

Table S1: Archive Entries For the B3LYP optimized Geometries**1a**

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1\1\GINC-N03\FOpt\UB3LYP\6-31G(d)\C8H14N5O5(2)\ROOT\04-Apr-2000\0\#\ O
PT UB3LYP/6-31G(D) FREQ=NORAMAN\TP2-m1-2-TS start at 2.4 for TS opt\
0,2\O,0.6276094352,-1.2664569871,-1.1695720655\C,0.8806913385,-0.93450
44721,0.1481537771\C,2.3416297105,-0.6026746042,0.3411778579\C,2.96789
48237,-1.0140108888,-1.0034038201\C,1.7716712673,-0.9021496827,-1.9709
128789\C,1.7895080878,-1.822532073,-3.1795560457\H,1.9057087361,-2.863
4731463,-2.8341734447\H,2.6513288016,-1.5780572815,-3.8119772829\O,0.6
408717096,-1.6647159992,-3.9902653078\H,-0.1260360001,-1.8100737413,-3
.4125140681\H,1.6685696864,0.142174877,-2.2969004741\H,3.3006838807,-2
.06222882,-0.9539185611\O,4.0457959694,-0.1526871866,-1.3278282683\H,4
.5533040952,-0.5531018116,-2.0499697765\H,2.7715743664,-1.1307740792,1
.1984528627\H,2.5268165537,0.4698858366,0.4868149357\N,0.1830375427,-1
.7067784574,1.0665489644\H,-0.7393876774,-1.9754681187,0.736349878\H,0
.136355553,-1.2495292937,1.9823580797\O,-0.0680550096,0.4716700553,2.9
790368409\C,-1.2590339512,2.0290796075,-0.0345062815\C,-0.3731110191,1
.5492403286,0.911897598\N,-0.8490495052,0.9492563243,2.0331799027\C,-2
.213573516,0.7756639199,2.1186198166\N,-3.0921500306,1.2019880046,1.21
80618735\N,-2.6016690604,1.8387887962,0.1210499807\O,-3.4218100042,2.2
488995903,-0.728529326\N,-2.6239477193,0.0901579488,3.2075174256\H,-3
.6007597903,0.1423378218,3.4549672888\H,-1.912330717,-0.006750554,3.924
4788914\H,0.6864342781,1.7513581583,0.894557768\H,-0.9651676104,2.5474
632445,-0.9345882532\Version=IBM-RS6000-G98RevA.7\HF=-962.9196167\S2=
0.755412\S2-1=0.\S2A=0.750018\RMSD=7.809e-09\RMSF=3.415e-06\Dipole=1.1
386329,-0.7732141,0.6381723\PG=C01 [X(C8H14N5O5)]\@

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1b

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1\1\GINC-SP\FTS\UB3LYP\6-31G(d)\C8H14N5O5(2)\ROOT\04-Jul-2000\0\#\OPT=
(RCFC,TS,NOEIGEN) GUESS=READ GEOM=CHECK SCF=(DIRECT) UB3LYP/6-31G*\1a
ts 6-31G(d) opt \0,2\O,0.7012022918,-0.2367243223,-1.0066590676\C,0.
0597365334,-1.3000059209,-0.4071316361\C,0.8974535229,-1.8264377588,0.
7397893356\C,2.269325013,-1.1848614879,0.4785033204\C,1.8787518374,0.1
258910131,-0.2324650179\C,2.8884417256,0.6924077808,-1.2168739016\H,3.
180477998,-0.0979366928,-1.9282460921\H,3.7866483913,1.0106243048,-0.6
748805712\O,2.3949839058,1.8384985131,-1.8857270646\H,1.5678446222,1.5
653056029,-2.3146459411\H,1.6088856806,0.8825850151,0.5141424476\H,2.8
503073592,-1.8139323517,-0.2149441713\O,2.9598771196,-1.0007994696,1.6
98411394\H,3.8753247812,-0.7508646505,1.5007802212\H,0.930448251,-2.91
84628215,0.7626655853\H,0.5245634304,-1.4589723472,1.7020502517\N,-0.5
100279308,-2.1899051464,-1.307253714\H,-1.135620084,-1.7226768211,-1.9
68667853\H,-1.0498662385,-2.8895543043,-0.803656985\C,-1.9288192231,1.
4921587401,-0.8475296362\N,-2.2186647305,0.2003945166,-0.6391875898\C,
-1.6963900737,-0.4030710631,0.540612293\N,-1.1899422298,0.3583932002,1
.5534187502\N,-0.8442843854,1.6158793328,1.2725914125\C,-1.2252804387,
2.2181618889,0.0920899412\H,-2.290930044,1.9133711208,-1.7765336345\O,
-0.1962070884,2.2673208374,2.1260111735\O,-2.8861625745,-0.5356453181,
-1.479123923\N,-2.3502144106,-1.5856637505,0.9140351078\H,-2.642333954
9,-1.5573864004,1.8857238957\H,-3.1227035463,-1.7553459224,0.270744739
9\H,-0.9399734523,3.2528981229,-0.0150279479\Version=IBM-RS6000-G98Re
vA.7\HF=-962.9084154\S2=0.786389\S2-1=0.\S2A=0.750554\RMSD=6.494e-09\R
MSF=4.830e-06\Dipole=0.0764173,-0.9362669,-0.7221026\PG=C01 [X(C8H14N5
O5)]\@

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1c

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1\1\GINC-N04\FOpt\UB3LYP\6-31G(d)\C8H14N5O5(2)\ROOT\13-Jul-2000\0\#\#OP
T=RCFC GUESS=READ GEOM=CHECK UB3LYP/6-31G*\ 1b 6-31G(d) opt\0,2\C,
2.0500029279,0.6429819933,1.7424737947\C,2.175666081,-0.6693796343,1.4
290792135\N,1.9330972774,-1.0889970678,0.160536697\C,1.3152940604,-0.1
19915414,-0.8410193634\N,1.5852930925,1.2640513085,-0.5210369591\N,1.8
019036392,1.5930349717,0.7067013334\O,2.1347696139,-2.2985757591,-0.20
20069771\N,1.829786216,-0.3702580437,-2.1621120037\O,1.9041467125,2.79
22352973,1.0414674479\C,-0.2469249271,-0.4167120685,-0.8511312851\O,-0
.6800935692,-0.2931492128,0.5004866255\C,-2.0383842564,0.2148515037,0.
5361022267\C,-2.4057839837,0.6036529329,-0.9165081762\C,-1.0485513433,
0.6331558575,-1.6270416788\N,-0.5772451583,-1.743030014,-1.3391815177\
O,-3.0206984031,1.8803503333,-1.0254078643\C,-2.9284490204,-0.85250483
92,1.1618817614\O,-2.4746720787,-1.2192696482,2.453798156\H,-2.9701692
098,-1.7213589456,0.4864915266\H,-3.947358206,-0.4651510512,1.28511151
39\H,-1.5398545641,-1.4569868217,2.3378939737\H,-2.0278249347,1.112862
9762,1.1646627055\H,-3.0477088836,-0.1709598475,-1.3589055338\H,-3.942
9688304,1.7977690291,-0.738778895\H,-1.1121084218,0.4141510772,-2.6943
963762\H,-0.6024757586,1.6221989643,-1.496849379\H,-0.053837831,-2.458
3490879,-0.835062252\H,-0.3436402728,-1.8205674814,-2.3270335618\H,2.4
862669083,-1.4315214056,2.1340390814\H,2.6842350647,0.1662331353,-2.29
65531035\H,2.053096495,-1.361299452,-2.2400738293\H,2.2096675435,1.079
8607553,2.7153832187\Version=IBM-RS6000-G98RevA.7\HF=-962.9266303\S2=
0.773157\S2-1=0.\S2A=0.750201\RMSD=4.879e-09\RMSF=2.617e-05\Dipole=0.2
907298,-1.2088416,-0.1362235\PG=C01 [X(C8H14N5O5)]\@

