$



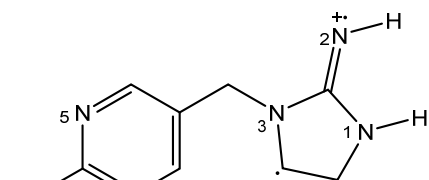
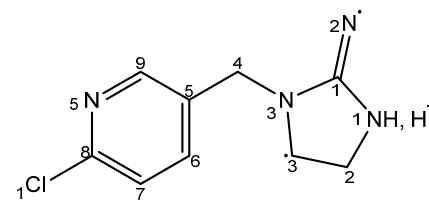
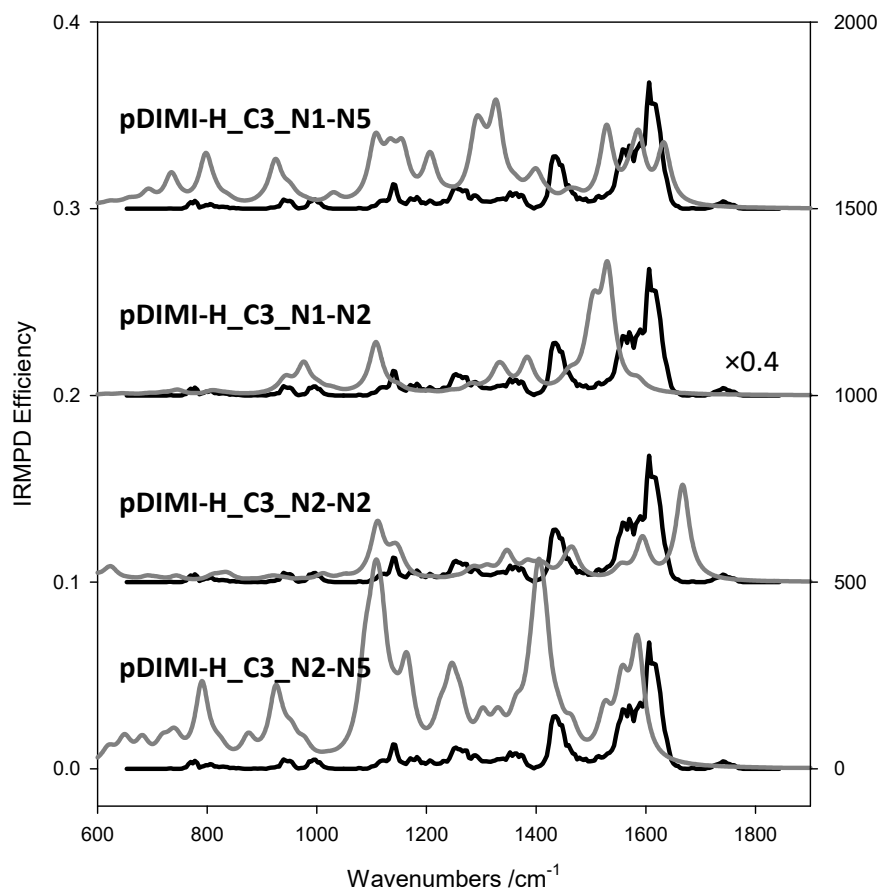
pDIMI-H_C2_N2-N3

$$\Delta_{rel}H = 385.5$$

$$\Delta_{rel}G = 381.2$$

Computed IR Intensity

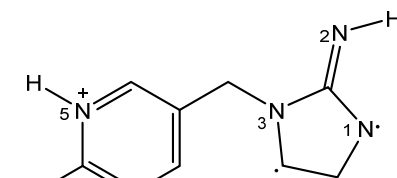
Figure S16. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the loss of NO_2^{\bullet} and $\bullet\text{H}$ from the C3 position of protonated imidacloprid (m/z 209)



pDIMI-H_C3_N1-N2

$$\Delta_{rel}H = 274.2$$

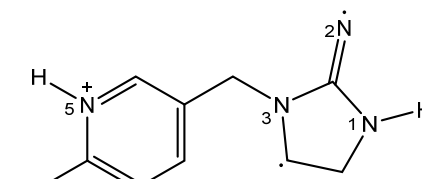
$$\Delta_{rel}G = 267.3$$



pDIMI-H_C3_N2-N5

$$\Delta_{rel}H = 259.7$$

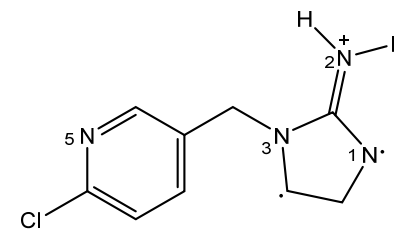
$$\Delta_{rel}G = 257.5$$



pDIMI-H_C3_N1-N5

$$\Delta_{rel}H = 293.9$$

$$\Delta_{rel}G = 290.9$$

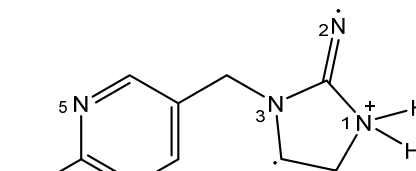
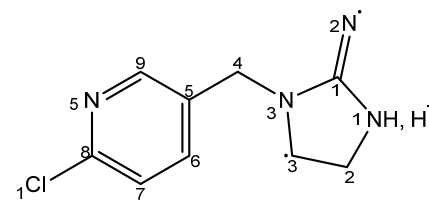
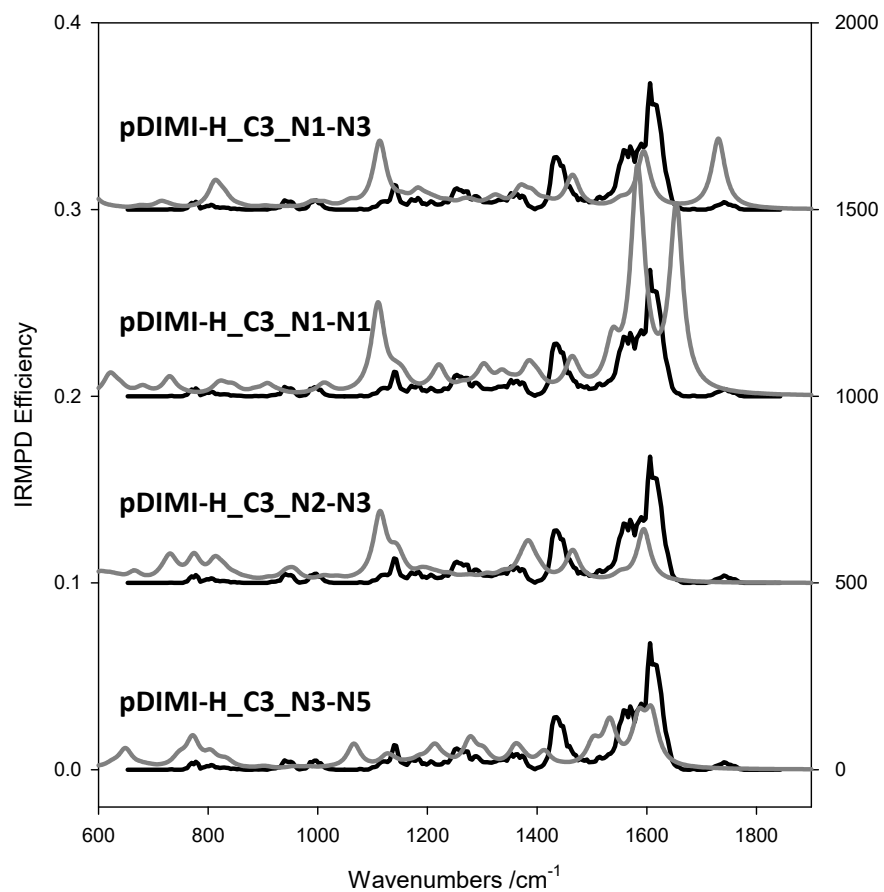


pDIMI-H_C3_N2-N2

$$\Delta_{rel}H = 268.6$$

$$\Delta_{rel}G = 259.8$$

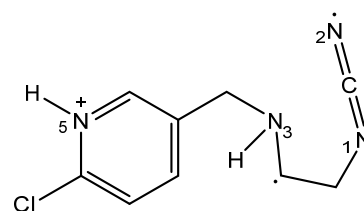
Figure S17. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the loss of NO_2^\bullet and $\bullet\text{H}$ from the C3 position of protonated imidacloprid (m/z 209)



pDIMI-H_C3_N1-N1

$$\Delta_{rel}H = 381.9$$

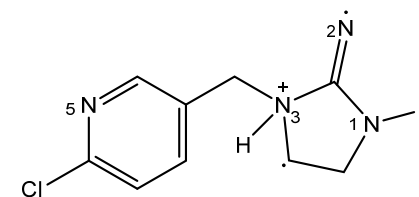
$$\Delta_{rel}G = 376.4$$



pDIMI-H_C3_N3-N5

$$\Delta_{rel}H = 312.7$$

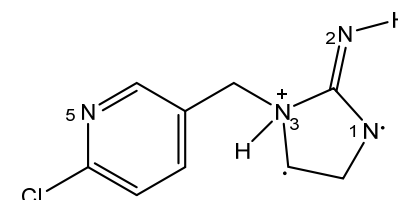
$$\Delta_{rel}G = 301.2$$



pDIMI-H_C3_N1-N3

$$\Delta_{rel}H = 406.3$$

$$\Delta_{rel}G = 400.1$$

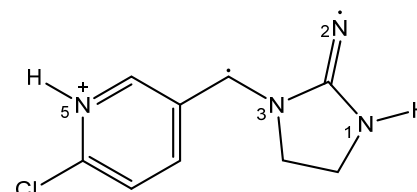
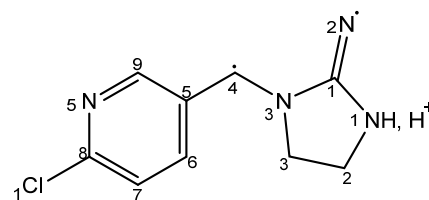
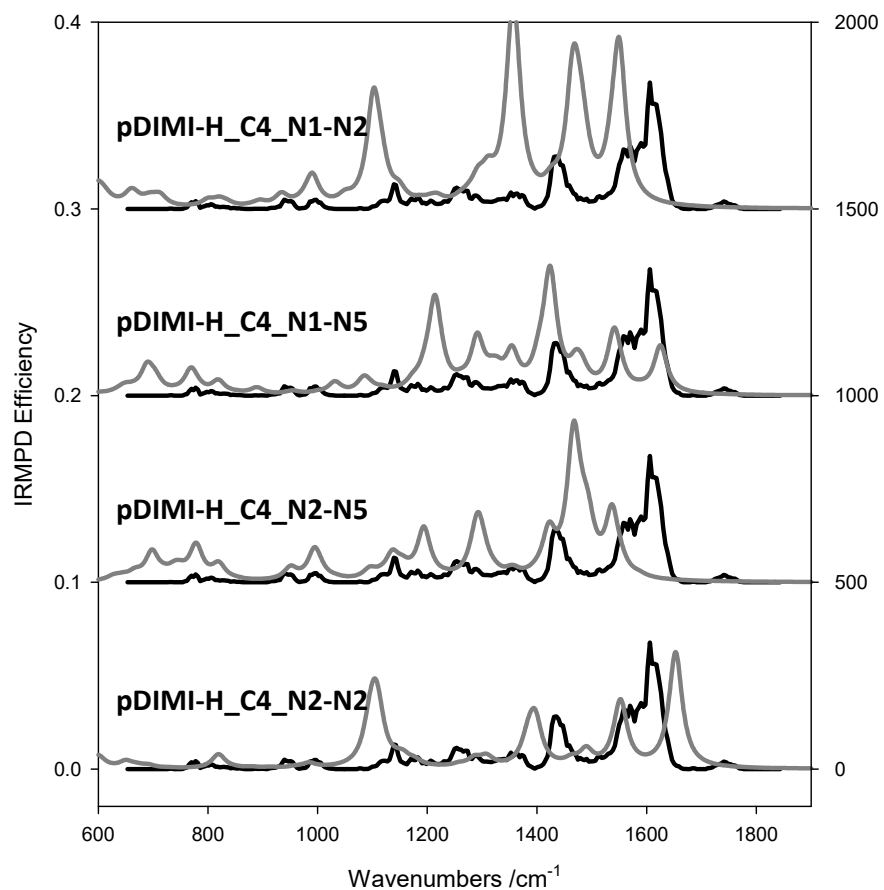


pDIMI-H_C3_N2-N3

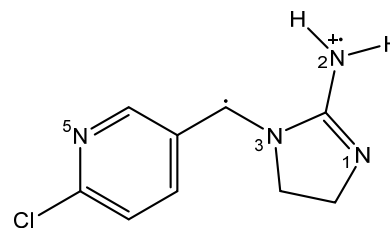
$$\Delta_{rel}H = 367.7$$

$$\Delta_{rel}G = 363.5$$

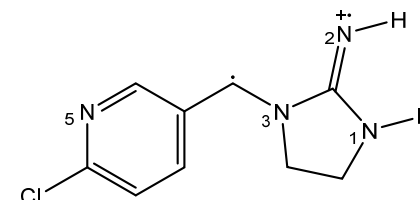
Figure S18. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the loss of NO_2^\bullet and $\bullet\text{H}$ from the C4 position of protonated imidacloprid (m/z 209)



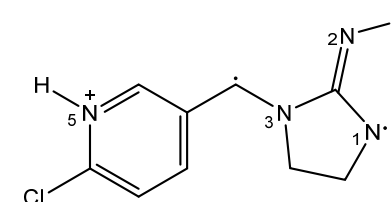
pDIMI-H_C4_N1-N5
 $\Delta_{rel}H = 238.6$
 $\Delta_{rel}G = 235.0$



pDIMI-H_C4_N2-N2
 $\Delta_{rel}H = 204.4$
 $\Delta_{rel}G = 198.7$

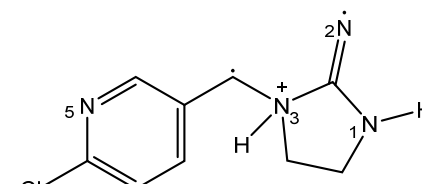
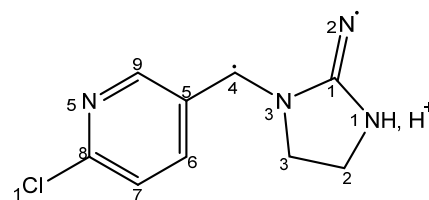
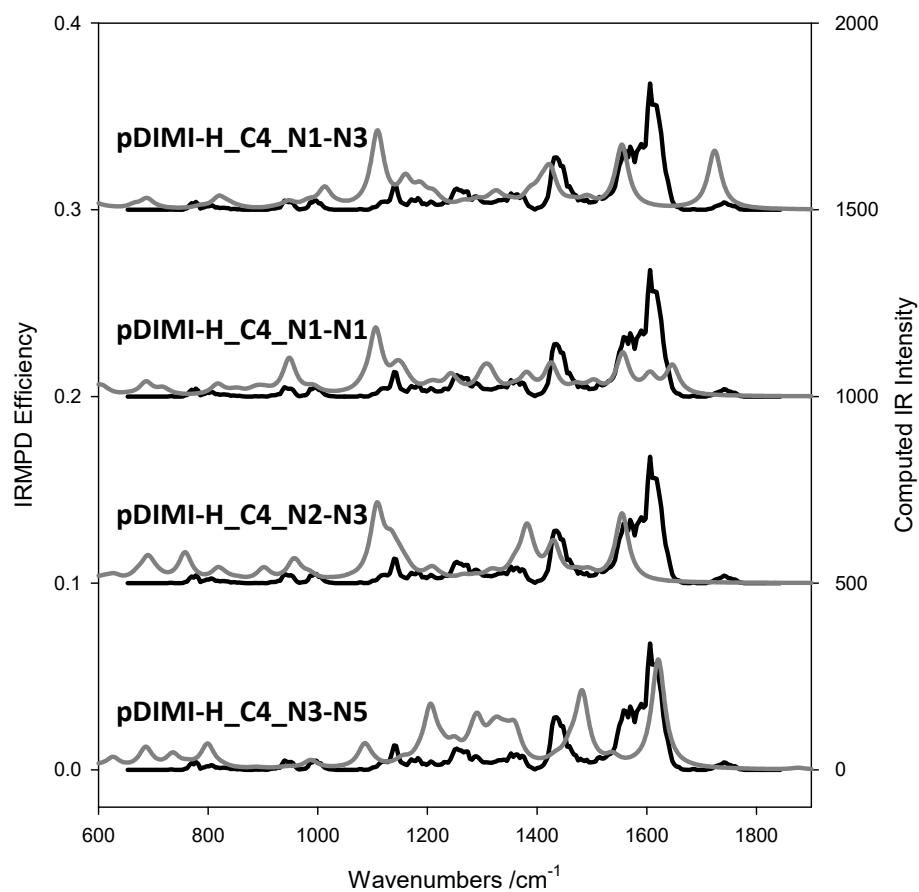


pDIMI-H_C4_N1-N2
 $\Delta_{rel}H = 240.3$
 $\Delta_{rel}G = 238.9$



pDIMI-H_C4_N2-N5
 $\Delta_{rel}H = 211.3$
 $\Delta_{rel}G = 206.4$

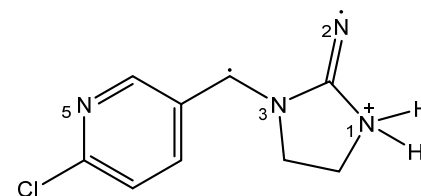
Figure S19. Comparison of the experimental IRMPD spectra (black trace) and the computed IR spectra (grey trace) for the loss of NO_2^\bullet and $\bullet\text{H}$ from the C4 position of protonated imidacloprid (m/z 209)



pDIMI-H_C4_N1-N3

$$\Delta_{rel}H = 367.2$$

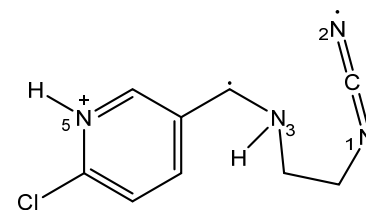
$$\Delta_{rel}G = 360.2$$



pDIMI-H_C4_N1-N1

$$\Delta_{rel}H = 359.9$$

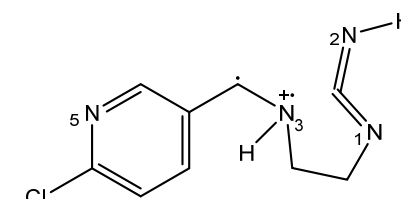
$$\Delta_{rel}G = 356.8$$



pDIMI-H_C4_N3-N5

$$\Delta_{rel}H = 255.3$$

$$\Delta_{rel}G = 241.9$$

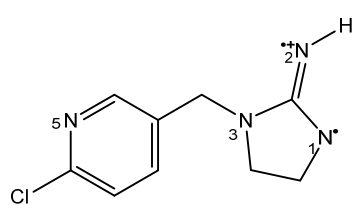


pDIMI-H_C4_N2-N3

$$\Delta_{rel}H = 332.3$$

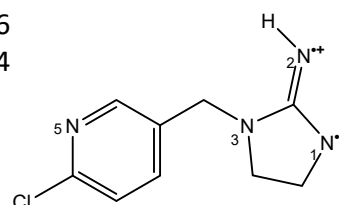
$$\Delta_{rel}G = 328.0$$

Figure S20. Energetics of formation of pIMI-NOOH_N2-N2a from pDIMI-H_N2.



pDIMI-H_N2
 $\Delta_{rel}H = 281.0$
 $\Delta_{rel}G = 276.7$

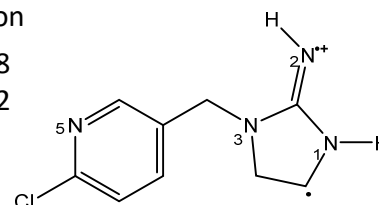
$\Delta_{rel}H = 328.6$
 $\Delta_{rel}G = 325.4$



pDIMI-H_N2
 $\Delta_{rel}H = 320.9$
 $\Delta_{rel}G = 315.2$

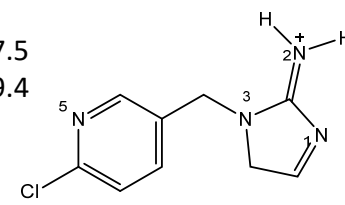
tautomerization

$\Delta_{rel}H = 490.8$
 $\Delta_{rel}G = 487.2$



pDIMI-H_N1-N2b
 $\Delta_{rel}H = 282.9$
 $\Delta_{rel}G = 276.5$

$\Delta_{rel}H = 507.5$
 $\Delta_{rel}G = 499.4$



pIMI-NOOH_N2-N2a
 $\Delta_{rel}H = 0.0$
 $\Delta_{rel}G = 0.0$

pIMI_N1-N5

1\1\GINC-GRA774\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\25-Oct-2018\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.104172549,-0.2469070833,-0.1727028542\C,-1.1941001956,-0.0099456231,1.2330632935\C,-0.6372401881,-1.1848607614,0.7425235747\C,-1.3617647197,-1.8911542331,-0.2225249436\C,-2.6009156926,-1.4327298068,-0.6826473428\H,-0.7047716288,0.6261239867,1.9574702541\H,-0.9529792712,-2.8074884623,-0.6384404952\H,-3.1676319162,-1.9726337098,-1.431122683\N,-2.3897766102,0.4172269068,0.77422386\C1,-4.5904848215,0.4454229792,-0.6633505511\C,0.7539584561,-1.6114016106,1.1812572008\H,0.991310222,-1.1699915346,2.1579308851\H,0.7808320135,-2.6984622073,1.2912391054\C,2.9653815635,-2.0801006269,-0.024670234\C,3.7831601005,-1.1995827899,-0.9896818319\H,2.7064282745,-3.050482834,-0.4520683069\H,3.4947880966,-2.2325695663,0.9261729848\H,3.5678523173,-1.4391862341,-2.0376717358\H,4.8581688815,-1.270506204,-0.8177968039\N,1.7602093548,-1.2539417021,0.1826099588\C,2.0913270696,0.066089354,-0.0379283613\N,1.2357025698,0.9820000003,0.3937821277\N,1.4502937699,2.3062935031,0.0709142495\N,3.2802520685,0.1369042195,-0.6533456932\H,3.6023603238,1.0176632421,-1.0347442675\O,2.4498387438,2.661020726,-0.5745374545\O,0.5724425608,3.070391966,0.4700614648\H,-2.7528429235,1.303013896,1.1217792936\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.7077814\RMSD=4.889e-09\RMSF=6.977e-06\Dipole=-1.0782887,-3.3451948,0.2842364\Quadrupole=22.6862409,-13.4902029,-9.196038,-10.7260257,-2.9499054,2.7852113\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N1-N2

1\1\GINC-GRA781\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\23-Oct-2018\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.1097895365,-0.6060045357,0.0971847484\C,-1.0932861039,-1.631309584,-0.1948648647\C,-0.583244327,-1.1168755135,1.0050635965\C,-1.4347780739,-0.3109390636,1.7780225308\C,-2.7239761825,-0.0472040581,1.3256961291\H,-0.480678765,-2.2719153177,-0.8272623924\H,-1.0990976406,0.1026803871,2.7259332288\H,-3.4119138368,0.5677373142,1.8934033208\N,-2.3231051953,-1.3768002002,-0.6463674682\C1,-4.7047824915,-0.2863354461,-0.5146337747\C,0.8231090283,-1.4486063111,1.4565020016\H,1.0693768838,-0.923700927,2.3880008586\H,0.9160980555,-2.5202943511,1.6541101069\C,3.1132292535,-1.9393466195,0.3876423053\C,3.896221697,-1.2538573908,-0.7496545438\H,2.8901098272,-2.9871226517,0.181157367\H,3.6274577724,-1.8615768382,1.3527446043\H,3.7767362776,-1.7710916409,-1.7069349211\H,4.9575988507,-1.1394070465,-0.5277208136\N,1.8551399416,-1.1521927041,0.4383693794\C,2.0595620597,0.0155404764,-0.1868191538\N,1.1468608364,1.028205044,-0.1274009508\N,1.1673505105,2.1989291378,-0.9511685043\N,3.233165309,0.0627910153,-0.8088473933\O,2.1788913077,2.4063033276,-1.601720881\O,0.15798376,2.86090336,-0.874274139\H,3.4722388949,0.8151349025,-1.4433937538\H,0.2217483372,0.856378295,0.2651177371\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6965338\RMSD=3.986e-09\RMSF=5.989e-06\Dipole=3.9398578,-1.3384164,1.3719693\Quadrupole=16.2645171,-9.6735204,-6.5909967,-10.5084084,-7.0109921,-0.2523199\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N1-02

1\1\GINC-CDR667\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\19-Apr-2019\0\#\ opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,3.3660427963,-0.6054912317,0.1074866615\C,1.1726616492,-0.9073476889,0.6400286516\C,1.0424243259,0.3983443508,1.1263726914\C,2.1797492508,1.2167710915,1.0958195811\C,3.3708091811,0.7145226944,0.5826520719\H,0.326773453,-1.5922684266,0.6652574524\H,2.1425547873,2.232995213,1.4807474094\H,4.2750834785,1.3102172569,0.5487059709\N,2.3062020244,-1.4028208021,0.134366234\C1,4.8336555056,-1.2673661474,-0.5631541967\C,-0.293651543,0.8915323939,1.6340162642\H,-0.7948432654,0.141429417,2.2468882485\H,-0.1808771274,1.7986424804,2.2336516035\C,-0.9332090291,2.3695141865,-0.3836698362\C,-2.0985717545,2.2915499655,-1.3976703643\H,0.0445251882,2.2198508565,-0.8544394078\H,-0.919189213,3.3039253166,0.1805641605\H,-1.7724652708,2.4188252646,-2.4306971014\H,-2.8911886275,3.0131574257,-1.1760475524\N,-1.2065281757,1.232840792,0.5211787302\C,-2.103816979,0.4232930218,-0.0383635834\N,-2.3686349955,-0.7733324663,0.5889324267\N,-3.2614164775,-1.532372808,0.0738380184\N,-2.5986871782,0.9216553361,-1.1750619422\O,-3.9713078872,-1.3845040598,-0.9159879215\O,-3.3922541841,-2.6788627521,0.7947661666\H,-3.3847181332,0.5061758839,-1.6560870999\H,-4.0856994892,-3.1909886442,0.3279313131\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6929624\RMSD=3.571e-09\RMSF=4.150e-06\Dipole=-3.8556517,2.0166376,-0.2473626\Quadrupole=11.2892934,1.9878802,-13.2771737,10.5730031,6.6202439,-2.4361292\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N1-01

