Substituent: H

# TEST OPT HF DIRECT 6-311G**				
HF=-285.800493				
PG=CS [SG(C2H1N1) X(C4H6)]				
Atom	Charge	X	Y	Z
N1	7	-0.0437909	2.3250275	0.0000000
C2	6	0.0000000	0.9296582	0.0000000
C3	6	-0.0145395	-1.8685584	0.0000000
C4	6	-0.0049890	0.2197466	1.1974936
C5	6	-0.0049890	0.2197466	-1.1974936
C6	6	-0.0117913	-1.1627828	-1.1913808
C7	6	-0.0117913	-1.1627828	1.1913808
H8	1	-0.0093083	0.7540417	2.1320908
H9	1	-0.0093083	0.7540417	-2.1320908
H10	1	-0.0145461	-1.6912979	-2.1287428
H11	1	-0.0145461	-1.6912979	2.1287428
H12	1	-0.0195830	-2.9431518	0.0000000
H13	1	0.3312142	2.7461542	0.8207696
H14	1	0.3312142	2.7461542	-0.8207696

Substituent: m-amino

# TEST OPT HF DIRECT 6-311G**				
HF=-340.8487416				
PG=C02 [C2(H1C1C1H1) X(C4H6N2)]				
Atom	Charge	X	Y	Z
H1	1	-0.3692420	-3.1869362	-0.4912511
C2	6	0.0231015	1.2070320	1.1047043
C3	6	-0.0246786	-1.2087191	-0.2885302
C4	6	0.0000000	0.0000000	1.7765298
C5	6	0.0246786	1.2087191	-0.2885302
C6	6	0.0000000	0.0000000	-0.9741850
C7	6	-0.0231015	-1.2070320	1.1047043
H8	1	0.0000000	0.0000000	2.8529201
N9	7	0.0000000	2.4102848	-0.9926072
H10	1	0.0000000	0.0000000	-2.0514570
H11	1	-0.0331934	-2.1360784	1.6464804
N12	7	0.0000000	-2.4102848	-0.9926072
H13	1	-0.3788298	-2.3591135	-1.9117898
H14	1	0.0331934	2.1360784	1.6464804
H15	1	0.3692420	3.1869362	-0.4912511
H16	1	0.3788298	2.3591135	-1.9117898

Substituent: m-bromo

# TEST OPT HF DIRECT 6-311G**				
HF=-2857.5846924				
PG=C01 [X(C6H6Br1N1)]				
Atom	Charge	X	Y	Z
N1	7	3.00466883	-1.53532913	-0.07178419
C2	6	2.05973729	-0.51594363	-0.01181648
C3	6	0.14993276	1.53597816	0.00717373
C4	6	2.45289620	0.82005505	-0.00469386
C5	6	0.70045489	-0.81797787	-0.01169688
C6	6	-0.22355823	0.20679015	-0.00154309
C7	6	1.50517596	1.82362747	0.00487403
H8	1	3.49991205	1.06717040	-0.01287049
H9	1	0.37433121	-1.84101476	-0.02523344
Br10	35	-2.07458037	-0.23580415	0.00153117
H11	1	1.82528469	2.85043702	0.01076774
H12	1	-0.58521814	2.31633055	0.01523775
H13	1	3.90047082	-1.29364123	0.28854666
H14	1	2.69501737	-2.41400891	0.27866566

Substituent: m-chloro

# TEST OPT HF DIRECT 6-311G**				
HF=-744.7234025				
PG=C01 [X(C6H6Cl1N1)]				
Atom	Charge	X	Y	Z
N1	7	-2.5478901	-1.3602220	-0.0718680
C2	6	-1.5062805	-0.4405357	-0.0116414
C3	6	0.5991571	1.4089432	0.0075742
C4	6	-0.1844328	-0.8767875	-0.0111018
C5	6	-1.7638876	0.9283492	-0.0049353
C6	6	-0.7198663	1.8313803	0.0045984
C7	6	0.8370209	0.0497071	-0.0007366
H8	1	0.0427125	-1.9263592	-0.0245515
H9	1	-2.7807513	1.2793001	-0.0133703
H10	1	-0.9351356	2.8850929	0.0101703
Cl11	17	2.4865436	-0.5256818	0.0028230
H12	1	1.4122951	2.1078306	0.0157685
H13	1	-2.3288966	-2.2648855	0.2807023
H14	1	-3.4164990	-1.0291743	0.2838208

Substituent: m-cyano

# TEST OPT HF DIRECT 6-311G**				
HF=-377.5540839				
PG=C01 [X(C7H6N2)]				
Atom	Charge	X	Y	Z
N1	7	-2.437969	-1.401612	-0.071358
C2	6	-1.403724	-0.474019	-0.011007
C3	6	0.677172	1.407356	0.007127
C4	6	-0.078052	-0.890169	-0.011234
C5	6	-1.672675	0.893527	-0.004725
C6	6	-0.644779	1.815456	0.004862
C7	6	0.944133	0.047067	-0.001418
H8	1	0.160152	-1.938146	-0.023811
H9	1	-2.694264	1.231300	-0.012990
H10	1	-0.877923	2.864849	0.010442
C11	6	2.313961	-0.411607	0.001564
H12	1	1.479926	2.119360	0.015207
H13	1	-2.209486	-2.308575	0.269158
H14	1	-3.307876	-1.082686	0.292179
N15	7	3.385576	-0.771498	0.005472

