

Supplementary Information

Novel Structure of Grid Spirofluorene: A New Organic Semiconductor with Low Reorganization Energy

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Table S1. Optimized ground-state geometry of GSFs and DSFs

GSF1

C	0.31869900	-5.19932800	1.24473000
C	0.99264400	-4.02826200	1.96692000
C	2.07360200	-3.26539600	1.55108500
C	2.53782800	-2.20647300	2.35675600
C	1.88953900	-1.96132800	3.58389300
C	0.80781500	-2.73031900	4.00722800
C	0.34999800	-3.76648500	3.19180600
C	-0.76367700	-4.70795300	3.35370600
C	-1.69778100	-4.85734900	4.38148400
C	-2.67210900	-5.85117500	4.26791400
C	-2.71347100	-6.68422100	3.14419200
C	-1.77795900	-6.53702100	2.11411000
C	-0.80781400	-5.54867600	2.22516300
C	-0.17721000	-4.85734900	-0.16450700
C	-1.01722900	-3.82542700	-0.55455200
C	-1.34578200	-3.66324500	-1.91525900
C	-0.81636900	-4.57754900	-2.84805900
C	0.03300900	-5.61143500	-2.45934900
C	0.36317500	-5.74910000	-1.10981300
C	1.24255600	-6.69761900	-0.41651100
C	2.00986400	-7.75986000	-0.90024100

C	2. 77659100	-8. 50268400	-0. 00005200
C	2. 77765600	-8. 18943600	1. 36384200
C	2. 00827100	-7. 12696300	1. 85088500
C	1. 24522300	-6. 38597600	0. 95699000
C	5. 19932800	0. 31869900	-1. 24473000
C	6. 38597600	1. 24522300	-0. 95699000
C	7. 12696300	2. 00827100	-1. 85088500
C	8. 18943600	2. 77765600	-1. 36384200
C	8. 50268400	2. 77659100	0. 00005200
C	7. 75986000	2. 00986400	0. 90024100
C	6. 69761900	1. 24255600	0. 41651100
C	5. 74910000	0. 36317500	1. 10981300
C	5. 61143500	0. 03300900	2. 45934900
C	4. 57754900	-0. 81636900	2. 84805900
C	3. 66324500	-1. 34578200	1. 91525900
C	3. 82542700	-1. 01722900	0. 55455200
C	4. 85734900	-0. 17721000	0. 16450700
C	4. 02826200	0. 99264400	-1. 96692000
C	3. 26539600	2. 07360200	-1. 55108500
C	2. 20647300	2. 53782800	-2. 35675600
C	1. 96132800	1. 88953900	-3. 58389300
C	2. 73031900	0. 80781500	-4. 00722800
C	3. 76648500	0. 34999800	-3. 19180600
C	4. 70795300	-0. 76367700	-3. 35370600
C	4. 85734900	-1. 69778100	-4. 38148400
C	5. 85117500	-2. 67210900	-4. 26791400
C	6. 68422100	-2. 71347100	-3. 14419200
C	6. 53702100	-1. 77795900	-2. 11411000
C	5. 54867600	-0. 80781400	-2. 22516300
C	-5. 19932800	-0. 31869900	-1. 24473000
C	-4. 85734900	0. 17721000	0. 16450700
C	-3. 82542700	1. 01722900	0. 55455200
C	-3. 66324500	1. 34578200	1. 91525900
C	-4. 57754900	0. 81636900	2. 84805900
C	-5. 61143500	-0. 03300900	2. 45934900
C	-5. 74910000	-0. 36317500	1. 10981300
C	-6. 69761900	-1. 24255600	0. 41651100
C	-7. 75986000	-2. 00986400	0. 90024100
C	-8. 50268400	-2. 77659100	0. 00005200
C	-8. 18943600	-2. 77765600	-1. 36384200
C	-7. 12696300	-2. 00827100	-1. 85088500
C	-6. 38597600	-1. 24522300	-0. 95699000
C	-5. 54867600	0. 80781400	-2. 22516300
C	-6. 53702100	1. 77795900	-2. 11411000

C	-6.68422100	2.71347100	-3.14419200
C	-5.85117500	2.67210900	-4.26791400
C	-4.85734900	1.69778100	-4.38148400
C	-4.70795300	0.76367700	-3.35370600
C	-3.76648500	-0.34999800	-3.19180600
C	-2.73031900	-0.80781500	-4.00722800
C	-1.96132800	-1.88953900	-3.58389300
C	-2.20647300	-2.53782800	-2.35675600
C	-3.26539600	-2.07360200	-1.55108500
C	-4.02826200	-0.99264400	-1.96692000
C	-0.31869900	5.19932800	1.24473000
C	0.80781400	5.54867600	2.22516300
C	1.77795900	6.53702100	2.11411000
C	2.71347100	6.68422100	3.14419200
C	2.67210900	5.85117500	4.26791400
C	1.69778100	4.85734900	4.38148400
C	0.76367700	4.70795300	3.35370600
C	-0.34999800	3.76648500	3.19180600
C	-0.80781500	2.73031900	4.00722800
C	-1.88953900	1.96132800	3.58389300
C	-2.53782800	2.20647300	2.35675600
C	-2.07360200	3.26539600	1.55108500
C	-0.99264400	4.02826200	1.96692000
C	-1.24522300	6.38597600	0.95699000
C	-2.00827100	7.12696300	1.85088500
C	-2.77765600	8.18943600	1.36384200
C	-2.77659100	8.50268400	-0.00005200
C	-2.00986400	7.75986000	-0.90024100
C	-1.24255600	6.69761900	-0.41651100
C	-0.36317500	5.74910000	-1.10981300
C	-0.03300900	5.61143500	-2.45934900
C	0.81636900	4.57754900	-2.84805900
C	1.34578200	3.66324500	-1.91525900
C	1.01722900	3.82542700	-0.55455200
C	0.17721000	4.85734900	-0.16450700
H	2.57192700	-3.48965200	0.61212100
H	2.21916500	-1.12858100	4.19805800
H	0.31949500	-2.50732900	4.95254000
H	-1.67092600	-4.21182900	5.25576600
H	-3.40590500	-5.97826200	5.05947300
H	-3.47884000	-7.45201800	3.07002900
H	-1.81139600	-7.18543900	1.24261000
H	-1.39238800	-3.11908800	0.18055100
H	-1.09123500	-4.48337100	-3.89459200

H	0.42781100	-6.29893700	-3.20311200
H	2.01437400	-8.00590400	-1.95909200
H	3.37928700	-9.33125300	-0.36252100
H	3.38107300	-8.77605500	2.05131000
H	2.00915300	-6.88641500	2.91072000
H	6.88641500	2.00915300	-2.91072000
H	8.77605500	3.38107300	-2.05131000
H	9.33125300	3.37928700	0.36252100
H	8.00590400	2.01437400	1.95909200
H	6.29893700	0.42781100	3.20311200
H	4.48337100	-1.09123500	3.89459200
H	3.11908800	-1.39238800	-0.18055100
H	3.48965200	2.57192700	-0.61212100
H	1.12858100	2.21916500	-4.19805800
H	2.50732900	0.31949500	-4.95254000
H	4.21182900	-1.67092600	-5.25576600
H	5.97826200	-3.40590500	-5.05947300
H	7.45201800	-3.47884000	-3.07002900
H	7.18543900	-1.81139600	-1.24261000
H	-3.11908800	1.39238800	-0.18055100
H	-4.48337100	1.09123500	3.89459200
H	-6.29893700	-0.42781100	3.20311200
H	-8.00590400	-2.01437400	1.95909200
H	-9.33125300	-3.37928700	0.36252100
H	-8.77605500	-3.38107300	-2.05131000
H	-6.88641500	-2.00915300	-2.91072000
H	-7.18543900	1.81139600	-1.24261000
H	-7.45201800	3.47884000	-3.07002900
H	-5.97826200	3.40590500	-5.05947300
H	-4.21182900	1.67092600	-5.25576600
H	-2.50732900	-0.31949500	-4.95254000
H	-1.12858100	-2.21916500	-4.19805800
H	-3.48965200	-2.57192700	-0.61212100
H	1.81139600	7.18543900	1.24261000
H	3.47884000	7.45201800	3.07002900
H	3.40590500	5.97826200	5.05947300
H	1.67092600	4.21182900	5.25576600
H	-0.31949500	2.50732900	4.95254000
H	-2.21916500	1.12858100	4.19805800
H	-2.57192700	3.48965200	0.61212100
H	-2.00915300	6.88641500	2.91072000
H	-3.38107300	8.77605500	2.05131000
H	-3.37928700	9.33125300	-0.36252100
H	-2.01437400	8.00590400	-1.95909200