1\1\GINC-GRA310\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\15-Dec-2018\0\#\ opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,3.3997818659,-0.5703248259,0.1151651089\C,1.2014861133,-0.898076643,0.6118054179\C,1.0539979254,0.3989438636,1.1163953212\C,2.1851009155,1.2266013457,1.1149342858\C,3.3874108939,0.7418809147,0.6113946389\H,0.3614635207,-1.5905179807,0.6149181409\H,2.1342149229,2.2363445413,1.5150716227\H,4.2873381471,1.3449749588,0.60011896\N,2.3461321101,-1.3761598783,0.114403176\C1,4.8817733401,-1.2097247908,-0.5455649992\C,-0.2925077158,0.8748785736,1.6127320232\H,-0.7949972304,0.1146647573,2.2113793072\H,-0.1945449452,1.7770621383,2.2224064563\C,-0.904530727,2.3628132428,-0.400738868\C,-2.0650978865,2.3041029697,-1.4182008686\H,0.0736289461,2.207168167,-0.8687904307\H,-0.8830051072,3.2920604676,0.1717376788\H,-1.7358486924,2.4512950672,-2.4475399078\H,-2.8584114146,3.0213441079,-1.184323626\N,-1.1937379454,1.2214735762,0.4913368496\C,-2.0899095965,0.4167850064,-0.0807818741\N,-2.3387539854,-0.7772461907,0.5498272165\N,-3.2217249801,-1.6106548542,0.1539902429\N,-2.5636689761,0.929324011,-1.2232108837\O,-4.0130651686,-1.2737915286,-0.961915777\O,-3.4395658045,-2.6781571852,0.6710139778\H,-3.361291184,0.5444356389,-1.7066190174\H,-4.5981341513,-2.0509655605,-1.0801956524\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.68553\RMSD=7.054e-09\RMSF=5.377e-06\Dipole=-4.1010188,2.4658635,-0.8361259\Quadrupole=15.7310265,-4.4629814,-11.2680451,7.361231,13.0177581,0.8806152\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N1-N3

```
1\1\GINC-CDR621\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\16-Apr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\N,1.8692106668,1.3188984545,-0.7929298484\C,1.0448120704,2.4345025456,-0.3263820803\H,1.456537909,3.3868142109,-0.6662625385\H,0.0183534555,2.3314782191,-0.6882551529\C,1.146061974,2.2840751728,1.2001448512\H,1.9707542232,2.869318113,1.6098861645\H,0.2241971885,2.5187059863,1.7289834112\N,1.4904143683,0.8162645216,1.4011714009\C,2.1251148549,0.387967161,0.1176572142\N,2.7379400588,-0.7457096466,0.1942955075\N,3.3195629016,-1.2379225665,-1.0149749031\C,0.2979967121,-0.1194275694,1.7959226606\H,0.763099988,-1.0969058762,1.9342363828\H,-0.0416060422,0.269033152,2.758684953\O,3.1551324335,-0.599539591,-2.0646633952\O,3.9271021671,-2.2757820655,-0.8908174327\C,-0.7786923489,-0.1244901501,0.7601410431\C,-0.7370094821,-0.9905547479,-0.3483918853\C,-1.7431626296,-0.9237376854,-1.3011521645\C,-1.8724254767,0.7445102512,0.8620897937\C,-2.7643197508,0.024086089,-1.1072653675\C1,-4.0201738876,0.1661173875,-2.2967661697\N,-2.8388285417,0.8300244666,-0.0541853509\H,-1.9880995205,1.3962496601,1.7278621087\H,-1.7549698595,-1.5778284379,-2.1648280749\H,0.0658150269,-1.7145002555,-0.4559772914\H,2.1701818365,1.1571291816,-1.7502858518\H,2.1958143247,0.7049994491,2.1378995958\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6669083\RMSD=5.486e-09\RMSF=1.664e-05\Dipole=1.1834386,2.3892547,2.5629272\Quadrupole=-9.778354,2.2275898,7.5507641,13.8210845,8.0299127,4.8509203\PG=C01 [X(C9H11Cl1N5O2)]\@\
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pIMI_N1-N1

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1\1\GINC-GRA785\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\02-Nov-2018\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,3.449444835,-0.3951165425,-0.0778258361\C,1.265261011,-0.80727324,0.4227775703\C,1.1220012364,0.4144700991,1.0920522005\C,2.2466407019,1.247112339,1.17291036\C,3.4406116895,0.84100737,0.586305773\H,0.4309152552,-1.5044151193,0.3581618122\H,2.1987562699,2.1962981662,1.7012806055\H,4.336611318,1.4481207441,0.6348429133\N,2.3998330687,-1.2034889086,-0.159991835\C1,4.9167500801,-0.9284305167,-0.8507096992\C,-0.2149093693,0.8068173319,1.673533013\H,-0.6661312218,-0.0009883869,2.2524874055\H,-0.1311127433,1.6865413549,2.3181479929\C,-1.0032035107,2.32618069,-0.2643732732\C,-1.8178857144,1.9569375701,-1.5109033369\H,0.0554475731,2.4619989783,-0.4962805162\H,-1.378599548,3.2237405912,0.2403104947\H,-1.2268780802,1.3862510481,-2.2292507808\H,-2.3061630622,2.7954758036,-2.0061773958\N,-1.1770350589,1.1458457556,0.5941895475\C,-2.1857295347,0.3621629357,0.2303186148\N,-2.5308526711,-0.7544126336,0.7879923716\N,-3.5320592055,-1.5348423877,0.1734987312\N,-2.8556697968,1.0154324085,-0.9445474791\H,-3.2034637717,0.2174127739,-1.5309227753\O,-3.8524568291,-1.3169461025,-1.0225290037\O,-3.9910768468,-2.4124068918,0.8592833297\H,-3.6967376544,1.5104038092,-0.6207447044\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6592936\RMSD=5.677e-09\RMSF=2.339e-06\Dipole=-2.6376072,4.49965,-0.5775502\Quadrupole=7.1336063,-1.864097,-5.2695093,-10.8894365,9.8819846,-2.9833286\PG=C01 [X(C9H11Cl1N5O2)]\@\
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pIMI-NO_N1-N2

1\1\GINC-CDR669\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\16-A
pr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldis
persion=gd3\Title Card Required\1,2\C,-3.1874451882,-0.6118878591,0.
3716722185\C,-1.3965859341,-0.3154894773,1.7524018936\C,-0.6101259667,
-1.2244269985,1.0367464714\C,-1.197137354,-1.86128922,-0.0717664172\C,
-2.5046927797,-1.5568978247,-0.4184145382\H,-1.0013891808,0.190631356,
2.6324273803\H,-0.6365251889,-2.5884518275,-0.6534422194\H,-2.99685739
13,-2.0268538422,-1.2615278312\N,-2.6583843453,-0.0076331256,1.4247836
407\C1,-4.8234266242,-0.1950522814,-0.0419995975\C,0.8043938808,-1.525
3557662,1.4690951397\H,1.0461909316,-1.0079454854,2.4057647857\H,0.927
7246768,-2.5975076711,1.647306926\C,3.1473260755,-1.8665358001,0.45832
6279\C,3.907689857,-1.1674571647,-0.6921370675\H,3.0150524789,-2.93740
81244,0.2956800679\H,3.6269036101,-1.7067594697,1.4310904926\H,3.87475
56135,-1.744781644,-1.6216089255\H,4.945011809,-0.9452779965,-0.439557
9833\N,1.8264120983,-1.183226111,0.4526981587\C,1.9502072954,-0.047798
5421,-0.2396198946\N,0.9912879617,0.933394199,-0.3577903799\N,3.126204
2685,0.0726920313,-0.8443189506\H,0.0827385252,0.8321704993,0.10356430
24\H,3.3021006886,0.8069197331,-1.5201890101\O,1.2255817125,1.95697854
28,-1.0891444218\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.7553894\
S2=0.754126\S2-1=0.\S2A=0.750012\RMSD=6.384e-09\RMSF=1.510e-05\Dipole=
4.4088158,-1.5642161,-0.3277821\Quadrupole=17.9627291,-10.0235224,-7.9
392066,-2.0570188,-0.7559325,0.137181\PG=C01 [X(C9H11Cl1N4O1)]\@\

pIMI-NO_N1-O1

1\1\GINC-CDR622\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\22-A
pr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldis
persion=gd3\Title Card Required\1,2\C,3.5595168088,-0.3847647909,0.0
063937691\C,1.347179969,-0.7934958509,0.3565880854\C,1.1725442359,0.39
91787186,1.0679315771\C,2.2933972273,1.2214522016,1.2420211407\C,3.516
9883085,0.8285425658,0.7103400293\H,0.5116409891,-1.4754987442,0.20439
53128\H,2.2179116339,2.1537252833,1.7960793556\H,4.4106735125,1.429322
5059,0.8290246464\N,2.5119546093,-1.1806206977,-0.169604071\C1,5.06891
0286,-0.9039655989,-0.6918511765\C,-0.1910143991,0.7699284596,1.605218
0227\H,-0.6306232515,-0.0362466999,2.1951754017\H,-0.1361076959,1.6619
886603,2.2382454005\C,-0.9481672748,2.2265758393,-0.3990306386\C,-2.02
94572055,1.9969952341,-1.487388859\H,0.0679198143,2.2376375425,-0.7979
586731\H,-1.1155606324,3.1440779139,0.1762054107\H,-1.5996464817,1.635
0106536,-2.4262857222\H,-2.6210177341,2.8923892787,-1.6831254938\N,-1.
1214581508,1.067162727,0.5018231445\C,-2.236137708,0.4115482125,0.1817
991117\N,-2.6183386171,-0.6824676828,0.9186811117\N,-2.8609925195,0.94
42339816,-0.8727919011\H,-3.6441276944,0.4921899901,-1.3246647709\O,-3
.7699401608,-1.1544621249,0.4008500679\H,-4.0010549491,-1.9310945883,0.
.9433921582\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.7518814\S2=0.
759673\S2-1=0.\S2A=0.750046\RMSD=5.760e-09\RMSF=9.727e-06\Dipole=-4.33
24634,1.6368259,0.205402\Quadrupole=17.1344038,-6.4136452,-10.7207586,
7.5876416,5.7715034,-3.9917\PG=C01 [X(C9H11Cl1N4O1)]\@\

pIMI-NO_N1-N5

1\1\GINC-CDR556\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\16-A

pr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldis
persion=gd3\Title Card Required\1,2\C,-3.0513619772,-0.1821218129,-0
.1593329955\C,-1.1601333226,-0.0683588316,1.2916819688\C,-0.6402133046
, -1.2441679869,0.7585023817\C,-1.3665487276,-1.8834652804,-0.245770133
7\C,-2.580117012,-1.3565072853,-0.7133174766\H,-0.6769029345,0.4975999
132,2.0748848732\H,-0.9818696713,-2.7955079507,-0.6923673617\H,-3.1472
299675,-1.8403632724,-1.4986926969\N,-2.3396286144,0.412362158,0.84037
9155\C1,-4.5039995679,0.5869962034,-0.6430562332\C,0.7351120393,-1.717
671927,1.1885256281\H,0.965373021,-1.3529242356,2.1988353564\H,0.75495
42201,-2.8100464445,1.2168351244\C,3.000951612,-2.0544083516,0.0364998
59\C,3.805306995,-1.1195963196,-0.8934482941\H,2.798712887,-3.02932895
51,-0.4110798472\H,3.5108640825,-2.1970980467,0.9994791991\H,3.6289819
63,-1.3538110857,-1.9502836064\H,4.8773580839,-1.149436733,-0.69242640
99\N,1.7507931216,-1.2898879095,0.2285781829\C,2.0262237097,0.03616765
23,0.0229809752\N,1.1571967075,1.0077089907,0.3834237809\N,3.229798459
,0.1835075595,-0.5468895809\H,-2.6941330407,1.2819718605,1.2313945379\
O,1.5507284593,2.1930052317,0.038128689\H,3.4999582592,1.0807388692,-0
.9297209356\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.7484843\S2=0.
756069\S2-1=0.\S2A=0.750026\RMSD=6.102e-09\RMSF=1.253e-05\Dipole=-0.42
05373,-2.050776,0.2916228\Quadrupole=21.0684713,-11.9513985,-9.1170727
, -10.8413995,-3.8362656,2.5393738\PG=C01 [X(C9H11Cl1N4O1)]\@\

pIMI-NO_N2-N5

1\1\GINC-CDR521\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\02-M
ay-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldis
persion=gd3\Title Card Required\1,2\C,-3.3156070912,-0.8240526051,0.
0907389223\C,-1.0210494654,-1.0041503011,-0.533478272\C,-0.6092063223,
-0.9149330862,0.7851843317\C,-1.6035697173,-0.7823094246,1.7655599225\
C,-2.956768291,-0.7370299481,1.4287545983\H,-0.3255972154,-1.100530454
1,-1.3560203634\H,-1.3204255232,-0.7022927104,2.811812631\H,-3.7294417
076,-0.6305370744,2.1802458341\N,-2.3391103771,-0.9599047426,-0.840007
3245\C1,-4.9345953545,-0.7724376107,-0.4651269896\C,0.8612112493,-0.91
24354315,1.1547207095\H,1.0811669788,0.0436211853,1.6458626138\H,1.026
6125334,-1.6961299679,1.9021280591\C,2.7849909948,-2.2304819488,0.1927
516196\C,3.873333145,-1.795247228,-0.8201955254\H,2.3589247601,-3.2140
516342,-0.0171641867\H,3.171758313,-2.2225924961,1.2211581413\H,3.7884
847457,-2.3423209723,-1.7676038847\H,4.8891121707,-1.9430179909,-0.445
7369157\N,1.7591990603,-1.1625171277,0.0302543238\C,2.4572497091,-0.12
26147438,-0.6035203426\N,1.8756617758,1.1243585652,-0.782938245\N,3.62
07383634,-0.3719756529,-1.0874471363\O,0.6489706914,1.3847837428,-0.51
29958273\H,2.4562033497,1.8364933676,-1.2338333229\H,-2.6144337955,-1.
0126937496,-1.8183465809\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.
7441284\S2=0.764622\S2-1=0.\S2A=0.750095\RMSD=5.978e-09\RMSF=9.958e-06
\Dipole=-1.5681094,-1.1047211,0.614087\Quadrupole=13.6296474,-11.81383
42,-1.8158132,-2.2908863,1.6423377,0.1456806\PG=C01 [X(C9H11Cl1N4O1)]\
\@

pIMI-NO_N5-01

1\1\GINC-CDR752\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\16-A
pr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldis

persion=gd3\\Title Card Required\\1,2\C,-3.1911425137,-0.3013469086,-0.0666654503\C,-1.2780884029,-0.069270493,1.3364125372\C,-0.6636926889,-1.1632719305,0.7518127283\C,-1.3511525223,-1.8199056024,-0.279886\C,-2.6173148371,-1.401472619,-0.6899506141\H,-0.8140293256,0.5337799046,2.1060273219\H,-0.8826618651,-2.6633064125,-0.7783047918\H,-3.1581710368,-1.9046491656,-1.4820340034\N,-2.5070793832,0.3241260421,0.9233145321\C1,-4.7303996767,0.3245980462,-0.4768161118\C,0.7374013075,-1.5786272266,1.1564142762\H,1.0155319021,-1.0988539027,2.1067183849\H,0.7519475496,-2.6600174585,1.320551023\C,2.9261870868,-2.0779382296,-0.0285566318\C,3.7977733295,-1.1450062093,-0.9059162192\H,2.7298638696,-3.0503003879,-0.485493523\H,3.3773272299,-2.2308637608,0.9635277312\H,3.6935397594,-1.3823746299,-1.9732500939\H,4.8603901028,-1.1863021984,-0.657488408\N,1.6816701321,-1.281273635,0.0859550661\C,2.0992301549,0.0412790208,-0.1246690829\N,1.2715942878,1.0762499437,0.2480211601\N,3.2617686307,0.2041659444,-0.6755178057\H,-2.9302651447,1.1420525901,1.3568184988\O,1.7999958207,2.2755274125,-0.0565973405\H,2.6794925934,2.1193022459,-0.4872714235\\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.7337074\S2=0.768913\S2-1=0.\S2A=0.750109\RMSD=4.819e-09\RMSF=2.336e-05\Dipole=-1.7269103,-1.294153,0.7672929\Quadrupole=15.9467036,-7.3359541,-8.6107495,-8.5256793,-1.4556961,3.8023639\PG=C01 [X(C9H11Cl1N4O1)]\\@

pIMI-NO_N2-01

1\1\GINC-CDR701\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\09-Jul-2019\0\\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,2\C,3.5299676163,-0.4630809745,0.0234698317\C,1.3288639042,-0.7427288496,0.5330725394\C,1.229938351,0.5298065515,1.1079599289\C,2.3834076897,1.3258200741,1.1200951502\C,3.5623407669,0.8268750024,0.5774882713\H,0.4649969977,-1.4055460211,0.4977318073\H,2.3681166347,2.3197237972,1.5599154108\H,4.4788411182,1.4046593939,0.5757323704\N,2.4484840217,-1.232806084,-0.0019403511\C1,4.9792730433,-1.1172991503,-0.6822591098\C,-0.088919099,1.0089165524,1.6758505385\H,-0.5007796911,0.3186649712,2.4078618994\H,0.0219149032,1.9864174761,2.1529001354\C,-0.9817567423,2.3241774365,-0.3303422622\C,-2.0692753459,1.9975357872,-1.3692944101\H,0.0284223009,2.3646490704,-0.7496432786\H,-1.1689941299,3.2499541368,0.2240466586\H,-1.6732019373,1.8569777166,-2.3862261911\H,-2.8444992887,2.7709352266,-1.4586790545\N,-1.0833233295,1.1781229244,0.5916947232\C,-2.0450610641,0.3487877841,0.1642972368\N,-2.4140176516,-0.8525795118,0.6597861191\N,-2.6940695489,0.7622388352,-0.9551969194\O,-2.1141765899,-1.1570820184,1.9830234866\H,-3.3287790498,-1.1806569238,0.3534630853\H,-1.7276647499,-2.0506252031,1.9665539538\\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.7210635\S2=0.762011\S2-1=0.\S2A=0.750057\RMSD=9.557e-09\RMSF=5.053e-06\Dipole=-3.1392579,1.7337134,0.5584755\Quadrupole=8.5959778,0.9056232,-9.501601,3.7706013,2.3010041,-5.6678817\PG=C01 [X(C9H11Cl1N4O1)]\\@

pIMI_U_N1-N5

1\1\GINC-GRA101\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N3O1(1+)\KJM408\14-Dec-2018\0\\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C,-3.1003343178,-0.2304069456,-0.1340760296\C,-1.1379431143,-0.0088707481,1.2025374539\C,-0.6303877405,-

1.210542382,0.7284995642\C,-1.4012969112,-1.916801983,-0.202372839\C,-
2.6409344951,-1.4374977067,-0.6359997988\H,-0.6021932196,0.6294560668,
1.8920364761\H,-1.0277399682,-2.8526409196,-0.6077202453\H,-3.24386249
67,-1.9787013974,-1.3546890825\N,-2.3386605939,0.4383127317,0.77039429
49\C1,-4.5901642271,0.4834764025,-0.5863652263\C,0.7518852589,-1.67475
91472,1.1496764201\H,0.9937639472,-1.2737473553,2.1442870541\H,0.75882
05124,-2.7654723724,1.2219345083\C,2.9641503868,-2.0755652234,-0.05003
99336\C,3.7924821418,-1.1336369825,-0.947919158\H,2.7461836525,-3.0321
286088,-0.5302424664\H,3.4758468369,-2.2602036615,0.9057284621\H,3.582
9267185,-1.3138964903,-2.0100670576\H,4.8655153495,-1.2305664893,-0.77
28900209\N,1.7418638198,-1.2844156834,0.1561971046\C,2.0488230607,0.07
62274856,0.0377296785\N,3.2904175321,0.1710168385,-0.5186189664\H,3.59
28422107,1.0477292424,-0.9181364479\H,-2.6792455065,1.3322321128,1.117
8870808\O,1.3096152633,0.9928751262,0.3985274747\\Version=ES64L-G16Rev
B.01\State=1-A\HF=-1049.1043544\RMSD=7.617e-09\RMSF=1.203e-05\Dipole=-
0.7912198,-0.953039,0.1686895\Quadrupole=18.5290095,-7.8657214,-10.663
2881,-8.1661533,-3.9548011,2.2468595\PG=C01 [X(C9H11Cl1N3O1)]\@

pIMIU_N1-01

1\1\GINC-GRA702\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N3O1(1+)\KJM408\11-Apr
-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,1\C,-3.1697557147,-0.5486560214,0.35
05628437\C,-1.3362887378,-0.2247908042,1.667859041\C,-0.6003446172,-1.
2138338649,1.0031074573\C,-1.2396974842,-1.9043095993,-0.0456974474\C,
-2.5419572811,-1.5737775092,-0.384735427\H,-0.9019611708,0.3251909498,
2.5017153617\H,-0.7209395603,-2.6935983296,-0.5833333841\H,-3.07227115
76,-2.0830960552,-1.1805355787\N,-2.5931971059,0.1086766201,1.34486279
58\C1,-4.7990471743,-0.1015734469,-0.0549139976\C,0.8081885158,-1.5534
037842,1.4346663765\H,1.0618136,-1.0425671082,2.3718371726\H,0.9007367
468,-2.6289209902,1.6107390737\C,3.1786435961,-1.8412654029,0.47076597
88\C,3.9238693818,-1.1398809761,-0.6893010761\H,3.1082717936,-2.922273
2508,0.3403582967\H,3.6329797187,-1.6240789207,1.444407726\H,3.9319536
611,-1.7471864188,-1.5998547848\H,4.9454870027,-0.8632211631,-0.427361
7201\N,1.8289768555,-1.2278715945,0.4146432576\C,1.9020904011,-0.10377
46601,-0.3045884606\N,3.0866199259,0.0565564138,-0.8877181317\H,0.1333
379806,0.5441429713,-0.018721421\H,3.2347926856,0.7539936517,-1.605884
3907\O,0.9647124285,0.7918130737,-0.4752892117\\Version=ES64L-G16RevB.
01\State=1-A\HF=-1049.088204\RMSD=3.214e-09\RMSF=5.359e-06\Dipole=4.40
97801,-1.1266685,-0.6291455\Quadrupole=18.5143823,-10.1938328,-8.32054
94,0.3887043,-2.217223,-1.4430079\PG=C01 [X(C9H11Cl1N3O1)]\@

pIMIU_N1-N3

1\1\GINC-GRA23\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N3O1(1+)\KJM408\02-Apr
-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldisper
sion=gd3\\Title Card Required\\1,1\N,1.6687303397,1.3604398173,-1.0731
487926\C,0.9321476173,2.4275646073,-0.3983352061\H,1.339665617,3.40650
63269,-0.6569977346\H,-0.128334228,2.3930423699,-0.6629154686\C,1.1670
449124,2.0964493966,1.0879252152\H,2.0453113131,2.6134298669,1.4773385
33\H,0.3051229135,2.3092500851,1.71832982\N,1.4692143596,0.6178745036,
1.0967085621\C,1.947327283,0.2750370648,-0.3449197334\C,0.322228498,-

0.3306253732,1.5190318795\H,0.7570758269,-1.3305401784,1.4557194342\H,
0.1187114178,-0.0884246433,2.5645981939\C,-0.8871225621,-0.1739545505,
0.6496312519\C,-1.020446955,-0.8710652192,-0.5651226471\C,-2.146290741
, -0.6603302713,-1.3489299892\C,-1.9304763783,0.6816801868,1.0231187957
\C,-3.1043993196,0.2571975464,-0.882643665\C1,-4.5094638626,0.57630533
43,-1.8540459685\N,-3.0111783865,0.9057514046,0.2716074834\H,-1.907048
9334,1.205066975,1.9786075993\H,-2.2953495621,-1.1842678226,-2.2855179
808\H,-0.2571198607,-1.5745568031,-0.886792135\H,2.2634227676,0.410240
9953,1.7102801657\H,1.8414413815,1.3442760509,-2.0711350623\O,2.428318
3968,-0.7964590501,-0.5814026609\\Version=ES64L-G16RevB.01\State=1-A\H
F=-1049.078613\RMSD=5.821e-09\RMSF=1.952e-05\Dipole=3.262957,1.15036,1
.3568946\Quadrupole=-1.0119194,-3.237012,4.2489314,11.0661802,8.422618
,0.4071108\PG=C01 [X(C9H11C11N301)]\ \@

pIMIU_N1-N1

1\1\GINC-GRA1039\FOpt\RB3LYP\6-31+G(d,p)\C9H11C11N301(1+)\KJM408\11-Dec-
2018\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldisp
ersion=gd3\\Title Card Required\\1,1\C,3.4511760703,-0.4281259561,-0.0
50709797\C,1.2553058979,-0.7744712162,0.4449849741\C,1.1446474015,0.45
17813266,1.1112641193\C,2.2924311998,1.251514919,1.1914652845\C,3.4759
670927,0.8096302627,0.6087744072\H,0.4009717239,-1.4472685392,0.378021
531\H,2.2694582764,2.2047927775,1.7139130759\H,4.3882543297,1.39206132
43,0.6558235657\N,2.3790684712,-1.2061097892,-0.1340834207\C1,4.905852
8997,-1.0067087898,-0.8177570703\C,-0.1803579254,0.8817250855,1.692867
1982\H,-0.6321641986,0.0987901424,2.3066473917\H,-0.0744378675,1.77941
48954,2.3096851474\C,-0.9655075077,2.2764320371,-0.3325988103\C,-1.902
744646,1.9092267129,-1.4951583137\H,0.07657103,2.31205404,-0.658326811
9\H,-1.2256276524,3.2352416468,0.1304862027\H,-1.4032399919,1.26521692
33,-2.220551686\H,-2.3455962529,2.7666711618,-2.0012781228\N,-1.158929
7812,1.181713375,0.6195443889\C,-2.2578441148,0.4468508065,0.449989687
4\N,-2.9625530801,1.0806990482,-0.8188826843\H,-3.3347917029,0.3162217
91,-1.3913067094\H,-3.7653717744,1.6326423541,-0.4957933668\O,-2.75672
95573,-0.4890013198,1.0036810393\\Version=ES64L-G16RevB.01\State=1-A\H
F=-1049.0726918\RMSD=8.450e-09\RMSF=3.631e-06\Dipole=-4.6206847,3.3393
4,-1.0509662\Quadrupole=19.3774953,-10.7191412,-8.6583541,-9.6255378,1
5.3902409,-1.6968264\PG=C01 [X(C9H11C11N301)]\ \@

pDIMI_N2-N2

1\1\GINC-GRA44\FOpt\UB3LYP\6-31+G(d,p)\C9H11C11N4(1+,2)\KJM408\09-Jan-
2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldisper
sion=gd3\\Title Card Required\\1,2\C,-3.0959347701,-0.8210879715,0.296