Substituent: m-fluoro

# TEST OPT HF DIRECT 6-311G**				
HF=-384.6805853				
PG=C01 [X(C6H6F1N1)]				
Atom	Charge	X	Y	Z
N1	7	-2.432291	-0.881636	-0.071251
C2	6	-1.197346	-0.248622	-0.011802
C3	6	1.300081	1.027561	0.007944
C4	6	-0.024225	-0.997585	-0.009731
C5	6	-1.110823	1.143344	-0.005346
C6	6	0.124510	1.760448	0.004283
C7	6	1.185916	-0.343965	0.000054
H8	1	-0.044148	-2.071969	-0.022118
H9	1	-2.009888	1.733603	-0.014237
H10	1	0.173923	2.834789	0.009579
F11	9	2.289977	-1.078262	0.004666
H12	1	2.267833	1.490764	0.016143
H13	1	-2.445436	-1.813247	0.278267
H14	1	-3.194720	-0.345216	0.276721

Substituent: m-hydroxy

# TEST OPT HF DIRECT 6-311G**				
HF=-360.6826239				
PG=C01 [X(C6H7N1O1)]				
Atom	Charge	X	Y	Z
N1	7	-2.410639	-0.949206	-0.072476
C2	6	-1.198598	-0.268458	-0.012384
C3	6	1.252386	1.079780	0.009282
C4	6	-0.000136	-0.979121	-0.009110
C5	6	-1.163270	1.121933	-0.005950
C6	6	0.058351	1.772509	0.004199
C7	6	1.209638	-0.306980	0.001377
H8	1	-0.017373	-2.056833	-0.024420
H9	1	-2.080317	1.683721	-0.015521
H10	1	0.076816	2.848375	0.009406
O11	8	2.385361	-0.966638	0.005577
H12	1	2.201661	1.580369	0.017726
H13	1	-2.392915	-1.868807	0.307838
H14	1	-3.191960	-0.431143	0.261738
H15	1	2.245446	-1.896112	-0.018525

Substituent: m-methoxy

# TEST OPT HF DIRECT 6-311G**				
HF=-399.7110093				
PG=C01 [X(C7H9N1O1)]				
Atom	Charge	X	Y	Z
H1	1	-2.845906	1.172335	-0.591293
C2	6	1.425333	-0.099134	0.861231
C3	6	-1.220616	0.712947	0.521003
C4	6	0.735269	-0.426309	-0.304174
C5	6	0.778151	0.626012	1.835124
C6	6	-0.537283	1.039084	1.682252
C7	6	-0.577763	-0.025331	-0.476489
O8	8	1.427398	-1.137053	-1.212389
H9	1	1.305341	0.881118	2.737931
H10	1	-1.026958	1.601002	2.457698
H11	1	-1.124131	-0.279802	-1.364391
N12	7	-2.557887	1.068583	0.355958
H13	1	2.443161	-0.421097	0.971996
H14	1	-2.847085	1.844169	0.908765
C15	6	0.820212	-1.533716	-2.407750
H16	1	-0.037602	-2.174204	-2.225346
H17	1	1.567070	-2.090941	-2.954076
H18	1	0.512306	-0.677554	-3.001056

Substituent: m-methyl

# TEST OPT HF DIRECT 6-311G**				
HF=-324.8468075				
PG=C01 [X(C7H9N1)]				
Atom	Charge	X	Y	Z
H1	1	0.330962	0.439521	3.020489
C2	6	-0.020071	-0.363561	-1.585002
C3	6	0.003067	-0.381028	1.202747
C4	6	-0.019471	0.838043	-0.890745
C5	6	-0.008600	-1.559783	-0.886362
C6	6	0.002966	-1.579827	0.493561
C7	6	-0.010063	0.816644	0.497131
C8	6	-0.005014	2.158093	-1.625104
H9	1	-0.011131	-2.491163	-1.425567
H10	1	0.002504	-2.516439	1.023812
H11	1	-0.021172	1.745969	1.042636
N12	7	-0.039009	-0.382287	2.597447
H13	1	-0.031264	-0.366983	-2.660322
H14	1	0.336058	-1.203026	3.018062
H15	1	0.998679	2.575132	-1.644695
H16	1	-0.653604	2.882232	-1.143162
H17	1	-0.334846	2.039281	-2.650740