H	-0.42781100	6.29893700	-3.20311200
H	1.09123500	4.48337100	-3.89459200
H	1.39238800	3.11908800	0.18055100

GSF2

C	0.00000000	6.32485900	0.00000000
C	1.19357200	5.49426500	0.48648600
C	1.96260800	4.59072700	-0.23082100
C	3.06227800	3.96013900	0.38443800
C	3.32965500	4.24668500	1.73849400
C	2.55231400	5.14726500	2.46397800
C	1.48531300	5.78775100	1.83153500
C	0.54567100	6.80993900	2.30721200
C	0.42068900	7.43496200	3.55024100
C	-0.57208600	8.40201800	3.72214800
C	-1.42841200	8.74047400	2.66825300
C	-1.30660800	8.11380200	1.42297200
C	-0.31917600	7.15179800	1.24943500
C	-1.19357200	5.49426500	-0.48648600
C	-1.96260800	4.59072700	0.23082100
C	-3.06227800	3.96013900	-0.38443800
C	-3.32965500	4.24668500	-1.73849400
C	-2.55231400	5.14726500	-2.46397800
C	-1.48531300	5.78775100	-1.83153500
C	-0.54567100	6.80993900	-2.30721200
C	-0.42068900	7.43496200	-3.55024100
C	0.57208600	8.40201800	-3.72214800
C	1.42841200	8.74047400	-2.66825300
C	1.30660800	8.11380200	-1.42297200
C	0.31917600	7.15179800	-1.24943500
C	6.32485900	0.00000000	0.00000000
C	7.15179800	-0.31917600	-1.24943500
C	8.11380200	-1.30660800	-1.42297200
C	8.74047400	-1.42841200	-2.66825300
C	8.40201800	-0.57208600	-3.72214800
C	7.43496200	0.42068900	-3.55024100
C	6.80993900	0.54567100	-2.30721200
C	5.78775100	1.48531300	-1.83153500
C	5.14726500	2.55231400	-2.46397800
C	4.24668500	3.32965500	-1.73849400
C	3.96013900	3.06227800	-0.38443800
C	4.59072700	1.96260800	0.23082100
C	5.49426500	1.19357200	-0.48648600
C	5.49426500	-1.19357200	0.48648600

C	4. 59072700	-1. 96260800	-0. 23082100
C	3. 96013900	-3. 06227800	0. 38443800
C	4. 24668500	-3. 32965500	1. 73849400
C	5. 14726500	-2. 55231400	2. 46397800
C	5. 78775100	-1. 48531300	1. 83153500
C	6. 80993900	-0. 54567100	2. 30721200
C	7. 43496200	-0. 42068900	3. 55024100
C	8. 40201800	0. 57208600	3. 72214800
C	8. 74047400	1. 42841200	2. 66825300
C	8. 11380200	1. 30660800	1. 42297200
C	7. 15179800	0. 31917600	1. 24943500
C	3. 06227800	-3. 96013900	-0. 38443800
C	3. 32965500	-4. 24668500	-1. 73849400
C	1. 96260800	-4. 59072700	0. 23082100
C	2. 55231400	-5. 14726500	-2. 46397800
C	1. 19357200	-5. 49426500	-0. 48648600
C	1. 48531300	-5. 78775100	-1. 83153500
C	0. 54567100	-6. 80993900	-2. 30721200
C	-0. 31917600	-7. 15179800	-1. 24943500
C	0. 42068900	-7. 43496200	-3. 55024100
C	-1. 30660800	-8. 11380200	-1. 42297200
C	-0. 57208600	-8. 40201800	-3. 72214800
C	-1. 42841200	-8. 74047400	-2. 66825300
C	-3. 96013900	3. 06227800	0. 38443800
C	-4. 24668500	3. 32965500	1. 73849400
C	-4. 59072700	1. 96260800	-0. 23082100
C	-5. 14726500	2. 55231400	2. 46397800
C	-5. 49426500	1. 19357200	0. 48648600
C	-5. 78775100	1. 48531300	1. 83153500
C	-6. 80993900	0. 54567100	2. 30721200
C	-7. 15179800	-0. 31917600	1. 24943500
C	-7. 43496200	0. 42068900	3. 55024100
C	-8. 11380200	-1. 30660800	1. 42297200
C	-8. 40201800	-0. 57208600	3. 72214800
C	-8. 74047400	-1. 42841200	2. 66825300
C	-6. 32485900	0. 00000000	0. 00000000
C	-5. 49426500	-1. 19357200	-0. 48648600
C	-7. 15179800	0. 31917600	-1. 24943500
C	-4. 59072700	-1. 96260800	0. 23082100
C	-5. 78775100	-1. 48531300	-1. 83153500
C	-8. 11380200	1. 30660800	-1. 42297200
C	-6. 80993900	-0. 54567100	-2. 30721200
C	-3. 96013900	-3. 06227800	-0. 38443800
C	-5. 14726500	-2. 55231400	-2. 46397800

C	-8.74047400	1.42841200	-2.66825300
C	-7.43496200	-0.42068900	-3.55024100
C	-4.24668500	-3.32965500	-1.73849400
C	-8.40201800	0.57208600	-3.72214800
C	0.00000000	-6.32485900	0.00000000
C	-1.19357200	-5.49426500	0.48648600
C	0.31917600	-7.15179800	1.24943500
C	-1.96260800	-4.59072700	-0.23082100
C	-1.48531300	-5.78775100	1.83153500
C	1.30660800	-8.11380200	1.42297200
C	-0.54567100	-6.80993900	2.30721200
C	-3.06227800	-3.96013900	0.38443800
C	-2.55231400	-5.14726500	2.46397800
C	1.42841200	-8.74047400	2.66825300
C	-0.42068900	-7.43496200	3.55024100
C	-3.32965500	-4.24668500	1.73849400
C	0.57208600	-8.40201800	3.72214800
H	1.71798200	4.36613800	-1.26513800
H	4.18933700	3.78643000	2.21632300
H	2.79750600	5.36319600	3.50077800
H	1.08397700	7.17665300	4.37185000
H	-0.68009000	8.89708000	4.68362000
H	-2.19492000	9.49613000	2.81767200
H	-1.97395700	8.37612500	0.60628700
H	-1.71798200	4.36613800	1.26513800
H	-4.18933700	3.78643000	-2.21632300
H	-2.79750600	5.36319600	-3.50077800
H	-1.08397700	7.17665300	-4.37185000
H	0.68009000	8.89708000	-4.68362000
H	2.19492000	9.49613000	-2.81767200
H	1.97395700	8.37612500	-0.60628700
H	8.37612500	-1.97395700	-0.60628700
H	9.49613000	-2.19492000	-2.81767200
H	8.89708000	-0.68009000	-4.68362000
H	7.17665300	1.08397700	-4.37185000
H	5.36319600	2.79750600	-3.50077800
H	3.78643000	4.18933700	-2.21632300
H	4.36613800	1.71798200	1.26513800
H	4.36613800	-1.71798200	-1.26513800
H	3.78643000	-4.18933700	2.21632300
H	5.36319600	-2.79750600	3.50077800
H	7.17665300	-1.08397700	4.37185000
H	8.89708000	0.68009000	4.68362000
H	9.49613000	2.19492000	2.81767200

H	8.37612500	1.97395700	0.60628700
H	4.18933700	-3.78643000	-2.21632300
H	1.71798200	-4.36613800	1.26513800
H	2.79750600	-5.36319600	-3.50077800
H	1.08397700	-7.17665300	-4.37185000
H	-1.97395700	-8.37612500	-0.60628700
H	-0.68009000	-8.89708000	-4.68362000
H	-2.19492000	-9.49613000	-2.81767200
H	-3.78643000	4.18933700	2.21632300
H	-4.36613800	1.71798200	-1.26513800
H	-5.36319600	2.79750600	3.50077800
H	-7.17665300	1.08397700	4.37185000
H	-8.37612500	-1.97395700	0.60628700
H	-8.89708000	-0.68009000	4.68362000
H	-9.49613000	-2.19492000	2.81767200
H	-4.36613800	-1.71798200	1.26513800
H	-8.37612500	1.97395700	-0.60628700
H	-5.36319600	-2.79750600	-3.50077800
H	-9.49613000	2.19492000	-2.81767200
H	-7.17665300	-1.08397700	-4.37185000
H	-3.78643000	-4.18933700	-2.21632300
H	-8.89708000	0.68009000	-4.68362000
H	-1.71798200	-4.36613800	-1.26513800
H	1.97395700	-8.37612500	0.60628700
H	-2.79750600	-5.36319600	3.50077800
H	2.19492000	-9.49613000	2.81767200
H	-1.08397700	-7.17665300	4.37185000
H	-4.18933700	-3.78643000	2.21632300
H	0.68009000	-8.89708000	4.68362000

GSF3

C	0.00000000	0.00000000	-5.79340900
C	1.07112600	0.69829400	-4.94327800
C	0.92216300	1.78489000	-4.09510400
C	2.04490700	2.31732800	-3.43038000
C	3.29330800	1.68923500	-3.61904100
C	3.44706900	0.60520000	-4.48083100
C	2.33293200	0.11809200	-5.16709000
C	2.19801800	-0.92557300	-6.19046700
C	3.14825800	-1.76644900	-6.77426600
C	2.73979800	-2.65747500	-7.76899700
C	1.40165400	-2.70926900	-8.17506300
C	0.44668400	-1.87186800	-7.58768100
C	0.85060200	-0.98268300	-6.59930100