1276051\C,-1.3671011494,-0.2825193015,1.6812204286\C,-0.5071614334,-1.
2032119136,1.0747765139\C,-1.0200938247,-1.9737399181,0.0169910939\C,-
2.3342650512,-1.789275298,-0.3850901131\H,-1.0301143813,0.3256522963,2
.5204518639\H,-0.40141349,-2.7140137297,-0.4838202972\H,-2.7717621944,
-2.3656948389,-1.1914591061\N,-2.6355047912,-0.0891005541,1.2993182171
\C1,-4.74178683,-0.5480557767,-0.1933680092\C,0.9148700869,-1.36385687
15,1.5627075606\H,1.1219081121,-0.6712322282,2.3885063759\H,1.09375180
71,-2.3758793856,1.9352338398\C,3.0205631391,-2.0637965806,0.231124494
1\C,3.7811274356,-1.3214600497,-0.8843631913\H,2.6218722204,-3.0356186

742, -0.0784351914\H, 3.6164074041, -2.2084171455, 1.1393932088\H, 3.814436
3772, -1.8747771015, -1.8345959055\H, 4.830220195, -1.1099357947, -0.633001
796\N, 1.9168849452, -1.1329156112, 0.5048742673\C, 2.0268575428, -0.040362
2573, -0.2712891357\N, 1.2126920663, 1.0130108001, -0.2590802848\N, 3.10150
38517, -0.0673504473, -1.1115681079\H, 0.3478055085, 1.024345138, 0.2649591
521\H, 1.4007945033, 1.7629381651, -0.912351533\\Version=ES64L-G16RevB.01
\State=2-A\HF=-1028.5653594\S2=0.761227\S2-1=0.\S2A=0.750052\RMSD=7.44
6e-09\RMSF=8.794e-06\Dipole=4.0199648, -0.7711237, -0.1704614\Quadrupole
=11.3805987, -3.1936666, -8.1869321, -2.9520134, 1.8445666, 0.3627792\PG=C0
1 [X(C9H11Cl1N4)]\@

pDIMI_N1-N2a

1\1\GINC-GRA123\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4(1+,2)\KJM408\27-Feb
-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,2\C, 3.4376981574, -0.482305611, -0.044
3008368\C, 1.2127240483, -0.745045759, 0.3532357885\C, 1.1407161196, 0.4597
535788, 1.0798294203\C, 2.3138567821, 1.2153422329, 1.2167836057\C, 3.49329
00481, 0.7381767003, 0.6616484755\H, 0.3275758631, -1.3653886918, 0.2292575
14\H, 2.3116321831, 2.1513911292, 1.7685775275\H, 4.429695015, 1.2750055898
, 0.7571758106\N, 2.3352999296, -1.2089009437, -0.1948846958\C1, 4.88300121
, -1.0876696671, -0.7809069972\C, -0.1885706153, 0.8976825824, 1.6512687351
\H, -0.6490910799, 0.1288051201, 2.2751297747\H, -0.0906805184, 1.816594193
5, 2.2392015989\C, -1.0123833739, 2.3375224308, -0.3349256689\C, -2.0042816
715, 1.9962453276, -1.4674650132\H, 0.0107201106, 2.4974182581, -0.68003494
06\H, -1.3301231646, 3.2126906994, 0.2483732413\H, -1.4902911485, 1.5774723
688, -2.3399990136\H, -2.591472106, 2.8621122164, -1.7758623123\N, -1.09186
72472, 1.1576252262, 0.5348899549\C, -2.20991039, 0.4137720718, 0.239049249
8\N, -2.4813527787, -0.6420322121, 0.9708707507\N, -2.8510704723, 0.9809178
084, -0.8194505428\H, -3.5335171523, 0.4530704069, -1.3459582899\H, -3.3721
495283, -1.0759161566, 0.7192961635\\Version=ES64L-G16RevB.01\State=2-A\
HF=-1028.5503111\S2=0.771095\S2-1=0.\S2A=0.750135\RMSD=5.822e-09\RMSF=
8.828e-06\Dipole=-2.908235, 2.106871, -0.1093153\Quadrupole=18.0658394, -
8.6523187, -9.4135208, -0.2387385, 8.7883792, -0.3493995\PG=C01 [X(C9H11Cl
1N4)]\@

pDIMI_N2-N5a

1\1\GINC-GRA14\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4(1+,2)\KJM408\01-Mar-
2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldisper
sion=gd3\\Title Card Required\\1,2\C, -3.0683497904, -0.3862201535, -0.16
6193915\C, -1.1331733053, -0.0438116902, 1.1861896275\C, -0.5655267, -1.229
8778591, 0.744081427\C, -1.2892974156, -1.9892009591, -0.1842932332\C, -2.5
444010503, -1.5789728642, -0.6411409613\H, -0.6338176205, 0.6308264399, 1.8
68476858\H, -0.8664475703, -2.914394021, -0.564993495\H, -3.1126102658, -2.
162300935, -1.355184618\N, -2.3507197645, 0.336342948, 0.7315895814\C1, -4.
5869016759, 0.2427619792, -0.646993149\C, 0.8270410399, -1.6304337007, 1.19
80977935\H, 1.0633508309, -1.1342790089, 2.1503873958\H, 0.854899045, -2.71
02637185, 1.3657525254\C, 2.954099214, -2.1622871453, -0.1166573268\C, 3.79
30253807, -1.2172692634, -1.0068364511\H, 2.6462481122, -3.0790206062, -0.6
266348175\H, 3.4943219155, -2.4339562917, 0.8019981693\H, 3.6139944963, -1.
4012704578, -2.0783887375\H, 4.8733263134, -1.3020797222, -0.8530763511\N,

1.8054218327,-1.2988526975,0.178142141\C,2.1831821248,0.0317128715,-0.0076266937\N,1.4894462031,1.0261910125,0.4684087931\N,3.3534798986,0.1373869193,-0.7210635499\H,-2.7415955284,1.2161958144,1.0614705637\H,1.93965033,1.9013422595,0.1965263132\\Version=ES64L-G16RevB.01\State=2-A\HF=-1028.5493723\S2=0.768892\S2-1=0.\S2A=0.750107\RMSD=6.999e-09\RMSF=8.319e-06\Dipole=-1.3874497,-0.9051097,0.5141378\Quadrupole=13.4956074,-3.8637936,-9.6318138,-11.0691983,-0.466121,4.5277974\PG=C01 [X(C9H11C11N4)]\ \@

pDIMI_N1-N2b

1\1\GINC-GRA1034\FOpt\UB3LYP\6-31+G(d,p)\C9H11C11N4(1+,2)\KJM408\12-Dec-2018\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,2\N,2.8772480663,1.4257838869,-0.6455622299\C,1.9937077414,2.5950923396,-0.5728835414\H,2.5419865452,3.48582359,-0.2622900818\H,1.5284500648,2.7809302615,-1.5477531154\C,0.9626296171,2.1319757825,0.4810958926\H,1.2086110256,2.4831943627,1.4912395585\H,-0.0603959936,2.4238264786,0.2407533331\N,1.1039359572,0.6592711601,0.4477869629\C,2.2727288366,0.3270394266,-0.155516568\N,2.8501797088,-0.8768189014,-0.2673109522\C,0.2432516497,-0.2139930381,1.2417328787\H,0.6563869051,-1.2276617727,1.2203649517\H,0.2810342986,0.1168995502,2.2868987487\C,-1.1731772807,-0.1818662584,0.7169227747\C,-2.2643070397,0.1457374448,1.5331043792\C,-3.5431411629,0.145686084,0.9900312201\C,-1.4332003895,-0.4866121071,-0.6287169178\C,-3.6729430658,-0.170978413,-0.3751026844\C1,-5.2509821422,-0.1560481125,-1.0959383652\N,-2.6523829368,-0.4805762391,-1.1674510872\H,-0.621767364,-0.7529179587,-1.304374897\H,-4.4163896874,0.3859806752,1.5846500462\H,-2.1208242917,0.3899687333,2.5822516168\H,3.6716940141,1.3426759104,-1.2673057703\H,2.2145583336,-1.6413802656,-0.0246377026\\Version=ES64L-G16RevB.01\State=2-A\HF=-1028.5441366\S2=0.763126\S2-1=0.\S2A=0.750059\RMSD=3.395e-09\RMSF=1.111e-05\Dipole=3.0557675,1.296627,1.2456128\Quadrupole=11.2999339,-3.5121321,-7.7878019,7.5996337,-7.0092101,-2.6061172\PG=C01 [X(C9H11C11N4)]\ \@

pDIMI_N1-N5

1\1\GINC-GRA101\FOpt\UB3LYP\6-31+G(d,p)\C9H11C11N4(1+,2)\KJM408\14-Dec-2018\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,2\C,-3.0729506621,-0.1821933202,-0.1032841623\C,-1.1647735704,-0.084223965,1.3195389003\C,-0.625988093,-1.2237357496,0.742305292\C,-1.3515491848,-1.8369044775,-0.2878076164\C,-2.5798959354,-1.3269908281,-0.7122333126\H,-0.667736487,0.4833359436,2.0955666319\H,-0.9431689054,-2.7155880788,-0.7779614367\H,-3.1492288444,-1.7926571454,-1.5071885795\N,-2.356218395,0.3944998533,0.8947137404\C1,-4.5544362747,0.5589227775,-0.5351896262\C,0.7549243743,-1.7052168779,1.1389323914\H,1.0325586795,-1.2922193276,2.120789542\H,0.7488239241,-2.7955905512,1.2263663534\C,3.0169195735,-2.0412281255,0.0657322919\C,3.7939623527,-1.1671193969,-0.9255767606\H,2.8938454102,-3.0718688525,-0.2747730422\H,3.4987198792,-2.0379636585,1.0546929287\H,3.5862510158,-1.4659139621,-1.9615663563\H,4.8713300572,-1.1896240252,-0.7509756746\N,1.7155231728,-1.3473740868,0.1040341176\C,1.9550383598,0.0271966613,-0.1244975666\N,1.1053089488,0.9598460791,0.1204840093\N,3.23718

91745,0.1537418748,-0.612394345\H,3.4701283836,0.9667057369,-1.1656175
193\H,-2.7172571638,1.2482280925,1.3147618296\\Version=ES64L-G16RevB.0
1\State=2-A\HF=-1028.5412543\S2=0.756969\S2-1=0.\S2A=0.750034\RMSD=8.2
77e-09\RMSF=4.138e-06\Dipole=-0.7714303,-0.9178636,0.3966937\Quadrupol
e=18.0605006,-8.938617,-9.1218836,-8.4903739,-4.3913641,2.5444637\PG=C
01 [X(C9H11C11N4)]\@\

pDIMI_N2-N5b

1\1\GINC-GRA650\FOpt\UB3LYP\6-31+G(d,p)\C9H11C11N4(1+,2)\KJM408\21-Feb
-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,2\C,-3.1933717883,-0.9294700998,0.08
44066319\C,-0.8825260538,-1.3366453098,-0.3491358855\C,-0.5255387116,-
0.9322051509,0.9273146565\C,-1.5573190883,-0.5160534313,1.7870537635\C
, -2.889353673,-0.5190323069,1.3782211434\H,-0.1598099477,-1.6658058574
, -1.0850398932\H,-1.3162322501,-0.181359269,2.7926596028\H,-3.68996803
37,-0.2044463504,2.0366405623\N,-2.1840559378,-1.3209796557,-0.7299884
534\C1,-4.7813007147,-0.9664694364,-0.5482303222\C,0.9290346283,-0.931
8051531,1.374336263\H,1.1453110819,0.0405534074,1.8491663372\H,1.04653
34882,-1.691817795,2.1541686051\C,3.0336434857,-2.0661025162,0.5322319
213\C,3.7849296173,-1.8509989896,-0.7996124792\H,2.7557815629,-3.10793
63756,0.7134305149\H,3.6185108861,-1.7012318518,1.3887951847\H,3.58910
03501,-2.66534381,-1.5155662059\H,4.872623863,-1.7932493542,-0.6906567
396\N,1.8477728215,-1.2294244485,0.3030838977\C,2.1651139898,-0.260489
7926,-0.6823860597\N,1.5242046653,0.8336502939,-0.9727395955\N,3.28140
19957,-0.6248662321,-1.3890006822\H,-2.4166151222,-1.6049810431,-1.679
921875\H,0.7626335855,1.026423838,-0.3195994327\\Version=ES64L-G16RevB
.01\State=2-A\HF=-1028.5308091\S2=0.771316\S2-1=0.\S2A=0.750123\RMSD=6
.770e-09\RMSF=1.058e-05\Dipole=-2.1352048,-1.5123652,1.6265379\Quadrup
ole=16.1417107,-12.4178247,-3.723886,-9.733012,6.7711755,8.0213523\PG=C
01 [X(C9H11C11N4)]\@\

pIMI-NOOH_N2-N2a restricted

1\1\GINC-GRA401\FOpt\RB3LYP\6-31+G(d,p)\C9H10C11N4(1+)\KJM408\16-Jul-2
019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispers
ion=gd3\\Title Card Required\\1,1\C,-0.0677052607,3.8394586139,-2.5420
208295\C,0.4604325643,3.1963182935,-0.419399077\C,0.4955040195,1.84259
29554,-0.7664985723\C,0.2095812053,1.5061482387,-2.1010049693\C,-0.079
6693923,2.5120640557,-3.0106817721\H,0.6518352609,3.5135549076,0.60522
72478\H,0.2094648279,0.4683363114,-2.4244519253\H,-0.3114311318,2.2967
435155,-4.0469429282\N,0.1916095795,4.1794544956,-1.2887795352\C1,-0.4
064554485,5.1290223072,-3.659123823\C,0.8177699747,0.7924114571,0.2691
922345\C,2.175230011,-1.4155458809,0.1996335663\C,3.6177926919,-1.6163
379049,-0.1459837741\H,1.5028870645,-1.9985274312,-0.4431208583\H,1.95
93199255,-1.6731394942,1.245554879\N,2.0455189134,0.0232064044,-0.040
8650888\C,3.2435651055,0.4837843332,-0.4098336126\N,3.5820867267,1.730
547013,-0.683272109\N,4.2132282484,-0.5260561838,-0.4918232993\H,2.906
5290897,2.48402187,-0.699653841\H,0.9311213706,1.245953194,1.260485017
2\H,0.0135875896,0.0543980193,0.3363089517\H,4.134106956,-2.5713355818
, -0.1193967885\H,4.5379290082,1.9130185412,-0.9637754218\\Version=ES64
L-G16RevB.01\State=1-A\HF=-1027.9978638\RMSD=5.926e-09\RMSF=8.824e-06\

Dipole=1.5191445,-3.68719,1.6973938\Quadrupole=-4.7535954,7.6638508,-2.9102554,-3.5252409,4.6621631,-9.5896238\PG=C01 [X(C9H10Cl1N4)]\ \@

pIMI-NOOH_N2-N2a unrestricted

1\1\GINC-GRA112\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+)\KJM408\10-Feb-2020\0\# opt freq ub3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-2.768793,-0.02716,-0.106271\C,-1.109024,-0.520982,1.376763\C,-0.217394,-0.880588,0.361894\C,-0.678001,-0.807165,-0.964117\C,-1.972556,-0.376935,-1.213261\H,-0.813794,-0.57966,2.423916\H,-0.032431,-1.087021,-1.792725\H,-2.369759,-0.311174,-2.219153\N,-2.358948,-0.09508,1.151055\Cl,-4.391462,0.535698,-0.381556\C,1.181117,-1.340972,0.695967\C,3.490224,-0.96889,-0.423047\C,4.204828,0.319551,-0.687655\H,3.323005,-1.553363,-1.33709\H,4.028401,-1.60193,0.295667\N,2.234886,-0.462749,0.136078\C,2.318757,0.869242,0.184557\N,1.425344,1.719665,0.656125\N,3.525301,1.357939,-0.337146\H,0.515386,1.422452,0.984776\H,1.320449,-1.405057,1.781181\H,1.37144,-2.334976,0.281707\H,5.193024,0.40026,-1.130669\H,1.63811,2.708572,0.607077\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9978638\S2=0.\S2-1=0.\S2A=0.\RMSD=3.921e-09\RMSF=8.827e-06\Dipole=4.2673876,-0.6322941,-0.4170454\Quadrupole=13.5324637,-5.3915002,-8.1409635,-5.1226522,0.9112289,2.1718187\PG=C01 [X(C9H10Cl1N4)]\ \@

pIMI-NOOH_N1-N2b restricted

1\1\GINC-GRA1107\FOpt\RB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+)\KJM408\14-Jul-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.0421904529,-0.2472520521,-0.347528131\C,-0.923239396,-0.7950062067,0.3003813217\C,-0.3634200004,0.3184295322,-0.3774370214\C,-1.2707918449,1.1920359902,-1.0352391211\C,-2.6220136286,0.910890822,-1.0299611871\H,-0.3130465682,-1.4760604953,0.8817797538\H,-0.9020030933,2.0750381484,-1.5493916706\H,-3.3418688495,1.54920668,-1.5277606109\N,-2.2203815985,-1.0663082266,0.3127826954\Cl,-4.7158906374,-0.6571565174,-0.3348301185\C,1.0221914842,0.6693738976,-0.4321743524\C,2.1982044288,-1.3799076035,0.4572956927\C,3.6933509307,-1.7016981498,0.2777377156\H,1.550691488,-2.0595065716,-0.0990808147\H,1.9109524658,-1.373204806,1.5131584781\H,3.8682260768,-2.274571042,-0.6405067325\H,4.0889502469,-2.2607441779,1.127583583\N,2.0813558917,-0.0101363014,-0.0775685322\C,3.41635035,0.6047943468,-0.1939600554\N,3.5022996137,1.8073787188,-0.5710023189\N,4.2847447027,-0.3687201908,0.201468765\H,5.2788518079,-0.2383865319,0.0774580028\H,4.4504761245,2.1656877228,-0.6506811157\H,1.2882977281,1.6505667743,-0.829766726\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9837744\RMSD=3.634e-09\RMSF=9.147e-06\Dipole=2.9671543,-0.1382074,-0.2030856\Quadrupole=25.9552737,-10.457715,-15.4975588,-9.6086554,5.6014707,-4.0252355\PG=C01 [X(C9H10Cl1N4)]\ \@

pIMI-NOOH_N1-N2b unrestricted

1\1\GINC-GRA740\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+)\KJM408\10-Feb-2020\0\# opt freq ub3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.083264,0.04541,-0.008025\C,-0.948616,0.80919,-0.272017\C,-0.395356,-0.475321,-0.0343\C,-1.31217,-1.5

37996,0.187933\C,-2.66841,-1.282936,0.208656\H,-0.327222,1.663182,-0.514425\H,-0.947198,-2.548178,0.350353\H,-3.395978,-2.066213,0.383482\N,-2.250222,1.058132,-0.258363\C1,-4.764548,0.420724,0.035314\C,0.994491,-0.813555,-0.033729\C,2.159461,1.426071,-0.008462\C,3.633451,1.663322,0.368788\H,1.464682,1.840075,0.724044\H,1.929317,1.819376,-1.003324\H,3.743181,1.84544,1.444302\H,4.058339,2.505286,-0.180608\N,2.051972,-0.044791,-0.040389\C,3.395269,-0.650906,-0.085911\N,3.494038,-1.906118,-0.188116\N,4.256409,0.404343,-0.030322\H,5.245683,0.241844,0.094356\H,4.446111,-2.26291,-0.193491\H,1.265897,-1.870835,-0.0223\\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9837744\S2=0.\S2-1=0.\S2A=0.\RMSD=3.825e-09\RMSF=9.024e-06\Dipole=2.9471349,0.0661377,0.4175727\Quadrupole=25.8666499,-8.2408748,-17.6257751,11.2396311,1.0804277,-0.4291186\PG=C01 [X(C9H10C11N4)]\ \@

pIMI-NOOH_N2-N5a restricted

1\1\GINC-GRA1086\FOpt\RB3LYP\6-31+G(d,p)\C9H10C11N4(1+)\KJM408\23-Jul-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C,-2.9775504822,0.0451504283,0.5183805443\C,-0.7286804907,0.7380992381,0.9161833737\C,-0.4035718823,0.5884997364,-0.4286672476\C,-1.4169753633,0.1608988349,-1.2972506171\C,-2.7068696187,-0.111855557,-0.8329192678\H,0.0224255938,1.0364543438,1.6497928635\H,-1.2054828469,0.0386863778,-2.3559475562\H,-3.4960165227,-0.4407203755,-1.4980173912\N,-1.9825200347,0.462475413,1.3422116223\C1,-4.5097254669,-0.2562160174,1.2214269392\C,1.0177077515,0.8860437572,-0.887710093\C,2.7899423559,-0.9403093322,-1.2704044471\C,3.8532860502,-1.3530597989,-0.2837934836\H,3.2240070157,-0.3896825991,-2.1188935704\H,2.2448821339,-1.8065628129,-1.669717065\N,1.9742527389,-0.0959300024,-0.4113537141\C,2.5778873288,0.0166108898,0.8358856299\N,2.1268797994,0.7628653356,1.7744482889\N,3.731454562,-0.8213840458,0.876442954\H,2.741265827,0.7156592086,2.5856886383\H,1.0479929695,0.9093808914,-1.979944166\H,1.3079401077,1.8787304752,-0.5199138625\H,-2.193538005,0.5749724855,2.3319783635\H,4.6583525992,-2.0431465344,-0.521874476\\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9805311\RMSD=5.590e-09\RMSF=3.343e-06\Dipole=-1.5217511,-0.0733523,-1.1978299\Quadrupole=12.29792,-12.3285115,0.0305915,-4.1726887,-10.6045127,3.5435025\PG=C01 [X(C9H10C11N4)]\ \@

pIMI-NOOH_N2-N5a unrestricted

1\1\GINC-GRA106\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+)\KJM408\10-Feb-2020\0\#\# opt freq ub3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C,-2.848997,0.030652,-0.124055\C,-0.703757,-0.721141,0.602991\C,-0.231685,0.585228,0.688113\C,-1.119273,1.618415,0.357995\C,-2.429787,1.350644,-0.047811\H,-0.054015,-1.572201,0.814867\H,-0.791461,2.652525,0.418487\H,-3.1224,2.143492,-0.302643\N,-1.974324,-0.954946,0.20227\C1,-4.422874,-0.439609,-0.608226\C,1.20705,0.82913,1.12382\C,3.125095,1.287911,-0.529498\C,4.104962,0.263594,-1.044377\H,3.607958,1.986227,0.171026\H,2.682281,1.875705,-1.345187\N,2.171141,0.405939,0.125019\C,2.633352,-0.903739,0.063781\N,2.039487,-1.889699,0.626286\N,3.828806,-0.943803,-0.713317\H,2.568086,-2.747913,0.478433\H,1.348986,1.894037,1.32448\H,1.391965,0.281426,2.056967\H,-2.29

3873, -1.919953, 0.143344\H, 4.973805, 0.513398, -1.647489\\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9805311\S2=0.\S2-1=0.\S2A=0.\RMSD=8.649e-09\RMSF=3.377e-06\Dipole=-1.3810808, 1.3587656, 0.0477392\Quadrupole=14.8356844, -1.5277258, -13.3079586, 9.6007143, -1.2609968, -0.7134614\PG=C01 [X(C9H10Cl1N4)]\@

pIMI-NOOH_N2-N2b restricted

1\1\GINC-GRA378\FOpt\RB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+)\KJM408\14-Jul-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C, -3.1453511625, 0.1638723439, 0.0255255085\C, -1.345606166, 1.3240941137, -0.7364840292\C, -0.4257330631, 0.4691072538, -0.0738766003\C, -0.9738947269, -0.5845785167, 0.7042841038\C, -2.3442048836, -0.7391862109, 0.7575192865\H, -0.9837583742, 2.1622426813, -1.3302374421\H, -0.3492623507, -1.2545161497, 1.2800640407\H, -2.8044079908, -1.5232296199, 1.3467210898\N, -2.6612404834, 1.1726893738, -0.6980339893\C1, -4.8576810062, -0.0170578452, 0.0620495928\C, 0.9563433195, 0.7919477652, -0.2503806713\C, 2.1386344756, -1.2789888432, 0.5817398697\C, 3.6153985283, -1.6155955623, 0.2471666946\H, 1.4145621756, -1.9160945277, 0.0716148095\H, 1.9490734143, -1.2860948092, 1.6594170292\H, 3.6896187159, -2.2631132669, -0.6337206803\H, 4.1217865479, -2.1190081281, 1.0734368433\N, 2.0253117334, 0.1080303992, 0.0770453974\C, 3.3944927592, 0.5713649637, -0.1535700464\N, 3.5679460338, 1.8689587243, -0.5567685309\N, 4.2691636728, -0.3413916313, -0.0319413069\H, 3.1761106414, 2.5928464689, 0.0369587763\H, 1.1758191467, 1.732543202, -0.7522982568\H, 4.5289061932, 2.0678379114, -0.8146337185\\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9800741\RMSD=2.859e-09\RMSF=1.596e-05\Dipole=1.979161, -0.1569011, 0.6816738\Quadrupole=8.2545223, 1.7995151, -10.0540374, 6.4616459, -1.80778, -3.6272757\PG=C01 [X(C9H10Cl1N4)]\@

pIMI-NOOH_N2-N2b unrestricted

1\1\GINC-GRA43\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+)\KJM408\10-Feb-2020\0\#\# opt freq ub3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C, 3.0998213895, 0.0031549869, -0.0105068301\C, 1.3166519376, -1.3877893681, -0.2372027371\C, 0.3857588068, -0.3562572098, 0.0553852275\C, 0.9198237719, 0.9244611472, 0.3568595158\C, 2.2873033938, 1.1075040801, 0.3262513911\H, 0.9662452935, -2.3957107362, -0.4546604959\H, 0.287085968, 1.7559864607, 0.6373621563\H, 2.7370669587, 2.0651691881, 0.5592001975\N, 2.6294187919, -1.2142233495, -0.2793974916\C1, 4.8086710643, 0.2087777113, -0.0709204769\C, -0.9912262797, -0.7424499751, 0.0373391545\C, -2.2069818568, 1.4712538386, 0.0182159853\C, -3.6925842659, 1.6297204333, -0.3988969633\H, -1.4995335829, 1.8711409109, -0.7098160401\H, -2.090328036, 1.8988867054, 1.0057930019\H, -3.7861436181, 1.8837620631, -1.46071182\H, -4.2022453024, 2.4065725194, 0.1749725932\N, -2.0706990708, -0.0010472247, 0.0893924301\C, -3.4324006413, -0.5378773438, 0.0764877902\N, -3.5837716118, -1.8926650018, 0.2103666241\N, -4.3236093136, 0.3374014279, -0.1527238737\H, -3.1737798923, -2.3235297671, 1.0327188144\H, -1.1963053045, -1.8072484661, -0.0572857113\H, -4.5426048323, -2.1902290307, 0.0634885582\\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9800741\S2=0.\S2-1=0.\S2A=0.\RMSD=6.081e-09\RMSF=1.108e-05\Dipole=-1.9765342, 0.3805197, 0.5957436\Quadrupole=8.0347376, 2.8017093, -10.8364469, 6.7079092, -1.0812774, -1.

8095939\PG=C01 [X(C9H10C11N4)]\@

pIMI_N1-N5

