

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