C	-1.07112600	-0.69829400	-4.94327800
C	-0.92216300	-1.78489000	-4.09510400
C	-2.04490700	-2.31732800	-3.43038000
C	-3.29330800	-1.68923500	-3.61904100
C	-3.44706900	-0.60520000	-4.48083100
C	-2.33293200	-0.11809200	-5.16709000
C	-2.19801800	0.92557300	-6.19046700
C	-3.14825800	1.76644900	-6.77426600
C	-2.73979800	2.65747500	-7.76899700
C	-1.40165400	2.70926900	-8.17506300
C	-0.44668400	1.87186800	-7.58768100
C	-0.85060200	0.98268300	-6.59930100
C	-0.55200900	5.60295900	-0.41974200
C	0.00000000	6.95505500	0.05522700
C	-0.62969200	7.92749300	0.82236600
C	0.07334200	9.09351400	1.14474700
C	1.38851200	9.27765100	0.70277100
C	2.02249700	8.30167000	-0.06861500
C	1.32166100	7.13721700	-0.39187000
C	1.71461500	5.96250200	-1.17675100
C	2.89870700	5.66473900	-1.85192300
C	2.99143300	4.47088500	-2.56248200
C	1.92646600	3.54819100	-2.60802800
C	0.74303400	3.85529300	-1.90474500
C	0.64083200	5.05144200	-1.20809000
C	-1.03050600	4.73458700	0.74852700
C	-0.29255600	4.24441700	1.81368100
C	-0.92823500	3.50803500	2.83398900
C	-2.31710000	3.28872300	2.73327400
C	-3.05782200	3.76176100	1.65202700
C	-2.41244900	4.48824400	0.64953500
C	-2.91416600	5.10205300	-0.58527500
C	-4.19313400	5.12274700	-1.14626900
C	-4.38641900	5.78547200	-2.36020100
C	-3.31812900	6.41876900	-3.00512400
C	-2.03657000	6.40200200	-2.44344500
C	-1.84163900	5.74282200	-1.23608400
C	0.55200900	-5.60295900	-0.41974200
C	1.03050600	-4.73458700	0.74852700
C	0.29255600	-4.24441700	1.81368100
C	0.92823500	-3.50803500	2.83398900
C	2.31710000	-3.28872300	2.73327400
C	3.05782200	-3.76176100	1.65202700
C	2.41244900	-4.48824400	0.64953500

C	2.91416600	-5.10205300	-0.58527500
C	4.19313400	-5.12274700	-1.14626900
C	4.38641900	-5.78547200	-2.36020100
C	3.31812900	-6.41876900	-3.00512400
C	2.03657000	-6.40200200	-2.44344500
C	1.84163900	-5.74282200	-1.23608400
C	0.00000000	-6.95505500	0.05522700
C	0.62969200	-7.92749300	0.82236600
C	-0.07334200	-9.09351400	1.14474700
C	-1.38851200	-9.27765100	0.70277100
C	-2.02249700	-8.30167000	-0.06861500
C	-1.32166100	-7.13721700	-0.39187000
C	-1.71461500	-5.96250200	-1.17675100
C	-2.89870700	-5.66473900	-1.85192300
C	-2.99143300	-4.47088500	-2.56248200
C	-1.92646600	-3.54819100	-2.60802800
C	-0.74303400	-3.85529300	-1.90474500
C	-0.64083200	-5.05144200	-1.20809000
C	0.00000000	0.00000000	6.47916800
C	-1.26757400	0.03329400	7.34523900
C	-1.65621600	0.98557700	8.27915700
C	-2.85359800	0.79654800	8.97835700
C	-3.64344400	-0.33504300	8.74567000
C	-3.25365200	-1.29413800	7.80855800
C	-2.06113500	-1.10503500	7.10614400
C	-1.41923900	-1.91095900	6.06188800
C	-1.80399900	-3.10464700	5.44934200
C	-1.01763400	-3.62535100	4.42436800
C	0.14742500	-2.97010500	3.97564400
C	0.53600100	-1.77940900	4.62279200
C	-0.23359500	-1.26907400	5.65671000
C	1.26757400	-0.03329400	7.34523900
C	1.65621600	-0.98557700	8.27915700
C	2.85359800	-0.79654800	8.97835700
C	3.64344400	0.33504300	8.74567000
C	3.25365200	1.29413800	7.80855800
C	2.06113500	1.10503500	7.10614400
C	1.41923900	1.91095900	6.06188800
C	1.80399900	3.10464700	5.44934200
C	1.01763400	3.62535100	4.42436800
C	-0.14742500	2.97010500	3.97564400
C	-0.53600100	1.77940900	4.62279200
C	0.23359500	1.26907400	5.65671000
H	-0.04843700	2.25983100	-3.98607900

H	4. 15916100	2. 05855400	-3. 07765000
H	4. 42773600	0. 15682100	-4. 61875500
H	4. 18952800	-1. 72862000	-6. 46453200
H	3. 46888200	-3. 31619900	-8. 23343000
H	1. 10074000	-3. 40626700	-8. 95255100
H	-0. 59292800	-1. 91628700	-7. 90142500
H	0. 04843700	-2. 25983100	-3. 98607900
H	-4. 15916100	-2. 05855400	-3. 07765000
H	-4. 42773600	-0. 15682100	-4. 61875500
H	-4. 18952800	1. 72862000	-6. 46453200
H	-3. 46888200	3. 31619900	-8. 23343000
H	-1. 10074000	3. 40626700	-8. 95255100
H	0. 59292800	1. 91628700	-7. 90142500
H	-1. 65058400	7. 78652500	1. 16730000
H	-0. 40674400	9. 86256900	1. 74384400
H	1. 92112800	10. 18881800	0. 96207800
H	3. 04396900	8. 44910200	-0. 41019700
H	3. 73351700	6. 36106900	-1. 84778100
H	3. 89468900	4. 26442500	-3. 12828400
H	-0. 08459300	3. 15155200	-1. 90431300
H	0. 78031900	4. 40762900	1. 84884000
H	-2. 82919600	2. 75422800	3. 52757700
H	-4. 12724000	3. 57300700	1. 60370300
H	-5. 02569500	4. 62962900	-0. 65087500
H	-5. 37590400	5. 80799800	-2. 80919500
H	-3. 48409600	6. 92775500	-3. 95072100
H	-1. 20846500	6. 89513100	-2. 94563000
H	-0. 78031900	-4. 40762900	1. 84884000
H	2. 82919600	-2. 75422800	3. 52757700
H	4. 12724000	-3. 57300700	1. 60370300
H	5. 02569500	-4. 62962900	-0. 65087500
H	5. 37590400	-5. 80799800	-2. 80919500
H	3. 48409600	-6. 92775500	-3. 95072100
H	1. 20846500	-6. 89513100	-2. 94563000
H	1. 65058400	-7. 78652500	1. 16730000
H	0. 40674400	-9. 86256900	1. 74384400
H	-1. 92112800	-10. 18881800	0. 96207800
H	-3. 04396900	-8. 44910200	-0. 41019700
H	-3. 73351700	-6. 36106900	-1. 84778100
H	-3. 89468900	-4. 26442500	-3. 12828400
H	0. 08459300	-3. 15155200	-1. 90431300
H	-1. 04310500	1. 86378800	8. 46332300
H	-3. 17211300	1. 53542700	9. 70875100
H	-4. 56976900	-0. 46785700	9. 29831100

H	-3.87196300	-2.17000200	7.62893000
H	-2.70472300	-3.62714800	5.76145700
H	-1.30669100	-4.56620400	3.96637800
H	1.41508200	-1.23913200	4.28443200
H	1.04310500	-1.86378800	8.46332300
H	3.17211300	-1.53542700	9.70875100
H	4.56976900	0.46785700	9.29831100
H	3.87196300	2.17000200	7.62893000
H	2.70472300	3.62714800	5.76145700
H	1.30669100	4.56620400	3.96637800
H	-1.41508200	1.23913200	4.28443200

GSF4

C	-2.51335500	3.68759900	-3.84334300
C	-2.11653700	2.22820600	-3.57854300
C	-0.84621300	1.67501000	-3.55531300
C	-0.67578900	0.30803000	-3.25581300
C	-1.82603300	-0.45879700	-2.97604900
C	-3.10601000	0.09020900	-3.02291500
C	-3.25733700	1.44290700	-3.33477000
C	-4.45027200	2.28537900	-3.48381600
C	-5.80879200	1.98145000	-3.37041700
C	-6.74676400	2.99354000	-3.58568900
C	-6.33517600	4.29119200	-3.90935500
C	-4.97461100	4.59949200	-4.01965300
C	-4.03925700	3.59443600	-3.80720700
C	-1.92845200	4.62725400	-2.78013100
C	-2.16727300	4.62964600	-1.41585700
C	-1.48710400	5.53674000	-0.57719400
C	-0.57371400	6.42977300	-1.17733800
C	-0.35775000	6.45243400	-2.55390500
C	-1.04207900	5.54726700	-3.36731300
C	-1.03539000	5.33427200	-4.81951500
C	-0.35125600	5.99685900	-5.84125700
C	-0.54858700	5.58657100	-7.16151400
C	-1.41556900	4.52892900	-7.45797000
C	-2.09909200	3.86066700	-6.43582500
C	-1.90667200	4.26777600	-5.12139500
C	2.51335500	-3.68759900	-3.84334300
C	4.03925700	-3.59443600	-3.80720700
C	4.97461100	-4.59949200	-4.01965300
C	6.33517600	-4.29119200	-3.90935500
C	6.74676400	-2.99354000	-3.58568900
C	5.80879200	-1.98145000	-3.37041700