1\1\GINC-GRA774\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\25-Oct-2018\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C,-3.104172549,-0.2469070833,-0.1727028542\C,-1.1941001956,-0.0099456231,1.2330632935\C,-0.6372401881,-1.1848607614,0.7425235747\C,-1.3617647197,-1.8911542331,-0.2225249436\C,-2.6009156926,-1.4327298068,-0.6826473428\H,-0.7047716288,0.6261239867,1.9574702541\H,-0.9529792712,-2.8074884623,-0.6384404952\H,-3.1676319162,-1.9726337098,-1.431122683\N,-2.3897766102,0.4172269068,0.77422386\C1,-4.5904848215,0.4454229792,-0.6633505511\C,0.7539584561,-1.6114016106,1.1812572008\H,0.991310222,-1.1699915346,2.1579308851\H,0.7808320135,-2.6984622073,1.2912391054\C,2.9653815635,-2.0801006269,-0.024670234\C,3.7831601005,-1.1995827899,-0.9896818319\H,2.7064282745,-3.050482834,-0.4520683069\H,3.4947880966,-2.2325695663,0.9261729848\H,3.5678523173,-1.4391862341,-2.0376717358\H,4.8581688815,-1.270506204,-0.8177968039\N,1.7602093548,-1.2539417021,0.1826099588\C,2.0913270696,0.066089354,-0.0379283613\N,1.2357025698,0.9820000003,0.3937821277\N,1.4502937699,2.3062935031,0.0709142495\N,3.2802520685,0.1369042195,-0.6533456932\H,3.6023603238,1.0176632421,-1.0347442675\O,2.4498387438,2.661020726,-0.5745374545\O,0.5724425608,3.070391966,0.4700614648\H,-2.7528429235,1.303013896,1.1217792936\\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.7077814\RMSD=4.889e-09\RMSF=6.977e-06\Dipole=-1.0782887,-3.3451948,0.2842364\Quadrupole=22.6862409,-13.4902029,-9.196038,-10.7260257,-2.9499054,2.7852113\PG=C01 [X(C9H11Cl1N5O2)]\@

pIMI_N1-N5b

1\1\GINC-GRA105\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\13-Dec-2018\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C,-2.9752588406,-0.8944706096,-0.2853433589\C,-1.0284594414,-0.9451929066,1.0907304237\C,-0.9438162148,0.4452913649,1.0925806809\C,-1.9299526509,1.1524023279,0.3963342915\C,-2.9536083866,0.4910108766,-0.2921504846\H,-0.3180005974,-1.5887583741,1.590315774\H,-1.906425185,2.2382885649,0.3799533334\H,-3.7197549714,1.031958117,-0.8337713265\N,-2.0212992018,-1.5631810487,0.4151763245\C1,-4.146434234,-1.8315552871,-1.1089196294\C,0.2560167253,1.1228670838,1.7414804087\H,-0.044422593,2.0658450158,2.2037404402\H,0.6606877524,0.4821852087,2.5295489725\C,1.5074302379,2.7374103336,0.149231625\C,2.7173011016,2.4668930263,-0.7680914179\H,1.704909008,3.5087642183,0.8962367348\H,0.6206458423,3.0194234629,-0.4360643496\H,3.66181849,2.7054192781,-0.2654682706\H,2.6630559621,3.012192979,-1.7112857338\N,1.3180760758,1.4233451605,0.7843977261\C,1.8815366327,0.4504223838,0.0016916893\N,1.5817529306,-0.8075065417,0.294056771\N,2.0597260557,-1.8093602693,-0.5262206364\N,2.6005279341,1.0183119114,-0.9847562942\O,2.9823980574,-1.6020926986,-1.3283191453\O,1.4936562965,-2.8930647509,-0.3785489947\H,3.2596371617,0.4514486703,-1.5041339731\H,-2.0314022474,-2.5818445472,0.3990690395\\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.7067215\RMSD=9.966e-09\RMSF=5.858e-06\Dipole=-2.253983,2.590767,0.9667079\Quadrupole=8.9353291,0.8832788,-9.818608,17.3869699,1.0204059,-2.736542\PG=C01 [X(C9H11Cl1N5O2)]\@

pIMI_N1-N5c

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1\1\GINC-GRA774\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\25-Oct-2018\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.182642945,-0.6353791026,-0.0611285326\C,-1.2569137379,-2.038996636,0.0264211727\C,-0.6209101572,-1.1856817367,0.9046844987\C,-1.3109233475,-0.0241069358,1.3011607146\C,-2.5909265426,0.2530546398,0.8273264038\H,-0.8115003932,-2.9497770802,-0.3558563476\H,-0.8282391087,0.6819227341,1.9664989213\H,-3.1206730915,1.1529193213,1.1144964403\N,-2.5050982835,-1.7494206799,-0.4295429675\C1,-4.7406206421,-0.406615133,-0.7311576791\C,0.7984112572,-1.4737250301,1.3669238387\H,1.0205656221,-0.8637479673,2.2521441913\H,0.8830417921,-2.5246251661,1.657465918\C,3.052562894,-1.9823522975,0.2889176571\C,3.8311833396,-1.2341695681,-0.8091122476\H,2.892848768,-3.0365249256,0.0548600037\H,3.5564453787,-1.8999337556,1.262316785\H,3.6682863676,-1.680734471,-1.7973106162\H,4.9026224092,-1.1856284789,-0.6089581974\N,1.7746349705,-1.2429390558,0.3040989842\C,2.0158716063,0.0448609313,-0.1412840163\N,1.0851572003,0.9519481809,0.1069201443\N,1.2375396178,2.2216550289,-0.423827056\N,3.2173998274,0.0949857927,-0.7353857042\O,2.2172342415,2.5091700784,-1.1332933694\O,0.3332705573,3.0008562046,-0.1404657521\H,3.4831041708,0.9151274769,-1.2665066959\H,-2.9542393813,-2.3914246188,-1.0783223019\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.7038429\RMSD=2.375e-09\RMSF=8.260e-06\Dipole=-1.000721,-4.1587738,0.4440128\Quadrupole=24.0989339,-13.6317513,-10.4671826,-3.6236238,1.0967506,4.5301707\PG=C01 [X(C9H11Cl1N5O2)]\@\
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pIMI_N1-N5d

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1\1\GINC-GRA784\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\13-Dec-2018\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.0974681582,-0.7922834999,-0.2690384033\C,-1.9260943807,1.1741918915,0.4029091337\C,-0.9606337429,0.432584629,1.054264345\C,-1.1016326555,-0.9727096943,1.046027589\C,-2.1628106585,-1.5864271654,0.3828642672\H,-1.9284388118,2.2569856719,0.3581179049\H,-0.3645643033,-1.5860089921,1.5500714302\H,-2.2681851431,-2.6642708932,0.3587961226\N,-2.9586616674,0.5554069347,-0.2323740116\C1,-4.4435826124,-1.4192729136,-1.1190091002\C,0.248083384,1.102560881,1.6984948629\H,-0.0434294379,2.0386197086,2.1813019675\H,0.6487376625,0.4417708418,2.4716458196\C,1.4954671588,2.7275133071,0.1169706896\C,2.7419033318,2.4735522992,-0.7545404768\H,1.6532595532,3.5042915849,0.8680826435\H,0.6272130269,2.9958091755,-0.5033215995\H,3.663054267,2.7225233864,-0.214546537\H,2.7177788044,3.0217523377,-1.6973877934\N,1.3068392861,1.4134971065,0.7474575396\C,1.9073808989,0.4437708943,-0.0151622229\N,1.6211280247,-0.8156958807,0.2735815792\N,2.2057163018,-1.8143472617,-0.4878821616\N,2.6484155217,1.0257306812,-0.9791694445\O,3.1389565368,-1.5635314639,-1.2689358315\O,1.7267354257,-2.9302600834,-0.3125752647\H,3.3331255708,0.4654812746,-1.4724636423\H,-3.6625165934,1.1228326021,-0.6988286553\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.7020118\RMSD=4.449e-09\RMSF=8.681e-06\Dipole=-3.0004022,3.4713974,0.6445933\Quadrupole=13.3067471,-2.6238101,-10.6829369,13.3211516,2.6977204,-2.2759262\PG=C01 [X(C9H11Cl1N5O2)]\@\
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pIMI_N2-N5

1\1\GINC-CDR503\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\16-Jun-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,3.8830632715,-0.3887291738,0.2396365893\C,1.5641835385,-0.1832905221,-0.2795345409\C,1.3523231708,0.6591683895,0.8001090057\C,2.4602297762,0.9774594601,1.6004434151\C,3.7266467282,0.4589384227,1.3285235197\H,0.7652317731,-0.4900548947,-0.9415721852\H,2.3356967246,1.6382423756,2.4543233149\H,4.5862244917,0.6986722254,1.9424824538\N,2.8009632015,-0.6759651744,-0.5254652731\C1,5.3756762121,-1.0985711029,-0.2045150847\C,-0.0437688362,1.1630031078,1.1239926581\H,-0.4423201027,0.5450771137,1.935123298\H,0.0270482848,2.1888461856,1.5142878832\C,-1.0950867425,2.3040877458,-0.8771877581\C,-2.4627739748,2.0240529556,-1.560661783\H,-0.2666569057,2.3943761834,-1.5851086505\H,-1.1226530645,3.2107915209,-0.2557278423\H,-2.3383297875,1.6618508423,-2.5874770544\H,-3.1061736687,2.905934705,-1.5969837998\N,-0.9389045381,1.1112125614,-0.0117852795\C,-2.2084237321,0.5317059442,0.0387800149\N,-2.5286817612,-0.4487247832,1.0100156005\N,-1.857594032,-1.6816815428,1.0334786262\N,-3.0974168241,0.9543302213,-0.7699186263\O,-0.7011915181,-1.7009688194,0.604330985\O,-2.4651773077,-2.6076226316,1.5374969001\H,2.9256946249,-1.3065770939,-1.3149821478\H,-3.5291895422,-0.6084977017,1.1069411409\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6826152\RMSD=4.050e-09\RMSF=3.254e-06\Dipole=2.9456937,1.5318149,-0.1833177\Quadrupole=13.5442987,-9.4225542,-4.1217446,-7.8860169,0.1360127,4.8714355\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N2-N3

1\1\GINC-CDR855\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\18-Jun-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,4.0617166025,0.510537759,0.2617425322\C,2.2381943426,1.6750710278,0.9746692972\C,1.3899311959,0.5757718527,0.8019889121\C,1.9602790884,-0.6255986446,0.3430099016\C,3.3182394741,-0.6680143257,0.0646264483\H,1.8547109743,2.6196478048,1.3597113773\H,1.3527820451,-1.5191234592,0.2155425062\H,3.8018342024,-1.5724359519,-0.2844451798\N,3.5462853816,1.6480997263,0.7085181084\C1,5.7625473919,0.5000749834,-0.0903697958\C,-0.0734371436,0.6805858913,1.0904998458\H,-0.467810661,-0.2124945467,1.5788441442\H,-0.3304720353,1.5579707174,1.6879834782\C,-0.7532947504,2.1525404283,-0.936424589\C,-2.0522897045,2.8756982978,-0.5164957176\H,-0.7287979708,1.9534606066,-2.0090502225\H,0.1739063902,2.6374417702,-0.6352479138\H,-2.4701245018,3.4770047331,-1.32624161\H,-1.917952869,3.5328351694,0.3496431721\N,-0.8775513405,0.8150421846,-0.2295203801\C,-2.357998313,0.7316455589,-0.0086380539\N,-2.8796472,-0.4500022035,0.5003134031\N,-2.5464358478,-1.7104385646,-0.0653689608\N,-2.9928138317,1.8084486613,-0.156479266\O,-1.5032733562,-1.7590250185,-0.7218174296\O,-3.299137563,-2.6149459176,0.2046426346\H,-0.5935876693,0.0278882747,-0.8267768934\H,-3.8518830613,-0.4270849952,0.8036438708\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.662352\RMSD=6.542e-09\RMSF=1.233e-05\Dipole=-2.6609955,1.1074179,-0.1659351\Quadrupole=6.2337635,-1.5901514,-4.6436121,-9.6736559,-1.3661773,-3.1720014\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N2-N2

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1\1\GINC-CDR603\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\14-Jun-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-2.941638556,-0.278608255,-0.067075954\C,-1.0751931278,-1.5059769528,-0.5358137403\C,-0.5290060976,-1.2914926663,0.7370315348\C,-1.2914354728,-0.5412352587,1.6453979173\C,-2.523918324,-0.0261655358,1.2487059545\H,-0.5366079516,-2.101923356,-1.2699189362\H,-0.93298729,-0.36751324,2.6575435283\H,-3.1440993481,0.5522276778,1.9232751589\N,-2.2462621033,-1.0012960113,-0.9384197618\C1,-4.4500117621,0.3890519712,-0.6216131378\C,0.8399228767,-1.8375738678,1.0820098969\H,1.1291332255,-1.5484423566,2.103474371\H,0.8237916693,-2.9313490744,1.0540694672\C,3.1506710665,-2.1629103478,0.0537161525\C,4.0433909871,-1.1780846147,-0.7458779099\H,3.0171605019,-3.1295748136,-0.4355854491\H,3.5275871043,-2.3268631723,1.0723384856\H,4.1141851268,-1.4526966734,-1.8068818945\H,5.0636530211,-1.095340436,-0.3634857095\N,1.862152642,-1.4239910249,0.106834976\C,2.2006877213,-0.1246039352,-0.1815986059\N,1.2863086996,0.9427165121,-0.1188144106\N,0.2779875492,1.0234654098,-1.8083903822\N,3.3663379098,0.1259306801,-0.6742087854\O,0.8695783704,0.4310891216,-2.6303916223\O,-0.6932292059,1.6695176905,-1.6499266285\H,0.5112740662,0.8731351084,0.5450358713\H,1.7710290217,1.842957871,-0.1053958662\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6334828\RMSD=4.050e-09\RMSF=3.891e-06\Dipole=2.5999286,0.2291029,1.3813522\Quadrupole=3.5866458,-0.0650345,-3.5216114,-7.3911656,-2.7714793,-1.58065\PG=C01 [X(C9H11Cl1N5O2)]\@\
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pIMI_N2-O2

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1\1\GINC-CDR567\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\25-Apr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.1047586987,-0.2754636406,0.1735844796\C,-1.3049795134,-0.4041132945,1.5681110429\C,-0.6102097075,-1.26267798,0.7085435099\C,-1.2530378616,-1.6382759247,-0.4877205181\C,-2.5201684249,-1.1482370686,-0.7650600659\H,-0.8671774886,-0.0972865161,2.5173568007\H,-0.7580442749,-2.3059712144,-1.1871482379\H,-3.0530794004,-1.4201983378,-1.6685269501\N,-2.5243512437,0.0921019635,1.3044952844\C1,-4.6817287616,0.3832733577,-0.1589170598\C,0.7761838147,-1.7645713171,1.0528919978\H,1.0744994541,-1.4208778247,2.0548943887\H,0.7730302605,-2.8579644027,1.0786662168\C,3.0847747488,-2.1227422376,0.0643051315\C,4.0103360287,-1.1524774368,-0.7126218718\H,2.9772688228,-3.1005228507,-0.4085061177\H,3.41449966,-2.2596066824,1.1035845268\H,4.1070744503,-1.4330093245,-1.7684267161\H,5.015659853,-1.0771424019,-0.2937524404\N,1.7874530071,-1.3923819189,0.0440718675\C,2.1659197572,-0.0898165211,-0.2396785144\N,1.1573254752,0.9097353942,-0.1193249918\N,1.3420710906,2.1791231122,-0.3679733151\N,3.3410149335,0.1655057607,-0.6635294107\O,2.349422303,2.7240414809,-0.7010418611\O,0.1634770255,2.8567555553,-0.1855709112\H,0.2035030654,0.6490298024,0.1711746726\H,0.374013555,3.7982373079,-0.3695208171\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6285672\RMSD=4.204e-09\RMSF=1.497e-05\Dipole=2.1152819,0.233229,-0.2920537\Quadrupole=-2.8279111,12.8826651,-10.054754,-3.7802096,4.9420494,-1.3948251\PG=C01 [X(C9H11Cl1N5O2)]\@\
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pIMI_N2-01

1\1\GINC-GRA767\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\16-Jun-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.0557308242,-0.3220238317,0.6447165282\C,-1.2740621033,-1.0952290234,1.8411136368\C,-0.664107478,-1.6509769025,0.7110074041\C,-1.3433972025,-1.5273729411,-0.5155204089\C,-2.5588565565,-0.8541749855,-0.5602746931\H,-0.8013069119,-1.1757115636,2.8188011749\H,-0.9218558389,-1.9547343483,-1.4215817236\H,-3.1174490743,-0.7436608082,-1.4823127332\N,-2.440867224,-0.437391428,1.812701262\C1,-4.5600849608,0.5521846961,0.6232412327\C,0.6885452621,-2.3122223426,0.8043466133\H,0.9941182052,-2.4142012799,1.855962848\H,0.6427459877,-3.3199949242,0.3813149802\C,3.058538214,-2.2869509226,-0.0664819756\C,4.0416905409,-1.0989036933,-0.2643343857\H,3.0580393555,-2.9972928151,-0.8952941501\H,3.2550688952,-2.8300084185,0.8670005826\H,4.3767740707,-1.0094993923,-1.3033221417\H,4.9314023448,-1.1585816844,0.3668187706\N,1.735438385,-1.6046954125,0.0326809045\C,2.0762599217,-0.2770059804,0.2108171625\N,0.9910909891,0.652872425,0.3757067278\N,1.0093024851,1.775634272,1.0389319277\N,3.2731818396,0.1229214484,0.0562662177\O,2.1194797473,1.9713491371,1.7728223735\O,0.0970289826,2.5642128553,1.0352542958\H,1.9807216624,2.8412797808,2.2097940235\H,0.0916464456,0.4831034336,-0.0814026244\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6250649\RMSD=3.323e-09\RMSF=2.107e-05\Dipole=2.750336,-0.0840497,-0.1993495\Quadrupole=1.5778187,5.233122,-6.8109408,-0.1764318,6.4011113,7.2333091\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N5-02

1\1\GINC-CDR608\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\15-May-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.2621041271,-0.5348536371,0.075658964\C,-1.0046885221,-1.0364950787,-0.5054410832\C,-0.6127375939,-1.0275489648,0.8229117529\C,-1.5992785559,-0.7619048266,1.7852875852\C,-2.923607874,-0.5188590141,1.4224071147\H,-0.3096876851,-1.2176425173,-1.3152009655\H,-1.3292892202,-0.7346300462,2.837590882\H,-3.6891951978,-0.3108797052,2.1598437173\N,-2.2952663081,-0.7950890484,-0.8375031889\C1,-4.8443076026,-0.2411265605,-0.5102154469\C,0.8276016921,-1.2900274154,1.2173235216\H,1.114936963,-0.5596178087,1.9897950865\H,0.8721638483,-2.2794547867,1.6863659431\C,2.9391945471,-2.1645900836,0.1699102141\C,3.8775389911,-1.4788872694,-0.8504925833\H,2.6916871774,-3.1980434554,-0.0826527971\H,3.3635806938,-2.1351052932,1.1848011477\H,3.7971186825,-1.9370228881,-1.8448321945\H,4.928813766,-1.5086346597,-0.5564214158\N,1.7440603911,-1.2939617401,0.0883444652\C,2.247231866,-0.0646869952,-0.4142573505\N,1.3239031596,0.9814096002,-0.319928282\N,1.71833054,2.152047892,-0.6286072485\N,3.4097852047,-0.0853980827,-0.9470753555\O,2.7960618667,2.5969120963,-0.9773769648\O,0.6553060593,3.0587166509,-0.5163666142\H,-2.5536953358,-0.7945221201,-1.8219439554\H,1.069409584,3.9117621378,-0.7528416881\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.664977\RMSD=5.582e-09\RMSF=1.650e-05\Dipole=-2.7351444,-1.2822247,0.7624363\Quadrupole=7.1226752,-2.6380845,-4.4845906,-3.7404028,2.6901652,-1.3265318\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N5-01

1\1\GINC-CDR540\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\14-May-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-3.1199070124,-0.3611853834,-0.0944347931\C,-1.2211236377,-0.1212724966,1.3256730418\C,-0.5858497709,-1.1986773664,0.7317208263\C,-1.2573939337,-1.8519149482,-0.3122701607\C,-2.5272328047,-1.4467403311,-0.7253106118\H,-0.7717821791,0.4805429968,2.1048014255\H,-0.7725463332,-2.6811063302,-0.8187928311\H,-3.0559627528,-1.9484227205,-1.5264859281\N,-2.4512872735,0.2622085176,0.9069922945\Cl,-4.6641639224,0.2506336424,-0.5101874895\C,0.8174254951,-1.6012141755,1.1409558105\H,1.0906042918,-1.1126910138,2.0877580947\H,0.8321905788,-2.680603727,1.3188919582\C,2.9764133219,-2.1680173644,-0.0456749202\C,3.8852256327,-1.2584577742,-0.9048131067\H,2.7439643643,-3.127117983,-0.5140956843\H,3.4134670198,-2.3505653533,0.9481771592\H,3.788273661,-1.4867813396,-1.9741938532\H,4.9423882828,-1.3343331305,-0.6422847666\N,1.7691170588,-1.3227152014,0.0705154976\C,2.2423883127,-0.006443168,-0.1454707893\N,1.3264455438,0.9634352024,0.2731187504\N,1.4800105947,2.203688776,0.0686173831\N,3.3982394525,0.1149677255,-0.6808888241\O,2.5970709695,2.6518811168,-0.6109221279\O,0.6768157495,3.0612109813,0.4407086845\H,-2.8846618834,1.0732800641,1.3433752491\H,2.4657244044,3.6216677741,-0.6284545188\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6626647\RMSD=5.181e-09\RMSF=6.089e-06\Dipole=-2.0916775,-1.1708394,0.6887486\Quadrupole=11.0296536,-0.0802948,-10.9493588,-1.812078,-0.6090322,1.4286534\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N3-02

1\1\GINC-GRA744\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\14-May-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-2.9082415552,0.2472180231,-0.8476663897\C,-1.8526760346,1.6146173864,0.6372208632\C,-0.8746661501,0.6553810093,0.9276051154\C,-0.9817821738,-0.5922064548,0.2883315261\C,-2.0120343151,-0.8104004736,-0.6147353756\H,-1.850813026,2.5812133555,1.1400876158\H,-0.2733989152,-1.3870965725,0.5037601933\H,-2.1336725915,-1.7581362122,-1.1251305599\N,-2.8436409626,1.4233274775,-0.2366458883\Cl,-4.1939687201,0.0252227573,-1.9959392513\C,0.2378827206,0.9632533413,1.8798300178\H,-0.0151947036,1.7767419289,2.5634126335\H,0.5536790341,0.091764176,2.4568540799\C,1.3613123733,2.6391486931,0.2360501242\C,1.3585151265,2.002323596,-1.1741021786\H,2.2278963236,3.2846025314,0.3881384746\H,0.4505841914,3.1783323934,0.4903126727\H,1.9213845424,2.5992316532,-1.8952132808\H,0.3468582582,1.8633972998,-1.5693259375\N,1.5220379548,1.4395072845,1.1484523552\C,2.0787332292,0.3904095258,0.196549551\N,2.5423197595,-0.6849104782,0.9114664466\N,3.0617447114,-1.6496832343,0.2358316362\N,1.9815766948,0.688536202,-1.0266182277\O,3.2168372224,-1.7916876913,-0.9601709352\O,3.4864827146,-2.6444119024,1.0844361005\H,2.2205102493,1.6223250005,1.8763440207\H,3.8781046316,-3.3170599359,0.4899881278\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6525414\RMSD=6.340e-09\RMSF=1.440e-05\Dipole=2.8775642,0.7441723,1.8689806\Quadrupole=-0.7455082,9.8108038,-9.0652956,0.3127905,5.0736401,4.0639408\PG=C01 [X(C9H11Cl1N5O2)]\@\

pIMI_N3-01

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1\1\GINC-CDR680\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\13-May
-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\Title Card Required\1,1\C,-2.7702045289,0.0521445704,-0.87
13925143\C,-1.7906016287,1.5900535456,0.495228663\C,-0.836692813,0.672
8135585,0.953815783\C,-0.9191305943,-0.6453141713,0.4692565623\C,-1.89
96850207,-0.9713422745,-0.4563010343\H,-1.8140897529,2.6093726604,0.87
96105625\H,-0.2332568986,-1.4091168792,0.8254039471\H,-2.0044528439,-1
.9762033806,-0.8475687099\N,-2.7297991712,1.2948072666,-0.405725209\Cl
,-3.9870303218,-0.3050546861,-2.0572986373\C,0.224346716,1.0902910334,
1.9208970345\H,-0.0679707948,1.9532065576,2.523149922\H,0.5427117119,0
.2775577541,2.5764896612\C,1.3963476451,2.7182361503,0.2394200819\C,1.
4147924368,2.0509815243,-1.1558457427\H,2.2631552002,3.3627409857,0.39
33136032\H,0.4837235163,3.2675970797,0.462553341\H,2.0036284511,2.6247
679392,-1.8744524017\H,0.4098855868,1.9119374981,-1.5659437133\N,1.531
2825386,1.5423026463,1.1963608374\C,2.088934786,0.4690973684,0.3109982
068\N,2.5263745411,-0.606856866,1.0023335864\N,2.9907594526,-1.6286972
77,0.3028255789\N,2.0260320331,0.7400844597,-0.9334662764\O,3.02395994
39,-1.6144303358,-1.0560644374\O,3.3983759845,-2.6220963873,0.83645218
55\H,2.2161758599,1.7457248931,1.9329004736\H,2.6585807948,-0.71760220
32,-1.3674215442\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.6527673\
RMSD=3.833e-09\RMSF=9.030e-06\Dipole=1.9356606,2.5118309,1.4479446\Qua
drupole=-3.7553823,4.2478034,-0.4924211,13.3221335,1.0370622,6.4287043
\PG=C01 [X(C9H11Cl1N5O2)]\@
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pIMI_01-02