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1d

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1\1\GINC-N06\FOpt\UB3LYP\6-31G(d)\C8H15N5O5(1+,2)\ROOT\21-Nov-2000\0\#
#OPT=CALCFC GUESS=READ GEOM=CHECK UB3LYP/6-31G(D)\1c complex\1,2\C,2
.2883619423,-1.1118896766,-0.2786698962\C,2.0302569667,0.3476138967,-0
.0596229672\O,3.1092942463,1.0145741871,0.2593356794\C,4.2711412558,0.
0852540757,0.3975296506\C,3.6281363103,-1.3102436123,0.4656618644\C,-3
.7477149327,0.8783166728,0.2203465602\N,-4.7929871716,0.0633829509,-0.
2379428364\C,-4.4605257755,-1.2795081586,-0.4933399473\C,-3.159189076,
-1.6080818367,-0.6648277752\N,-2.1925171489,-0.6436141308,-0.506738359
4\N,-2.4822270008,0.5870195441,0.0552190736\O,-6.0091901395,0.23691920
06,0.4723800093\N,-4.1096163119,2.0508562151,0.78460451\O,-0.950202750
4,-0.8968868921,-0.756147097\N,0.8823094752,0.9370965193,-0.1717772643
\C,5.229840092,0.3412548477,-0.760383579\O,5.7648134917,1.6423374655,-
0.7264386251\O,3.4306339675,-1.596072147,1.8352710216\H,4.7383850956,0
.1129626127,-1.72065239\H,6.0749725512,-0.3467729085,-0.6519662607\H,5
.0703109544,2.2732426386,-0.9718477556\H,4.7325200831,0.3546879976,1.3
478904582\H,4.2588043616,-2.0612290988,-0.0260804047\H,3.1971195936,-2
.5324879643,1.937379508\H,2.3854062497,-1.2871252167,-1.3581766525\H,1
.4691007154,-1.7348359354,0.0874864761\H,0.8042595117,1.9344160785,0.0
00603588\H,0.0243023965,0.3534365126,-0.3990760823\H,-5.2868166107,-1.
9653179487,-0.6079934096\H,-5.0377493755,2.1069835035,1.181262652\H,-3
.3769359927,2.581417421,1.2345992318\H,-2.8075165431,-2.589612391,-0.9
479600319\H,-6.6255271058,0.5737752435,-0.2043961571\Version=IBM-RS60
00-G98RevA.7\HF=-963.3621888\S2=0.768054\S2-1=0.\S2A=0.750112\RMSD=7.8
77e-09\RMSF=5.663e-06\Dipole=-1.5362533,-0.0916143,-0.2090657\PG=C01 [
X(C8H15N5O5)]\@

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1e

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1\1\GINC-WALT\FOpt\RB3LYP\6-31G(d)\C5H12N1O4(1+)\KAT\18-Nov-2000\0\#

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OPT=FCCARDS RB3LYP/6-31G(D)\00000\1,1\O,-0.8765334899,-0.5936429374,
 -0.280413696\C,-0.8744861443,-0.4960701311,1.0082572983\C,0.4547136405
 , -0.1501496004,1.5977161429\C,1.3090473028,0.2243879376,0.3534692686\C
 , 0.4095568468,-0.1106809933,-0.8583170086\C,0.936359204,-1.1742716661,
 -1.8139277683\H,1.1187326052,-2.1139088456,-1.268861116\H,1.9031200968
 , -0.8169742329,-2.1870925353\O,0.1024956184,-1.3432763641,-2.932191958
 1\H,-0.6390952497,-1.9210243219,-2.6955771146\H,0.1443173563,0.7979201
 764,-1.3998296305\H,2.2247781814,-0.3767899518,0.3266027444\O,1.625961
 3474,1.6042010507,0.2803326034\H,2.4611087326,1.774628854,0.7445272313
 \H,0.849581404,-1.0204055126,2.1357015296\H,0.3654520861,0.6860724416,
 2.295079624\N,-1.9640231189,-0.7866726268,1.672650813\H,-2.8292195834,
 -0.9899882797,1.1814566768\H,-2.0001191844,-0.6937734328,2.6803976332\O,
 -1.0316192638,2.2055243893,0.87238201\H,-0.1552886882,2.5560350074,0
 .6351124714\H,-1.6687847205,2.8831740968,0.5998675238\Version=IBM-RS6
 000-G98RevA.4\HF=-553.1438429\RMSD=2.691e-09\RMSF=2.205e-06\Dipole=-0.
 5782124,-0.3959175,2.2673196\PG=C01 [X(C5H12N1O4)]\@

1f

1\1\GINC-N04\FTS\RB3LYP\6-31G(d)\C5H12N1O4(1+)\13-Mar-2001\0\# GUES
 S=READ GEOM=CHECK OPT=(READFC,TS,NOEIGEN) SCF=(DIRECT, CONVER=5) RB3LY
 P/6-31G(D)\1e-h2o-ts\1,1\O,0.1836382382,-0.8467072529,-0.4213877158\O,
 -1.0302898608,-0.5904402075,0.1027510111\C,-0.86190292,0.4507167362,
 1.1981995027\C,0.1285416638,1.3756720885,0.4831644112\C,1.0222169394,0
 .3742065446,-0.2909510953\C,2.3329837847,-0.0209376934,0.384811501\H,2
 .1333665858,-0.418484638,1.3931160776\H,2.9447172337,0.8805963956,0.50
 01181918\O,3.0783244095,-0.9113058176,-0.4080943582\H,2.6460651843,-1.
 7795213287,-0.3964824758\H,1.2231985321,0.7138062803,-1.3106516317\H,0
 .7016132066,2.0084301977,1.1686860266\O,-0.6896623462,2.165717872,-0.3
 867088912\H,-0.1460087804,2.7939692478,-0.890196328\H,-0.4056503297,-0
 .0208831865,2.0743968974\H,-1.7806100649,0.961626004,1.4933192824\N,-1
 .8693978568,-1.7768344513,0.3464492512\H,-1.4897723425,-2.619623291,-0
 .0918417891\H,-2.1000928256,-1.9564249083,1.3236426862\O,-2.0034064332
 , -0.1010370562,-0.9714547136\H,-2.0953846193,0.8826665633,-0.980065093
 2\H,-2.6461053719,-0.9969629507,-0.4758731554\Version=IBM-RS6000-G98R
 evA.7\HF=-553.0789082\RMSD=2.839e-06\RMSF=1.089e-05\Dipole=-1.9632245,
 -0.3848129,0.9735436\PG=C01 [X(C5H12N1O4)]\@

1g

1\1\GINC-N02\FOpt\RB3LYP\6-31G(d)\C5H12N1O4(1+)\ROOT\04-Nov-2000\0\#
 OPT=CALCFC RB3LYP/6-31G(D)\C1+2h2o-P\1,1\C,-0.7015387936,0.109814020
 9,-0.8801543153\O,-0.6934411436,0.1909678516,0.592451134\C,0.620810895
 6,0.1574284221,1.046198536\C,1.4146369463,-0.6162945485,-0.0112115582\O,
 0.792250329,0.0141652212,-1.2635745785\N,0.5273566702,-0.5326518959,
 2.4145013214\O,1.1504940777,1.3758650115,1.4038457177\O,1.3943644226,1
 .3083720354,-1.3567268839\C,-1.5836950081,-1.062117255,-1.3021100963\O
 , -2.9303916515,-0.8569781368,-0.9481511402\H,-1.1818516616,-2.00510228
 08,-0.8933278898\H,-1.5622863099,-1.1427391629,-2.3941449372\H,-2.9980
 329528,-0.8357445718,0.0193195547\H,-1.1481857805,1.0410492612,-1.2408
 442668\H,0.9653705099,-0.572324484,-2.1721531145\H,1.065143845,1.77614
 63301,-2.1419160189\H,1.1961819371,-1.6885507271,0.0252266389\H,2.4915
 600247,-0.4512073746,0.0517406003\H,-0.0646499052,0.058604634,3.014360
 5541\H,0.1025702009,-1.4631111948,2.3453729442\H,1.3652570139,1.844512
 0864,0.5670356209\H,1.4544345301,-0.5967585025,2.851582517\Version=IB
 M-RS6000-G98RevA.7\HF=-553.1304056\RMSD=2.957e-09\RMSF=7.077e-06\Dipol
 e=1.3132369,-1.032283,1.9999169\PG=C01 [X(C5H12N1O4)]\@