Substituent: m-nitro

# TEST OPT HF DIRECT 6-311G**				
HF=-489.3234116				
PG=C01 [X(C6H6N2O2)]				
Atom	Charge	X	Y	Z
N1	7	-2.749977	-1.382929	-0.075207
C2	6	-1.730280	-0.440077	-0.012022
C3	6	0.324282	1.476933	0.009135
C4	6	-0.399331	-0.838587	-0.012954
C5	6	-2.018616	0.923642	-0.002825
C6	6	-1.005538	1.861601	0.008596
C7	6	0.588405	0.124281	-0.001797
H8	1	-0.131401	-1.876097	-0.025948
H9	1	-3.045005	1.246374	-0.010271
H10	1	-1.254179	2.907119	0.016596
N11	7	1.989069	-0.321534	0.001153
H12	1	1.122555	2.189465	0.017687
H13	1	-2.504849	-2.290291	0.252207
H14	1	-3.623569	-1.082285	0.294774
O15	8	2.195703	-1.490206	0.014433
O16	8	2.830456	0.513981	-0.008867

Substituent: p-amino

# TEST OPT HF DIRECT 6-311G**				
HF=-340.8424716				
PG=C02H [SGH(C2N2) X(C4H8)]				
Atom	Charge	X	Y	Z
H1	1	-0.347694	-3.223639	0.814903
C2	6	-0.000733	0.691494	-1.187559
C3	6	0.000733	-0.691494	1.187559
C4	6	0.000733	-0.691494	-1.187559
C5	6	0.000733	1.409678	0.000000
C6	6	-0.000733	0.691494	1.187559
C7	6	-0.000733	-1.409678	0.000000
H8	1	0.007828	-1.216662	-2.127626
N9	7	-0.056042	2.815796	0.000000
H10	1	-0.007828	1.216662	2.127626
N11	7	0.056042	-2.815796	0.000000
H12	1	0.007828	-1.216662	2.127626
H13	1	-0.347694	-3.223639	-0.814903
H14	1	-0.007828	1.216662	-2.127626
H15	1	0.347694	3.223639	0.814903
H16	1	0.347694	3.223639	-0.814903

Substituent: p-bromo

# TEST OPT HF DIRECT 6-311G**				
HF=-2857.5843888				
PG=CS [SG(C2Br1N1) X(C4H6)]				
Atom	Charge	X	Y	Z
N1	7	0.099988	-3.850580	0.000000
C2	6	0.032545	-2.459901	0.000000
C3	6	0.000000	0.323388	0.000000
C4	6	0.025706	-1.747735	1.195959
C5	6	0.025706	-1.747735	-1.195959
C6	6	0.009179	-0.366096	-1.196949
C7	6	0.009179	-0.366096	1.196949
H8	1	0.039015	-2.276873	2.132774
H9	1	0.039015	-2.276873	-2.132774
H10	1	0.002936	0.167490	-2.128629
H11	1	0.002936	0.167490	2.128629
Br12	35	-0.025263	2.226442	0.000000
H13	1	-0.256758	-4.283803	0.822229
H14	1	-0.256758	-4.283803	-0.822229

Substituent: p-chloro

# TEST OPT HF DIRECT 6-311G**				
HF=-744.722564				
PG=CS [SG(C2Cl1N1) X(C4H6)]				
Atom	Charge	X	Y	Z
N1	7	0.068757	-3.204914	0.000000
C2	6	0.011403	-1.812802	0.000000
C3	6	0.000000	0.969486	0.000000
C4	6	0.010039	-1.100390	1.195574
C5	6	0.010039	-1.100390	-1.195574
C6	6	0.003910	0.281214	-1.196209
C7	6	0.003910	0.281214	1.196209
H8	1	0.019606	-1.629086	2.132597
H9	1	0.019606	-1.629086	-2.132597
H10	1	0.001960	0.818926	-2.125645
H11	1	0.001960	0.818926	2.125645
Cl12	17	-0.010131	2.718404	0.000000
H13	1	-0.294014	-3.634066	0.821747
H14	1	-0.294014	-3.634066	-0.821747

Substituent: p-cyano

# TEST OPT HF DIRECT 6-311G**				
HF=-377.5573752				
PG=CS [SG(C3N2) X(C4H6)]				
Atom	Charge	X	Y	Z
N1	7	0.060868	-3.082127	0.000000
C2	6	0.009379	-1.702077	0.000000
C3	6	0.000000	1.090083	0.000000
C4	6	0.008311	-0.991262	1.201613
C5	6	0.008311	-0.991262	-1.201613
C6	6	0.003594	0.385148	-1.198476
C7	6	0.003594	0.385148	1.198476
H8	1	0.016619	-1.524078	2.135728
H9	1	0.016619	-1.524078	-2.135728
H10	1	0.001829	0.920858	-2.129946
H11	1	0.001829	0.920858	2.129946
C12	6	-0.007398	2.528145	0.000000
H13	1	-0.259944	-3.529831	0.828014
H14	1	-0.259944	-3.529831	-0.828014
N15	7	-0.013977	3.659635	0.000000

Substituent: p-fluoro

# TEST OPT HF DIRECT 6-311G**				
HF=-384.6766404				
PG=CS [SG(C2F1N1) X(C4H6)]				
Atom	Charge	X	Y	Z
N1	7	-0.049342	2.768903	0.000000
C2	6	0.000000	1.370168	0.000000
C3	6	-0.008801	-1.400215	0.000000
C4	6	-0.003902	0.658147	1.194655
C5	6	-0.003902	0.658147	-1.194655
C6	6	-0.007429	-0.725146	-1.197351
C7	6	-0.007429	-0.725146	1.197351
H8	1	-0.009833	1.188152	2.130989
H9	1	-0.009833	1.188152	-2.130989
H10	1	-0.009462	-1.277180	-2.119048
H11	1	-0.009462	-1.277180	2.119048
F12	9	-0.010477	-2.732702	0.000000
H13	1	0.333529	3.187157	0.818728
H14	1	0.333529	3.187157	-0.818728