C	4.45027200	-2.28537900	-3.48381600
C	3.25733700	-1.44290700	-3.33477000
C	3.10601000	-0.09020900	-3.02291500
C	1.82603300	0.45879700	-2.97604900
C	0.67578900	-0.30803000	-3.25581300
C	0.84621300	-1.67501000	-3.55531300
C	2.11653700	-2.22820600	-3.57854300
C	1.92845200	-4.62725400	-2.78013100
C	2.16727300	-4.62964600	-1.41585700
C	1.48710400	-5.53674000	-0.57719400
C	0.57371400	-6.42977300	-1.17733800
C	0.35775000	-6.45243400	-2.55390500
C	1.04207900	-5.54726700	-3.36731300
C	1.03539000	-5.33427200	-4.81951500
C	0.35125600	-5.99685900	-5.84125700
C	0.54858700	-5.58657100	-7.16151400
C	1.41556900	-4.52892900	-7.45797000
C	2.09909200	-3.86066700	-6.43582500
C	1.90667200	-4.26777600	-5.12139500
C	-3.01952600	3.30140200	3.79953900
C	-2.41310800	1.91624400	3.56824200
C	-1.08361600	1.53199800	3.65157600
C	-0.71196300	0.20827300	3.34049400
C	-1.72246900	-0.70457900	2.97695000
C	-3.06124000	-0.32642300	2.90874800
C	-3.40990800	0.99424500	3.19470300
C	-4.70475400	1.68239900	3.16061100
C	-5.98559800	1.21511000	2.85657000
C	-7.05650400	2.11029300	2.89465000
C	-6.85157200	3.45300000	3.23182300
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C	-2.81443100	3.89538000	5.19692800
C	-3.10601000	3.32896700	6.43146200
C	-2.86513600	4.07458800	7.59092300
C	-2.34569600	5.37135000	7.50828900
C	-2.05386800	5.94392500	6.26837700
C	-2.28841500	5.19981200	5.10974000
C	-2.05935700	5.51767500	3.69556200
C	-1.55230800	6.65691900	3.06819400
C	-1.39888200	6.66090000	1.68325100
C	-1.71350300	5.53560500	0.89237300
C	-2.24359700	4.40126400	1.54306500
C	-2.42925900	4.40644500	2.91600500

C	3.01952600	-3.30140200	3.79953900
C	4.50310000	-3.03328200	3.50032600
C	5.56970600	-3.92253200	3.53844500
C	6.85157200	-3.45300000	3.23182300
C	7.05650400	-2.11029300	2.89465000
C	5.98559800	-1.21511000	2.85657000
C	4.70475400	-1.68239900	3.16061100
C	3.40990800	-0.99424500	3.19470300
C	3.06124000	0.32642300	2.90874800
C	1.72246900	0.70457900	2.97695000
C	0.71196300	-0.20827300	3.34049400
C	1.08361600	-1.53199800	3.65157600
C	2.41310800	-1.91624400	3.56824200
C	2.81443100	-3.89538000	5.19692800
C	3.10601000	-3.32896700	6.43146200
C	2.86513600	-4.07458800	7.59092300
C	2.34569600	-5.37135000	7.50828900
C	2.05386800	-5.94392500	6.26837700
C	2.28841500	-5.19981200	5.10974000
C	2.05935700	-5.51767500	3.69556200
C	1.55230800	-6.65691900	3.06819400
C	1.39888200	-6.66090000	1.68325100
C	1.71350300	-5.53560500	0.89237300
C	2.24359700	-4.40126400	1.54306500
C	2.42925900	-4.40644500	2.91600500
H	0.01422500	2.29129100	-3.79770100
H	-1.71423300	-1.50288000	-2.70078900
H	-3.97039800	-0.53354000	-2.80959000
H	-6.13446000	0.97475700	-3.12121300
H	-7.80715600	2.77058300	-3.50211100
H	-7.07790000	5.06673100	-4.07580500
H	-4.65635600	5.60836500	-4.26877100
H	-2.89462100	3.93937900	-1.00136800
H	-0.00249800	7.10948700	-0.55357600
H	0.34818400	7.16166000	-2.97878900
H	0.32172200	6.82059700	-5.61693800
H	-0.02450400	6.09466600	-7.96669600
H	-1.55932700	4.22296600	-8.49068200
H	-2.76994200	3.03778500	-6.66802500
H	4.65635600	-5.60836500	-4.26877100
H	7.07790000	-5.06673100	-4.07580500
H	7.80715600	-2.77058300	-3.50211100
H	6.13446000	-0.97475700	-3.12121300
H	3.97039800	0.53354000	-2.80959000

H	1. 71423300	1. 50288000	-2. 70078900
H	-0. 01422500	-2. 29129100	-3. 79770100
H	2. 89462100	-3. 93937900	-1. 00136800
H	0. 00249800	-7. 10948700	-0. 55357600
H	-0. 34818400	-7. 16166000	-2. 97878900
H	-0. 32172200	-6. 82059700	-5. 61693800
H	0. 02450400	-6. 09466600	-7. 96669600
H	1. 55932700	-4. 22296600	-8. 49068200
H	2. 76994200	-3. 03778500	-6. 66802500
H	-0. 32865800	2. 24895300	3. 96100600
H	-1. 44681500	-1. 71850500	2. 70356700
H	-3. 81502200	-1. 05020000	2. 60953100
H	-6. 14969200	0. 17307300	2. 59386700
H	-8. 05848400	1. 76105500	2. 65973200
H	-7. 69506000	4. 13764600	3. 25623100
H	-5. 41331400	4. 96512200	3. 80210500
H	-3. 51181500	2. 32292800	6. 49709200
H	-3. 08322400	3. 64211000	8. 56364000
H	-2. 16527800	5. 93788000	8. 41803300
H	-1. 64728100	6. 95048600	6. 21055800
H	-1. 28175200	7. 53803100	3. 64461100
H	-1. 03642600	7. 56542800	1. 20572100
H	-2. 48210300	3. 50626900	0. 97785700
H	5. 41331400	-4. 96512200	3. 80210500
H	7. 69506000	-4. 13764600	3. 25623100
H	8. 05848400	-1. 76105500	2. 65973200
H	6. 14969200	-0. 17307300	2. 59386700
H	3. 81502200	1. 05020000	2. 60953100
H	1. 44681500	1. 71850500	2. 70356700
H	0. 32865800	-2. 24895300	3. 96100600
H	3. 51181500	-2. 32292800	6. 49709200
H	3. 08322400	-3. 64211000	8. 56364000
H	2. 16527800	-5. 93788000	8. 41803300
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H	1. 28175200	-7. 53803100	3. 64461100
H	1. 03642600	-7. 56542800	1. 20572100
H	2. 48210300	-3. 50626900	0. 97785700

GSF5

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C	-0. 51875100	0. 53359100	-3. 84975300
C	-1. 87071200	0. 22412000	-4. 11039200

C	-2.85217200	1.20905600	-4.19079100
C	-2.48928900	2.54824700	-4.03934800
C	-3.27044600	3.78543700	-4.14393000
C	-4.63313600	3.99392500	-4.36914900
C	-5.11356700	5.30361400	-4.43119800
C	-4.24607500	6.38999600	-4.27126900
C	-2.88043600	6.18345400	-4.04648800
C	-2.39978900	4.88114500	-3.98342400
C	-0.29315500	4.97159800	-2.50561700
C	-0.76320800	4.97840200	-1.20013800
C	0.00022100	5.58032000	-0.17796600
C	1.24678900	6.14415600	-0.52044200
C	1.71180900	6.15898900	-1.83257800
C	0.93219600	5.58265000	-2.83574600
C	1.12785800	5.50612500	-4.28703200
C	2.16254800	5.97567400	-5.09991900
C	2.07492900	5.78390600	-6.48016500
C	0.96993100	5.13277400	-7.04051500
C	-0.06537100	4.65863800	-6.22746000
C	0.01944900	4.84976400	-4.85378000
C	0.96291800	-4.40358600	-3.76131400
C	2.39978900	-4.88114500	-3.98342400
C	2.88043600	-6.18345400	-4.04648800
C	4.24607500	-6.38999600	-4.27126900
C	5.11356700	-5.30361400	-4.43119800
C	4.63313600	-3.99392500	-4.36914900
C	3.27044600	-3.78543700	-4.14393000
C	2.48928900	-2.54824700	-4.03934800
C	2.85217200	-1.20905600	-4.19079100
C	1.87071200	-0.22412000	-4.11039200
C	0.51875100	-0.53359100	-3.84975300
C	0.17850900	-1.89088500	-3.66348200
C	1.14638200	-2.87700200	-3.78027500
C	0.29315500	-4.97159800	-2.50561700
C	0.76320800	-4.97840200	-1.20013800
C	-0.00022100	-5.58032000	-0.17796600
C	-1.24678900	-6.14415600	-0.52044200
C	-1.71180900	-6.15898900	-1.83257800
C	-0.93219600	-5.58265000	-2.83574600
C	-1.12785800	-5.50612500	-4.28703200
C	-2.16254800	-5.97567400	-5.09991900
C	-2.07492900	-5.78390600	-6.48016500
C	-0.96993100	-5.13277400	-7.04051500
C	0.06537100	-4.65863800	-6.22746000