1h

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1\1\GINC-N05\FOpt\RB3LYP\6-31G(d)\C5H14N1O5(1+)\ROOT\07-Nov-2000\0\#\#
OPT=CALCFC GUESS=READ GEOM=CHECK RB3LYP/6-31G(D)\C1+2h2o-RC\1,1\O,0.
9855952742,-0.7767786179,-0.7367108663\C,-0.1614167109,-0.9353576743,-
0.128982247\C,-0.372301811,0.05988984,0.9737045787\C,0.5340852898,1.20
30723004,0.508595413\C,1.6616771452,0.4578899351,-0.2372967983\C,2.885
0443382,0.0568858266,0.5850534129\H,2.5841564336,-0.5553400274,1.44988
1949\H,3.3383362206,0.9748190244,0.9760048956\O,3.8624839615,-0.568850
1618,-0.2081035762\H,3.5986573847,-1.4865446254,-0.3776085031\H,1.9823
174897,0.9746160754,-1.1441340983\H,0.9183239412,1.8060471468,1.338525
7169\O,-0.2604457532,1.9845441356,-0.38100977\H,0.2377751595,2.7650813
296,-0.6742635182\H,-0.0155882464,-0.3841503876,1.9115905925\H,-1.4139
207132,0.3520015472,1.1083922615\N,-0.986740205,-1.8710587997,-0.48161
45058\H,-0.7516438202,-2.4859823258,-1.2559219881\H,-1.9665846489,-1.8
458928675,-0.0894929091\O,-3.1440707269,1.3320586995,-0.4688817747\H,-
2.255935692,1.7167539422,-0.5908807849\H,-3.7144957004,2.0655964684,-0
.1936743086\O,-3.3478686669,-1.2060305919,0.5481317196\H,-4.2058562785
,-1.6564303671,0.5411011674\H,-3.4764423121,-0.3169924104,0.1379290533
\\Version=IBM-RS6000-G98RevA.7\HF=-629.5880609\RMSD=3.043e-09\RMSF=3.3
32e-06\Dipole=-1.2578271,0.0604586,0.242006\PG=C01 [X(C5H14N1O5)]\@e

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1i

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1\1\GINC-N05\FTS\RB3LYP\6-31G(d)\C5H14N1O5(1+)\ROOT\02-Nov-2000\0\#\#OP
T=(CALCFC,TS,NOEIGEN) GUESS=READ GEOM=CHECK RB3LYP/6-31G*\01\1,1\O,-
0.5001105404,-0.2395183111,-0.8866325013\C,-0.6213563235,-0.1755247445
,0.4908312745\C,0.7873788353,-0.4012453569,1.0504720436\C,1.6071265068
,0.3893812185,0.027018049\C,0.8727052632,0.0839642943,-1.2943265201\C,
1.424088406,-1.0877114729,-2.1049510638\H,1.4684304977,-1.9926842758,-
1.4762095304\H,2.4467996341,-0.8521561856,-2.4183960001\O,0.6830368819
,-1.2931204673,-3.2837850685\H,-0.2133202735,-1.5698623165,-3.03557093
16\H,0.8158858333,0.966851085,-1.9395111505\H,2.6657898856,0.113015357
9,0.007223517\O,1.4554099739,1.7706488724,0.4083491634\H,1.9265902191,
2.3434271545,-0.2196237835\H,1.0421404867,-1.4648682218,1.0063325868\H
,0.9233882353,-0.0414050567,2.0724140773\N,-1.6723463364,-1.0479605287
,0.9866652623\H,-2.438444198,-1.047103845,0.3088632198\H,-1.3330519332
,-2.0070513628,1.0490550503\O,-1.0887511649,1.1818598486,0.8603131478\
H,-0.3118205762,1.7873541187,0.7207593526\H,-1.6466242035,1.1323063159
,2.0627815491\O,-2.1499396873,0.6307304874,2.9444292947\H,-3.040243044
6,0.9872535142,3.1277270786\H,-2.2159160409,-0.2773396531,2.4718431401
\\Version=IBM-RS6000-G98RevA.7\HF=-629.5515741\RMSD=8.067e-09\RMSF=9.9
13e-06\Dipole=-1.4139961,0.1812181,2.1973214\PG=C01 [X(C5H14N1O5)]\@e