Substituent: p-hydroxy

# TEST OPT HF DIRECT 6-311G**				
HF=-360.6771269				
PG=C01 [X(C6H7N1O1)]				
Atom	Charge	X	Y	Z
N1	7	0.061696	-0.035777	-2.793077
C2	6	0.005056	-0.015459	-1.388946
C3	6	0.003636	0.008841	1.412011
C4	6	0.005147	1.178309	-0.686944
C5	6	0.008052	-1.201394	-0.659177
C6	6	0.005477	-1.191662	0.720148
C7	6	0.003960	1.191445	0.700432
H8	1	0.011479	2.113013	-1.220816
H9	1	0.018126	-2.144225	-1.178675
H10	1	0.006501	-2.111991	1.274856
H11	1	0.002771	2.135602	1.219669
O12	8	-0.000336	-0.040572	2.768826
H13	1	-0.354735	-0.848124	-3.192960
H14	1	-0.317816	0.782998	-3.215760
H15	1	0.016519	0.827266	3.129469

Substituent: p-methoxy

# TEST OPT HF DIRECT 6-311G**				
HF=-399.7061904				
PG=C01 [X(C7H9N1O1)]				
Atom	Charge	X	Y	Z
O1	8	0.313114	0.702832	-2.203057
C2	6	0.121392	0.327400	-0.916034
C3	6	-0.359349	-0.240820	1.789920
C4	6	0.402309	-0.922207	-0.401724
C5	6	-0.402086	1.297197	-0.067059
C6	6	-0.635061	1.020173	1.259506
C7	6	0.160702	-1.198049	0.941047
H8	1	0.807142	-1.700106	-1.019997
H9	1	-0.618013	2.269327	-0.470856
H10	1	-1.031028	1.790639	1.898714
H11	1	0.391665	-2.179050	1.319796
N12	7	-0.552335	-0.497354	3.157923
C13	6	0.848140	-0.212030	-3.111119
H14	1	0.206650	-1.081918	-3.226883
H15	1	1.841535	-0.536807	-2.812595
H16	1	0.916271	0.303145	-4.058400
H17	1	-1.299379	0.028515	3.556397
H18	1	-0.669690	-1.464906	3.365589

Substituent: p-methyl

# TEST OPT HF DIRECT 6-311G**				
HF=-324.845281				
PG=CS [SG(C3H1N1) X(C4H8)]				
Atom	Charge	X	Y	Z
H1	1	0.310667	3.250750	-0.816650
C2	6	0.011081	-1.389747	0.000088
C3	6	-0.012497	1.431617	-0.000100
C4	6	0.015346	-0.665739	-1.183770
C5	6	-0.003534	-0.665739	1.183864
C6	6	-0.016252	0.717155	1.192013
C7	6	0.002759	0.717155	-1.192121
H8	1	0.031031	-1.188623	-2.125339
H9	1	-0.002866	-1.188623	2.125564
H10	1	-0.031517	1.245780	2.130042
H11	1	0.002455	1.245780	-2.130274
N12	7	-0.074665	2.829329	-0.000595
C13	6	-0.005544	-2.901013	-0.000044
H14	1	0.297604	3.250750	0.821500
H15	1	-1.022909	-3.285303	-0.008157
H16	1	0.488026	-3.298971	0.880502
H17	1	0.502005	-3.298971	-0.872607

Substituent: p-nitro

# TEST OPT HF DIRECT 6-311G**				
HF=-489.3281769				
PG=CS [SG(C2N2) X(C4H6O2)]				
Atom	Charge	X	Y	Z
N1	7	0.065649	-3.436665	0.000000
C2	6	0.014284	-2.061466	0.000000
C3	6	0.000000	0.706706	0.000000
C4	6	0.011740	-1.351208	1.204020
C5	6	0.011740	-1.351208	-1.204020
C6	6	0.004390	0.024234	-1.204116
C7	6	0.004390	0.024234	1.204116
H8	1	0.020633	-1.884544	2.137468
H9	1	0.020633	-1.884544	-2.137468
H10	1	0.001394	0.572077	-2.125076
H11	1	0.001394	0.572077	2.125076
N12	7	-0.010625	2.158954	0.000000
H13	1	-0.235304	-3.892311	0.830615
H14	1	-0.235304	-3.892311	-0.830615
O15	8	-0.014868	2.712861	1.052026
O16	8	-0.014868	2.712861	-1.052026