C	-0.01944900	-4.84976400	-4.85378000
C	-2.58433400	3.65460000	3.83675400
C	-2.15902800	2.19877500	3.64196400
C	-0.89642500	1.64650600	3.79144400
C	-0.68220400	0.29075500	3.47591600
C	-1.78368200	-0.48678800	3.06456000
C	-3.05624800	0.06298000	2.92540000
C	-3.24191900	1.42054400	3.19123800
C	-4.41466800	2.28813700	3.03403300
C	-5.71511300	2.00601600	2.60944000
C	-6.63821000	3.05034300	2.52477100
C	-6.26829600	4.35789100	2.85903300
C	-4.96716900	4.64211300	3.28842700
C	-4.04723600	3.60449800	3.37260500
C	-2.47001400	4.18751600	5.27034200
C	-3.01721600	3.66638500	6.43607600
C	-2.80968900	4.34539600	7.64182500
C	-2.06975400	5.53286300	7.67227200
C	-1.52026600	6.05927800	6.50139800
C	-1.72159400	5.38023300	5.29740200
C	-1.24961900	5.66612900	3.93788100
C	-0.44096300	6.68652000	3.43499600
C	-0.07403400	6.66142000	2.09173600
C	-0.47966100	5.62330600	1.22674100
C	-1.32818700	4.62221800	1.74148700
C	-1.71180900	4.65566600	3.07400000
C	2.58433400	-3.65460000	3.83675400
C	4.04723600	-3.60449800	3.37260500
C	4.96716900	-4.64211300	3.28842700
C	6.26829600	-4.35789100	2.85903300
C	6.63821000	-3.05034300	2.52477100
C	5.71511300	-2.00601600	2.60944000
C	4.41466800	-2.28813700	3.03403300
C	3.24191900	-1.42054400	3.19123800
C	3.05624800	-0.06298000	2.92540000
C	1.78368200	0.48678800	3.06456000
C	0.68220400	-0.29075500	3.47591600
C	0.89642500	-1.64650600	3.79144400
C	2.15902800	-2.19877500	3.64196400
C	2.47001400	-4.18751600	5.27034200
C	3.01721600	-3.66638500	6.43607600
C	2.80968900	-4.34539600	7.64182500
C	2.06975400	-5.53286300	7.67227200
C	1.52026600	-6.05927800	6.50139800

C	1. 72159400	-5. 38023300	5. 29740200
C	1. 24961900	-5. 66612900	3. 93788100
C	0. 44096300	-6. 68652000	3. 43499600
C	0. 07403400	-6. 66142000	2. 09173600
C	0. 47966100	-5. 62330600	1. 22674100
C	1. 32818700	-4. 62221800	1. 74148700
C	1. 71180900	-4. 65566600	3. 07400000
H	0. 84518900	2. 17278000	-3. 43818600
H	-2. 15746000	-0. 80588700	-4. 29403400
H	-3. 88112500	0. 93070800	-4. 40396100
H	-5. 31144100	3. 15351500	-4. 49272000
H	-6. 17178300	5. 48082200	-4. 60407800
H	-4. 63583900	7. 40311300	-4. 32103100
H	-2. 20874900	7. 02873900	-3. 92208900
H	-1. 73625900	4. 55301000	-0. 97250100
H	1. 87036400	6. 56707200	0. 26088100
H	2. 67082200	6. 61572500	-2. 06382100
H	3. 02117900	6. 48480200	-4. 66939700
H	2. 87126200	6. 14522800	-7. 12547700
H	0. 91494900	4. 99371900	-8. 11684000
H	-0. 92077900	4. 15072100	-6. 66475700
H	2. 20874900	-7. 02873900	-3. 92208900
H	4. 63583900	-7. 40311300	-4. 32103100
H	6. 17178300	-5. 48082200	-4. 60407800
H	5. 31144100	-3. 15351500	-4. 49272000
H	3. 88112500	-0. 93070800	-4. 40396100
H	2. 15746000	0. 80588700	-4. 29403400
H	-0. 84518900	-2. 17278000	-3. 43818600
H	1. 73625900	-4. 55301000	-0. 97250100
H	-1. 87036400	-6. 56707200	0. 26088100
H	-2. 67082200	-6. 61572500	-2. 06382100
H	-3. 02117900	-6. 48480200	-4. 66939700
H	-2. 87126200	-6. 14522800	-7. 12547700
H	-0. 91494900	-4. 99371900	-8. 11684000
H	0. 92077900	-4. 15072100	-6. 66475700
H	-0. 06906100	2. 26043300	4. 13600200
H	-1. 62500700	-1. 52642200	2. 79440200
H	-3. 87862500	-0. 55482800	2. 57391500
H	-6. 00644000	0. 99246500	2. 34573100
H	-7. 65316000	2. 84583000	2. 19434400
H	-6. 99737900	5. 16023800	2. 78487100
H	-4. 68330000	5. 65793300	3. 55047100
H	-3. 59568700	2. 74664300	6. 41361100
H	-3. 22734800	3. 94675700	8. 56239400

H	-1.91926300	6.04927000	8.61661700
H	-0.94307700	6.98001300	6.53144400
H	-0.09244600	7.49125700	4.07740900
H	0.53600000	7.46983500	1.70092500
H	-1.64478400	3.79853200	1.10846200
H	4.68330000	-5.65793300	3.55047100
H	6.99737900	-5.16023800	2.78487100
H	7.65316000	-2.84583000	2.19434400
H	6.00644000	-0.99246500	2.34573100
H	3.87862500	0.55482800	2.57391500
H	1.62500700	1.52642200	2.79440200
H	0.06906100	-2.26043300	4.13600200
H	3.59568700	-2.74664300	6.41361100
H	3.22734800	-3.94675700	8.56239400
H	1.91926300	-6.04927000	8.61661700
H	0.94307700	-6.98001300	6.53144400
H	0.09244600	-7.49125700	4.07740900
H	-0.53600000	-7.46983500	1.70092500
H	1.64478400	-3.79853200	1.10846200

GSF6

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C	-2.79623900	2.85947600	-2.18908300
C	-2.68567400	2.26876300	-3.46330100
C	-3.44741900	1.15965100	-3.82250700
C	-4.34733800	0.62830600	-2.89784100
C	-5.30861000	-0.47361400	-3.01410000
C	-5.58114700	-1.34598600	-4.07044900
C	-6.57763300	-2.31032100	-3.90769800
C	-7.29197800	-2.40155100	-2.70762900
C	-7.02016900	-1.52854700	-1.64873500
C	-6.02888700	-0.56821000	-1.80916800
C	-5.12466300	-0.12857900	0.52910300
C	-4.14999600	-1.08719600	0.76400900
C	-3.99029900	-1.63846700	2.05375800
C	-4.82736500	-1.15509200	3.08252600
C	-5.78035000	-0.16544500	2.85955000
C	-5.94085900	0.34716300	1.57226600
C	-6.88527500	1.32918200	1.03096700
C	-7.87297900	2.09432400	1.65575700
C	-8.64321500	2.96321200	0.88033800
C	-8.43105100	3.06567400	-0.49927000