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1j

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1\1\GINC-N05\FOpt\RB3LYP\6-31G(d)\C5H14N1O5(1+)\ROOT\05-Nov-2000\0\#\#O
PT=RCFC GUESS=READ GEOM=CHECK FREQ=NORAMAN RB3LYP/6-31G*\C1+2h2o-PC\1,
1\C,-1.034739953,-0.0232174485,-1.2080679442\O,-1.0105838645,0.01403
31437,0.2615897796\C,0.3144005141,0.0729645422,0.6908544184\C,1.114132
5008,-0.6993580779,-0.3642830331\C,0.4536266352,-0.1170386575,-1.62107
69582\N,0.3170420948,-0.5157115838,2.0853890383\O,0.7838008371,1.36530
05038,0.9107527172\O,1.0375318819,1.1830316001,-1.7838522642\C,-1.9249
665073,-1.1765647439,-1.6604150694\O,-3.2653404431,-0.9862985502,-1.27
39837905\O,2.5760588192,0.6457614688,2.9801615669\H,-1.5156337836,-2.1
349931993,-1.3000790121\H,-1.9221296511,-1.2073289998,-2.7554767287\H,
-3.3190973664,-1.043007531,-0.3071670741\H,-1.4783218995,0.9200271054,
-1.5429653601\H,0.6124136723,-0.7297705869,-2.5142699763\H,0.667548419
6,1.6188050995,-2.5692690746\H,0.9208945654,-1.7751026738,-0.298891288

```

2\H,2.1886254869,-0.5129509951,-0.3266347608\H,-0.5089714865,-0.154942
6247,2.578380506\H,0.2586773196,-1.538091806,2.0714702436\H,0.90516495
96,1.762326038,0.0173347648\H,2.5992856273,1.245271171,2.2138419125\H,
2.6724989914,1.2226815835,3.7561070091\H,1.1932934971,-0.1782805121,2.
6004830172\\Version=IBM-RS6000-G98RevA.7\HF=-629.5704187\RMSD=3.937e-0
9\RMSF=3.415e-04\Dipole=1.2599726,-0.1960743,1.7139716\PG=C01 [X(C5H14
N105)]\\@

1k

1\1\GINC-N05\FTS\RB3LYP\6-31G(d)\C5H12N1O4(1+)\ROOT\13-Nov-2000\0\# O
PT=(CALCFC,TS,NOEIGEN) RB3LYP/6-31G(D)\C1+2h2o-P-dbreak1-fix-dft\\1,1
\C,0.4911883341,0.8476582066,0.3356868443\O,0.831434206,-0.5963748093,
0.1315564445\C,0.0670353702,-1.1174976209,-0.806766316\C,-0.7709652392
, -0.0817216465,-1.4993655978\C,-0.8210296488,1.0554725407,-0.464106816
\N,-1.3261197937,-2.1059804205,0.2542715687\O,0.5511603136,-2.13972522
77,-1.4864119149\O,-0.8537718029,2.287349412,-1.1361958864\C,0.4474475
972,1.1434825832,1.8255429677\O,1.7126997103,1.091875675,2.4349295845\
H,-0.2895271065,0.4856008236,2.3160250314\H,0.0899504654,2.1736688006,
1.9410193805\H,1.9831102795,0.1660259659,2.5347056644\H,1.3050529429,1.
4024983192,-0.1380098948\H,-1.6897779763,0.9369141713,0.2012520964\H,
-1.2612695087,2.9657610174,-0.5759503478\H,-1.7383499478,-0.4426123909
, -1.8496286891\H,-0.2019849326,0.2660017284,-2.3718973251\H,-0.8459161
433,-2.6687966989,0.9593268075\H,-2.0251563012,-1.5388744717,0.7378555
245\H,1.3592026995,-2.4862662343,-1.0593872782\H,-1.8167338121,-2.7474
228663,-0.3721842652\\Version=IBM-RS6000-G98RevA.7\HF=-553.1212574\RMS
D=4.423e-09\RMSF=1.007e-05\Dipole=0.8506245,-1.5679243,1.852001\Polar=
71.5944177,0.0808937,66.2265893,3.3007286,-0.8713904,79.3259354\PG=C01
[X(C5H12N1O4)]\\@

1l

1\1\GINC-N04\FOpt\RB3LYP\6-31G(d)\C5H12N1O4(1+)\ROOT\26-Feb-2001\0\#B
3LYP/6-31G* OPT=FCCARDS\\1k-ro\\1,1\C,0.5197283394,0.8729486729,0.3239
989513\O,0.9743682686,-0.525415691,-0.0350068099\C,0.2777280515,-0.972
0083461,-1.0131893251\C,-0.6994459399,-0.0144795042,-1.5837499989\C,-0
.7954047721,1.0555722117,-0.4639618421\N,-1.6290828939,-2.1423856386,0
.501772931\O,0.5651769283,-2.1052761483,-1.5576549009\O,-0.8117378857,
2.3781228451,-0.93134567\C,0.4410047773,0.9923607299,1.8355781744\O,1.
7079585644,0.9927568966,2.4444202767\H,-0.2311171611,0.2187612143,2.23
55489555\H,-0.0157440562,1.9683563335,2.039315431\H,2.0028371636,0.079
6246068,2.5804418406\H,1.3000648502,1.5249789646,-0.0748982566\H,-1.65
27715429,0.8348298947,0.1836350245\H,-1.725913064,2.6810622339,-1.0453
313144\H,-1.6322709463,-0.4986382946,-1.8737314238\H,-0.2456333147,0.4
365663907,-2.4789323849\H,-1.2064454684,-2.6248925728,1.296680676\H,-2
.4740358284,-1.7085413828,0.8773012182\H,1.3013896355,-2.557724873,-1.
0942214998\H,-1.964569751,-2.8855488488,-0.1135777083\\Version=IBM-RS6
000-G98RevA.7\HF=-553.1244995\RMSD=5.315e-09\RMSF=5.858e-06\Dipole=-1.
1292648,-1.9349815,-0.5189369\PG=C01 [X(C5H12N1O4)]\\@

1m

1\1\GINC-N06\FOpt\RB3LYP\6-31G(d)\C5H12N1O4(1+)\ROOT\27-Nov-2000\0\#
OPT=CALCFC FREQ=NORAMAN RB3LYP/6-31G(D)\C1+2h2o-P-H1-calcfc\\1,1\C,-0
.4991863434,0.0600296166,-1.226550651\O,-0.4970416459,0.1285249269,0.2
531444258\C,0.7280654841,-0.0738366448,0.7323086654\C,1.7083742844,-0.
3559703079,-0.3763357238\C,0.9935084074,0.198086335,-1.6117281979\N,-0
.5760837658,0.819179582,3.8882504585\O,0.9618062533,-0.0315841455,1.93
83645538\O,1.382825387,1.555272349,-1.7131540221\C,-1.1869981716,-1.23

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12149598,-1.6589150819\O,-2.5400271472,-1.2712846344,-1.2629453951\H,-
0.620902243,-2.104959794,-1.2973394812\H,-1.1823941124,-1.2689813173,-
2.753536677\H,-2.5736232008,-1.4169088884,-0.3052372672\H,-1.087605200
1,0.9212397109,-1.5497749864\H,1.2265023197,-0.3660542436,-2.523400194
7\H,1.071480046,1.9176304612,-2.558135483\H,1.8695442095,-1.439304443,
-0.4351369622\H,2.6709110574,0.1264513199,-0.1972031354\H,-1.433704615
7,1.2963200164,3.5939378383\H,-0.8206239774,0.0430718123,4.5113629201\
H,-0.024369259,0.4458188198,3.0185690625\H,0.0142865925,1.4814272687,4
.4021905925\\Version=IBM-RS6000-G98RevA.7\HF=-553.1692358\RMSD=7.354e-
09\RMSF=3.323e-06\Dipole=-0.4535674,0.7550406,3.7779824\PG=C01 [X(C5H1
2N1O4)]\\@

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2a

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1\1\GINC-N03\FTS\UB3LYP\6-31G(d)\C8H14N5O5(2)\ROOT\27-Mar-2000\0\\# OP
T=(RCFC, TS, NOEIGENTEST) GUESS=READ GEOM=CHECK UB3LYP/6-31G(D)\\TP2-m
1-2-TS start at 2.4 for TS opt\\0,2\O,-1.7072501521,0.6726635165,0.683
