

1.gjf

C	-1.20740100	2.02568400	0.12347900
C	-0.00070800	2.71099000	0.14284800
C	1.18770800	1.99928600	0.09574000
C	1.18595600	0.60307700	0.02545200
C	-0.02004800	-0.10819400	0.00315500
C	-1.18945000	0.64476100	0.05879900
N	-2.50206700	-0.03879000	0.13080800
O	-3.43985000	0.52436700	-0.38239300
O	-2.53959100	-1.07854200	0.74294100
C	-0.13340800	-1.59697700	-0.33251300
O	-0.71869800	-1.91006300	-1.32318600
O	0.41255700	-2.47117000	0.49677700
C	2.50720800	-0.10993200	0.08687600
O	2.69408700	-1.07368300	0.77437200
O	3.50687000	0.42919800	-0.61965000
H	-2.16016500	2.53710400	0.15762200
H	0.01072300	3.79098900	0.20839900
H	2.13216400	2.53009900	0.14617800
H	1.06059200	-2.04406900	1.07798200
H	3.16901100	1.08439200	-1.23973600

2.gjf

C	-1.37040900	1.93069800	0.06737500
C	-0.21986700	2.71761400	0.11277300
C	1.02895100	2.12226200	0.08188900
C	1.13191900	0.73220900	0.04864300
C	-0.00527100	-0.07403200	0.01397900
C	-1.24678200	0.55812500	-0.00406000
N	-2.49738600	-0.20872600	-0.19194800
O	-2.54179500	-0.94124300	-1.14730500
O	-3.39422400	0.02015500	0.58597900
C	0.12448400	-1.54858100	0.19757900
O	-0.77782200	-2.26395300	0.55372300
C	2.49143500	0.13005000	-0.05334600
O	3.49578800	0.78455500	-0.21336600
H	-2.35960000	2.37044400	0.07520500
H	-0.31074900	3.79533800	0.15738200
H	1.94317700	2.70246200	0.08432800
H	1.53613100	-2.93081400	0.48034900
H	3.34165900	-1.65827400	-0.44054000
N	1.39236800	-2.05086100	-0.00117400
N	2.53174000	-1.23831700	-0.00373000

3.gjf

C	-2.26197900	1.29784000	-0.00079800
C	-1.37541800	2.35459000	-0.04351800
C	0.00149100	2.13777500	-0.05361100
C	0.46290600	0.83465300	-0.02715800
C	-0.41460300	-0.26311600	0.02117900
C	-1.81429300	-0.03838000	0.03234300
N	-2.71115800	-1.05548100	0.10583500
C	0.11810200	-1.63311200	0.00154400
O	-0.55577300	-2.64858300	-0.09365600
C	1.93660700	0.62951400	-0.00581200
O	2.74364700	1.52740200	0.07910400
H	-3.33036200	1.48404700	0.01107200
H	-1.76152700	3.36680800	-0.06843100
H	0.71758400	2.94757300	-0.07882200
H	1.82798700	-2.62540100	-0.29016000
H	3.28149300	-0.83385700	0.27927600
N	1.48491200	-1.75756400	0.10172000
N	2.35538500	-0.67794700	-0.09758000
H	-3.68430200	-0.85132000	-0.03777300
H	-2.37471300	-2.00003300	-0.01358300

TS-1.gjf

C	1.37984300	-0.30007900	-0.10718300
O	0.58172000	-1.29648100	-0.24702700
C	2.48353400	-0.18149900	-1.16023100
C	3.19177600	-1.53956600	-1.30616400
C	3.49482800	0.94217100	-0.93274400
H	1.96010800	-0.00293300	-2.10400200
H	2.46491200	-2.33251800	-1.47564900
H	3.87528800	-1.49831900	-2.15657400
H	3.77691600	-1.78943200	-0.41930000
H	3.02269900	1.91507500	-0.78836800
H	4.12634700	0.74466700	-0.06395400
H	4.15322200	1.01781600	-1.80029500
C	1.63199600	0.18676300	1.31812400
C	2.68774200	-0.73696800	1.95832000
C	0.36406700	0.13614300	2.16911900
H	2.01951300	1.20749200	1.28188700
H	3.66357000	-0.65300800	1.48235600
H	2.80659300	-0.47867600	3.01216900
H	2.35873900	-1.77689600	1.89421800
H	-0.42396900	0.80273300	1.79879400
H	-0.01727500	-0.88668800	2.22940800

H	0.57576700	0.46723000	3.18686000
Mg	-1.00036000	-0.19827100	-0.32353200
Br	-3.33740900	-0.38344000	-0.15505800
C	0.13976200	1.58493800	-0.83112000
C	-0.29101500	2.73266300	0.09123300
H	-0.56746500	1.52952900	-1.68879400
H	1.07291300	1.84106300	-1.32154500
H	-0.27844000	3.70226800	-0.41699000
H	-1.30375900	2.59778900	0.48623000
H	0.37899400	2.81690600	0.95306000

P1.gjf

C	1.55309700	0.26560300	0.07126100
O	0.45766600	-0.02551800	-0.73806300
C	2.74231200	0.66091700	-0.86034700
C	2.92492700	-0.21828100	-2.10189100
C	4.06539400	0.82916400	-0.11102800
H	2.44600500	1.64443900	-1.24466700
H	1.95585400	-0.49878500	-2.51326200
H	3.47474000	0.34335700	-2.86183200
H	3.49606200	-1.12438400	-1.89948300
H	3.96973700	1.47595800	0.76545200
H	4.45017600	-0.13813100	0.22479500
H	4.81974700	1.26898500	-0.76767900
C	1.86200700	-0.95549300	0.99502500
C	2.20957200	-2.22427500	0.21326800
C	0.69572100	-1.26446300	1.94103000
H	2.71699800	-0.68140600	1.62352800
H	3.22296100	-2.19656800	-0.18504900
H	2.13735100	-3.10337400	0.85829000
H	1.51482700	-2.34975600	-0.62063800
H	0.43729200	-0.42878300	2.59399200
H	-0.19896800	-1.57360600	1.38273300
H	0.94813000	-2.10841300	2.58610500
Mg	-1.31757700	0.07346800	-0.36912700
Br	-3.64406000	-0.10854800	-0.28061000
C	1.26460200	1.51398900	0.99082400
C	-0.21167700	1.86850900	1.18306400
H	1.74621200	2.39731200	0.56366400
H	1.72146000	1.36852600	1.97382100
H	-0.33167900	2.70438300	1.87421000
H	-0.66747600	2.21301000	0.24380700
H	-0.80345200	1.05490900	1.63035200