```
1\1\GINC-GRA710\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N5O2(1+)\KJM408\24-May
-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\Title Card Required\1,1\N,3.0389129233,1.6797146906,-0.551
8967508\C,2.1088887478,2.8243402743,-0.5698961254\H,2.5888673676,3.702
2385818,-0.1308332117\H,1.900316268,3.0570049115,-1.622574644\C,0.8327
624273,2.3571715226,0.1814929961\H,0.8103248306,2.6989881901,1.2261006
324\H,-0.0959929672,2.6557800628,-0.306662486\N,0.9942032846,0.8852436
552,0.1470973158\C,2.3165662469,0.6868639524,-0.1576972732\N,2.7698116
245,-0.651431455,-0.1508329106\N,3.9537940932,-0.953723061,-0.23340917
08\C,0.1841604011,0.0412145935,1.0280040642\H,0.5793491015,-0.97895442
97,0.9745012596\H,0.2922828792,0.3790995619,2.0696939081\O,5.001892102
,-0.127854965,-0.2909470025\O,4.3526692297,-2.2497346827,-0.2774276497
\C,-1.2737199953,0.0611491277,0.6248400313\C,-2.2939627291,0.297196515
1,1.554111936\C,-3.6205520347,0.2830711485,1.1349644475\C,-1.652132453
,-0.1748973035,-0.7011784948\C,-3.8680163567,0.0341125209,-0.222073433
8\Cl,-5.5192119578,0.0117765978,-0.7913712029\N,-2.9205834425,-0.18765
37263,-1.1230280406\H,-0.8984119862,-0.3519753949,-1.4659479199\H,-4.4
386854788,0.4622636,1.8220931412\H,-2.0589117106,0.4921130179,2.597417
3313\H,5.8067870731,-0.6912613405,-0.324459401\H,3.5370775016,-2.79625
49062,-0.2621171356\Version=ES64L-G16RevB.01\State=1-A\HF=-1233.60370
53\RMSD=5.036e-09\RMSF=3.519e-06\Dipole=5.6264476,-1.1463062,1.2209932
\Quadrupole=24.2892358,-4.8867054,-19.4025305,-17.8756838,-8.1470786,0
.6330936\PG=C01 [X(C9H11Cl1N5O2)]\@
```

pIMI-NO_N2-N3

1\1\GINC-CDR856\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\08-Jul-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,2\C,-0.2885092896,-5.9785626232,0.4004726803\C,1.3996656629,-4.5793026681,1.0182342308\C,0.5946516215,-3.4429018233,0.8781809978\C,-0.7448824276,-3.6341548892,0.4927484766\C,-1.202965234,-4.9201578659,0.2470044248\H,2.43298803,-4.4922717814,1.3534059831\H,-1.4245057608,-2.7893670216,0.4032859939\H,-2.2281159238,-5.1158227086,-0.0436800453\N,0.9725390192,-5.8216703686,0.7815153206\C1,-0.8199452278,-7.601556809,0.0839415034\C,1.1402999798,-2.0741375016,1.1280503511\H,0.4115552805,-1.4178543004,1.6052117823\H,2.0662647656,-2.0808759908,1.7067603975\C,2.7590794368,-1.8950713408,-0.8897030602\C,3.8269583234,-0.8766181395,-0.4234349834\H,2.5991703426,-1.8473772283,-1.9683024912\H,2.9295352055,-2.9282873786,-0.5914452268\H,4.5632687109,-0.6707375562,-1.2032531972\H,4.3739348356,-1.2058968844,0.4675486926\N,1.4987046774,-1.3746335712,-0.2180142086\C,1.8554507001,0.0613921623,-0.0230671525\N,0.7981896573,0.9014792048,0.2352195117\N,3.0865078474,0.3487555722,-0.0993228246\O,-0.4067688844,0.4718300636,0.2071851127\H,0.9869906242,1.8930578083,0.4136729814\H,0.6709427473,-1.4563025105,-0.820158601\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.7236745\S2=0.764403\S2-1=0.\S2A=0.750081\RMSD=8.410e-09\RMSF=1.663e-05\Dipole=1.347641,3.0996609,-0.6207457\Quadrupole=2.2899687,4.1905197,-6.4804884,9.1605873,-2.2766805,-0.5715521\PG=C01 [X(C9H11Cl1N4O1)]\@\

pIMI-NO_N3-01

1\1\GINC-CDR700\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\01-Aug-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,2\C,3.197745934,-0.045363079,-0.5825193806\C,2.0559885459,1.4098479393,0.7473268915\C,1.0578296345,0.469710298,1.0325803719\C,1.1990727969,-0.8147545531,0.4775366799\C,2.2836165011,-1.0866126014,-0.3438033291\H,2.0250628942,2.4056475284,1.1887120628\H,0.4726940358,-1.5954001031,0.6858997814\H,2.4314984814,-2.0630441438,-0.7890611603\N,3.099110383,1.166111796,-0.0487856806\C1,4.5517334167,-0.335948397,-1.631128093\C,-0.1084133305,0.8372974709,1.8935478829\H,-0.4482535723,0.0143021066,2.5224915576\H,0.1003638953,1.7064898914,2.5212951883\C,-1.130283663,2.3802642329,0.0741282551\C,-0.9589527406,1.6362008837,-1.2703305587\H,-0.2659797236,2.9666109723,0.3817631095\H,-2.0244709502,3.0061275621,0.079411429\H,0.093626117,1.4726127952,-1.5305646574\H,-1.4233442565,2.1707245832,-2.1033826998\N,-1.3601818339,1.2494085974,1.0593388204\C,-1.8531521656,0.138276683,0.1414977113\N,-2.4910000412,-0.9435913006,0.6226777313\N,-1.5994936408,0.3402146448,-1.1050672685\O,-2.6698366422,-0.8092478786,1.9711610785\H,-3.177909556,-1.5968413854,2.2338067848\H,-2.0971687495,1.4834152765,1.732990412\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.7157735\S2=0.7777\S2-1=0.\S2A=0.750166\RMSD=5.450e-09\RMSF=9.526e-06\Dipole=-3.4372035,0.9699566,2.1266988\Quadrupole=2.5952807,0.9575369,-3.5528177,-6.4313243,-11.1812927,-2.4975979\PG=C01 [X(C9H11Cl1N4O1)]\@\

pIMI-NO_N1-N3

1\1\GINC-CDR448\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\30-A

pr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,2\C,-0.2396554967,-5.9616666644,0.2062974259\C,1.257519701,-4.5475028078,1.1817545414\C,0.4799878725,-3.4200273329,0.8910788444\C,-0.7455984201,-3.6264924972,0.2333464502\C,-1.1211891729,-4.9151555857,-0.1190311573\H,2.197067926,-4.4507707086,1.7244593676\H,-1.4104621322,-2.7927305695,0.0174312657\H,-2.0610313235,-5.1207816217,-0.6171445907\N,0.9119232671,-5.7916486904,0.8435685193\C1,-0.6631893307,-7.5871853919,-0.23572994\C,0.9473790142,-2.0470553646,1.2598516218\H,0.1271741618,-1.3762480912,1.5238657171\H,1.6838516065,-2.0416207841,2.0658989651\C,2.9386313466,-2.0495618754,-0.3979548643\C,3.7271916477,-0.8973829868,-1.026241868\H,2.6990848366,-2.8724478827,-1.0689559141\H,3.4310201897,-2.4281913793,0.4986410553\H,3.4463221959,-0.734964194,-2.0752649614\H,4.8025148822,-1.0754418065,-0.9689366525\N,1.6498171852,-1.3736350934,0.0603226896\C,2.0470376208,0.0372142484,0.2953839886\N,1.2082967606,0.8290440452,0.8343212277\N,3.3298516675,0.2152596638,-0.1610082718\H,3.6577266251,1.158068372,-0.3327331112\O,1.3651723903,2.0444654375,1.1115886294\H,0.9818803488,-1.3934405787,-0.7196191675\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.7081195\S2=0.75772\S2-1=0.\S2A=0.750039\RMSD=8.376e-09\RMSF=2.033e-05\Dipole=1.4918762,2.3807935,-1.2439801\Quadrupole=9.2129186,-4.4401587,-4.7727599,13.4329126,-3.3849619,-5.0060353\PG=C01 [X(C9H11Cl1N4O1)]\@\

pIMI-NO_N1-N1

1\1\GINC-CDR439\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\30-A pr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,2\C,3.4367155838,-0.3248794343,-0.1116433592\C,2.1813776945,1.2860903056,0.8958458251\C,1.1052540454,0.415644213,1.0901085382\C,1.2499756218,-0.9125583071,0.6544040312\C,2.4363754511,-1.3002672477,0.0470517548\H,2.1349249392,2.316676299,1.2472148129\H,0.4488713039,-1.6325055154,0.8010939616\H,2.5991132111,-2.3164222155,-0.2918331122\N,3.3247101583,0.9295473941,0.3002276792\C1,4.9278012276,-0.768234475,-0.8955208494\C,-0.1792073077,0.9003646259,1.7139139051\H,-0.6423641313,0.1423391696,2.3484160133\H,-0.0270030732,1.8068119318,2.3059909853\C,-1.0941115886,2.4701789545,-0.1429642191\C,-1.8939600474,2.1106531143,-1.4082880892\H,-0.0513099946,2.6982776981,-0.3771037507\H,-1.5274120332,3.3095353463,0.4124454871\H,-1.2588037093,1.6616726642,-2.1733203834\H,-2.4681584033,2.933454708,-1.8325869936\N,-1.1723064089,1.242110921,0.6613974516\C,-2.0947220802,0.3931339759,0.219668901\N,-2.3794192124,-0.8370212235,0.6216462954\N,-2.8279501439,1.0223630765,-0.9131967024\H,-3.0650900766,0.2669306177,-1.5782748365\O,-3.3233566654,-1.3675797383,-0.0879577274\H,-3.7316987705,1.3875579512,-0.5850133987\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.7071331\S2=0.762803\S2-1=0.\S2A=0.750044\RMSD=5.588e-09\RMSF=1.411e-05\Dipole=-4.3005301,2.8439252,-1.0059674\Quadrupole=6.3493177,-2.1478667,-4.201451,-21.400577,10.1938623,-1.5429305\PG=C01 [X(C9H11Cl1N4O1)]\@\

pIMI-NO_N3-N5

1\1\GINC-CDR502\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\23-Jul-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,2\C,-2.848690958,-0.0255762598,-0.

2353919116\C, -1.1842817953, -0.3628923439, 1.4394469002\C, -0.5829150089, -1.3635035266, 0.6757917461\C, -1.1367940821, -1.6652920038, -0.5662471369\C, -2.2813865129, -0.9999612703, -1.0326573936\H, -0.8481678233, -0.0690152291, 2.4236446214\H, -0.6679362592, -2.4087033152, -1.203630586\H, -2.7090753635, -1.2140761867, -2.0035943496\N, -2.3103686487, 0.2377701179, 0.9878722365\C1, -4.2252885096, 0.8851859259, -0.6860250808\C, 0.7483098367, -1.9244044755, 1.1024880787\H, 0.7876043395, -2.1498884105, 2.1710122847\H, 0.9648030886, -2.8386783992, 0.5479832153\C, 3.193815411, -1.6278678692, 0.5098449016\C, 3.1348527233, -1.774441411, -1.0321743194\H, 3.2821044862, -2.562112466, 1.0667425278\H, 3.9900892213, -0.944307075, 0.811060869\H, 2.699911246, -2.7351810524, -1.3411084538\H, 4.1321989548, -1.7199489701, -1.4761239567\N, 1.8855140179, -0.9541176243, 0.8066223512\C, 1.6511615048, -0.1610942717, -0.5300947645\N, 0.8898156924, 0.9559726308, -0.4440892549\N, 2.3077240555, -0.6721327989, -1.5093787237\H, -2.7167467308, 0.9884110072, 1.5399539305\H, 1.9172085626, -0.2421374625, 1.5463694261\O, 0.4834870717, 1.2056863798, 0.7697226226\\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.6993722\S2=0.765268\S2-1=0.\S2A=0.750091\RMSD=9.178e-09\RMSF=2.487e-05\Dipole=-0.1196587, -2.390872, 2.0272693\Quadrupole=17.8472876, -10.8437827, -7.0035049, -14.3894198, 5.6046846, 3.2097152\PG=C01 [X(C9H11Cl1N4O1)]\@

pIMI-NO_01-01

1\1\GINC-CDR594\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\30-Jul-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,2\C, -3.0345961236, -0.6010806905, -0.3198276229\C, -1.0213804454, -1.658893183, -0.3662080576\C, -0.633269262, -1.1127837056, 0.8658952267\C, -1.5376981608, -0.2594772498, 1.5115467286\C, -2.7690662818, -0.0019033398, 0.9228258665\H, -0.3609670772, -2.337713281, -0.9040811613\H, -1.283171995, 0.1986032158, 2.4630044133\H, -3.5014184392, 0.6458133437, 1.3894578481\N, -2.1922368215, -1.4093277996, -0.9532218991\C1, -4.5520104191, -0.2763334844, -1.1061157196\C, 0.7224678904, -1.4477900842, 1.4500871997\H, 0.8770732236, -0.9181084723, 2.3976893821\H, 0.823317748, -2.5174960675, 1.6515665916\C, 2.7804199226, -2.0119915587, -0.0529351591\C, 3.5307781351, -1.1054249386, -1.0571556107\H, 2.2761195482, -2.8586205545, -0.5293927011\H, 3.4414293138, -2.3999029557, 0.7314480767\H, 3.3371154493, -1.3816676271, -2.1049939247\H, 4.6206266374, -1.1178451081, -0.9348188143\N, 1.7962245439, -1.0865476304, 0.5205911593\C, 2.0144758995, 0.1667700535, 0.0579799696\N, 1.3257225982, 1.2423210662, 0.4416560896\N, 3.0337382822, 0.2372661745, -0.8412797997\O, 1.8714630507, 2.3340699439, -0.478195122\H, 2.675142315, 1.895523894, -0.9428802014\H, 2.1304288678, 3.0737790291, 0.1049038015\\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.6730205\S2=0.759943\S2-1=0.\S2A=0.750048\RMSD=5.274e-09\RMSF=7.970e-06\Dipole=4.5274534, 0.8511248, 0.9255465\Quadrupole=12.1481838, 1.4523922, -13.600576, 0.9297413, -6.9880014, -0.4147069\PG=C01 [X(C9H11Cl1N4O1)]\@

pIMI-NO_N2-N2

1\1\GINC-CDR507\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4O1(1+,2)\KJM408\02-May-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,2\C, -3.1080539087, -0.30471112, -0.0168651715\C, -1.0908463376, -1.1611510428, -0.6157414745\C, -0.5477237624, -0.9635846555, 0.6951816332\C, -1.4483553186, -0.5059068009, 1.6995009827\

C, -2.7304706901, -0.1637568942, 1.3461592186\H, -0.4752317533, -1.61953204
34, -1.3871837136\H, -1.107054115, -0.3943566056, 2.7238521542\H, -3.444142
6611, 0.2132492106, 2.0693404203\N, -2.3171201591, -0.8122784393, -0.967529
3862\C1, -4.6804859885, 0.1860372494, -0.4990981592\C, 0.7901962991, -1.544
7913031, 1.0704538046\H, 1.1342167321, -1.0957333286, 2.0127099935\H, 0.665
5083075, -2.6202374056, 1.2473789667\C, 3.0685974843, -2.174925322, 0.19059
16547\C, 4.0825590957, -1.334102773, -0.6375553321\H, 2.9467269692, -3.1973
951633, -0.1712267157\H, 3.3330465647, -2.200474406, 1.2558292314\H, 4.2783
013319, -1.7772078111, -1.6194982019\H, 5.040841089, -1.1946221282, -0.1340
280059\N, 1.7996126608, -1.4062809168, 0.0184229901\C, 2.23193627, -0.19030
09124, -0.4667416957\N, 1.2591868195, 0.8929936336, -0.6863718082\N, 3.4247
099181, -0.0245765537, -0.8564255308\O, 0.2977387552, 1.018599404, 0.319659
9015\H, 0.8004183876, 0.7712671211, -1.6030365337\H, 1.8074702195, 1.766705
0569, -0.7364049327\\Version=ES64L-G16RevB.01\State=2-A\HF=-1103.673072
9\S2=0.76208\S2-1=0.\S2A=0.750093\RMSD=5.956e-09\RMSF=1.016e-05\Dipole
=1.3661167, -0.4354449, 0.6342571\Quadrupole=11.4829415, -5.7719564, -5.71
09851, -7.1360717, -5.2795513, -3.6245787\PG=C01 [X(C9H11Cl1N401)]\@

pIMIU_N1-N5

1\1\GINC-GRA101\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N301(1+)\KJM408\14-Dec
-2018\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,1\C, -3.1003343178, -0.2304069456, -0.1
340760296\C, -1.1379431143, -0.0088707481, 1.2025374539\C, -0.6303877405, -
1.210542382, 0.7284995642\C, -1.4012969112, -1.916801983, -0.202372839\C, -
2.6409344951, -1.4374977067, -0.6359997988\H, -0.6021932196, 0.6294560668,
1.8920364761\H, -1.0277399682, -2.8526409196, -0.6077202453\H, -3.24386249
67, -1.9787013974, -1.3546890825\N, -2.3386605939, 0.4383127317, 0.77039429
49\C1, -4.5901642271, 0.4834764025, -0.5863652263\C, 0.7518852589, -1.67475
91472, 1.1496764201\H, 0.9937639472, -1.2737473553, 2.1442870541\H, 0.75882
05124, -2.7654723724, 1.2219345083\C, 2.9641503868, -2.0755652234, -0.05003
99336\C, 3.7924821418, -1.1336369825, -0.947919158\H, 2.7461836525, -3.0321
286088, -0.5302424664\H, 3.4758468369, -2.2602036615, 0.9057284621\H, 3.582
9267185, -1.3138964903, -2.0100670576\H, 4.8655153495, -1.2305664893, -0.77
28900209\N, 1.7418638198, -1.2844156834, 0.1561971046\C, 2.0488230607, 0.07
62274856, 0.0377296785\N, 3.2904175321, 0.1710168385, -0.5186189664\H, 3.59
28422107, 1.0477292424, -0.9181364479\H, -2.6792455065, 1.3322321128, 1.117
8870808\O, 1.3096152633, 0.9928751262, 0.3985274747\\Version=ES64L-G16Rev
B.01\State=1-A\HF=-1049.1043544\RMSD=7.617e-09\RMSF=1.203e-05\Dipole=-
0.7912198, -0.953039, 0.1686895\Quadrupole=18.5290095, -7.8657214, -10.663
2881, -8.1661533, -3.9548011, 2.2468595\PG=C01 [X(C9H11Cl1N301)]\@

pIMIU_N1-N5b

1\1\GINC-GRA782\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N301(1+)\KJM408\14-Dec
-2018\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,1\C, -3.1456695349, -0.6707537328, -0.3
260398087\C, -1.0580973177, -0.8891531452, 0.8094030168\C, -1.0003888683, 0
.479697174, 1.0529565102\C, -2.0667234247, 1.2637415599, 0.5883325979\C, -3
.1427821577, 0.6981597158, -0.1007300487\H, -0.2685897915, -1.5707630705, 1
.1023625035\H, -2.0648295252, 2.3350641779, 0.7686424012\H, -3.9705310608,
1.2971909031, -0.4602465984\N, -2.1097898552, -1.4145933105, 0.1386304777\

C1, -4.3944357698, -1.4932804516, -1.1600101751\C, 0.2310538672, 1.0691678371, 1.726814797\H, -0.0308781599, 1.9889669576, 2.2553328869\H, 0.6209750425, 0.3596902149, 2.4616548154\C, 1.3916126789, 2.6196032577, 0.0245381576\C, 2.6402904508, 2.3434820703, -0.8408818627\H, 1.5212042814, 3.4759062721, 0.6907814931\H, 0.5058531266, 2.7861236583, -0.6080542518\H, 3.5526338143, 2.6578170642, -0.318551149\H, 2.5928318354, 2.8393452057, -1.8119208109\N, 1.2851881454, 1.3673891743, 0.7756694773\C, 1.888116373, 0.328464298, 0.0736575952\N, 2.5735359192, 0.8862011649, -0.9748307185\H, 3.3135874187, 0.3475393356, -1.403344371\H, -2.1227368513, -2.4180033472, -0.0341715934\O, 1.7709185734, -0.8647455834, 0.3511749485\\Version=ES64L-G16RevB.01\State=1-A\HF=-1049.103545\RMSD=3.417e-09\RMSF=7.063e-06\Dipole=-1.4342062, 0.6266426, 0.0707784\Quadrupole=8.5916222, 1.876761, -10.4683831, 12.9479304, -1.7825877, 0.9971281\PG=C01 [X(C9H11Cl1N3O1)]\@

pIMIU_N1-N5c

1\1\GINC-GRA766\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N3O1(1+)\KJM408\14-Dec-2018\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C, -3.1584181535, -0.595148231, -0.0438581858\C, -1.2720780858, -2.0497403177, 0.0367929948\C, -0.6058072578, -1.2103288129, 0.9080693842\C, -1.2562941285, -0.0252947982, 1.2947960179\C, -2.5333205377, 0.2836244114, 0.8306635204\H, -0.8519246205, -2.9727990493, -0.344468653\H, -0.7435609946, 0.6719801598, 1.9474434309\H, -3.0387731219, 1.1974634638, 1.1173738783\N, -2.5141975539, -1.7286735662, -0.4115057442\C1, -4.7185615415, -0.3305410982, -0.6990334516\C, 0.8048715197, -1.5407394401, 1.3602510092\H, 1.0455213598, -0.9509076641, 2.2564430573\H, 0.8633677845, -2.5976204732, 1.6369187756\C, 3.0703217751, -1.9721110267, 0.3015011605\C, 3.8253134564, -1.1914871368, -0.7933725725\H, 2.9844134456, -3.0380046547, 0.0782270203\H, 3.5583208689, -1.847422704, 1.2794094829\H, 3.6786727755, -1.6503917121, -1.7796533831\H, 4.894990362, -1.1184327581, -0.588285176\N, 1.7574036085, -1.309117178, 0.2836807022\C, 1.9231998814, 0.0163024702, -0.1545277568\N, 3.1674224014, 0.1105940549, -0.7057613787\H, 3.3958124066, 0.8981526983, -1.2949839483\H, -2.9849159289, -2.3613176155, -1.054092404\O, 1.0788019993, 0.9002789982, -0.0313209106\\Version=ES64L-G16RevB.01\State=1-A\HF=-1049.1016229\RMSD=4.598e-09\RMSF=9.226e-06\Dipole=-0.7271338, -1.7726856, -0.0049553\Quadrupole=20.2046236, -9.8302651, -10.3743586, -2.3937221, -0.3868968, 2.6098443\PG=C01 [X(C9H11Cl1N3O1)]\@

pIMIU_N1-N5d

1\1\GINC-GRA782\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N3O1(1+)\KJM408\14-Dec-2018\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C, -3.2454380372, -0.5550891504, -0.3102861508\C, -2.1383308894, 1.2806390625, 0.7350269903\C, -1.0203041756, 0.5138855589, 1.0063099242\C, -1.0431055788, -0.8385794289, 0.5972057318\C, -2.1488067476, -1.373024465, -0.060056177\H, -2.2359658464, 2.3237507402, 1.013547023\H, -0.1674783046, -1.4536056518, 0.7891816634\H, -2.1763773995, -2.408557141, -0.3773292179\N, -3.2077413676, 0.7367380093, 0.0935854864\C1, -4.6640607595, -1.0905693891, -1.1042474999\C, 0.2081639715, 1.1058760559, 1.6870622295\H, -0.0520968055, 2.0329923736, 2.205667937\H, 0.5737900653, 0.3937687229, 2.4321122536\C, 1.352753516, 2.5473084894, -0.1083025278\C, 2.6768329329, 2.2901338123, -0.8606673438\H, 1.370837628, 3.4761207977, 0.46

79027018\H,0.5023736945,2.5754139748,-0.8082289025\H,3.522242571,2.7368031603,-0.3221863739\H,2.6577482345,2.6752669571,-1.8817607303\N,1.2897633412,1.3763187012,0.7649226533\C,2.0249304705,0.3214086637,0.2231524006\N,2.7357746836,0.8276185743,-0.8359704094\H,3.5446688099,0.3131635307,-1.156033899\H,-4.0211583217,1.3202769205,-0.0896575909\O,1.9887684146,-0.8381870689,0.6241002482\\Version=ES64L-G16RevB.01\State=1-A\HF=-1049.1003095\RMSD=6.718e-09\RMSF=3.670e-06\Dipole=-2.1787327,1.543733,-0.1667073\Quadrupole=14.2840203,-2.8494528,-11.4345674,8.8098286,-2.9399261,2.4356219\PG=C01 [X(C9H11Cl1N3O1)]\ \@

pIMIU_N3-N5

1\1\GINC-GRA745\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N3O1(1+)\KJM408\15-Apr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C,-2.7564048364,-0.7757971301,-0.3366604358\C,-0.7008458677,-0.3974585795,0.7954777173\C,-1.0926595522,0.8721163533,1.1914474916\C,-2.3763066617,1.2949067889,0.8172651407\C,-3.2175221223,0.4724674981,0.063514742\H,0.2731174115,-0.8060844887,1.0231464704\H,-2.7239701308,2.2838243688,1.1032504982\H,-4.2076561653,0.7924379833,-0.2373141208\N,-1.5168815764,-1.1680760327,0.0452694849\Cl,-3.6635511828,-1.8551099234,-1.3068597079\C,-0.0962000032,1.7288442637,1.9574640482\H,-0.4467486002,2.7725935909,1.9647245878\H,-0.0791462486,1.397405543,3.0019099121\C,1.5507390621,2.4367495785,0.2550201007\C,2.72819643,1.9035756302,-0.5701941208\H,1.7834819219,3.4662886241,0.5688334145\H,0.6672576565,2.4873905561,-0.3914494674\H,3.6059041498,1.7417927315,0.0669176824\H,3.0064667285,2.6418656028,-1.3263190986\N,1.2426093725,1.5615538494,1.392688377\C,1.831354036,-0.3684062903,-1.1377642681\N,2.415507318,0.6686240066,-1.2498656125\H,-1.1467832665,-2.0536022857,-0.2998188949\H,1.9487219583,1.6556930875,2.1162067033\O,1.262371909,-1.4154819762,-1.1345831442\\Version=ES64L-G16RevB.01\State=1-A\HF=-1049.0752605\RMSD=8.255e-09\RMSF=1.765e-05\Dipole=-1.0054906,1.0687266,1.3620544\Quadrupole=8.0741085,-0.0967818,-7.9773267,9.0121983,4.6597704,3.7887848\PG=C01 [X(C9H11Cl1N3O1)]\ \@