7084131\C,-1.2033772264,-0.6064967192,0.5753053991\C,-2.1765201835,-1.
5134736384,-0.1225152503\C,-3.4613545831,-0.6673937901,-0.1587529488\C
,-2.9034189515,0.7708616736,-0.1225865455\C,-3.7886060191,1.8283919224
,0.5143545601\H,-4.0811934863,1.4918260182,1.5230607002\H,-4.701913753
8,1.9481546569,-0.080257269\O,-3.1639483045,3.0986021309,0.5491336335\
H,-2.3230995206,2.9754331431,1.0189951497\H,-2.623974192,1.0737224781,
-1.1405196708\H,-4.0559922758,-0.849785947,0.7501195968\O,-4.214873630
9,-0.9555265407,-1.3238360921\H,-5.1023875724,-0.5812852621,-1.2159117
294\H,-2.3058225139,-2.4671212193,0.401031744\H,-1.8650612203,-1.72618
0061,-1.1521524314\N,-0.4196487249,-0.9895717693,1.656988383\H,0.01145
45886,-0.1956256929,2.1212764054\H,0.2861125248,-1.6764243126,1.402380
5407\O,0.7327568952,-1.368473276,-1.1611770985\C,2.9414628618,1.419236
9918,-0.7190088829\C,1.8623271431,0.6903263657,-1.1547343946\N,1.74393
55216,-0.6257728305,-0.8130194238\C,2.7397529154,-1.1413049702,0.00057
35898\N,3.797784383,-0.4785135552,0.4205954294\N,3.9052142721,0.839005
4121,0.0610735142\O,4.9063598451,1.4806334977,0.4660470757\N,2.5253040
951,-2.4303005987,0.3899772012\H,3.3368714182,-2.9216602074,0.74005263
56\H,1.894634437,-2.9270308623,-0.2328926733\H,1.073685391,1.086792530
1,-1.7778960849\H,3.1026063856,2.4611764878,-0.9534132582\\Version=IBM
-RS6000-G98RevA.7\HF=-962.9122415\S2=0.793566\S2-1=0.\S2A=0.750461\RMS
D=5.697e-09\RMSF=1.104e-05\Dipole=-1.5192521,-0.906213,0.0156133\PG=C0
1 [X(C8H14N5O5)]\\@

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2b

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1\1\GINC-N05\FOpt\UB3LYP\6-31G(d)\C8H14N5O5(2)\ \23-Feb-2000\0\\# OPT=
RCFC GUESS=READ GEOM=CHECK B3LYP/6-31G(D) FREQ=NORAMAN\\TP2-m1-2-opt f
rom aml guess-opt\\0,2\O,0.9112281574,-0.7197567943,-0.8448286595\C,0.
826724037,-0.4977046221,0.5608186476\C,2.2762711389,-0.557859193,1.085
895632\C,3.1421563162,-0.7846423166,-0.1627809935\C,2.2125477415,-0.29
94835664,-1.2915730127\C,2.429330304,-0.9022901772,-2.669567695\H,-2.43
92876223,-2.0021151841,-2.5852938533\H,3.4007487136,-0.5840505785,-3.0
643913575\O,1.4535044601,-0.4612581544,-3.5961099531\H,0.5936048065,-0
.7159084876,-3.2237093232\H,2.2562759214,0.7969914661,-1.3477788235\H,
3.3426280121,-1.8592775305,-0.2984891347\O,4.3518414706,-0.0570169426,
-0.0430292198\H,4.9553691088,-0.3458522837,-0.7443643892\H,2.393312962
7,-1.3320077773,1.8485367273\H,2.5477814715,0.4036476347,1.5297406447\
N,-0.0777924761,-1.4120944606,1.1812460309\H,-0.9340827962,-1.48877906
3,0.6333724305\H,0.3386300821,-2.3400166889,1.2059322031\O,0.417272563
1,0.8812800269,0.8079279778\C,-2.7641352824,0.5696449213,-0.8460875146
\C,-1.474968243,0.9600480441,-0.7035090716\N,-0.9607449583,1.191610012

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5,0.5849925054\C,-1.8236840487,0.8969437876,1.6611552892\N,-3.06705114
 36,0.5394062955,1.5436962144\N,-3.5736267441,0.362296284,0.2521017565\
 O,-4.7804906925,-0.0110932921,0.1383186181\N,-1.3043541902,1.135674278
 4,2.9023753863\H,-1.8394391837,0.7157463745,3.6511828321\H,-0.30240569
 89,1.0191995486,2.9705951836\H,-0.8243583718,1.205949648,-1.5293812412
 \H,-3.2546655152,0.44304604,-1.8011729493\\Version=IBM-RS6000-G98RevA.
 7\HF=-962.9403981\S2=0.769967\S2-1=0.\S2A=0.750144\RMSD=8.293e-09\RMSF
 =1.559e-06\Dipole=2.8376033,-1.2842277,0.0343285\PG=C01 [X(C8H14N5O5)]
 \\@

2c

1\1\GINC-SP\FTS\UB3LYP\6-31G(d)\C8H14N5O5(2)\ROOT\05-May-2000\0\\#OPT=
 (CALCFC,TS,NOEIGEN) GUESS=READ GEOM=CHECK UB3LYP/6-31G(D)\\TP2-step2-
 TS\\0,2\O,-1.1795768937,0.5351255463,0.4511119043\C,-0.6658017833,-0.8
 092654191,0.4709692437\C,-1.9195155095,-1.7208267457,0.5218289146\C,-3
 .1160574646,-0.7653210442,0.3924343969\C,-2.4632438807,0.5037696533,-0
 .1895705506\C,-3.1450955881,1.8286143527,0.1097934951\H,-3.3286452958,
 1.9047766945,1.1948821212\H,-4.1128550181,1.8763359603,-0.4020148176\O
 ,-2.3825645608,2.9260059712,-0.3630690308\H,-1.5124863623,2.8425614412
 ,0.0600789951\H,-2.3425016584,0.3768094577,-1.274529803\H,-3.526999057
 4,-0.5340617795,1.388139834\O,-4.1078344475,-1.3492679766,-0.436274565
 2\H,-4.912581985,-0.8124113237,-0.3744445684\H,-1.9329458653,-2.318265
 6772,1.4373513799\H,-1.9165444031,-2.4032758385,-0.3316863071\N,0.2287
 887053,-0.9918222711,1.5789575091\H,0.9141725778,-0.2378909467,1.60365
 19782\H,-0.2985235586,-0.9197646703,2.4470067437\O,-0.0528909064,-1.12
 05697167,-0.7728635832\C,2.2940437307,1.6505202022,-0.2959659203\C,1.3
 057933449,1.0016659671,-0.9746388276\N,1.3259471375,-0.3719202216,-1.1
 202539142\C,2.396462373,-1.0173714418,-0.483730012\N,3.3792202244,-0.4
 280542046,0.1536811433\N,3.3432125164,0.9440537502,0.2477324109\O,4.29
 24511811,1.5218874639,0.8448316222\N,2.4194375617,-2.3701003394,-0.632
 2241804\H,3.0322780208,-2.854427722,0.0104059951\H,1.5057485964,-2.78
 45906159,-0.7673897\H,0.5051765813,1.5282003116,-1.4765315724\H,2.3742
 780932,2.7247442628,-0.2067862763\\Version=IBM-RS6000-G98RevA.7\HF=-96
 2.93785\S2=0.783919\S2-1=0.\S2A=0.750478\RMSD=9.820e-09\RMSF=2.520e-06
 \Dipole=-2.05505,-0.5952479,0.6710172\PG=C01 [X(C8H14N5O5)]\\@

2d

1\1\GINC-N02\FOpt\UB3LYP\6-31G(d)\C8H14N5O5(2)\ROOT\09-Jul-2000\0\\#UB
 3LYP/6-31G* OPT=RCFC FREQ=NORAMAN GUESS=READ GEOM=CHECK\\TP2-step2-PC-
 freq\\0,2\O,-2.0886694051,0.6972017365,0.2815246817\C,-1.4392767679,-0
 .5796114575,0.4582612597\C,-2.6374252769,-1.6172281697,0.5866920938\C,
 -3.8964755568,-0.7895905185,0.302196592\C,-3.3364413265,0.4731618099,-
 0.3815715864\C,-4.1582743677,1.7444255218,-0.24289397\H,-4.334659202,1
 .9393781728,0.8289079632\H,-5.1332594673,1.6138047925,-0.7273236469\O,