Substituent: 3-amino-4-hydroxy

# TEST OPT HF DIRECT 6-311G**				
HF=-415.7251406				
PG=C01 [X(C6H8N2O1)]				
Atom	Charge	X	Y	Z
N1	7	2.949326	0.402453	-0.053136
C2	6	1.595336	0.061454	-0.006222
C3	6	-1.111375	-0.591400	-0.007437
C4	6	0.626553	1.060123	0.004091
C5	6	1.196530	-1.268927	-0.029155
C6	6	-0.153919	-1.577355	-0.029270
C7	6	-0.724991	0.748060	-0.000325
H8	1	0.928473	2.094110	0.007052
H9	1	1.930359	-2.054664	-0.053491
H10	1	-0.477580	-2.602762	-0.051061
N11	7	-1.705872	1.735880	0.051662
O12	8	-2.451427	-0.906276	-0.037690
H13	1	3.163732	1.280115	0.365592
H14	1	3.557450	-0.310003	0.284572
H15	1	-1.398040	2.630364	-0.258864
H16	1	-2.552336	1.464249	-0.399137
H17	1	-2.813616	-0.811261	0.827081

Substituent: 3-bromo-4-methoxy

# TEST OPT HF DIRECT 6-311G**				
HF=-2971.4872014				
PG=C01 [X(C7H8Br1N1O1)]				
Atom	Charge	X	Y	Z
N1	7	3.570880	-1.089229	0.312526
C2	6	2.397189	-0.367434	0.084498
C3	6	0.026541	1.098250	-0.269274
C4	6	1.161653	-0.999251	0.112229
C5	6	2.433744	1.007704	-0.125640
C6	6	1.265607	1.718780	-0.300858
C7	6	-0.001322	-0.270155	-0.062266
H8	1	1.101797	-2.059626	0.271632
H9	1	3.379366	1.520027	-0.152590
H10	1	1.299428	2.778391	-0.480366
Br11	35	-1.658921	-1.194944	-0.039732
O12	8	-1.102111	1.817614	-0.480298
H13	1	3.505256	-2.057702	0.090020
H14	1	4.382806	-0.685496	-0.099255
C15	6	-1.668177	2.421698	0.658984
H16	1	-2.557728	2.937828	0.326919
H17	1	-0.980409	3.136990	1.101217
H18	1	-1.938972	1.678783	1.401718

Substituent: 3-bromo-4-methyl

# TEST OPT HF DIRECT 6-311G**				
HF=-2896.6289738				
PG=C01 [X(C7H8Br1N1)]				
Atom	Charge	X	Y	Z
N1	7	-3.238700	-1.486210	-0.070086
C2	6	-2.205480	-0.550988	-0.011488
C3	6	-0.096779	1.343142	0.002176
C4	6	-0.878437	-0.962224	-0.010562
C5	6	-2.470544	0.812815	-0.007982
C6	6	-1.433861	1.723971	-0.000716
C7	6	0.136693	-0.025446	-0.003347
H8	1	-0.638756	-2.008950	-0.021062
H9	1	-3.488683	1.160847	-0.016973
H10	1	-1.670782	2.773545	0.002642
Br11	35	1.925625	-0.691815	0.000656
C12	6	1.002658	2.376561	0.010166
H13	1	-3.002367	-2.384099	0.289660
H14	1	-4.102405	-1.165640	0.307659
H15	1	1.634897	2.276840	0.886430
H16	1	0.576893	3.372962	0.013195
H17	1	1.639721	2.284500	-0.863383

Substituent: 3-chloro-4-methyl

# TEST OPT HF DIRECT 6-311G**				
HF=-783.7682726				
PG=C01 [X(C7H8Cl1N1)]				
Atom	Charge	X	Y	Z
N1	7	-3.092136	-0.845974	-0.069970
C2	6	-1.840890	-0.233136	-0.011248
C3	6	0.707621	1.003141	0.002347
C4	6	-0.679794	-0.995655	-0.010237
C5	6	-1.718700	1.151285	-0.007990
C6	6	-0.470220	1.740340	-0.000946
C7	6	0.553264	-0.375551	-0.002943
H8	1	-0.733339	-2.068319	-0.020880
H9	1	-2.600983	1.767092	-0.017046
H10	1	-0.406864	2.814479	0.002228
Cl11	17	1.969343	-1.405704	0.001089
C12	6	2.056616	1.678459	0.010306
H13	1	-3.114783	-1.773068	0.292525
H14	1	-3.834878	-0.297069	0.302051
H15	1	1.935223	2.755157	0.014054
H16	1	2.640304	1.407078	-0.863387
H17	1	2.634058	1.400137	0.885995

Substituent: 3-chloro-5-methoxy

# TEST OPT HF DIRECT 6-311G**				
HF=-858.6345604				
PG=C01 [X(C7H8Cl1N1O1)]				
Atom	Charge	X	Y	Z
N1	7	-1.056950	3.038288	-0.068298
C2	6	-0.580157	1.736726	-0.011574
C3	6	0.373479	-0.895778	0.003475
C4	6	-1.482338	0.666707	-0.009922
C5	6	0.780166	1.483601	-0.006798
C6	6	1.253118	0.176960	-0.000456
C7	6	-0.982220	-0.609749	-0.001518
H8	1	-2.541349	0.839116	-0.023003
H9	1	1.494377	2.286074	-0.014900
O10	8	2.587738	0.047768	0.004364
Cl11	17	-2.105050	-1.947869	0.003426
H12	1	0.703605	-1.912819	0.010108
H13	1	-1.974184	3.168014	0.294805
H14	1	-0.424308	3.733115	0.258738
C15	6	3.170906	-1.226453	0.002382
H16	1	4.238735	-1.066406	0.001562
H17	1	2.893060	-1.786714	-0.884806
H18	1	2.894929	-1.788850	0.888889