C	-7.44309900	2.29901200	-1.12691100
C	-6.67450900	1.43462500	-0.35688400
C	0.21350000	5.71492400	0.86688900
C	0.78771300	7.08544600	0.47390800
C	1.62505300	7.91712800	1.20698600
C	2.02909700	9.13302200	0.64505300
C	1.59735000	9.50557300	-0.63309900
C	0.75610700	8.67040600	-1.37100900
C	0.35151400	7.45612000	-0.81114600
C	-0.50812700	6.39027200	-1.33709600
C	-1.15033900	6.25618000	-2.56858500
C	-1.88939200	5.10364200	-2.82292600
C	-2.00933100	4.07608900	-1.86648200
C	-1.36813800	4.22987300	-0.62183200
C	-0.62182900	5.37311800	-0.36868700
C	1.31563100	4.69718600	1.17942800
C	2.24666300	4.14960700	0.31285600
C	3.20521600	3.23269800	0.79027700
C	3.19713000	2.92212700	2.16614800
C	2.24352900	3.45014200	3.03449400
C	1.28150900	4.33145800	2.53707900
C	0.13134600	4.98639600	3.17160700
C	-0.35659000	4.92071400	4.47861600
C	-1.51219100	5.63439800	4.80389700
C	-2.17152800	6.40344000	3.83858200
C	-1.68125000	6.47623300	2.52971900
C	-0.53329400	5.76553600	2.20286400
C	-1.06433500	-5.61719300	0.56842000
C	0.08749400	-4.97705300	-0.22338900
C	1.24700100	-4.40369900	0.27059100
C	2.23157700	-3.92732400	-0.61696000
C	1.98450400	-4.01462200	-2.00141300
C	0.81169400	-4.58243600	-2.49981100
C	-0.13925600	-5.08279800	-1.60648900
C	-1.41492200	-5.77942200	-1.81884700
C	-2.08256100	-6.13131800	-2.99386100
C	-3.29596400	-6.81679600	-2.90167200
C	-3.83596000	-7.14740600	-1.65402000
C	-3.16993200	-6.79501800	-0.47470900
C	-1.96254400	-6.11259600	-0.56226900
C	-0.52686400	-6.68412300	1.52832800
C	0.10359800	-7.88502200	1.22826500
C	0.56525200	-8.68650700	2.27865300
C	0.40413300	-8.28050000	3.60815800

C	-0.22689400	-7.07219300	3.91213900
C	-0.69599700	-6.27441700	2.86575200
C	-1.42637000	-5.00220100	2.87463200
C	-1.86710700	-4.19274900	3.92201800
C	-2.64318900	-3.07253900	3.63535300
C	-3.03039600	-2.74479100	2.31812900
C	-2.52591000	-3.54304200	1.26866600
C	-1.72309700	-4.63823300	1.54786100
C	6.23403800	-0.66965100	-0.64344400
C	7.33208700	-0.64900300	0.43265500
C	8.41969000	0.20803400	0.54481300
C	9.30786200	0.03497100	1.61189600
C	9.10566500	-0.98499800	2.54880600
C	8.01314900	-1.84716800	2.43674300
C	7.12442700	-1.67457000	1.37259600
C	5.90455100	-2.40155800	1.00692900
C	5.26235600	-3.47742000	1.62003400
C	4.07899700	-3.96149100	1.06963300
C	3.50905900	-3.38900900	-0.08582800
C	4.17746800	-2.31279000	-0.70396600
C	5.36142800	-1.83088500	-0.16128700
C	6.83283500	-0.82859200	-2.04589800
C	7.55005000	-1.89746100	-2.56828100
C	8.04379700	-1.80592100	-3.87463100
C	7.82573900	-0.65428400	-4.63908600
C	7.10683600	0.42238500	-4.11518400
C	6.60746600	0.33092200	-2.81390500
C	5.80416400	1.26807600	-2.02031600
C	5.30309100	2.53807300	-2.31091700
C	4.50019800	3.18300500	-1.37282700
C	4.15559500	2.57915600	-0.14539900
C	4.69967000	1.31112700	0.14571200
C	5.52167400	0.67953200	-0.77359800
H	-3.80150700	2.75311700	-0.27567200
H	-1.97735400	2.68295400	-4.17512600
H	-3.34239500	0.72388400	-4.81282300
H	-5.02854600	-1.27869800	-5.00417800
H	-6.80019600	-2.99689600	-4.72020700
H	-8.06433800	-3.15778100	-2.59617900
H	-7.57561400	-1.60195200	-0.71757700
H	-3.51864200	-1.41626300	-0.05520000
H	-4.76068800	-1.58727200	4.07487100
H	-6.40950200	0.17423000	3.67837400
H	-8.04030100	2.01922900	2.72723500

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H	-7.27994000	2.38092900	-2.19821300
H	1.96084600	7.63017300	2.19986300
H	2.68364600	9.79391100	1.20687500
H	1.91939700	10.45388600	-1.05514900
H	0.42292300	8.96424500	-2.36321800
H	-1.07974500	7.03571100	-3.32290400
H	-2.40605600	4.99992400	-3.77271800
H	-1.42999700	3.43682800	0.11866400
H	2.20508500	4.39635800	-0.74316500
H	3.95358300	2.25453500	2.56642800
H	2.25423600	3.16959500	4.08466400
H	0.14845600	4.32052400	5.23118600
H	-1.90490100	5.58939500	5.81627500
H	-3.07217200	6.94909500	4.10676100
H	-2.19254300	7.07683800	1.78204200
H	1.39824500	-4.31762600	1.34249800
H	2.74270800	-3.66724600	-2.69754700
H	0.65940200	-4.65431800	-3.57378200
H	-1.66768900	-5.87799600	-3.96615700
H	-3.82584200	-7.09615400	-3.80849500
H	-4.78061100	-7.68164100	-1.59940800
H	-3.59187500	-7.05142400	0.49353000
H	0.23351300	-8.19958000	0.19617300
H	1.05295100	-9.63248300	2.05923400
H	0.76990500	-8.91351400	4.41232000
H	-0.35549700	-6.76480700	4.94690400
H	-1.62058600	-4.43010100	4.95386300
H	-2.96010600	-2.44265800	4.45959400
H	-2.80009000	-3.33487500	0.23963700
H	8.57915600	1.00006500	-0.18199200
H	10.16222500	0.69872500	1.71352000
H	9.80507000	-1.10672100	3.37169700
H	7.85946100	-2.63719600	3.16755700
H	5.67588400	-3.93970900	2.51270700
H	3.59165300	-4.81524300	1.53054600
H	3.74717800	-1.84125700	-1.58336800
H	7.72395400	-2.79094000	-1.97446300
H	8.60182100	-2.63664600	-4.29815000
H	8.21728700	-0.59800100	-5.65135000
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H	4.13377500	4.17958000	-1.59747200

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GSF7

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C	-6. 20492600	1. 29432700	-1. 25147300
C	-6. 21462400	2. 67299900	-1. 46806100
C	-5. 58621800	3. 51025000	-0. 54362300
C	-5. 42847900	4. 97060600	-0. 49826400
C	-5. 89700800	5. 97089700	-1. 35270100
C	-5. 60492500	7. 30399000	-1. 05511800
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C	-4. 37981800	6. 63356700	0. 93412200
C	-4. 67049000	5. 30662200	0. 64167800
C	-2. 72852800	3. 82084100	1. 42188400
C	-1. 84654600	3. 81052200	0. 35335800
C	-0. 48153200	3. 53010400	0. 56570700
C	-0. 05743600	3. 26050400	1. 88397000
C	-0. 93808900	3. 29759500	2. 96327900
C	-2. 28508500	3. 58694300	2. 73551300
C	-3. 42780400	3. 71475600	3. 64824700
C	-3. 50944000	3. 60421000	5. 03818100
C	-4. 74581700	3. 79585100	5. 65901000
C	-5. 88550700	4. 09325300	4. 90356500
C	-5. 80753600	4. 20018200	3. 51025000
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C	-4. 24696100	-4. 04762200	-1. 39810000
C	-4. 67049000	-5. 30662200	-0. 64167800
C	-4. 37981800	-6. 63356700	-0. 93412200
C	-4. 85437500	-7. 63419500	-0. 07867300
C	-5. 60492500	-7. 30399000	1. 05511800
C	-5. 89700800	-5. 97089700	1. 35270100
C	-5. 42847900	-4. 97060600	0. 49826400
C	-5. 58621800	-3. 51025000	0. 54362300
C	-6. 21462400	-2. 67299900	1. 46806100
C	-6. 20492600	-1. 29432700	1. 25147300
C	-5. 60114000	-0. 73654500	0. 10978700
C	-4. 97120000	-1. 58819800	-0. 81434000
C	-4. 95059300	-2. 95545100	-0. 58180400
C	-2. 72852800	-3. 82084100	-1. 42188400
C	-1. 84654600	-3. 81052200	-0. 35335800
C	-0. 48153200	-3. 53010400	-0. 56570700

C	-0.05743600	-3.26050400	-1.88397000
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C	-3.42780400	-3.71475600	-3.64824700
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C	-5.80753600	-4.20018200	-3.51025000
C	-4.57883500	-4.01110300	-2.88990600
C	4.24696100	4.04762200	-1.39810000
C	4.95059300	2.95545100	-0.58180400
C	4.97120000	1.58819800	-0.81434000
C	5.60114000	0.73654500	0.10978700
C	6.20492600	1.29432700	1.25147300
C	6.21462400	2.67299900	1.46806100
C	5.58621800	3.51025000	0.54362300
C	5.42847900	4.97060600	0.49826400
C	5.89700800	5.97089700	1.35270100
C	5.60492500	7.30399000	1.05511800
C	4.85437500	7.63419500	-0.07867300
C	4.37981800	6.63356700	-0.93412200
C	4.67049000	5.30662200	-0.64167800
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C	5.80753600	4.20018200	-3.51025000
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C	0.05743600	3.26050400	-1.88397000
C	0.48153200	3.53010400	-0.56570700
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C	2.72852800	3.82084100	-1.42188400
C	4.24696100	-4.04762200	1.39810000
C	4.67049000	-5.30662200	0.64167800
C	4.37981800	-6.63356700	0.93412200
C	4.85437500	-7.63419500	0.07867300
C	5.60492500	-7.30399000	-1.05511800
C	5.89700800	-5.97089700	-1.35270100
C	5.42847900	-4.97060600	-0.49826400
C	5.58621800	-3.51025000	-0.54362300
C	6.21462400	-2.67299900	-1.46806100
C	6.20492600	-1.29432700	-1.25147300