 -3.5370095108,2.8461710551,-0.8770957004\H,-2.623940393,2.8672833431,-
 0.5460566111\H,-3.1659813053,0.2494157274,-1.4443842681\H,-4.374199156
 7,-0.5069132469,1.2538976524\O,-4.7873270139,-1.5413081818,-0.50545747
 25\H,-5.6302774615,-1.0647332579,-0.5547009016\H,-2.579460309,-2.05866
 8694,1.5836478478\H,-2.5526475303,-2.4175308971,-0.1540311977\N,-0.555
 5080996,-0.5633398231,1.5861808929\H,0.3290397287,-0.1168356538,1.3253
 413853\H,-0.9800121635,-0.0297534419,2.3416459948\O,-0.8120557016,-0.9
 776989434,-0.6756431322\C,4.4422057006,1.3086192875,0.4960868908\C,3.1
 073806391,1.2722578554,0.8338899252\N,2.2803822702,0.2859433313,0.4811
 441411\C,2.8668109412,-0.6904666299,-0.2512010761\N,4.1615757908,-0.74
 74605641,-0.6410717056\N,4.9465348782,0.2650523639,-0.2517933628\O,6.1
 440258316,0.2484309177,-0.5844484384\N,2.1048916412,-1.7368117556,-0.6

294398453\H,2.5045676737,-2.4001303143,-1.2762402644\H,1.0947144775,-1.6743233271,-0.5410150689\H,2.6854932981,2.0849782866,1.4210832498\H,5.1527489336,2.0785647777,0.7542867442\\Version=IBM-RS6000-G98RevA.7\HF=-962.9804597\S2=0.753303\S2-1=0.\S2A=0.750008\RMSD=4.757e-09\RMSF=1.815e-06\Dipole=-1.8326483,0.286792,1.1651588\PG=C01 [X(C8H14N5O5)]\\@

2e

1\1\GINC-SP\FOpt\UB3LYP\6-31G(d)\C5H10N1O4(2)\ROOT\09-Jul-2000\0\#OPT=RCFC FREQ=NORAMAN GUESS=READ GEOM=CHECK UB3LYP/6-31G(D)\sugar-nh2-O radical\\0,2\O,-1.1913140213,-0.8105348779,-1.8107470555\C,-1.0597372327,-0.9316030017,-0.4745826405\O,0.3257847375,-0.9284056223,-0.0549718265\C,0.7570119206,0.4338513575,0.014610805\C,-0.43355178,1.1620768045,0.6684261431\C,-1.6469037593,0.426531344,0.0870430076\N,-1.7249455271,-2.1121877609,0.0265736182\O,-0.5160596631,2.5426506996,0.3540315615\C,2.0709292908,0.4572603914,0.7781924378\O,3.0836400263,-0.2711465326,0.1097853672\H,1.8977820066,0.0695586238,1.7968863116\H,2.4335185467,1.4883539425,0.8664728088\H,2.6974237437,-1.1379892765,-0.0979422892\H,0.9021489208,0.8373943316,-0.9978117127\H,-0.3964807278,1.0103582998,1.7591285431\H,0.1807870657,3.0079048108,0.8418985374\H,-2.4318686767,0.1793173247,0.8046335871\H,-2.0858003106,1.0256291937,-0.7161366307\H,-1.5369313077,-2.8901542617,-0.6031939122\H,-1.3288598432,-2.3542693712,0.9331265378\\Version=IBM-RS6000-G98RevA.7\HF=-552.0920098\S2=0.753041\S2-1=0.\S2A=0.750007\RMSD=3.453e-09\RMSF=1.388e-06\Dipole=-0.0453695,-0.0767825,1.1034473\PG=C01 [X(C5H10N1O4)]\\@

2f

1\1\GINC-N06\FOpt\RB3LYP\6-31G(d)\C3H4N4O1\ROOT\04-Jul-2000\0\# OPT RB3LYP/6-31G(D)\TP2-2step-1NO\\0,1\C,-1.5016360328,-0.0841855358,-0.5164917358\C,-1.4617922955,-0.0373612535,0.8617288919\N,-0.3323413353,0.0335880738,1.5678778184\C,0.7798306196,0.0529029801,0.8063469665\N,0.8613534785,0.0248470253,-0.5405484986\N,-0.3055577226,-0.0473393404,-1.1992137826\O,-0.2823131631,-0.0763272529,-2.441960752\N,1.9721942972,0.0826985772,1.4544498451\H,2.8067830092,0.2722516572,0.9204358297\H,1.9619588452,0.2905731537,2.4412083236\H,-2.3942502842,-0.0562964956,1.4220525248\H,-2.3839410377,-0.1406077878,-1.1354730738\\Version=IBM-RS6000-G98RevA.7\HF=-410.8746147\RMSD=8.576e-09\RMSF=6.898e-05\Dipole=-0.0422911,0.2519742,1.2979339\PG=C01 [X(C3H4N4O1)]\\@

2g

1\1\GINC-N02\FOpt\RB3LYP\6-31G(d)\C8H15N5O5\ROOT\30-Aug-2000\0\# OPT=RCFC GUESS=READ GEOM=CHECK RB3LYP/6-31G(D)\tp4-2-p-fre.log\\0,1\O,0.9056242283,-0.9941674298,-0.9774597316\C,0.9055122768,-0.9943069757,0.4570387208\C,2.3889273888,-0.9945296603,0.8772445752\C,3.1787408147,-0.9580811572,-0.4396018521\C,2.1348158683,-0.3958755056,-1.422407779\C,2.2976425635,-0.7418434726,-2.8921868796\H,2.386057274,-1.83578625,-3.0001977809\H,3.2145743102,-0.2867088535,-3.2831692991\O,1.2297626249,-0.2271276243,-3.6689401461\H,0.418432014,-0.611932376,-3.2990127699\H,2.0917248997,0.6965635933,-1.3017139723\H,3.4529136196,-1.9793582119,-0.7483219215\O,4.3329753002,-0.149931013,-0.2872195683\H,4.9111227668,-0.2923466714,-1.0520324487\H,2.6202264565,-1.8576419142,1.5052136782\H,2.6085371819,-0.0877200504,1.447693961\N,0.1318318104,-2.0771654337,0.9772707855\H,-0.8161964685,-2.0004975241,0.6100691016\H,0.5193910913,-2.9565154073,0.6415513428\O,0.3769326441,0.2608151303,0.9174534188\C,-2.4826317034,1.8570297031,-0.4451169906\C,-1.2820809629,1.2566854665,-0.3835310553\N,-1.0213243657,0.3663558531,0.6450491462\C,-1.746763515,0.7732257874,1.9045876942\N,-3.1762952605,0.8466783339,1.6078612485\N

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, -3.4777082672, 1.4639359277, 0.520021619\O, -4.6623316679, 1.6963022401, 0
.2052422472\N, -1.5829838183, -0.1190115843, 2.9995761698\H, -2.0443572922
, -1.0044274073, 2.8033193584\H, -0.596295828, -0.3031930411, 3.1592330959\
H, -0.512946477, 1.3961366386, -1.1330622555\H, -2.8487179168, 2.4934268053
, -1.2348588114\H, -1.3477877446, 1.7634934531, 2.1880675762\Version=IBM-
RS6000-G98RevA.7\HF=-963.5464\RMSD=2.962e-09\RMSF=2.399e-06\Dipole=2.6
171253, -1.3150155, -1.0023999\PG=C01 [X(C8H15N5O5)]\@
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2h

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1\1\GINC-N03\FTS\RB3LYP\6-31G(d)\C8H15N5O5\ROOT\20-Aug-2000\0\# OPT=(
CALCFC, TS, NOEIGEN) GUES=READ GEOM=CHECK RB3LYP/6-31G(D) SCF=(DIRECT, CO
NVER=6)\S4-4ringts-aml\0, 1\O, 1.9633705338, 0.1937165094, -0.8471306627
\C, 0.9886845837, -0.7953865348, -0.401439178\C, 1.7378611296, -1.602723583
8, 0.7094864095\C, 3.0670908216, -0.8619708152, 0.9186394684\C, 2.794521338
6, 0.5091525129, 0.271257481\C, 3.9998648838, 1.2652445113, -0.2641530234\H
, 4.5673373676, 0.6020784095, -0.9397078559\H, 4.661887357, 1.5541107599, 0.
5607744663\O, 3.6167595834, 2.4626955224, -0.9173639315\H, 2.909686543, 2.2