pIMIU_N5-01

1\1\GINC-GRA290\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N3O1(1+)\KJM408\20-Apr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C,-3.1968433622,-0.4852455338,0.019772042\C,-0.9769335878,-1.1656584442,-0.5257078314\C,-0.5457576794,-0.9606594054,0.7745085094\C,-1.492609906,-0.5000482379,1.7040575526\C,-2.8169325959,-0.2647072205,1.3380155392\H,-0.3140818668,-1.5030549515,-1.3124913541\H,-1.1901601595,-0.3146116163,2.7312174491\H,-3.5517867053,0.091572882,2.0496042247\N,-2.2677939037,-0.9270493683,-0.8618848238\Cl,-4.7840627352,-0.2261198337,-0.5666249176\C,0.8918497216,-1.2301639805,1.1734081321\H,1.220441384,-0.4388329721,1.8651876722\H,0.9150457953,-2.1713478967,1.7342146802\C,3.0023165979,-2.2016306506,0.1914462588\C,3.9153271708,-1.6147306004,-0.917681977\H,2.7772281109,-3.2629387965,0.0653141132\H,3.4356347529,-2.042370551,1.1897207627\H,3.8523589739,-2.2037389939,-1.8407652651\H,4.9644148359,-1.5740185448,-0.6176827475\N,1.7799427118,-1.3744657445,0.0311136482\C,2.2469311538,-0.2226981341,-0.6265548299\N,3.3914348382,-0.2595032168,-1.1772009061\H,-2.55

60392647, -1.0768752611, -1.8266268941\H, 1.8219165947, 1.5455039875, -1.1212182229\O, 1.3845381248, 0.8183637052, -0.6483015949\\Version=ES64L-G16RevB.01\State=1-A\HF=-1049.0665872\RMSD=4.906e-09\RMSF=6.618e-06\Dipole=-2.1005778, -0.5525398, 0.6796203\Quadrupole=10.2685988, -8.4655865, -1.8030124, -6.5762033, 3.6783054, 1.350537\PG=C01 [X(C9H11Cl1N3O1)]\@

pIMIU_N3-01

1\1\GINC-GRA116\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N3O1(1+)\KJM408\18-Apr-2019\0\#\# opt=tight freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C, -2.7200852473, -0.0950125721, -0.8308521595\C, -1.8262865667, 1.4740987701, 0.5577719246\C, -0.82364698, 0.6036611735, 1.0038669494\C, -0.8300622792, -0.7077449806, 0.4962934056\C, -1.7906606281, -1.0731263844, -0.4354139871\H, -1.9027078376, 2.4858837177, 0.9550525121\H, -0.0996463725, -1.4369860698, 0.8356588617\H, -1.8358638305, -2.0741995697, -0.8469832524\N, -2.7496925457, 1.140224205, -0.3458959086\Cl, -3.9191373434, -0.5033014542, -2.0193841528\C, 0.2080136903, 1.0670512517, 1.9815301325\H, -0.1242328843, 1.9313779317, 2.5604160822\H, 0.5327871242, 0.2776800112, 2.6625142047\C, 1.3551757462, 2.6336700858, 0.2272232631\C, 1.5020882652, 1.8590410025, -1.1079598149\H, 2.1668472612, 3.3472958152, 0.3766997852\H, 0.3963450239, 3.1315232487, 0.359383955\H, 2.1010927932, 2.4146539405, -1.8319232636\H, 0.5342372075, 1.633583239, -1.5648769653\N, 1.5145104683, 1.5426016421, 1.2761588361\C, 2.1700025525, 0.4533641139, 0.4788184425\N, 2.1693852376, 0.5991339536, -0.7657702029\H, 2.1561764622, 1.8401572928, 2.0194119696\H, 3.061227928, -1.2034935688, 0.7260806979\O, 2.618222215, -0.5207731454, 1.260163875\\Version=ES64L-G16RevB.01\State=1-A\HF=-1049.0498907\RMSD=5.624e-09\RMSF=3.220e-07\Dipole=3.4436247, 1.0223638, 2.0282844\Quadrupole=1.6463709, 2.9150707, -4.5614415, 6.6168223, 6.3900726, 3.6193639\PG=C01 [X(C9H11Cl1N3O1)]\@

pIMIU_01-01

1\1\GINC-GRA47\FOpt\RB3LYP\6-31+G(d,p)\C9H11Cl1N3O1(1+)\KJM408\22-Apr-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C, -3.0192088577, -0.151749948, 0.1626873841\C, -1.0958832713, -0.2181933973, 1.3927555401\C, -0.5882899829, -1.3108354769, 0.6737995929\C, -1.3959085195, -1.8375328739, -0.3573143547\C, -2.6299417007, -1.265743635, -0.6140631605\H, -0.5454776618, 0.1946880517, 2.2390065434\H, -1.0528389672, -2.6876647238, -0.9397397488\H, -3.2857593684, -1.6482110936, -1.3874696196\N, -2.2834189442, 0.3619133674, 1.1349427597\Cl, -4.5446063144, 0.6069830629, -0.163680219\C, 0.78165735, -1.8745634338, 0.9782553145\H, 1.1266356978, -1.534705272, 1.9657768492\H, 0.7375844309, -2.9662348117, 1.0039906195\C, 3.1618706548, -2.0884855673, 0.0957895072\C, 4.0426656063, -1.0352774834, -0.6478641037\H, 3.2128902767, -3.0871411613, -0.3405035175\H, 3.4080270277, -2.1478228389, 1.1634707435\H, 4.3299271256, -1.3736901277, -1.6474294125\H, 4.9478839321, -0.7698797399, -0.1000050095\N, 1.7801636821, -1.5274447069, -0.0587726757\C, 2.0463386005, -0.2470280608, -0.46010379\N, 3.1753952406, 0.165131842, -0.8120370252\H, 1.2042741537, 1.5855520692, -0.6698722259\O, 0.9110349193, 0.6501140273, -0.617599576\H, 0.1270838102, 0.4459123016, -0.0021869056\\Version=ES64L-G16RevB.01\State=1-A\HF=-1048.9905514\RMSD=5.340e-09\RMSF=2.744e-05\Dipole=2.3238358, -0.7097568, -0.1266413\Quadrupole=9.7302915, -0.978771, -8.7515206, -2

.2303651,4.2587108,-0.9709631\PG=C01 [X(C9H11Cl1N3O1)]\ \@

pDIMI_N3-N5

1\1\GINC-GRA21\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4(1+,2)\KJM408\12-Feb-2019\0\#\ opt=(Tight) freq b3lyp/6-31+g(d,p) geom=connectivity empiric aldispersion=gd3\Title Card Required\1,2\C,-3.203705233,-1.149476268 3,0.4504573141\C,-0.9864291194,-0.3392347678,0.1025025091\C,-1.3247714 554,0.9201765685,0.5819359136\C,-2.6519193596,1.1204786427,0.992914177 5\C,-3.5951815862,0.092792339,0.9323701645\H,0.0099307547,-0.607591050 1,-0.2379769919\H,-2.9603134935,2.0939528051,1.3642726095\H,-4.6214771 245,0.2414269675,1.2452093381\N,-1.9180194716,-1.3197346137,0.05542512 29\C1,-4.2580365804,-2.491255254,0.317426043\C,-0.267416297,2.00535850 81,0.6722071583\H,-0.7600318573,2.9896985225,0.7271695395\H,0.26316753 82,1.8773914351,1.6246907036\C,1.9681092092,2.5984723054,-0.2140715829 \C,3.0180168908,1.7364913708,0.5397926283\H,1.8539731114,3.5343198672, 0.3542800316\H,2.3742887658,2.8590417722,-1.1944196233\H,2.6051713806, 1.4130916384,1.5052312082\H,3.9034440154,2.3475793695,0.7253631891\N,0 .7032394595,1.8947940776,-0.4090696438\C,2.6198018943,-0.3917013386,-0 .3993835386\N,1.9425356064,-1.3582356616,-0.5873883212\N,3.4247799235, 0.5925540883,-0.2594472195\H,-1.6321291731,-2.233229725,-0.2944947066\ H,0.2854080809,2.1381273911,-1.3012714229\Version=ES64L-G16RevB.01\St ate=2-A\HF=-1028.5269064\S2=0.770962\S2-1=0.\S2A=0.750138\RMSD=3.151e- 09\RMSF=4.772e-07\Dipole=-1.9289928,1.2436511,0.7010688\Quadrupole=7.5 839807,3.2606518,-10.8446325,13.6863491,0.1505424,0.8321941\PG=C01 [X(C9H11Cl1N4)]\ \@

pDIMI_N2-N3a

1\1\GINC-GRA396\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4(1+,2)\KJM408\13-Mar -2019\0\#\ opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe rsion=gd3\Title Card Required\1,2\C,1.9797141732,0.5593368898,-0.909 9575982\C,0.3126407987,1.7741430692,0.0582959367\C,-0.0944880161,0.701 1019699,0.8613358716\C,0.6419984093,-0.4935425755,0.7676776561\C,1.699 4728606,-0.5745901391,-0.1271256833\H,-0.1816640578,2.7425700081,0.129 7852122\H,0.3981427485,-1.3450824511,1.3966508115\H,2.2979643416,-1.47 24450477,-0.2239578736\N,1.3177120152,1.7062444086,-0.8176753875\C1,3. 2707927859,0.4860168383,-2.0693517069\C,-1.2710129543,0.8350426544,1.7 767793767\H,-1.1769036005,0.2237158391,2.6769227418\H,-1.4613026103,1. 8727562715,2.0599145864\C,-2.9678249235,1.015322547,-0.1871270083\C,-2 .5682220331,-0.0440407836,-1.2395220032\H,-2.4484228035,1.9664512452,- 0.2889159316\H,-4.0459049239,1.1849180401,-0.1745906385\H,-1.574772762 2,0.147688904,-1.6713334801\H,-3.2698323063,-0.1006477965,-2.078008306 5\N,-2.5901419301,0.3498117232,1.1169031662\C,-2.5354952395,-1.1334064 071,0.7513972754\N,-2.4963141915,-1.9575213546,1.7477369199\N,-2.51208 20017,-1.3198442129,-0.5606008488\H,-3.3272012192,0.4696538944,1.81868 10358\H,-2.4696972895,-2.9256871848,1.4127558762\Version=ES64L-G16Rev B.01\State=2-A\HF=-1028.5265613\S2=0.780502\S2-1=0.\S2A=0.750165\RMSD= 7.327e-09\RMSF=3.740e-06\Dipole=-3.5705213,-0.104931,1.551771\Quadrupo le=10.2727545,-4.6928352,-5.5799193,-6.2809474,-3.0325387,1.0716132\PG =C01 [X(C9H11Cl1N4)]\ \@

pDIMI_N2-N3b

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1\1\GINC-GRA21\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4(1+,2)\KJM408\10-Mar-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,2\C,3.1045213795,0.1224828033,-0.7200379773\C,2.0418225617,1.4957958156,0.7553594543\C,0.9997956138,0.5818852349,0.957960444\C,1.0751829708,-0.6491333226,0.2809483369\C,2.1416491918,-0.8919795462,-0.5724464954\H,2.0630962929,2.4441882512,1.2916057962\H,0.3135505577,-1.4116865467,0.4181142454\H,2.2399612014,-1.827972651,-1.1089945644\N,3.0670665071,1.2803445214,-0.0714482414\Cl,4.4365533759,-0.1303624524,-1.8039500831\C,-0.1437393225,0.927542748,1.8599412395\H,-0.5223915605,0.0588696095,2.4052422687\H,0.1206923751,1.7052330009,2.5802466893\C,-1.0853869806,2.6798684501,0.2010742697\C,-0.9941977603,2.0512124498,-1.2076092636\H,-0.1770829425,3.185373564,0.5254119229\H,-1.9351903246,3.3596255459,0.284696247\H,0.0443145984,1.8571902746,-1.513970053\H,-1.4348063473,2.6841397043,-1.9851647226\N,-1.3632434967,1.486348766,1.0845000208\C,-1.9446576731,0.4315749337,0.0818940526\N,-2.5579839309,-0.641542539,0.4545549448\N,-1.6810724096,0.7853061282,-1.1657281326\H,-2.0834945828,1.7184610719,1.7747358835\H,-2.6767822345,-0.7420907856,1.4656327076\Version=ES64L-G16RevB.01\State=2-A\HF=-1028.5140264\S2=0.780216\S2-1=0.\S2A=0.750167\RMSD=4.807e-09\RMSF=1.677e-05\Dipole=-3.2549441,1.4620187,2.35948\Quadrupole=0.5420709,-0.2307538,-0.3113171,-11.769838,-11.8829002,0.5455634\PG=C01 [X(C9H11Cl1N4)]\@
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pDIMI_N1-N3

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1\1\GINC-GRA284\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4(1+,2)\KJM408\14-Mar-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,2\N,3.0691249173,1.7069181871,0.0669987733\C,2.0907360365,2.7448319457,-0.2647783156\H,2.2670462959,3.6477129863,0.3227406038\H,2.1053804279,3.003332144,-1.3311232712\C,0.7863345489,2.0559285611,0.1419521535\H,0.6182893811,2.1211567118,1.21770886\H,-0.1006627435,2.3883893957,-0.3952846249\N,1.0587876994,0.5948367397,-0.1741667515\C,2.5723513977,0.4482126763,-0.0768932308\N,3.0822828979,-0.7068318247,-0.1368790165\C,0.2838870436,-0.4311348114,0.6790363177\H,0.6900381957,-1.4050402027,0.3964750302\H,0.562907097,-0.218876488,1.7130883541\C,-1.1859619566,-0.3139649423,0.4260649468\C,-1.7960396332,-0.9553530392,-0.6668390541\C,-3.1570916607,-0.7899948752,-0.8804592266\C,-2.00309398,0.4501966435,1.2680458252\C,-3.8633351659,0.0248928721,0.0227261011\Cl,-5.564733073,0.2739302132,-0.221617198\N,-3.3117461542,0.623648789,1.070888979\H,-1.5912676133,0.9367813963,2.1514416746\H,-3.6698363386,-1.274287016,-1.7028175764\H,-1.2190681739,-1.5949987215,-1.3314912921\H,4.0671379654,1.8583385687,-0.0097912985\H,0.8135750285,0.4128624103,-1.1547623631\Version=ES64L-G16RevB.01\State=2-A\HF=-1028.5142943\S2=0.758093\S2-1=0.\S2A=0.750037\RMSD=6.441e-09\RMSF=8.000e-06\Dipole=3.4148532,1.3968204,-0.8187519\Quadrupole=8.9344963,-1.7285908,-7.2059054,18.0246442,2.0991119,0.7009869\PG=C01 [X(C9H11Cl1N4)]\@
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pDIMI_N1-N1

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1\1\GINC-GRA1111\FOpt\UB3LYP\6-31+G(d,p)\C9H11Cl1N4(1+,2)\KJM408\11-De
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c-2018\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,2\C,-3.242494238,-0.4348234962,-0.2337688636\C,-2.0366279607,1.2740752734,0.6656405791\C,-1.0111182259,0.4199650115,1.0838147209\C,-1.1626966932,-0.9516543903,0.8228752766\C,-2.2972145713,-1.3974183258,0.1561545569\H,-1.9887534384,2.3426896305,0.8737799895\H,-0.4070042904,-1.6634749769,1.1450081476\H,-2.4598419925,-2.4474446605,-0.0554587837\N,-3.1284631452,0.8625161087,0.0120284148\C1,-4.6684270654,-0.9528743469,-1.0941870556\C,0.2283198843,0.9711817521,1.7450029133\H,0.0168028197,1.8930352281,2.2927040361\H,0.6652496127,0.2544169668,2.4462947581\C,1.1645086253,2.4532320234,-0.1403859047\C,2.5160359398,2.4417589792,-0.8587232498\H,1.0219957393,3.3719022636,0.4330661875\H,0.3220095997,2.3351464501,-0.8346754039\H,3.2997247711,2.9022157893,-0.2565779941\H,2.5077758389,2.8634308396,-1.8637669019\N,1.2912044517,1.3058542065,0.763263015\C,2.0391685798,0.3146481252,0.2134495651\N,2.1853956306,-0.9219237629,0.4380047601\N,2.8254240636,0.9513296836,-0.933006088\H,3.8244065866,0.7366267803,-0.8413273385\H,2.5043641477,0.5294787878,-1.8127676968\Version=ES64L-G16RevB.01\State=2-A\HF=-1028.5084786\S2=0.757555\S2-1=0.\S2A=0.750034\RMSD=3.521e-09\RMSF=1.195e-05\Dipole=5.5537111,2.1200602,-0.9479785\Quadrupole=14.1287563,-5.4560086,-8.6727477,16.7949151,-12.7341901,-1.3255212\PG=C01 [X(C9H11C11N4)]\@

pIMI-NOOH_N2-N2c

1\1\GINC-GRA50\FOpt\RB3LYP\6-31+G(d,p)\C9H10C11N4(1+)\KJM408\27-Jul-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-2.9134829654,-0.6851871332,-0.2236266351\C,-1.144709099,-0.0235996988,1.0523018068\C,-0.4353796835,0.4413853192,-0.0610722964\C,-1.0485817213,0.3311407224,-1.3204724361\C,-2.3112771337,-0.2380064117,-1.4132052383\H,-0.725780251,0.0602866509,2.0546305396\H,-0.5514360181,0.696259861,-2.2158083907\H,-2.826507322,-0.3331311509,-2.3614920429\N,-2.3557531744,-0.5817626125,0.9758716261\C1,-4.4866415668,-1.4194630797,-0.3006360298\C,0.9368454199,1.0266828163,0.0989187101\C,1.9036802361,-1.2812084493,-0.1616263568\C,3.2670661371,-1.8605834429,-0.2719108972\H,3.3819020144,-2.393699097,-1.229390333\H,3.4457148828,-2.6141841698,0.5105598327\N,2.022483619,0.0028677165,-0.024817498\C,3.4615807591,0.3102756718,-0.0303775137\N,3.8493037717,1.6062864603,0.0066625423\N,4.1777810226,-0.7431274938,-0.1594886347\H,3.307240781,2.2933672593,0.5109869177\H,1.1537889206,1.7802498336,-0.6641417655\H,0.9386139955,-1.7734528844,-0.192267862\H,1.0632544261,1.4846303385,1.0858275568\H,4.8511046993,1.7562028443,0.0165036783\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.973157\RMSD=9.553e-09\RMSF=1.086e-05\Dipole=3.382483,0.8324798,-0.3529994\Quadrupole=6.17375,1.8463668,-8.0201168,4.1417421,7.1453369,3.152517\PG=C01 [X(C9H10C11N4)]\@

pIMI-NOOH_N1-N2c

1\1\GINC-GRA1088\FOpt\RB3LYP\6-31+G(d,p)\C9H10C11N4(1+)\KJM408\25-Jul-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,1\C,-2.8651341448,-0.6056609453,-0.2233097504\C,-1.0747467107,0.0416420119,1.0290618406\C,-0.3905179308,0.5352439618,-0.0881325753\C,-1.0310194964,0.4478899941,-1.3355382414\C,-

2.2926084985, -0.1271145265, -1.4145802496\H, -0.6365281329, 0.110895804, 2.0241052854\H, -0.5559335209, 0.838988792, -2.2318551291\H, -2.8283791413, -0.202979748, -2.3531724647\N, -2.2832427237, -0.5252355574, 0.9661452155\C1, -4.4351739977, -1.3521717709, -0.2838416655\C, 0.97807438, 1.1297136519, 0.0568682531\C, 1.9435056001, -1.1700189271, -0.2224835988\C, 3.2816303603, -1.8206943174, -0.2822993888\H, 3.4087571732, -2.3539137795, -1.2362852614\H, 3.3842372371, -2.5591267639, 0.5272139411\N, 2.0592836037, 0.1014647651, -0.0667081976\C, 3.4761625782, 0.5054437937, 0.0029493804\N, 3.7428956217, 1.7264196166, 0.159060712\N, 4.1571948953, -0.6760053643, -0.137937389\H, 5.1640672839, -0.7360202118, -0.1118092163\H, 4.734949832, 1.9506069939, 0.2013161671\H, 1.2062423408, 1.8812831168, -0.7027487161\H, 0.97878109, -1.6607348403, -0.293087604\H, 1.1408720812, 1.6004662904, 1.0301501029\\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9717898\RMSD=7.984e-09\RMSF=4.857e-06\Dipole=4.6546341, -0.7508904, -0.7947527\Quadrupole=21.806639, -9.4908081, -12.315831, -7.5866105, 4.7907668, 0.6930118\PG=C01 [X(C9H10Cl1N4)]\@

pIMI-NOOH_N1-N2a

1\1\GINC-GRA1023\FOpt\RB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+)\KJM408\16-Jul-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C, -2.8680096821, -0.4307216527, 0.2429471739\C, -1.2391528696, 0.371698919, -1.1323930492\C, -0.393351697, 0.6772873719, -0.0636260731\C, -0.8603122184, 0.4044649905, 1.23274401\C, -2.1188900501, -0.1560202371, 1.4010137641\H, -0.9366340953, 0.5815649068, -2.1576006672\H, -0.2492073236, 0.6370310849, 2.1014654026\H, -2.5231378859, -0.3719387912, 2.3827748894\N, -2.4518999691, -0.176930736, -0.9878981661\C1, -4.4457750707, -1.1514536344, 0.4130296608\C, 0.9799688298, 1.251354615, -0.3070936643\C, 1.9262186306, -1.1136772237, -0.6218943297\C, 3.2540398257, -1.6844307181, -0.2779097342\H, 1.7696123512, -1.151816679, -1.713341071\H, 1.1104017995, -1.6937505682, -0.1648060207\N, 2.0281330145, 0.2364827766, -0.0948738856\C, 3.277273351, 0.5022233019, 0.4070529277\N, 3.9182785384, 1.4680460295, 0.9053201498\N, 3.97121668, -0.7814947028, 0.290301537\H, 3.4153012662, 2.3511657882, 0.9525289923\H, 1.0603062707, 1.6503281881, -1.3256515994\H, 1.1856616524, 2.0697161176, 0.3888584878\H, 3.6018256453, -2.6959996938, -0.4629034855\H, 4.9289485067, -0.874368123, 0.6309768009\\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9593792\RMSD=3.772e-09\RMSF=1.939e-06\Dipole=5.0254549, -1.1472283, -0.073734\Quadrupole=13.7311985, -3.2098324, -10.5213661, -13.4999962, -7.4432199, 0.9869248\PG=C01 [X(C9H10Cl1N4)]\@

pIMI-NOOH_N2-N3a

1\1\GINC-GRA726\FOpt\RB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+)\KJM408\24-Jul-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,1\C, -1.3859146794, 0.7281127625, 2.9694392448\C, -1.0544923807, 0.1765137522, 0.7852336957\C, 0.0345642783, 1.0490422226, 0.6588848638\C, 0.3761985965, 1.8245846418, 1.782630825\C, -0.3406179405, 1.6688340893, 2.959792764\H, -1.4049251874, -0.4035326453, -0.0688752932\H, 1.182788433, 2.5494008306, 1.7294328642\H, -0.116571565, 2.2514865383, 3.8452500633\N, -1.7453539709, 0.0076997834, 1.914570184\C1, -2.2850950682, 0.4818827867, 4.4348879428\C, 0.7753664618, 1.158467213, -0.6359872351\

C,1.825067291,-1.2104533078,-0.4237221054\C,2.6455191536,-1.4249297801,0.8264499955\H,2.1906821432,-1.8045511974,-1.2665608951\H,0.7666578219,-1.4267196436,-0.266684488\N,2.0433117946,0.2554718225,-0.6773660728\C,3.0903668307,0.6671367666,0.3792248199\N,3.548028016,1.8268267585,0.3075069481\N,3.3121465737,-0.4104942515,1.2362025314\H,4.2404795159,2.0210460282,1.0337359655\H,0.1721490692,0.8368123438,-1.488113075\H,1.1634489654,2.162334803,-0.8183877768\H,2.6730874872,-2.3781457484,1.3480311175\H,2.4785946702,0.4064039912,-1.592621514\\Version=ES64L-G16RevB.01\State=1-A\HF=-1027.9506912\RMSD=5.501e-09\RMSF=4.970e-06\Dipole=2.6190494,-0.706595,-3.0336165\Quadrupole=-4.865101,-1.5100464,6.3751474,-4.6456168,-6.8938772,7.8321945\PG=C01 [X(C9H10Cl1N4)]\@\

pDIMI-H_N2

1\1\GINC-CDR688\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\30-Aug-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,3\C,-1.6517678754,1.1434401419,-2.8962555845\C,-1.1477788846,0.122530305,-0.9212710478\C,-0.0566549781,0.9812786897,-0.6952914699\C,0.2249460739,1.9641597526,-1.6607058495\C,-0.5936877049,2.0688846775,-2.773374416\H,-1.4240549754,-0.6334461782,-0.1877338298\H,1.0631082924,2.6417596059,-1.5263205175\H,-0.4301002004,2.8205832238,-3.5364059293\N,-1.9307701163,0.2070594514,-1.9939332923\Cl,-2.6493554357,1.1906075121,-4.3071542573\C,0.7949546379,0.827604609,0.5513549475\C,1.9576204637,-1.4548109855,0.1530197572\C,3.3499346361,-1.7561622869,-0.4530786426\H,1.1192674955,-1.8399098842,-0.4360222817\H,1.8410113277,-1.8140580455,1.1841892694\N,1.9411013036,0.0053234034,0.1614576616\C,3.1556768354,0.4977539508,-0.3208344546\N,3.341533666,1.8054867986,-0.393974486\N,4.0158422002,-0.4856476095,-0.6618068447\H,3.2927563918,-2.2783748533,-1.4181305843\H,1.1706559429,1.7850769106,0.9141149191\H,3.9765467597,-2.3823682606,0.1939951087\H,0.2604916396,0.3102566419,1.3511722414\H,4.2892154444,1.9943462294,-0.7369419971\\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8868559\S2=2.033117\S2-1=0.\S2A=2.000306\RMSD=7.561e-09\RMSF=5.822e-06\Dipole=2.0865864,-0.8540417,1.8531067\Quadrupole=-1.6377943,1.341784,0.2960103,-6.653487,6.4626468,-8.5709751\PG=C01 [X(C9H10Cl1N4)]\@\