C	5.60114000	-0.73654500	-0.10978700
C	4.97120000	-1.58819800	0.81434000
C	4.95059300	-2.95545100	0.58180400
C	4.57883500	-4.01110300	2.88990600
C	5.80753600	-4.20018200	3.51025000
C	5.88550700	-4.09325300	4.90356500
C	4.74581700	-3.79585100	5.65901000
C	3.50944000	-3.60421000	5.03818100
C	3.42780400	-3.71475600	3.64824700
C	2.28508500	-3.58694300	2.73551300
C	0.93808900	-3.29759500	2.96327900
C	0.05743600	-3.26050400	1.88397000
C	0.48153200	-3.53010400	0.56570700
C	1.84654600	-3.81052200	0.35335800
C	2.72852800	-3.82084100	1.42188400
H	-4.47833200	1.16620400	1.68604300
H	-6.69094900	0.63389000	-1.96455100
H	-6.70612900	3.08159900	-2.34747500
H	-6.48281500	5.72077300	-2.23360900
H	-5.96564100	8.09261400	-1.71018100
H	-4.63745800	8.67634400	0.29701600
H	-3.79459300	6.89143300	1.81285700
H	-2.20684600	4.04459700	-0.64359300
H	0.98005400	2.99879800	2.06612700
H	-0.57277000	3.09185900	3.96627300
H	-2.62692000	3.37673900	5.63068300
H	-4.82275900	3.71549700	6.74013600
H	-6.83922400	4.24300700	5.40243700
H	-6.69374000	4.42991000	2.92445900
H	-3.79459300	-6.89143300	-1.81285700
H	-4.63745800	-8.67634400	-0.29701600
H	-5.96564100	-8.09261400	1.71018100
H	-6.48281500	-5.72077300	2.23360900
H	-6.70612900	-3.08159900	2.34747500
H	-6.69094900	-0.63389000	1.96455100
H	-4.47833200	-1.16620400	-1.68604300
H	-2.20684600	-4.04459700	0.64359300
H	0.98005400	-2.99879800	-2.06612700
H	-0.57277000	-3.09185900	-3.96627300
H	-2.62692000	-3.37673900	-5.63068300
H	-4.82275900	-3.71549700	-6.74013600
H	-6.83922400	-4.24300700	-5.40243700
H	-6.69374000	-4.42991000	-2.92445900
H	4.47833200	1.16620400	-1.68604300

H	6. 69094900	0. 63389000	1. 96455100
H	6. 70612900	3. 08159900	2. 34747500
H	6. 48281500	5. 72077300	2. 23360900
H	5. 96564100	8. 09261400	1. 71018100
H	4. 63745800	8. 67634400	-0. 29701600
H	3. 79459300	6. 89143300	-1. 81285700
H	6. 69374000	4. 42991000	-2. 92445900
H	6. 83922400	4. 24300700	-5. 40243700
H	4. 82275900	3. 71549700	-6. 74013600
H	2. 62692000	3. 37673900	-5. 63068300
H	0. 57277000	3. 09185900	-3. 96627300
H	-0. 98005400	2. 99879800	-2. 06612700
H	2. 20684600	4. 04459700	0. 64359300
H	3. 79459300	-6. 89143300	1. 81285700
H	4. 63745800	-8. 67634400	0. 29701600
H	5. 96564100	-8. 09261400	-1. 71018100
H	6. 48281500	-5. 72077300	-2. 23360900
H	6. 70612900	-3. 08159900	-2. 34747500
H	6. 69094900	-0. 63389000	-1. 96455100
H	4. 47833200	-1. 16620400	1. 68604300
H	6. 69374000	-4. 42991000	2. 92445900
H	6. 83922400	-4. 24300700	5. 40243700
H	4. 82275900	-3. 71549700	6. 74013600
H	2. 62692000	-3. 37673900	5. 63068300
H	0. 57277000	-3. 09185900	3. 96627300
H	-0. 98005400	-2. 99879800	2. 06612700
H	2. 20684600	-4. 04459700	-0. 64359300

GSF8

C	5. 13447600	-1. 54122700	1. 21264800
C	4. 46387500	-0. 33104700	1. 87355600
C	4. 31465900	0. 95575500	1. 37570000
C	3. 76039900	1. 96070000	2. 19237600
C	3. 36672100	1. 62881100	3. 50342300
C	3. 50240700	0. 33460300	4. 00097700
C	4. 05297600	-0. 65215400	3. 18196000
C	4. 33456700	-2. 06981100	3. 43440200
C	4. 08964900	-2. 86908500	4. 55344600
C	4. 46415500	-4. 21371200	4. 51620100
C	5. 07501700	-4. 75243200	3. 37818700
C	5. 32408600	-3. 95253900	2. 25753800
C	4. 95185300	-2. 61432000	2. 29262200
C	4. 60974000	-1. 96197600	-0. 16614800
C	3. 33486600	-2. 38364600	-0. 52310000

C	3.07872000	-2.82568300	-1.83912100
C	4.14071200	-2.79762700	-2.76778200
C	5.41274100	-2.35317700	-2.42165400
C	5.65480600	-1.94392900	-1.11082900
C	6.88927800	-1.50185000	-0.45581000
C	8.17907500	-1.31271500	-0.95846500
C	9.18548300	-0.88958300	-0.08829800
C	8.90790400	-0.65921400	1.26419100
C	7.61670700	-0.84757300	1.76855000
C	6.61417900	-1.26837000	0.90344800
C	2.01156900	5.28569700	-1.29584500
C	1.92287500	6.79836700	-1.08709700
C	1.37062700	7.75876100	-1.92572000
C	1.40766900	9.10145500	-1.53313000
C	1.99309700	9.47147600	-0.31720700
C	2.54920700	8.50844100	0.52768400
C	2.51297600	7.16764500	0.13844700
C	2.99253500	5.95399600	0.81244400
C	3.56676100	5.75782100	2.07081700
C	3.83737900	4.45853700	2.49772500
C	3.55735000	3.34128700	1.68568000
C	3.01837900	3.55595300	0.40392100
C	2.73216800	4.84677900	-0.01463700
C	0.67306900	4.55123300	-1.42820800
C	-0.36045400	4.49610000	-0.50760100
C	-1.44681100	3.62194700	-0.71184400
C	-1.46761200	2.86629900	-1.90423000
C	-0.45031700	2.95181300	-2.85198300
C	0.64261200	3.78503600	-2.60626300
C	1.89151200	4.00480000	-3.34503500
C	2.33477200	3.50263900	-4.57072300
C	3.59682800	3.87767400	-5.03650700
C	4.40602900	4.74068300	-4.28920300
C	3.96458000	5.24464900	-3.06047600
C	2.70928200	4.87378700	-2.59515900
C	-1.26854500	-5.45776500	-0.94084000
C	-2.14399900	-4.55251200	-0.05905400
C	-2.99924800	-3.53797200	-0.45804100
C	-3.76906800	-2.85188400	0.50051300
C	-3.62378500	-3.20132300	1.85744100
C	-2.76574100	-4.22488400	2.25938700
C	-2.03073300	-4.91744000	1.29393000
C	-1.11780900	-6.06364100	1.39513200
C	-0.68702500	-6.79749400	2.50249400