067790044, -1.5326617935\H, 2.2450114798, 1.1355690603, 0.9890954424\H, 3.8
72654185, -1.3685683163, 0.3628949085\O, 3.374253697, -0.8052421259, 2.3035
513455\H, 4.2761314882, -0.4628233011, 2.4002908237\H, 1.8579940649, -2.646
1405728, 0.4062575342\H, 1.1637457432, -1.5770737989, 1.6385466122\N, 0.594
5832447, -1.6164274262, -1.532723862\H, 0.1377561222, -1.0008829083, -2.205
6444172\H, 1.4269775569, -1.9938940061, -1.9844628544\O, -0.0888970741, -0.
1584607789, 0.1338747025\C, -3.0648825913, 1.7550227545, 0.1521863642\C, -2
.1005113888, 1.4492359678, -0.7614745607\N, -1.8194456936, 0.1762932964, -1
.1114351248\C, -2.4458176077, -0.8264804794, -0.3082613836\N, -3.545057840
2, -0.5287024977, 0.5582685865\N, -3.8148803449, 0.7264288156, 0.7718392208
\O, -4.7615002597, 1.0707318685, 1.5112089951\N, -2.613203671, -2.112525296
4, -0.9224746216\H, -3.2638280451, -2.0559986467, -1.7034120978\H, -1.70308
35784, -2.4168180466, -1.2698874547\H, -1.5652100856, 2.241368051, -1.27839
69092\H, -3.3809453345, 2.7497260822, 0.4333890063\H, -1.5128435896, -0.942
9939756, 0.4080321406\Version=IBM-RS6000-G98RevA.7\HF=-963.4709842\RMS
D=6.612e-07\RMSF=3.062e-06\Dipole=1.1916983, 0.2929574, -1.5701681\PG=C0
1 [X(C8H15N5O5)]\@
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2i

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1\1\GINC-N05\Fopt\RB3LYP\6-31G(d)\C8H15N5O5\ROOT\29-Aug-2000\0\#OPT=R
CFC GUESS=READ GEOM=CHECK RB3LYP/6-31G(D)\S4-4ringts-pc\0, 1\N, -4.329
2109023, 1.028509747, 0.478487704\C, -3.0530856288, 1.3395004233, 0.8950525
887\C, -2.0214332502, 0.5045758289, 0.5205321755\N, -2.2012279001, -0.58463
86668, -0.2361172991\C, -3.4835204593, -0.8044727715, -0.5870041245\N, -4.5
634680744, -0.0644779574, -0.2659916108\N, -3.7389265644, -1.8833880234, -1
.3754125364\O, -5.2942995311, 1.7465664888, 0.7905788418\O, 0.9523145852, -
0.7417449763, 1.2547025553\C, 1.6431031053, -1.0267503937, 0.0502937728\O,
1.899340107, 0.2423412485, -0.5514960454\C, 3.1150983017, 0.7997293836, -0.
0180334643\C, 3.8858535953, -0.3632229499, 0.6687356306\C, 3.0521308009, -1
.593026975, 0.3043482785\N, 0.8168481412, -1.8709921068, -0.755015406\O, 3.
927449652, -0.2540127983, 2.0862810999\C, 3.8572768088, 1.4339554782, -1.18
97206084\O, 3.0499717384, 2.3714816489, -1.8751044492\H, 4.2095778843, 0.63
42370853, -1.8651196881\H, 4.7394397124, 1.9752011646, -0.828023747\H, 2.20
91345256, 1.9149923092, -2.0466508291\H, 2.8577549161, 1.5664652407, 0.7250
851288\H, 4.9088755737, -0.4383805189, 0.2675312342\H, 4.3698589714, 0.5793
84739, 2.3109554597\H, 3.4286894321, -2.0545578523, -0.6152606407\H, 3.0694
925652, -2.3407837852, 1.1002474952\H, -0.1117483739, -1.4523621538, -0.845
5383608\H, 1.2209731374, -1.9939371092, -1.680734981\H, -4.7015165789, -2.1
703468941, -1.4767734986\H, -3.0223367602, -2.5915865804, -1.4309912177\H,
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-1.0035927566,0.7036509169,0.8466558911\H,-2.9724602664,2.2300566386,1.4996370573\H,0.6590030658,-1.5959051856,1.6124032236\\Version=IBM-RS6000-G98RevA.7\HF=-963.64423\RMSD=6.891e-09\RMSF=7.743e-05\Dipole=1.2347643,-1.5094578,-0.2230689\PG=C01 [X(C8H15N5O5)]\\@

2j

1\1\GINC-N05\FOpt\UB3LYP\6-31G(d)\C5H11N1O4\ROOT\05-Jun-2000\0\\# OPT=(RCFC) GUESS=READ GEOM=CHECK FREQ=NORAMAN UB3LYP/6-31G(D)\\sugar-nh2-o-h-ro\\0,1\O,-0.8957749011,-1.039209851,-1.8590487985\C,-1.0241132895,-0.899700932,-0.45868163\O,0.3094007211,-0.9017733453,0.050143268\C,0.7805749006,0.4528027051,0.0733267433\C,-0.4390798012,1.2477792453,0.5783220597\C,-1.6142863484,0.4769538756,-0.0414773057\N,-1.7887966309,-2.0115294919,0.0338503412\O,-0.4704828091,2.6037287336,0.158874016\C,2.0201123526,0.4787104031,0.9510979786\O,3.056121184,-0.3301443815,0.4248679327\H,1.7394921302,0.1638421739,1.9711747627\H,2.4175702304,1.4992049459,1.0101302018\H,2.644440096,-1.1846741406,0.2142334793\H,1.032006839,0.7840968818,-0.9440159553\H,-0.4801889371,1.1818190717,1.6776427703\H,0.2088294278,3.0888494873,0.6520385503\H,-2.4590766608,0.3647086615,0.6434821468\H,-1.9608668227,1.0138141871,-0.9283271746\H,-1.2906013367,-2.8709260273,-0.1956915527\H,-1.8713468722,-1.9652202737,1.0477757289\H,-1.7920421215,-1.1948895532,-2.1996137671\\Version=IBM-RS6000-G98RevA.7\HF=-552.7602269\S2=0.\S2-1=0.\S2A=0.\RMSD=9.810e-09\RMSF=2.139e-06\Dipole=-0.7296459,-0.0629091,0.8031922\PG=C01 [X(C5H11N1O4)]\\@

2k

1\1\GINC-N04\FOpt\UB3LYP\6-31G(d)\C3H5N4O1(2)\ \05-Mar-2001\0\\# B3LYP/6-31G(D) GEOM=CHECK GUESS=READ OPT=CALCFC FREQ=NORAMAN TEST\\2h-cleave drug\\0,2\C,-1.2437596014,0.9573026779,-0.1354104714\C,-0.0629101591,1.7080369036,-0.1443583289\N,1.1172920641,1.1952519871,0.096470791\C,1.1481275201,-0.228428966,0.4060076807\N,-0.0479184185,-1.0591394378,0.2363991177\N,-1.1756523085,-0.4450845503,0.0343097741\O,-2.2473532934,-1.0807232322,-0.0688096414\N,2.2242277856,-0.9091349214,-0.3007679049\H,2.0069901503,-0.919937084,-1.2971469796\H,3.0738346492,-0.3572885048,-0.1891092453\H,-0.1251719715,2.7743472048,-0.3636857648\H,-2.2428194078,1.3310127696,-0.3056696355\H,1.3916025102,-0.2770637636,1.4837730278\\Version=IBM-RS6000-G98RevA.7\HF=-411.3888422\S2=0.817036\S2-1=0.\S2A=0.752225\RMSD=4.103e-09\RMSF=6.233e-06\Dipole=0.4251346,1.6761844,-0.2686653\PG=C01 [X(C3H5N4O1)]\\@

8 (sugar-C₁'')