Substituent: 3-methoxy-5-nitro

# TEST OPT HF DIRECT 6-311G**				
HF=-603.2342105				
PG=C01 [X(C7H8N2O3)]				
Atom	Charge	X	Y	Z
N1	7	0.025933	3.315840	-0.072938
C2	6	0.118745	1.933615	-0.013364
C3	6	0.308484	-0.866772	0.003298
C4	6	-1.043906	1.156715	-0.012886
C5	6	1.351430	1.305441	-0.006787
C6	6	1.449283	-0.081559	0.000733
C7	6	-0.907385	-0.206114	-0.003154
H8	1	-2.016220	1.605054	-0.024851
H9	1	2.261204	1.877240	-0.013628
O10	8	2.696204	-0.571319	0.007801
N11	7	-2.132117	-1.024041	0.001471
H12	1	0.333024	-1.933886	0.009598
H13	1	-0.822599	3.699388	0.277574
H14	1	0.824313	3.809611	0.256609
C15	6	2.904308	-1.959024	0.007513
H16	1	2.480964	-2.421041	0.893615
H17	1	3.974530	-2.099813	0.009098
H18	1	2.483538	-2.420093	-0.880227
O19	8	-2.005469	-2.203438	-0.021264
O20	8	-3.173388	-0.456851	0.028509

Substituent: 3-methyl-4-nitro

# TEST OPT HF DIRECT 6-311G**				
HF=-528.3701785				
PG=C01 [X(C7H8N2O2)]				
Atom	Charge	X	Y	Z
N1	7	-3.524341	-0.071794	-0.053723
C2	6	-2.152236	-0.148961	-0.007409
C3	6	0.619972	-0.269460	-0.002209
C4	6	-1.507459	-1.386601	-0.009150
C5	6	-1.378290	1.010792	-0.005121
C6	6	0.006515	0.990688	-0.002797
C7	6	-0.137546	-1.433832	-0.005990
H8	1	-2.078809	-2.296975	-0.017934
H9	1	-1.878556	1.962471	-0.011041
C10	6	0.725306	2.320340	-0.000971
H11	1	0.368855	-2.377243	-0.005865
N12	7	2.065755	-0.437169	0.003577
H13	1	-4.024943	-0.876593	0.245798
H14	1	-3.933427	0.783285	0.245357
H15	1	1.362040	2.421568	-0.869428
H16	1	1.359031	2.421928	0.869703
H17	1	-0.003506	3.121103	-0.002724
O18	8	2.751678	0.534922	0.003706
O19	8	2.496052	-1.546748	0.008674

Substituent: 3_4-dimethyl

# TEST OPT HF DIRECT 6-311G**				
HF=-363.8905178				
PG=C01 [X(C8H11N1)]				
Atom	Charge	X	Y	Z
N1	7	-3.001811	0.373071	-0.071329
C2	6	-1.644077	0.042144	-0.012209
C3	6	1.098749	-0.590856	0.002750
C4	6	-1.227270	-1.278917	-0.008673
C5	6	-0.673160	1.040357	-0.010306
C6	6	0.679082	0.744890	-0.002166
C7	6	0.125317	-1.574971	-0.001420
H8	1	-1.952541	-2.074318	-0.017428
H9	1	-0.986627	2.070832	-0.021936
H10	1	0.425322	-2.609123	0.001845
C11	6	1.686345	1.871122	0.000141
C12	6	2.564581	-0.959773	0.011550
H13	1	-3.604853	-0.330854	0.293102
H14	1	-3.219346	1.261449	0.323010
H15	1	2.333797	1.821299	-0.870836
H16	1	2.323416	1.828135	0.879233
H17	1	1.191966	2.835044	-0.006942
H18	1	2.687071	-2.036753	0.015198
H19	1	3.074148	-0.568040	0.888342
H20	1	3.082925	-0.573154	-0.862293

Substituent: 3_5-dibromo

# TEST OPT HF DIRECT 6-311G**				
HF=-5429.3669897				
PG=CS [SG(C2H1N1) X(C4H4Br2)]				
Atom	Charge	X	Y	Z
N1	7	0.061349	-3.529583	0.000000
C2	6	0.008305	-2.143254	0.000000
C3	6	0.000586	0.662624	0.000000
C4	6	0.007537	-1.438530	1.201373
C5	6	0.007537	-1.438530	-1.201373
C6	6	0.003219	-0.060480	-1.177846
C7	6	0.003219	-0.060480	1.177846
H8	1	0.015913	-1.964775	2.136923
H9	1	0.015913	-1.964775	-2.136923
Br10	35	-0.001033	0.881558	-2.826978
Br11	35	-0.001033	0.881558	2.826978
H12	1	-0.003566	1.732989	0.000000
H13	1	-0.283911	-3.966771	0.824614
H14	1	-0.283911	-3.966771	-0.824614