pDIMI-H_N1

1\1\GINC-GRA650\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\03-Sep-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,3\C,0.9627150396,4.8880036848,0.2002225977\C,0.8651126026,2.9259277772,-0.9481364204\C,0.7493558593,2.1686021842,0.2337887521\C,0.7014223626,2.8688642252,1.4537756074\C,0.8131417823,4.2503037199,1.4467662641\H,0.8686955726,2.4341742205,-1.9198290177\H,0.5807742133,2.3368491093,2.3934597574\H,0.7812044415,4.8310324421,2.3607371105\N,0.9789275893,4.2523950237,-0.9661762025\Cl,1.1226130156,6.6138408007,0.1550550255\C,0.6378970358,0.6676271394,0.1711570691\C,2.1207009926,-1.4481575309,-0.055572176\C,3.6354576738,-1.6079707366,-0.3476054\H,1.4863716073,-1.87331243,-0.8365498724\H,1.8302531798,-1.8777065027,0.9105299227\N,1.9497511924,0.0190447088,0.0019266662\C,3.14515651,0.6181809336,0.0892737987\N,3.3416582336,1.9583366686,0.2525000098\N,4.1485982244,-0.2697960241,-0.0008116265\H,3.8341565444,-1.82

08565644, -1.4032804621\H, 0.1837796166, 0.2687734473, 1.0864651125\H, 4.104016588, -2.3767961543, 0.268586138\H, 0.0161899887, 0.3483523541, -0.6729188625\H, 5.1139215439, 0.0188241635, -0.0965263915\\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8840145\S2=2.015103\S2-1=0.\S2A=2.00011\RMSD=4.044e-09\RMSF=1.360e-05\Dipole=0.9559255, -4.6493629, 0.4550032\Quadrupole=-3.5386769, 15.7364302, -12.1977533, -11.1298699, -3.528224, 6.9094734\PG=C01 [X(C9H10C11N4)]\ \@

pDIMI-H_N5

1\1\GINC-GRA1045\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\23-Aug-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,3\C,0.8599509036,4.9595366794,-0.2081900566\C,0.8091687752,3.0691620459,1.2422374702\C,0.714733165,2.1969236226,0.1714069098\C,0.7046032289,2.7494289085,-1.1195514407\C,0.7683480617,4.1278216459,-1.3178143749\H,0.8635712534,2.7458253782,2.274293473\H,0.6606473151,2.0886478921,-1.9801161735\H,0.7576991331,4.5651767568,-2.3086763964\N,0.8733990939,4.4058730223,1.0292324888\C1,0.9586334876,6.6638161105,-0.3095773751\C,0.7269564931,0.6960161913,0.3849593466\C,2.1008918392,-1.2893625869,-0.3971206886\C,3.6340700009,-1.4577412405,-0.4222336359\H,1.6200279297,-1.5151440854,-1.3521001209\H,1.6428837729,-1.9060568434,0.3905348158\N,1.9921073923,0.1469278732,-0.0806376042\C,3.1801186109,0.4845793419,0.6110303411\N,3.3036541983,1.5468550019,1.3667352511\N,4.1834786649,-0.4036404623,0.4285922679\H,4.043977415,-1.3072727574,-1.4330052942\H,0.9648064842,5.0252348962,1.8320024887\H,0.5344361415,0.4613997476,1.4436195708\H,3.9825280575,-2.4347271208,-0.0764584165\H,-0.075462978,0.2414557824,-0.2035691263\\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8789411\S2=2.042724\S2-1=0.\S2A=2.000365\RMSD=6.095e-09\RMSF=6.956e-06\Dipole=-2.2384973,0.7327532,-0.3972446\Quadrupole=-16.2372107,20.5147689,-4.2775582,-4.6700482,-4.2790397,5.1615462\PG=C01 [X(C9H10C11N4)]\ \@

pDIMI-H_N3

1\1\GINC-CDR608\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\04-Sep-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,3\C,0.6550191745,4.926946561,0.0444930879\C,0.4618642201,2.8724341116,-0.9169933119\C,0.7370439011,2.211906556,0.2891882308\C,0.9515749199,3.0032202525,1.4317732961\C,0.9059072282,4.3849742708,1.3163212477\H,0.2383255092,2.3088809413,-1.8244977918\H,1.1496634754,2.5459881578,2.3966720497\H,1.0617348124,5.0328490812,2.1703165302\N,0.4331033574,4.1979733458,-1.0455650857\C1,0.6187807121,6.6507841112,-0.1464553884\C,0.7766831667,0.7149276137,0.3299933246\C,2.0936756915,-1.3412867183,-0.4997289734\C,3.5740361438,-1.7056982907,-0.2541302814\H,1.719061978,-1.5940293648,-1.4920142738\H,1.4404557706,-1.7735067035,0.2607199868\N,2.0645277376,0.1615616404,-0.3096871661\C,3.3651401883,0.4219231277,0.4916093679\N,3.5665787205,1.6037180003,1.0206567163\N,4.155924234,-0.6205213721,0.5174576595\H,4.1524109345,-1.7948947037,-1.1850276319\H,0.752883757,0.3157047243,1.3459950012\H,3.695336198,-2.6504899077,0.2836486583\H,-0.0347285383,0.2658891825,-0.2498893105\H,2.1794303173,0.6376665225,-1.2128672324\\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8516749\S2=2.044232\S2-1=0.\S2A=2.000373\

RMSD=5.885e-09\RMSF=7.021e-05\Dipole=0.1141044,-4.6538848,-0.2810486\Quadrupole=-12.9944761,20.4905945,-7.4961184,-5.0211087,-4.8459102,10.1482571\PG=C01 [X(C9H10C11N4)]\ \@

pDIMI-H_C2_N1-N2

1\1\GINC-CDR721\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\13-Feb-2020\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,-1.6445508013,1.0135737344,-2.8623723851\C,0.2804543992,1.6018748077,-1.8001275282\C,-0.0730195588,0.840967013,-0.641004361\C,-1.2885878186,0.1844478464,-0.6444680288\C,-2.104911024,0.2557201516,-1.7644710362\H,1.216918056,2.1540780843,-1.840510638\H,-1.606314923,-0.3843973589,0.2251455807\H,-3.0643321217,-0.2461500373,-1.8070928244\N,-0.490121266,1.6716872476,-2.8852793659\Cl,-2.6219884969,1.0959588339,-4.2883718408\C,0.8774726939,0.8599798627,0.5363174705\C,2.0562098623,-1.3837821188,-0.0077127357\C,3.4780368333,-1.6505129614,-0.3984969736\H,1.3139931052,-1.6868960489,-0.7647385655\H,1.7500762653,-1.847799847,0.9445980095\N,2.0487603478,0.0777052701,0.1448830588\C,3.2775371003,0.6209278493,-0.1841993473\N,3.4527210482,1.9185447635,-0.115120187\N,4.0968448293,-0.4133624851,-0.537364034\H,4.4075812179,2.2039899083,-0.3409421217\H,1.2254783836,1.8560892893,0.8138643479\H,0.4258399044,0.3801289378,1.4097212238\H,3.8770024811,-2.5430669831,-0.8534901985\H,5.0649776424,-0.2825485677,-0.7968889994\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.892292\S2=2.025265\S2-1=0.\S2A=2.000213\RMSD=3.798e-09\RMSF=6.990e-06\Dipole=2.4092422,-1.647379,2.0558029\Quadrupole=20.4174345,-9.4052539,-11.0121807,-2.2684977,4.451425,-1.7871143\PG=C01 [X(C9H10C11N4)]\ \@

pDIMI-H_C2_N1-N5

1\1\GINC-CDR603\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\13-Feb-2020\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,-0.0938729825,3.6524715951,2.8541154203\C,0.6758851522,3.1029008887,0.6676222709\C,0.3536066417,1.7678046354,0.8463862078\C,-0.2021884855,1.3896266597,2.077262702\C,-0.4370823615,2.327028615,3.08350229\H,1.1472726136,3.4887921902,-0.227188032\H,-0.4369197395,0.3448416641,2.257360928\H,-0.8661264946,2.0474932854,4.0378379018\N,0.4427121817,3.9970245441,1.6568998501\Cl,-0.3108376412,4.8996061473,4.0058815166\C,0.7076695216,0.7410489666,-0.2102872772\C,2.094390917,-1.3795936496,-0.3631751094\C,3.513403833,-1.6223816348,0.0567330454\H,1.9804412615,-1.3321918272,-1.4644431593\H,1.3888442239,-2.1250504864,0.0195471945\N,1.834702643,-0.0560344387,0.245546737\C,3.0636081851,0.5918793472,0.4705532815\N,3.2115881705,1.8412963689,0.7448557263\N,4.0479156301,-0.3660182021,0.3425398303\H,-0.1396620326,0.0658527983,-0.3615455054\H,0.9126453596,1.2393159903,-1.1702127142\H,4.1528616054,-2.4120895418,-0.3111787137\H,4.9974433452,-0.1938218362,0.639716826\H,0.7139989425,4.9672625503,1.513032763\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8823326\S2=2.013711\S2-1=0.\S2A=2.000092\RMSD=5.495e-09\RMSF=2.418e-06\Dipole=-1.1737455,0.3924195,-0.2790571\Quadrupole=-4.639902,9.5554886,-4.9155865,-10.3105281,-6.5836938,9.302008\PG=C01 [X(C9H10C11N4)]\ \@

pDIMI-H_C2_N2-N2

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1\1\GINC-CDR686\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\10-Feb-2020\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,-1.5230660481,1.0200783368,-2.8687795022\C,0.2841243702,1.7208318652,-1.6768525338\C,-0.070705588,0.9145884463,-0.5667857954\C,-1.2067238925,0.0939452385,-0.679457053\C,-1.9661153219,0.156256327,-1.83521506\H,1.1745078558,2.3439324196,-1.6395322254\H,-1.5130352032,-0.5490533519,0.1408141181\H,-2.8711095426,-0.426951996,-1.9599299172\N,-0.435505286,1.7843349844,-2.7924097196\C1,-2.4213011957,1.0857731711,-4.334814522\C,0.8228467657,0.8896467266,0.6590046949\C,1.9499929829,-1.3666098336,0.065081885\C,3.1813307847,-1.536853639,-0.7953716551\H,1.0113232538,-1.6918500922,-0.4051896519\H,2.0127802701,-1.8578092326,1.0519614602\N,1.9705180412,0.0950409154,0.252232592\C,3.1873598157,0.5873773478,-0.3691081673\N,3.4505840594,1.9304021096,-0.3665563386\N,3.8532252868,-0.3627365132,-0.9544733157\H,1.1461509595,1.8878369586,0.9550649033\H,0.3336254138,0.4094792009,1.5104902746\H,3.5409840875,-2.4679952144,-1.206996897\H,3.3742612587,2.4261304364,0.5162791755\H,4.3011881525,2.1649839686,-0.8687689667\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8797991\S2=2.018418\S2-1=0.\S2A=2.000173\RMSD=5.552e-09\RMSF=7.063e-06\Dipole=0.1997733,-0.347808,2.5154561\Quadrupole=4.317484,-2.826745,-1.490739,6.2125121,8.7010936,1.1748834\PG=C01 [X(C9H10Cl1N4)]\@\
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pDIMI-H_C2_N2-N5

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1\1\GINC-GRA1091\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\14-Feb-2020\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,-1.8000642186,0.9912834179,-2.8627296761\C,0.0092879252,1.9944750565,-1.6359951973\C,-0.0783806794,1.0182735749,-0.6742796977\C,-1.0526969137,-0.0103161945,-0.8014467247\C,-1.9093993075,-0.006118647,-1.9250630284\H,0.7387747006,2.7954024757,-1.6103347612\H,-1.2001685631,-0.7389310897,-0.0121034956\H,-2.666253233,-0.7695034253,-2.0586606284\N,-0.852879782,1.9901761023,-2.7071123442\C1,-2.7864668203,1.1035474012,-4.2681613936\C,0.9235414661,1.008463245,0.4595516789\C,1.9336405236,-1.334980287,0.0461522365\C,3.2847821413,-1.682555738,-0.4945738072\H,1.0878119386,-1.612184118,-0.6171111494\H,1.7100603775,-1.7643141257,1.035391903\N,2.0364422224,0.1123428938,0.120542689\C,3.2699956444,0.4681468276,-0.3488864677\N,3.5712902545,1.7771546823,-0.4445371427\N,4.022890379,-0.6173392356,-0.7123811293\H,1.3489701971,1.9951347797,0.640963234\H,0.4686426152,0.6385037582,1.3841128115\H,3.6310076257,-2.6873890304,-0.7027269128\H,4.5273507363,1.8697148779,-0.8065004099\H,-0.8202949199,2.7417105982,-3.3849112766\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8787408\S2=2.024012\S2-1=0.\S2A=2.000282\RMSD=8.384e-09\RMSF=8.050e-06\Dipole=0.4155972,-0.295693,0.9403523\Quadrupole=-0.3547438,2.0187629,-1.664019,-1.7623855,7.895416,-8.5925762\PG=C01 [X(C9H10Cl1N4)]\@\
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pDIMI-H_C2_N1-N3

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1\1\GINC-CDR546\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\10-Feb-2020\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,-2.9456722715,-0.4017050876,0.20
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35547782\C, -1.0937360151, 0.0486405033, -1.0455890008\C, -0.4082093103, 0.5893864235, 0.0492384663\C, -1.0849001345, 0.6407490427, 1.2811413055\C, -2.3756536264, 0.1395585301, 1.3701545277\H, -0.6322074748, 0.0192794965, -2.0319342689\H, -0.6176654078, 1.0867660535, 2.1566743116\H, -2.9376012719, 0.168395067, 2.2959449423\N, -2.3324127868, -0.442675352, -0.9728988586\C1, -4.5520025577, -1.0567432277, 0.2775697011\C, 0.9971762389, 1.0830449995, -0.0916021076\C, 2.0077046652, -1.2808765479, -0.5029365028\C, 3.4058913332, -1.7642644215, -0.2973061479\H, 1.8029391488, -0.9660260395, -1.5361254186\H, 1.2186727542, -1.9567880285, -0.1721800297\N, 1.9899143081, -0.0098555467, 0.3467257104\C, 3.4382075592, 0.4425556524, 0.3871831176\N, 3.737145981, 1.618407559, 0.7582063675\N, 4.1719834101, -0.6454663968, 0.0118428104\H, 1.2673594722, 1.3297280606, -1.1201498923\H, 1.213377577, 1.94367534, 0.5458523977\H, 3.8526811065, -2.6291966611, -0.7639779921\H, 5.183625438, -0.6360558097, 0.0651609556\H, 1.7478406441, -0.2740208291, 1.3112924475\\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8543009\S2=2.019891\S2-1=0.\S2A=2.000137\RMSD=9.715e-09\RMSF=1.340e-05\Dipole=3.7656006, -0.5764365, 0.3273692\Quadrupole=17.3095631, -10.1333694, -7.1761937, -10.4653141, -8.2056052, 1.1568051\PG=C01 [X(C9H10Cl1N4)]\@

pDIMI-H_C2_N2-N3

1\1\GINC-GRA767\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\14-Feb-2020\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,3\C,1.0316200353,4.9627406151,0.2983553376\C,1.1159550753,3.0930547616, -1.0004664505\C,0.8546997982,2.2467716434,0.0895360512\C,0.6372157815,2.8488524785,1.3434706506\C,0.7261995112,4.2259779855,1.4600454557\H,1.2478418396,2.6820734392, -2.0009127144\H,0.388725712,2.2495784876,2.2165619315\H,0.5636775616,4.7316710224,2.4042393402\N,1.2140852467,4.4192165606, -0.8995513851\C1,1.1746909761,6.685358447,0.4103332859\C,0.7881562155,0.7604960087, -0.1039715741\C,2.1217352837, -1.4276469271,0.2037166339\C,3.5172677926, -1.597060257, -0.3528361617\H,1.3407815399, -1.7172820041, -0.5079619192\H,1.9453062054, -1.9462180297,1.1498658633\N,2.0561332647,0.0785114189,0.4097163306\C,3.3532000267,0.571704695, -0.2513312634\N,3.7021411587,1.8665619476,0.0415821124\N,4.1243081885, -0.4389898185, -0.5826956946\H, -0.0413338425,0.3049456614,0.4445974263\H,0.7095401499,0.4891280972, -1.1588864271\H,3.9605720561, -2.5481847647, -0.616964323\H,2.1403644284,0.3010273091,1.4103150572\H,3.7312340251,2.5080027122, -0.7593374033\\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8470512\S2=2.025204\S2-1=0.\S2A=2.000196\RMSD=3.900e-09\RMSF=1.735e-05\Dipole=-0.7748441, -3.9180401,0.8184667\Quadrupole=-12.0395709,18.6949155, -6.6553446, -0.85718, -2.8496404,1.9454865\PG=C01 [X(C9H10Cl1N4)]\@

pDIMI-H_C2_N3-N5

1\1\GINC-CDR405\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\11-Feb-2020\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,3\C,0.8041462564,4.9824631034,0.3386800718\C,0.968562715,3.056825487, -1.0962566228\C,0.7246937459,2.2230061965, -0.0292860913\C,0.5198903579,2.7780820097,1.2698831\C,0.5755242718,4.1822209337,1.4272829648\H,1.1592065138,2.7029039213, -2.1013853632\H,0.2522721756,2.1489538567,2.1125069133\H,0.4294023289,4.6447973784,2

.3957395513\N,0.974149646,4.4144761845,-0.9234014424\C1,0.8942763639,6
.6995528069,0.399166312\C,0.7824902799,0.7448260371,-0.2062354786\C,2.
2337717803,-1.306728477,0.4391004084\C,3.3538746534,-1.5463580807,-0.5
494224029\H,1.2882270644,-1.7733243285,0.1522889426\H,2.4960492389,-1.
6280965171,1.4518938181\N,2.1096606899,0.1984205683,0.4006132999\C,3.3
311518475,0.6342697491,-0.4350366735\N,3.5713451852,1.8765732194,-0.54
02117406\N,3.9270739646,-0.4740444002,-0.9871636484\H,-0.0117801748,0.
2328812582,0.3428355144\H,0.7761303644,0.421875656,-1.2486143723\H,3.6
670648653,-2.536971896,-0.8610523312\H,2.1921625111,0.6162801157,1.335
3992506\H,1.1522760748,5.0234290076,-1.71167489\\Version=ES64L-G16RevB
.01\State=3-A\HF=-1027.8442842\S2=2.018965\S2-1=0.\S2A=2.00021\RMSD=3.
353e-09\RMSF=7.630e-06\Dipole=-1.0114183,-2.8571996,0.3888418\Quadrupo
le=-18.1359019,23.943036,-5.8071341,-4.5986682,2.0872666,-5.6572081\PG
=C01 [X(C9H10C11N4)]\@

pDIMI-H_C2_N1-N1

1\1\GINC-CDR540\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\10-Feb
-2020\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,3\C,0.982647587,4.9253466437,-0.1001
788634\C,0.860254789,3.0310002654,1.1503074947\C,0.8050177764,2.207437
929,0.0115982698\C,0.8259440562,2.8349452326,-1.2474378066\C,0.9216990
232,4.2139877733,-1.3161318379\H,0.8322960429,2.5957684679,2.146942522
4\H,0.7659460135,2.2453040107,-2.1582458533\H,0.9389097945,4.741909159
8,-2.2620243291\N,0.9465004378,4.3612822614,1.0974111448\C1,1.10040600
23,6.6582212264,-0.1527553433\C,0.7129789131,0.7094534162,0.1466589548
\C,2.1199965416,-1.385915893,-0.2514451181\C,3.5893727787,-1.599916874
4,-0.3478443729\H,1.5845939942,-1.8026396951,-1.1150126128\H,1.6984755
561,-1.857917966,0.6548872031\N,1.9961859059,0.073255766,-0.2116075997
\C,3.1565045216,0.7128113673,0.1353907717\N,3.4792274918,1.8588733735,
0.531141363\N,4.281611468,-0.333437422,-0.1091251489\H,0.4407579829,0.
4286453359,1.1729030487\H,-0.0438215339,0.2997424342,-0.5297790049\H,4
.1586184372,-2.5053744449,-0.5021576531\H,4.8996948842,-0.3413922807,0.
.7149652933\H,4.8580773759,-0.0269838273,-0.9063870424\\Version=ES64L-
G16RevB.01\State=3-A\HF=-1027.8315344\S2=2.012489\S2-1=0.\S2A=2.000094
\RMSD=5.619e-09\RMSF=8.009e-06\Dipole=2.1309705,-5.7826616,-1.0298577\
Quadrupole=-0.6254637,16.6621148,-16.0366511,-18.3805317,-0.5534942,-3
.3929079\PG=C01 [X(C9H10C11N4)]\@

pDIMI-H_C3_N2-N5

1\1\GINC-GRA139\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\13-Feb
-2020\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,3\C,-1.6046456618,1.042372136,-2.949
9011273\C,0.0067103686,2.0400636789,-1.4927467857\C,-0.1030309738,0.99
55176102,-0.5972470723\C,-0.9939658968,-0.0605778459,-0.9064590449\C,-
1.7339649268,-0.0378806193,-2.0923346962\H,0.6968484244,2.8644400903,-
1.3576381243\H,-1.1278272828,-0.8810127844,-0.2097921224\H,-2.42064940
08,-0.8351414671,-2.3498726246\N,-0.7449378226,2.0537793875,-2.6241198
3\C1,-2.4778438428,1.2071499768,-4.4164483184\C,0.8336052999,0.9087614
873,0.5847823187\C,1.9462228681,-1.3155980448,0.2274817181\C,3.2016238
912,-1.7544526987,-0.473707538\H,3.0419488659,-2.4515151857,-1.3118708

462\H,3.9172222598,-2.2685358978,0.1926323251\N,1.9558274876,0.0484845
037,0.2172734949\C,3.0350533001,0.4977265588,-0.5773265525\N,3.1674050
031,1.7644558135,-0.8848860212\N,3.8200955324,-0.5321540049,-0.9740047
761\H,1.2297313582,1.887330383,0.858694986\H,1.3284330914,-1.873721501
4,0.9174176632\H,0.3363794575,0.4749305379,1.4566574957\H,4.0315243262
,1.8835542099,-1.4193718922\H,-0.6671128661,2.8431228963,-3.2594432593
\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.895311\S2=2.034253\S2-1=
0.\S2A=2.000397\RMSD=4.234e-09\RMSF=8.969e-06\Dipole=-0.9727025,0.0883
59,0.2651079\Quadrupole=-1.6066401,2.0797401,-0.4731,-3.6801281,7.6393
358,-8.6861936\PG=C01 [X(C9H10C11N4)]\@

pDIMI-H_C3_N2-N2

1\1\GINC-GRA772\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\12-Feb
-2020\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\Title Card Required\1,3\C,-0.1643028178,3.6239304905,2.772
9914402\C,0.433613289,3.2503618086,0.6045196088\C,0.4259080479,1.86207
79716,0.7715948162\C,0.0778284553,1.3608810874,2.0385557887\C,-0.22636
76243,2.2469093558,3.0608718335\H,0.6683354898,3.6937235711,-0.3629947
717\H,0.0399832409,0.2897822551,2.2203806407\H,-0.506676019,1.90416318
78,4.0497789629\N,0.1529528568,4.1181077552,1.585725729\C1,-0.51648905
7,4.7643233881,4.0369750069\C,0.7674581621,0.9472521414,-0.3786073646\
C,2.0815814603,-1.2407263488,-0.4917517463\C,3.4834025092,-1.671733205
5,-0.1544089294\H,4.0880401595,-1.9884063056,-1.0242546995\H,3.5583121
966,-2.5085983867,0.5608510056\N,1.9698608889,0.1156318867,-0.11981474
37\C,3.1495822202,0.5193928458,0.3722168317\N,3.4880020097,1.731499780
7,0.7868730442\N,4.1072707398,-0.4914328718,0.4327980879\H,-0.04337338
32,0.2413171994,-0.5741821438\H,1.1992577212,-1.830840299,-0.689042737
5\H,0.9382246625,1.5151259262,-1.2999173514\H,4.4240945043,1.860093091
6,1.1567763448\H,2.8264060872,2.5002871546,0.8213922667\Version=ES64L
-G16RevB.01\State=3-A\HF=-1027.8917318\S2=2.012675\S2-1=0.\S2A=2.00008
5\RMSD=7.347e-09\RMSF=5.547e-06\Dipole=1.693255,-2.8741191,-1.7441243\
Quadrupole=-0.9356327,2.5797226,-1.64409,-2.6754959,-4.9615528,7.52529
87\PG=C01 [X(C9H10C11N4)]\@

pDIMI-H_C3_N1-N2

1\1\GINC-GRA703\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\11-Feb
-2020\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\Title Card Required\1,3\C,0.0883876928,3.6013544164,2.7538
305802\C,0.6488427747,3.1848144022,0.5900242537\C,0.5124227888,1.78330
61368,0.7608678654\C,0.1240573218,1.3178206445,2.0345878529\C,-0.08690
895,2.2280036837,3.052691627\H,0.9449156882,3.5884737869,-0.3743139315
\H,-0.0147184996,0.255003678,2.2125041252\H,-0.3932802882,1.9198153838
,4.0453870936\N,0.445133373,4.0687486381,1.5630693122\C1,-0.1832183451