1\1\GINC-N06\FOpt\UB3LYP\6-31G(d)\C5H10N1O3(2)\ \09-Mar-2000\0\\#UB3LYP/6-31G(D) OPT=FCCARDS FREQ=NORAMAN\\ 6-31G(d) structure of 8-neutral re-optimized \\0,2\O,-0.9784486678,-0.1127171619,-0.3245032245\C,-0.9825372937,-0.3126832195,1.0635953268\C,0.4245056557,-0.2355690899,1.5667084228\C,1.087242485,0.7248827979,0.5613572853\C,0.2698497224,0.4998500187,-0.7247394517\C,0.9298984008,-0.4456391834,-1.7259524387\H,1.2711874842,-1.3549654527,-1.1995891555\H,1.8107213291,0.0342380715,-2.1669234882\O,0.0538816901,-0.7637379366,-2.789631243\H,-0.7853938997,-1.0144225173,-2.367368726\H,0.0442413722,1.4593780394,-1.2000304088\H,2.1499823674,0.4845386736,0.4029526459\O,0.9356566599,2.093740618,0.917829388\H,1.3783482631,2.2304889138,1.7698431568\H,0.9257541149,-1.223451062,1.5381004868\H,0.4878945853,0.1252736646,2.5989330866\N,-1.9029571758,-1.2194359816,1.5837609384\H,-2.8140001236,-1.1266964372,1.1433642439\H,-1.6105065413,-2.2016621214,1.5190173584\\Version=IBM-RS6000-G98RevA.7\HF=-476.8808847\S2=0.753134\S2-1=0.\S2A=0.750008\RMSD=5.826e-09\RMSF=2.262e-05\Dipole=0.5001031,-0.5468862,0.8582904\PG=C01 [X(C5H

10N1O3)]\\@

8-cation

1\\1\GINC-N03\FOpt\RB3LYP\6-31G(d)\C5H10N1O3(1+)\ROOT\08-Jul-2000\0\\#
 RB3LYP/6-31G(D) OPT=FCCARDS FREQ=NORAMAN\\8-cation 6-31G(d)\\1,1\O,-0
 .9926465404,-0.1778544524,-0.2554167726\C,-0.8769616888,-0.5972988215,
 0.9613789382\C,0.4843034951,-0.3814793471,1.5443690733\C,1.0566992636,
 0.715161068,0.6053226434\C,0.2772318958,0.4984802775,-0.7048691846\C,0
 .9356161354,-0.3671142963,-1.7750712256\H,1.1954345826,-1.3571201546,-
 1.3669719972\H,1.8734024229,0.1274580045,-2.0528927045\O,0.1559515793,
 -0.4447544985,-2.9406788368\H,-0.5374872272,-1.1121049405,-2.825414112
 6\H,-0.059580684,1.4454561033,-1.1266336605\H,2.1334208902,0.582250616
 4,0.4499784151\O,0.7322745523,2.0042653455,1.0695283104\H,1.4226469906
 ,2.3243104323,1.6718304868\H,1.0447455223,-1.3237717955,1.4759536923\H
 ,0.4569933852,-0.0705708973,2.5917140739\N,-1.9026559274,-1.1613252752
 ,1.5484669197\H,-2.7914757412,-1.2554705398,1.0638657734\H,-1.84547998
 58,-1.4909043425,2.5050585197\\Version=IBM-RS6000-G98RevA.7\HF=-476.71
 37052\RMSD=3.443e-09\RMSF=2.298e-05\Dipole=-0.5358143,-1.4169634,2.411
 6247\PG=C01 [X(C5H10N1O3)]\\@

9 (3-amino-1,2,4-triazine)

1\\1\GINC-N03\FOpt\UB3LYP\6-31G(d)\C3H4N4O2\ROOT\08-Mar-2000\0\\# OPT U
 B3LYP/6-31G(D) FREQ=NORAMAN\\ --8-- \\0,1\N,-1.494807693,-0.008131020
 3,-0.5091350042\C,-1.4689494433,-0.024784572,0.8588063908\C,-0.2636649
 738,-0.0243101854,1.5267196173\N,0.9039482071,-0.0033390864,0.85028236
 16\C,0.8013023355,0.0203903961,-0.5438645489\N,-0.3401689561,0.0140485
 3,-1.2150217477\H,-0.1784391584,-0.0416596626,2.6050051017\H,-2.433223
 122,-0.0409413492,1.3436992394\N,1.9839829084,0.0601267044,-1.17198121
 25\H,2.7998717397,-0.0065228703,-0.5739278428\H,2.0269310868,-0.005073
 6959,-2.1761318537\O,-2.5726762277,-0.0131208141,-1.1410373381\O,2.072
 9325625,-0.0084432045,1.4000843155\\Version=IBM-RS6000-G98RevA.7\HF=-4
 86.0274591\S2=0.\S2-1=0.\S2A=0.\RMSD=6.669e-09\RMSF=4.457e-05\Dipole=0
 .6028736,-0.0814443,0.354572\PG=C01 [X(C3H4N4O2)]\\@

9-anion

1\\1\GINC-N02\FOpt\UB3LYP\6-31G(d)\C3H4N4O2(1-,2)\ROOT\18-Oct-2000\0\\#
 OPT UB3LYP/6-31G(D)\\ 9-anion \\-1,2\N,-1.5110298499,-0.0224566
 073,-0.5195704008\C,-1.4792043066,-0.0585554803,0.8413570559\C,-0.3010
 666215,-0.0383292775,1.5425965767\N,0.9018905837,0.0216960401,0.834524
 5063\C,0.8040305193,0.0792122998,-0.5234113325\N,-0.3023171723,0.06672
 8703,-1.2548180748\H,-0.2136019203,-0.0677624433,2.618244206\H,-2.4529
 474482,-0.1072604772,1.3129364495\N,2.0372591092,0.1690327199,-1.15014
 65953\H,2.7391018904,-0.119114702,-0.4626245863\H,2.0540748957,-0.3076
 77252,-2.0428105189\O,-2.614022036,-0.0580418531,-1.1919774273\O,2.095
 2965785,-0.0591026927,1.4471117524\\Version=IBM-RS6000-G98RevA.7\HF=-4
 86.0371505\S2=0.769396\S2-1=0.\S2A=0.750171\RMSD=8.922e-09\RMSF=2.223e
 -05\Dipole=0.5110991,-0.3885236,0.4166376\PG=C01 [X(C3H4N4O2)]\\@

Deoxyribonolactone

1\\1\GINC-MAX\FOpt\RB3LYP\6-31G(d)\C5H8O4\KAT\14-Jul-2000\0\\# OPT=CALC
 FC GUESS=READ GEOM=CHECK RB3LYP/6-31G(D)\\final product\\0,1\C,-1.6851
 656113,0.6337348782,0.0354885984\C,-1.4478368473,-0.8693944872,-0.0081
 505791\O,-0.1067364684,-1.1016959082,-0.1785925675\C,0.6289139389,0.14
 33743511,-0.2822713825\C,-0.3053662374,1.2176692978,0.3208218299\O,-2.
 2447739585,-1.7625515705,0.0815045573\C,1.9624949009,-0.0565980225,0.4
 204583709\O,2.7394339339,-1.0700454303,-0.1845823382\O,-0.1687711329,2

.4916225187,-0.2824448648\H,1.775188701,-0.266137597,1.4871305239\H,2.
5504271359,0.8668171796,0.3572550308\H,2.1975737735,-1.8764361186,-0.1
779079041\H,0.7907527378,0.3588249763,-1.3455615239\H,-0.1403086002,1.
2777028539,1.4083164103\H,0.6355752424,2.9108931024,0.0597492503\H,-2.
4599404914,0.888651901,0.7607211228\H,-2.0207283551,0.96833072,-0.9548
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SF=3.518e-06\Dipole=0.4972142,1.2651651,0.510457\PG=C01 [X(C5H8O4)]\\@

O₄ protonated derivative of the 3-amino-1,2,4-triazine anion

1\1\GINC-SP\FOpt\UB3LYP\6-31G(d)\C3H5N4O2(2)\ROOT\05-Nov-2000\0\\# OPT
=RCFC GUESS=READ GEOM=CHECK FREQ=NORAMAN UB3LYP/6-31G(D)\\ld separate\
\0,2\N,-1.5299757593,-0.0491798636,-0.5140098755\C,-1.4879995751,-0.02
64618415,0.8656898644\C,-0.3190356022,0.159684252,1.51758655\N,0.87062
76709,0.4017830034,0.7953003529\C,0.7663855473,0.084650879,-0.58445106
24\N,-0.3415269595,-0.0900065682,-1.2348617612\H,-0.2394885391,0.23091
53827,2.5930248629\H,-2.4470999711,-0.1236428242,1.3544178483\N,1.9598
795699,0.0643902408,-1.2587868495\H,2.7348380014,-0.2956580444,-0.7165
110264\H,1.8815123815,-0.3174500907,-2.1931553806\O,-2.6191680106,-0.1
306012856,-1.1562388919\O,2.0006649763,-0.3091691645,1.3983247224\H,2.
5491285277,0.4278517536,1.7190918736\\Version=IBM-RS6000-G98RevA.7\HF=
-486.5952885\S2=0.770149\S2-1=0.\S2A=0.750185\RMSD=6.562e-09\RMSF=2.96
8e-06\Dipole=1.9269986,0.0778119,1.30715\PG=C01 [X(C3H5N4O2)]\\@