Substituent: 3_5-dimethoxy

# TEST OPT HF DIRECT 6-311G**				
HF=-513.6236428				
PG=C01 [X(C8H11N1O2)]				
Atom	Charge	X	Y	Z
N1	7	0.896673	2.992717	-0.070257
C2	6	0.437908	1.681636	-0.011716
C3	6	-0.453881	-0.958812	0.007037
C4	6	-0.914671	1.411685	-0.008922
C5	6	1.369780	0.632940	-0.005186
C6	6	0.912554	-0.667749	0.004289
C7	6	-1.352854	0.087419	-0.001683
H8	1	-1.645005	2.199105	-0.019619
H9	1	2.416847	0.862809	-0.021553
O10	8	1.715644	-1.744657	0.011385
O11	8	-2.685506	-0.072087	0.000148
H12	1	-0.750682	-1.986982	0.014445
H13	1	0.241021	3.675061	0.237796
H14	1	1.795393	3.138270	0.331562
C15	6	-3.235874	-1.359283	0.003119
C16	6	3.105524	-1.585822	-0.006980
H17	1	-2.942523	-1.917067	-0.880708
H18	1	-4.307955	-1.227123	0.000585
H19	1	-2.946137	-1.911639	0.891620
H20	1	3.433255	-1.064810	-0.901349
H21	1	3.521761	-2.582579	-0.004663
H22	1	3.455306	-1.052201	0.871668

Substituent: 3_5-dimethyl

# TEST OPT HF DIRECT 6-311G**				
HF=-363.8931597				
PG=C01 [X(C8H11N1)]				
Atom	Charge	X	Y	Z
N1	7	-0.001240	2.807215	-0.073182
C2	6	-0.000758	1.413257	-0.013026
C3	6	0.000829	-1.363827	0.006356
C4	6	-1.199381	0.707854	-0.024635
C5	6	1.198636	0.709478	0.006638
C6	6	1.206931	-0.676152	0.013679
C7	6	-1.206120	-0.677646	-0.012129
H8	1	-2.130612	1.248932	-0.048481
H9	1	2.129566	1.251649	0.007682
C10	6	-2.516497	-1.429067	0.013184
C11	6	2.518075	-1.426385	-0.003771
H12	1	0.001432	-2.440151	0.014418
H13	1	-0.825086	3.233188	0.288891
H14	1	0.817627	3.234061	0.298983
H15	1	2.872358	-1.550760	-1.023966
H16	1	2.411155	-2.413271	0.432156
H17	1	3.284084	-0.893019	0.548797
H18	1	-2.873113	-1.541268	1.034088
H19	1	-2.407451	-2.421252	-0.409917
H20	1	-3.281575	-0.903689	-0.548150

Substituent: 4-chloro-3-nitro

# TEST OPT HF DIRECT 6-311G**				
HF=-948.2291053				
PG=C01 [X(C6H5Cl1N2O2)]				
Atom	Charge	X	Y	Z
N1	7	-3.504999	0.533305	0.138246
C2	6	-2.204886	0.058541	0.050068
C3	6	0.436425	-0.907585	-0.018514
C4	6	-1.128200	0.932929	0.032892
C5	6	-1.938040	-1.308271	0.027797
C6	6	-0.643319	-1.775299	-0.017033
C7	6	0.163104	0.446831	0.013672
H8	1	-1.280526	1.994713	0.037517
H9	1	-2.751158	-2.011915	0.041920
H10	1	-0.457226	-2.831528	-0.055249
N11	7	1.223488	1.460381	0.039670
Cl12	17	2.032470	-1.572359	-0.136174
H13	1	-3.639422	1.466185	-0.181418
H14	1	-4.204783	-0.082460	-0.210199
O15	8	1.070921	2.409619	-0.658341
O16	8	2.134228	1.284935	0.771300

Substituent: 4-methyl-3-nitro

# TEST OPT HF DIRECT 6-311G**				
HF=-528.3643816				
PG=C01 [X(C7H8N2O2)]				
Atom	Charge	X	Y	Z
N1	7	-3.160427	-1.044984	0.160967
C2	6	-1.978883	-0.314950	0.050910
C3	6	0.439527	1.187145	-0.054117
C4	6	-1.992475	1.074962	-0.002561
C5	6	-0.747597	-0.947502	0.044811
C6	6	0.415588	-0.200475	0.001707
C7	6	-0.815621	1.790131	-0.061807
H8	1	-2.932043	1.599552	0.002096
H9	1	-0.678866	-2.016788	0.073329
N10	7	1.662436	-0.977564	0.018052
H11	1	-0.868394	2.862574	-0.116488
C12	6	1.677721	2.052295	-0.124948
H13	1	-3.961016	-0.594933	-0.223497
H14	1	-3.094389	-1.988855	-0.149213
O15	8	2.628690	-0.468880	0.482588
O16	8	1.629293	-2.079344	-0.424442
H17	1	1.389395	3.064186	-0.383559
H18	1	2.379373	1.697248	-0.868816
H19	1	2.198453	2.071019	0.823884