,4.7622679535,4.0032748892\C,0.6986103565,0.833861835,-0.4000225484\C,
2.1283721216,-1.2959351309,-0.5958613696\C,3.5292118086,-1.653254615,-
0.1857285084\H,4.1781517563,-1.9105038438,-1.0362895757\H,3.5846183348
, -2.4809439574,0.5367900868\N,1.8980253035,0.0141855377,-0.1898058873\
C,3.0134579641,0.5610288809,0.3554992589\N,3.0983619073,1.8723879295,0.
.5914511022\N,3.9644944199,-0.3930662201,0.4485827111\H,4.9226959372,-
0.1908931323,0.6983532184\H,3.6405874275,2.1398727885,1.4144780583\H,-

0.1517913452,0.1516240355,-0.4844680267\H,1.3203157414,-1.9603407743,-
0.8581959398\H,0.7933646201,1.3826380129,-1.3428457674\\Version=ES64L-
G16RevB.01\State=3-A\HF=-1027.8893531\S2=2.014302\S2-1=0.\S2A=2.000106
\RMSD=4.088e-09\RMSF=3.745e-06\Dipole=1.4283261,-3.039412,-0.8349949\Q
uadrupole=3.7892909,0.592845,-4.382136,-9.8551463,-3.9870683,9.0621748
\PG=C01 [X(C9H10C11N4)]\@

pDIMI-H_C3_N1-N5

1\1\GINC-GRA770\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\11-Feb
-2020\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,3\C,-1.6529891819,0.7832644626,2.872
5783541\C,-0.0234105027,1.9776987006,1.6012173106\C,-0.1522123367,1.09
88014785,0.538436963\C,-1.0646144504,0.0305266007,0.6724327924\C,-1.81
08097816,-0.1312356781,1.8408484012\H,0.6771091041,2.8039659213,1.6104
534973\H,-1.1985548306,-0.6709465697,-0.144545475\H,-2.5159775924,-0.9
448414898,1.9593793054\N,-0.7710564914,1.8090056985,2.718580493\C1,-2.
5194116144,0.7111186618,4.3487556909\C,0.8008359782,1.1816324498,-0.63
22202948\C,1.8797125229,-1.0922539912,-0.6937975373\C,3.0772097954,-1.
7244706951,-0.0482767237\H,3.8755116543,-1.9297249576,-0.7814595654\H,
2.8456394791,-2.6638797261,0.4675195616\N,1.910618402,0.2581125571,-0.
400876993\C,2.8483925136,0.5139949382,0.6271779836\N,2.9857405359,1.66
68024841,1.1781697639\N,3.4698947087,-0.6793271287,0.9066887068\H,4.37
80777627,-0.6770394029,1.3481431629\H,0.3114191412,0.8972053931,-1.566
6204863\H,1.3952678541,-1.4368831029,-1.5986681232\H,1.2057824677,2.18
93087732,-0.7495422052\H,-0.6625920179,2.4697905627,3.4844070971\\Vers
ion=ES64L-G16RevB.01\State=3-A\HF=-1027.8840817\S2=2.015551\S2-1=0.\S2
A=2.000128\RMSD=8.214e-09\RMSF=7.697e-06\Dipole=-0.9664061,-0.3360576,
-0.2772375\Quadrupole=2.332319,-3.4514376,1.1191187,-9.359905,-8.47285
23,7.3573108\PG=C01 [X(C9H10C11N4)]\@

pDIMI-H_C3_N3-N5

1\1\GINC-GRA644\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\17-Feb
-2020\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,3\C,0.9580547562,4.6804184139,-0.488
4328739\C,1.4315962219,2.5677438004,0.491607471\C,0.4239040009,1.94893
34168,-0.2275564833\C,-0.3422089562,2.750069021,-1.0875153526\C,-0.092
5283315,4.1204350655,-1.2057503265\H,2.0736494029,2.044163736,1.180404
6984\H,-1.13882174,2.3065109369,-1.6786920943\H,-0.6817674327,4.751432
811,-1.8597791411\N,1.6862094113,3.8860819717,0.3330631019\C1,1.398647
3615,6.3311614625,-0.5885410743\C,0.2026575313,0.4498760403,-0.0761491
175\C,2.5094792928,-0.3580428927,-0.3200988584\C,3.7422030233,-0.97539
89219,0.2285775932\H,4.350277595,-1.4114068883,-0.5747237224\H,3.52711
60536,-1.8039874358,0.9170584637\N,1.3766473041,-0.214385678,0.4650375
556\C,4.5153860445,1.1559074155,1.0481074644\N,4.3912517171,2.33661176
48,1.17711459\N,4.7003587542,-0.1093713292,0.9795222007\H,-0.638821299
6,0.2752091133,0.6019338676\H,2.5375917608,0.2071051661,-1.244799593\H
, -0.0813586555,0.0379400477,-1.0567981053\H,2.4997460389,4.266872193,0
.8184844762\H,1.2001496551,-0.9307588705,1.1592570701\\Version=ES64L-G
16RevB.01\State=3-A\HF=-1027.8747013\S2=2.026558\S2-1=0.\S2A=2.000259\
RMSD=3.222e-09\RMSF=2.314e-05\Dipole=-2.0784779,-0.4713026,-0.573996\Q

uadrupole=-5.0264989,14.081815,-9.0553161,-3.5190296,1.7107297,-4.0930337\PG=C01 [X(C9H10C11N4)]\ \@

pDIMI-H_C3_N2-N3

1\1\GINC-GRA26\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\11-Feb-2020\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,-1.079398285,0.8418665939,-3.0964785784\C,-0.7964847556,0.0051095915,-0.9966025196\C,0.1150106164,1.0104899684,-0.6484899177\C,0.3963842549,1.9951348779,-1.61190139\C,-0.2119804176,1.9218305956,-2.8572396627\H,-1.0856043758,-0.7574523132,-0.2744320506\H,1.0749403069,2.8126873616,-1.3844509917\H,-0.033009417,2.6649558778,-3.6249735314\N,-1.3734767512,-0.089305766,-2.1962809351\C1,-1.8315119943,0.6935345816,-4.6551610369\C,0.77093589,1.0102492862,0.6923794343\C,1.8647457368,-1.2823283411,0.3250455902\C,2.5426753236,-1.5316666487,-0.9829046867\H,1.8400439441,-1.7012182099,-1.8199776879\H,3.2015865982,-2.4144964851,-0.9791701726\N,2.0662001404,0.1086392233,0.6915732463\C,3.0961719625,0.5786130147,-0.3423182378\N,3.5603019474,1.7734706141,-0.1721655708\N,3.3241201475,-0.3434501901,-1.2669206096\H,1.1322571005,1.9939899809,0.9973851213\H,1.2063123875,-1.9087443285,0.9092500907\H,0.1435218345,0.5819765006,1.4769730855\H,4.2474007622,1.9984607321,-0.8987000526\H,2.4819006132,0.2031817525,1.6284443938\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8530283\S2=2.034947\S2-1=0.\S2A=2.000327\RMSD=4.194e-09\RMSF=1.200e-05\Dipole=2.41634,-0.5020079,3.0324705\Quadrupole=-4.313206,-0.8099926,5.1231986,-3.872299,5.4165589,-7.208735\PG=C01 [X(C9H10C11N4)]\ \@

pDIMI-H_C3_N1-N1

1\1\GINC-GRA135\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\10-Feb-2020\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,0.9427270349,4.9105213245,0.2280510378\C,0.775959798,3.0595929421,-1.0812746371\C,0.7665288313,2.1974294853,0.0298858346\C,0.8284139627,2.7819034225,1.3079883686\C,0.9246403712,4.1585137575,1.4200726239\H,0.7086737781,2.6583532554,-2.0905669178\H,0.7977622217,2.1629688242,2.2009121741\H,0.9733109762,4.6537440245,2.3823795459\N,0.8630845438,4.3869234949,-0.9863468472\C1,1.062290014,6.6403105001,0.3342069499\C,0.662886573,0.706430541,-0.1561138264\C,2.1941097919,-1.3003933286,0.1912753638\C,3.5975700475,-1.6324710011,-0.2042737443\H,3.7058859101,-1.9149001099,-1.261387325\H,4.1025871973,-2.3692346779,0.4227723819\N,1.9889794875,0.0483699995,-0.0574965352\C,3.1440409166,0.7574896068,-0.2688724177\N,3.43026493,1.9590487782,-0.5291417172\N,4.2657208008,-0.2682086573,-0.0524722884\H,0.03245228,0.2544568795,0.6150900454\H,1.3663865956,-1.993564866,0.1950292043\H,0.2381853056,0.4613220335,-1.1353879033\H,5.0267467056,-0.0991564749,-0.7175973665\H,4.6415115164,-0.1340995038,0.894617626\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8505992\S2=2.020488\S2-1=0.\S2A=2.000178\RMSD=8.203e-09\RMSF=5.059e-06\Dipole=2.1731117,-5.4956801,0.6459772\Quadrupole=0.5763909,14.138928,-14.7153189,-18.1477377,-0.8533245,6.2220335\PG=C01 [X(C9H10C11N4)]\ \@

pDIMI-H_C3_N1-N3

1\1\GINC-GRA704\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\11-Feb-2020\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,0.5720725942,3.0023765376,-2.9353888035\C,0.0181861163,1.1751344143,-1.694523634\C,0.648023244,1.6825261289,-0.5507643291\C,1.24351622,2.953588184,-0.6414298486\C,1.2023735518,3.6349129882,-1.8495618362\H,-0.4969994467,0.2154999595,-1.6666267939\H,1.7297675265,3.3997078721,0.2212622355\H,1.6373739699,4.6206043449,-1.9632633637\N,-0.0106853825,1.8106724338,-2.8674324725\C1,0.5342261704,3.8077180797,-4.4742254547\C,0.694525425,0.8819244757,0.7046863947\C,1.9869279032,-1.0779133259,-0.3493825637\C,3.0893001523,-0.7739258698,-1.3006410934\H,2.7079321335,-0.4544229596,-2.2823553768\H,3.7434304304,-1.6433936798,-1.4567435705\N,1.9542029087,-0.087259177,0.7211062684\C,3.2550444486,0.6841651278,0.5690884924\N,3.5787746016,1.5006154439,1.4824960336\N,3.7865782256,0.3157138979,-0.6189259258\H,4.6832070046,0.6731979189,-0.9180813841\H,0.8178159169,1.4888022639,1.603363311\H,1.1440378897,-1.7420041212,-0.4759172063\H,-0.1563585194,0.2066997419,0.8194900563\H,1.9617171056,-0.5382349197,1.646053355\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8401185\S2=2.011653\S2-1=0.\S2A=2.00074\RMSD=9.057e-09\RMSF=3.677e-05\Dipole=1.0346402,-2.8167812,2.2137626\Quadrupole=-3.7358138,9.0795356,-5.3437217,-3.8343494,-6.6723652,-8.8549597\PG=C01 [X(C9H10Cl1N4)]\@\

pDIMI-H_C4_N2-N2

1\1\GINC-GRA1087\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\06-Aug-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,-0.1899941884,3.5277096127,2.8526248368\C,1.0549021746,1.7445859958,2.1682717849\C,0.8343656354,2.0278310456,0.7845212395\C,0.0167914901,3.1640672688,0.4950541071\C,-0.4970478687,3.9155681443,1.5276046307\H,1.6499966583,0.884551817,2.467201554\H,-0.1971916936,3.4301890074,-0.5359477444\H,-1.1211237271,4.7822331936,1.3443586821\N,0.5617323722,2.4717868969,3.1607270757\C1,-0.8139716023,4.458993602,4.1706514854\C,1.369602167,1.2469056933,-0.2568256404\C,1.8040399803,-1.2653121504,-0.3571328308\C,3.0637398848,-2.0512549661,0.0589024505\H,1.5803755102,-1.3288066408,-1.4273041458\H,0.9060218274,-1.5393193273,0.2044892654\N,2.1976898326,0.1165586319,-0.0152380157\C,3.4611687823,0.135691344,0.4484304198\N,4.1309617948,1.2265445056,0.8030374282\N,4.0357191369,-1.1015304426,0.5474509644\H,3.5188625998,-2.6182226894,-0.7669911701\H,1.1191626004,1.4204624136,-1.2990207335\H,2.8773193419,-2.7922922579,0.8504168897\H,3.7250035841,2.1500433643,0.7311652496\H,5.0808113769,1.1256580877,1.1367200467\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.9164524\S2=2.033437\S2-1=0.\S2A=2.000613\RMSD=4.246e-09\RMSF=6.866e-06\Dipole=1.6111609,-1.8744745,-2.7398507\Quadrupole=-1.1505112,9.9299873,-8.7794761,-8.4807874,-2.3171228,8.0962965\PG=C01 [X(C9H10Cl1N4)]\@\

pDIMI-H_C4_N2-N5

1\1\GINC-GRA40\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\08-Aug-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,0.3587810237,5.0269312584,-0.0470734557\C,1.817218827,3.2023928504,0.4874821865\C,1.058949387,2.2869929

12, -0.2801861197\C, -0.0966821127, 2.8455424522, -0.9330710581\C, -0.43866
52368, 4.1771133728, -0.8212732876\H, 2.7007799491, 2.8933265915, 1.0366188
008\H, -0.7254955936, 2.19858579, -1.5373044907\H, -1.3113538984, 4.5808420
499, -1.3197264013\N, 1.4457393327, 4.4930582482, 0.5679161547\C1, 0.052014
3718, 6.6980770498, 0.1764357961\C, 1.3136045711, 0.9067502855, -0.47569414
9\C, 2.1840860583, -1.3726457186, -0.5056349772\C, 3.4738435698, -1.9952809
55, 0.0659720377\H, 2.1342264384, -1.4121171824, -1.5966246603\H, 1.2794312
986, -1.8284486376, -0.0902862451\N, 2.2800374134, 0.0381810609, -0.0513676
211\C, 3.3790837491, 0.1482069515, 0.8287339717\N, 3.7043894552, 1.24706668
84, 1.457202169\N, 4.0691008727, -1.0172037015, 0.9485951442\H, 4.209943950
1, -2.235005659, -0.7154100036\H, 0.5955392413, 0.4094480518, -1.1183453629
\H, 3.3023177676, -2.9266401746, 0.6176267909\H, 4.5257566296, 1.0516530939
, 2.0336976285\H, 2.0214271851, 5.1134298113, 1.1328259921\\Version=ES64L-
G16RevB.01\State=3-A\HF=-1027.9154035\S2=2.039803\S2-1=0.\S2A=2.000751
\RMSD=6.919e-09\RMSF=4.855e-06\Dipole=-0.4763514, -0.3353806, -0.5340748
\Quadrupole=-7.7562424, 20.4452069, -12.6889645, -7.0393156, 4.7651749, 6.1
587584\PG=C01 [X(C9H10Cl1N4)]\@

pDIMI-H_C4_N1-N5

1\1\GINC-GRA132\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\05-Aug
-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispe
rsion=gd3\\Title Card Required\\1,3\C,0.4345379033,5.0956623019,0.0545
744076\C,1.7519292232,3.1881629282,0.6543761445\C,1.1012550261,2.36078
6197,-0.2910188152\C,0.0689612096,3.0036490845,-1.0609960732\C,-0.2563
19578,4.333443234,-0.8946610947\H,2.5626945559,2.8442190399,1.28875859
\H,-0.4726920781,2.4246916301,-1.8028762234\H,-1.0338666259,4.80370075
05,-1.4840044319\N,1.4036369989,4.4813078377,0.781362227\C1,0.13719081
9,6.7553368956,0.3582056151\C,1.3425984022,0.9847743614,-0.5220822424\
C,2.0879240482,-1.3491189234,-0.2343743834\C,3.4871430918,-1.906032261
7,0.0400469593\H,1.7376611798,-1.5488939323,-1.2490354082\H,1.35318000
48,-1.7188572962,0.4884616639\N,2.2709105371,0.1131728021,-0.033297166
6\C,3.449902117,0.3272832609,0.7185014941\N,3.9231732973,1.4642248839,
1.0718408117\N,3.9945742862,-0.9122178825,0.9903255842\H,4.0894645,-1.
9448794035,-0.8768410513\H,4.9631685256,-0.9357170011,1.2825730029\H,1
.9059871461,5.0385503995,1.4691561488\H,0.6559050861,0.5016998457,-1.2
085995833\H,3.4564711038,-2.8978259221,0.4945677545\\Version=ES64L-G16
RevB.01\State=3-A\HF=-1027.9063351\S2=2.024856\S2-1=0.\S2A=2.000362\RM
SD=3.887e-09\RMSF=5.202e-06\Dipole=-0.4955595,-0.9169203,-0.4737416\Qu
adrupole=-8.5308577,22.8686343,-14.3377766,-13.7702709,5.1545899,4.599
0538\PG=C01 [X(C9H10Cl1N4)]\@

pDIMI-H_C4_N1-N2

1\1\GINC-GRA1134\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\05-Au
g-2019\0\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldisp
ersion=gd3\\Title Card Required\\1,3\C,0.4537787788,4.0946917179,-2.35
39439781\C,1.0498874724,1.9250572604,-2.0367817091\C,0.7955501243,1.98
46043157,-0.6165638039\C,0.2123182346,3.1812356484,-0.1324379375\C,0.0
428506855,4.2448124572,-0.9953673237\H,1.2724997002,0.9732322826,-2.50
97006055\H,-0.0548345401,3.2763247131,0.9152957379\H,-0.3706331925,5.1
885651182,-0.6581616543\N,0.9051637105,2.9587346198,-2.8604166215\C1,0

.3261711244,5.4536466692,-3.4103713798\C,1.0719393765,0.8886523335,0.2577907302\C,2.0212837239,-1.4529692474,0.4149851123\C,3.4343735593,-1.9534628505,0.0468157249\H,1.2350182696,-1.9654265984,-0.1483592733\H,1.80341572,-1.5282672763,1.4826749088\N,2.0612495293,-0.0351738918,-0.0035516103\C,3.1629167753,0.2056910909,-0.7831155392\N,3.4195142624,1.4289291394,-1.2042339409\N,3.8605770851,-0.9495988317,-0.9464069446\H,3.4220154304,-2.9522515301,-0.3916617546\H,4.8155898787,-0.9207093229,-1.279165009\H,0.5331805793,0.7543562721,1.1887845458\H,4.1063414659,-1.9465111035,0.9119526374\H,4.0629345864,1.4819066846,-1.9953953418\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.9035786\S2=2.016054\S2-1=0.\S2A=2.000129\RMSD=9.064e-09\RMSF=1.097e-05\Dipole=1.1188412,-2.7379835,1.8966432\Quadrupole=-2.3034144,13.8445038,-11.5410894,-16.7447891,-2.689868,-7.6954064\PG=C01 [X(C9H10C11N4)]\@\

pDIMI-H_C4_N3-N5

1\1\GINC-GRA644\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\09-Aug-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,0.6594625481,5.0204061077,0.2208963235\C,-0.1592728055,2.7778817865,0.1028685079\C,1.0757802997,2.2859976198,-0.3556253983\C,2.1264983648,3.2614421725,-0.5226219348\C,1.9084977161,4.596172812,-0.2363578833\H,-1.0184477232,2.1395623214,0.275389527\H,3.1089546942,2.9635531262,-0.8699866622\H,2.6953254382,5.3313334257,-0.3556863231\N,-0.3290472434,4.0778751843,0.3693102912\C1,0.2636732614,6.6416212637,0.6121050289\C,1.2006376304,0.8983474538,-0.5689970275\C,2.5037973396,-1.1768268298,-0.904802378\C,3.1478789459,-1.6616854136,0.4212028836\H,3.1473608336,-1.4871083444,-1.7328360552\H,1.5274997885,-1.6490314569,-1.0396784709\N,2.3315841814,0.2716845028,-0.9540316125\C,2.2771476492,-0.2256297512,2.0825960919\N,2.1860060597,0.8457822981,2.6046583712\N,2.2538599619,-1.3865145751,1.5401105829\H,4.1287230076,-1.1869182995,0.5501715009\H,-1.2337118754,4.3915192217,0.7119695265\H,0.3454866452,0.2539361222,-0.3942869083\H,3.2794172268,-2.7446955674,0.3548723657\H,3.1735425052,0.8176353398,-1.0866359873\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8979626\S2=2.041623\S2-1=0.\S2A=2.000932\RMSD=9.028e-09\RMSF=1.179e-05\Dipole=-0.2783369,-0.4879788,-1.6950079\Quadrupole=3.3811658,15.1598686,-18.5410344,-12.9659241,-5.2415263,6.5724863\PG=C01 [X(C9H10C11N4)]\@\

pDIMI-H_C4_N2-N3

1\1\GINC-CDR562\FOpt\UB3LYP\6-31+G(d,p)\C9H10C11N4(1+,3)\KJM408\08-Aug-2019\0\#\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\Title Card Required\1,3\C,-0.4071809263,3.5872139624,-2.7898358936\C,1.3285425227,2.272575404,-2.1180037253\C,0.4804975186,1.4069165661,-1.3623050057\C,-0.9081122934,1.7458544692,-1.3456563335\C,-1.3542081292,2.8365101835,-2.0562006678\H,2.4088411357,2.1339430053,-2.1336743028\H,-1.6078933607,1.1393068682,-0.7784659898\H,-2.4002146847,3.118831965,-2.0662371158\N,0.8960419839,3.3146693782,-2.8114141023\C1,-0.9410554233,4.9466513244,-3.716318716\C,0.9259819286,0.276164063,-0.6651000153\C,2.5457434463,-1.6440402368,-0.5776168407\C,3.8732961322,-1.7497830405,0.2014949831\H,2.556706847,-2.0835668871,-1.5747086185\H,1.7123643715,-2.0560849862,-0.00680201\N,2.3242772037,-0.1477912382,-0.

.678691515\C,3.2148785325,0.4109615083,0.4854056381\N,3.0545725951,1.6605463082,0.7640511743\N,4.0266237519,-0.5214600404,0.9534565057\H,4.7485374805,-1.8447264929,-0.4597848747\H,0.3002779551,-0.3017362322,0.021504558\H,3.9031652197,-2.6091099151,0.8783001959\H,3.6703356684,1.9409996812,1.5341445514\H,2.7572338643,0.1946145423,-1.5451906572\\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8675344\S2=2.055408\S2-1=0.\S2A=2.001573\RMSD=7.514e-09\RMSF=1.431e-05\Dipole=1.3447735,-3.7188044,1.5567199\Quadrupole=4.2485557,6.760446,-11.0090017,-14.2378945,5.396335,-5.5251086\PG=C01 [X(C9H10Cl1N4)]\\@

pDIMI-H_C4_N1-N1

1\1\GINC-GRA34\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\03-Aug-2019\0\\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,3\C,0.0508012987,3.9390100326,2.6665773615\C,1.0060448381,1.9183219446,2.2208658856\C,0.8005394592,2.0465726506,0.8178433858\C,0.1157400559,3.2173055475,0.387590072\C,-0.259913768,4.1718641596,1.3102807732\H,1.4401325865,1.0160434716,2.6401908336\H,-0.0957000938,3.3672373931,-0.667156535\H,-0.7714878182,5.0796677966,1.0134968565\N,0.6474909397,2.8392039712,3.1097177589\Cl,-0.3777787017,5.1376712696,3.8486857004\C,1.1661694386,1.0558583991,-0.1337561239\C,2.0782966538,-1.2361890054,-0.5879437681\C,3.5338089405,-1.7088972251,-0.5689143222\H,1.7014340918,-1.1356711063,-1.6087552902\H,1.411658623,-1.9053936722,-0.0322415408\N,2.1477395231,0.0835722872,0.0618526446\C,3.2719979686,0.2451759156,0.8218485927\N,3.7402890962,1.1664322102,1.5603489623\N,4.063793028,-1.0502978415,0.6909326862\H,4.1064715678,-1.3037496225,-1.4044712684\H,5.0662198096,-0.834654929,0.6501007251\H,0.7060574841,1.0273722944,-1.1155967194\H,3.6633988732,-2.7894364929,-0.5084125984\H,3.9139119554,-1.6298154683,1.526799798\\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8596486\S2=2.030969\S2-1=0.\S2A=2.000534\RMSD=5.535e-09\RMSF=2.450e-05\Dipole=2.6812685,-5.255706,-3.3520516\Quadrupole=-2.9323458,17.7223767,-14.7900309,-27.7810185,-4.9578358,10.4169328\PG=C01 [X(C9H10Cl1N4)]\\@

pDIMI-H_C4_N1-N3

1\1\GINC-GRA639\FOpt\UB3LYP\6-31+G(d,p)\C9H10Cl1N4(1+,3)\KJM408\05-Aug-2019\0\\# opt freq b3lyp/6-31+g(d,p) geom=connectivity empiricaldispersion=gd3\\Title Card Required\\1,3\C,-2.2816540564,1.0139150327,-2.7333167006\C,-0.1009654596,0.4854557653,-2.3374510475\C,-0.2776296249,0.479860213,-0.9202879198\C,-1.599044626,0.7636170314,-0.4514533246\C,-2.6008365745,1.0312465236,-1.3553407075\H,0.8647296508,0.259715695,-2.7917618239\H,-1.8045256349,0.7756926193,0.6146519957\H,-3.6107464445,1.255115559,-1.0328511187\N,-1.0660453648,0.7453742929,-3.206507353\Cl,-3.5181979286,1.3530603369,-3.8919580895\C,0.7433792471,0.2178786159,0.0018333586\C,2.5059824402,-1.5130954873,-0.6095615801\C,4.0171394533,-1.5006918112,-0.384744898\H,2.1791595846,-1.8460643292,-1.5945978629\H,1.9777574197,-2.060510626,0.171807632\N,2.1211843178,-0.0371498366,-0.432293954\C,3.1876849498,0.5150258837,0.5223853995\N,3.0301953904,1.6688120817,1.0126185208\N,4.1393052915,-0.4505691055,0.6288456365\H,4.5693964873,-1.2588482497,-1.3018030856\H,0.6103514953,0.1812364673,1.0743197574\H,4.3723961859,-2.4572851324,0.0031498245\H,5.0202608914,-0.2

301464602,1.0759642459\H,2.2825312192,0.4538510006,-1.3211260853\\Version=ES64L-G16RevB.01\State=3-A\HF=-1027.8560046\S2=2.034067\S2-1=0.\S2A=2.000637\RMSD=8.021e-09\RMSF=1.887e-06\Dipole=3.070498,-2.1174851,1.6013008\Quadrupole=24.0882034,-11.0669751,-13.0212283,-15.6277084,5.1445022,-5.1174716\PG=C01 [X(C9H10Cl1N4)]\ \@