Substituent: 3_5-dibromo-4-hydroxy

# TEST OPT HF DIRECT 6-311G**				
HF=-5504.2403538				
PG=C01 [X(C6H5Br2N1O1)]				
Atom	Charge	X	Y	Z
N1	7	-0.023612	3.669420	-0.072627
C2	6	-0.010142	2.272404	-0.011094
C3	6	-0.000019	-0.552760	0.000190
C4	6	-1.198618	1.550686	-0.010618
C5	6	1.181902	1.569281	-0.009948
C6	6	1.171216	0.186417	-0.003471
C7	6	-1.186471	0.173341	-0.003589
H8	1	-2.140554	2.065963	-0.021146
H9	1	2.120719	2.089917	-0.019947
Br10	35	2.841742	-0.730320	0.001431
Br11	35	-2.839265	-0.750584	0.001407
O12	8	-0.051340	-1.891042	0.008598
H13	1	-0.845083	4.083360	0.309587
H14	1	0.792345	4.099903	0.302983
H15	1	0.814681	-2.261313	-0.000044

Substituent: 3_5-dibromo-4-methoxy

# TEST OPT HF DIRECT 6-311G**				
HF=-5543.2667544				
PG=CS [SG(C3H1N1O1) X(C4H6Br2)]				
Atom	Charge	X	Y	Z
N1	7	-0.492323	-3.783844	0.000000
C2	6	-0.366878	-2.396408	0.000000
C3	6	0.000000	0.401797	0.000000
C4	6	-0.279380	-1.692204	1.193782
C5	6	-0.279380	-1.692204	-1.193782
C6	6	-0.102615	-0.323762	-1.180004
C7	6	-0.102615	-0.323762	1.180004
H8	1	-0.349139	-2.208544	2.132354
H9	1	-0.349139	-2.208544	-2.132354
Br10	35	-0.034628	0.583718	-2.844959
Br11	35	-0.034628	0.583718	2.844959
O12	8	0.134232	1.741232	0.000000
H13	1	-0.909665	-4.160967	0.821511
H14	1	-0.909665	-4.160967	-0.821511
C15	6	1.457131	2.240335	0.000000
H16	1	1.990657	1.917894	-0.886568
H17	1	1.990657	1.917894	0.886568
H18	1	1.375072	3.317268	0.000000

Substituent: 3_5-dibromo-4-methyl

# TEST OPT HF DIRECT 6-311G**				
HF=-5468.407559				
PG=C01 [X(C7H7Br2N1)]				
Atom	Charge	X	Y	Z
N1	7	0.028368	3.646313	-0.067799
C2	6	0.016968	2.256838	-0.011006
C3	6	-0.006679	-0.592656	-0.000575
C4	6	-1.181887	1.555328	-0.009857
C5	6	1.199510	1.533840	-0.009392
C6	6	1.169549	0.152131	-0.003802
C7	6	-1.169773	0.178009	-0.003868
H8	1	-2.116826	2.082396	-0.019174
H9	1	2.142841	2.045511	-0.018046
Br10	35	2.879141	-0.700325	0.001570
Br11	35	-2.874848	-0.677989	0.001437
C12	6	-0.060063	-2.101490	0.005927
H13	1	-0.788710	4.084827	0.294045
H14	1	0.856471	4.070909	0.285444
H15	1	-0.585949	-2.460480	0.883953
H16	1	0.928153	-2.531003	0.004899
H17	1	-0.590579	-2.467361	-0.866339

Substituent: 3_5-dimethyl-4-nitro

# TEST OPT HF DIRECT 6-311G**				
HF=-567.4116458				
PG=C01 [X(C8H10N2O2)]				
Atom	Charge	X	Y	Z
N1	7	3.587162	0.003428	-0.057425
C2	6	2.207710	0.001098	-0.008307
C3	6	-0.552492	0.000046	-0.001567
C4	6	1.500175	1.197442	0.059706
C5	6	1.500681	-1.195814	-0.075047
C6	6	0.119321	-1.222101	-0.058750
C7	6	0.118490	1.222668	0.050060
H8	1	2.040016	2.125770	0.114968
H9	1	2.041169	-2.122603	-0.146846
C10	6	-0.575730	-2.563066	-0.132291
C11	6	-0.577051	2.563317	0.124329
N12	7	-2.012537	-0.000918	0.005851
H13	1	4.034198	0.816505	0.300083
H14	1	4.034293	-0.838633	0.225098
H15	1	-0.980051	-2.837575	0.833370
H16	1	0.132433	-3.319735	-0.445566
H17	1	-1.398780	-2.553003	-0.835664
H18	1	-1.394773	2.555768	0.833981
H19	1	-0.988762	2.833192	-0.839460
H20	1	0.132964	3.322075	0.428258
O21	8	-2.565845	-0.791850	0.700483
O22	8	-2.574369	0.789241	-0.682483

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