C	0.18016200	-7.87393400	2.30292100
C	0.61207600	-8.21375600	1.01618500
C	0.18482000	-7.47805100	-0.09497600
C	-0.67935400	-6.40730200	0.09968000
C	-2.10787300	-6.09733800	-2.05128800
C	-3.16376600	-6.99282900	-1.93608400
C	-3.82948000	-7.40510800	-3.09602900
C	-3.44555200	-6.91539300	-4.34957200
C	-2.38685400	-6.01225200	-4.46724600
C	-1.71528900	-5.60603700	-3.31157100
C	-0.55669400	-4.72482500	-3.12840000
C	0.22982400	-4.03143500	-4.04905300
C	1.36587100	-3.36218700	-3.60179600
C	1.76320700	-3.38669700	-2.24801600
C	0.91800000	-4.03289600	-1.32085700
C	-0.23003400	-4.67820800	-1.75970700
C	-5.95216700	1.78505800	0.93928600
C	-6.96525100	2.36300700	-0.05046100
C	-7.56300900	3.61733200	-0.04683800
C	-8.47126700	3.93641800	-1.06251500
C	-8.77336300	3.00790200	-2.06488100
C	-8.17380900	1.74654300	-2.07111500
C	-7.26683500	1.42583700	-1.05851600
C	-6.48661100	0.20628400	-0.81351100
C	-6.37693900	-0.98345100	-1.53657700
C	-5.49800000	-1.96888700	-1.09102300
C	-4.72316200	-1.79732300	0.07408600
C	-4.86013000	-0.60262200	0.80544900
C	-5.72717800	0.38321500	0.35731400
C	-6.41965000	1.79403600	2.39746000
C	-7.58155500	1.25914500	2.93966500
C	-7.80403400	1.38124500	4.31602800
C	-6.87153200	2.03042200	5.13288100
C	-5.70216200	2.56805600	4.59062900
C	-5.47822100	2.44821000	3.21713700
C	-4.36145800	2.89827300	2.37848000
C	-3.15500500	3.52582800	2.69311500
C	-2.23120800	3.77067800	1.67988100
C	-2.48727300	3.43256600	0.33320000
C	-3.72760500	2.83552700	0.03059400
C	-4.63113600	2.55443600	1.04227500
H	4.65042300	1.20060300	0.37154600
H	2.91782700	2.39638600	4.12746800
H	3.17798000	0.10326500	5.01239800

H	3. 61237500	-2. 45598600	5. 43849500
H	4. 27744700	-4. 84837300	5. 37845600
H	5. 35802500	-5. 80146100	3. 36358600
H	5. 79906500	-4. 37304200	1. 37519400
H	2. 53647600	-2. 37810400	0. 21353800
H	3. 97783500	-3. 17468600	-3. 77193400
H	6. 21007500	-2. 36003500	-3. 16041600
H	8. 39883600	-1. 49030100	-2. 00816800
H	10. 19361800	-0. 73734800	-0. 46457100
H	9. 70209100	-0. 33011200	1. 92888200
H	7. 40321100	-0. 66646700	2. 81856500
H	0. 91741200	7. 47327000	-2. 87136100
H	0. 97834700	9. 86287800	-2. 17866900
H	2. 01514800	10. 51864000	-0. 02715300
H	3. 00236100	8. 80187100	1. 47126000
H	3. 78627400	6. 60063900	2. 72147400
H	4. 27966900	4. 29958800	3. 47728600
H	2. 76856000	2. 70582000	-0. 22466500
H	-0. 31191200	5. 11371400	0. 38332900
H	-2. 27218800	2. 15966800	-2. 07698300
H	-0. 49540300	2. 33887900	-3. 74853000
H	1. 71040200	2. 83161600	-5. 15511900
H	3. 95385700	3. 49541500	-5. 98919400
H	5. 38560100	5. 02259500	-4. 66575600
H	4. 59369300	5. 91610000	-2. 48207200
H	-3. 07440200	-3. 26465500	-1. 50668900
H	-4. 22384900	-2. 68594600	2. 60222700
H	-2. 69411100	-4. 49040900	3. 31111300
H	-1. 02007500	-6. 53928000	3. 50448300
H	0. 52248100	-8. 45379900	3. 15601100
H	1. 28563700	-9. 05519600	0. 87800000
H	0. 52367500	-7. 74149000	-1. 09347700
H	-3. 46692900	-7. 36958700	-0. 96281300
H	-4. 65196600	-8. 11144300	-3. 02200300
H	-3. 97411300	-7. 24374100	-5. 24063000
H	-2. 08911600	-5. 63937700	-5. 44402500
H	-0. 02453500	-4. 02182000	-5. 10596800
H	1. 96627100	-2. 81545200	-4. 32187100
H	1. 19523200	-4. 07746800	-0. 27180500
H	-7. 32975900	4. 33970700	0. 73091900
H	-8. 94565000	4. 91399800	-1. 07237800
H	-9. 48134800	3. 27087000	-2. 84637500
H	-8. 41187700	1. 02915900	-2. 85240500
H	-6. 96171300	-1. 14421900	-2. 43878600

H	-5.41676600	-2.90016000	-1.64415300
H	-4.25147500	-0.43845300	1.69041400
H	-8.30725600	0.75528000	2.30667000
H	-8.70933800	0.96893000	4.75338500
H	-7.05934800	2.11786200	6.19977800
H	-4.98164800	3.07227800	5.22963900
H	-2.91416200	3.79171300	3.71930100
H	-1.27144900	4.19658500	1.95146600
H	-3.97762300	2.57721800	-0.99330600

GSF9

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C	-2.07003900	2.77699300	2.32482200
C	-1.57395000	3.28508300	3.54327800
C	-0.58789900	4.26715500	3.58635700
C	-0.09447600	4.78991600	2.39089500
C	0.92907800	5.80609500	2.12911200
C	1.75023800	6.52788800	2.99866500
C	2.66823800	7.43334100	2.46300200
C	2.76389500	7.61596700	1.07876100
C	1.93855600	6.89764300	0.20654900
C	1.02615200	5.99484300	0.73791100
C	0.60810800	4.32869000	-1.16308800
C	1.56390900	3.32471100	-1.12534500
C	2.07003900	2.77699300	-2.32482200
C	1.57395000	3.28508300	-3.54327800
C	0.58789900	4.26715500	-3.58635700
C	0.09447600	4.78991600	-2.39089500
C	-0.92907800	5.80609500	-2.12911200
C	-1.75023800	6.52788800	-2.99866500
C	-2.66823800	7.43334100	-2.46300200
C	-2.76389500	7.61596700	-1.07876100
C	-1.93855600	6.89764300	-0.20654900
C	-1.02615200	5.99484300	-0.73791100
C	-5.72085000	0.00000000	0.00000000
C	-6.52748600	-1.11715500	0.66040900
C	-7.53765000	-1.89871400	0.11372900
C	-8.12757700	-2.89179500	0.90402300
C	-7.70391900	-3.09755600	2.22162800
C	-6.68761800	-2.31467800	2.77375600
C	-6.09993700	-1.32011500	1.98877500
C	-5.03881800	-0.35210000	2.29206000

C	-4.25386200	-0.15057300	3.42908200
C	-3.28904600	0.85467100	3.42117600
C	-3.09726300	1.70209900	2.30842100
C	-3.90274600	1.48573400	1.17238800
C	-4.83718900	0.46356300	1.16551000
C	-4.83718900	-0.46356300	-1.16551000
C	-3.90274600	-1.48573400	-1.17238800
C	-3.09726300	-1.70209900	-2.30842100
C	-3.28904600	-0.85467100	-3.42117600
C	-4.25386200	0.15057300	-3.42908200
C	-5.03881800	0.35210000	-2.29206000
C	-6.09993700	1.32011500	-1.98877500
C	-6.68761800	2.31467800	-2.77375600
C	-7.70391900	3.09755600	-2.22162800
C	-8.12757700	2.89179500	-0.90402300
C	-7.53765000	1.89871400	-0.11372900
C	-6.52748600	1.11715500	-0.66040900
C	5.72085000	0.00000000	0.00000000
C	4.83718900	-0.46356300	1.16551000
C	3.90274600	-1.48573400	1.17238800
C	3.09726300	-1.70209900	2.30842100
C	3.28904600	-0.85467100	3.42117600
C	4.25386200	0.15057300	3.42908200
C	5.03881800	0.35210000	2.29206000
C	6.09993700	1.32011500	1.98877500
C	6.68761800	2.31467800	2.77375600
C	7.70391900	3.09755600	2.22162800
C	8.12757700	2.89179500	0.90402300
C	7.53765000	1.89871400	0.11372900
C	6.52748600	1.11715500	0.66040900
C	6.52748600	-1.11715500	-0.66040900
C	7.53765000	-1.89871400	-0.11372900
C	8.12757700	-2.89179500	-0.90402300
C	7.70391900	-3.09755600	-2.22162800
C	6.68761800	-2.31467800	-2.77375600
C	6.09993700	-1.32011500	-1.98877500
C	5.03881800	-0.35210000	-2.29206000
C	4.25386200	-0.15057300	-3.42908200
C	3.28904600	0.85467100	-3.42117600
C	3.09726300	1.70209900	-2.30842100
C	3.90274600	1.48573400	-1.17238800
C	4.83718900	0.46356300	-1.16551000
C	0.00000000	-5.11865300	0.00000000
C	-1.02615200	-5.99484300	0.73791100

C	-1.93855600	-6.89764300	0.20654900
C	-2.76389500	-7.61596700	1.07876100
C	-2.66823800	-7.43334100	2.46300200
C	-1.75023800	-6.52788800	2.99866500
C	-0.92907800	-5.80609500	2.12911200
C	0.09447600	-4.78991600	2.39089500
C	0.58789900	-4.26715500	3.58635700
C	1.57395000	-3.28508300	3.54327800
C	2.07003900	-2.77699300	2.32482200
C	1.56390900	-3.32471100	1.12534500
C	0.60810800	-4.32869000	1.16308800
C	1.02615200	-5.99484300	-0.73791100
C	1.93855600	-6.89764300	-0.20654900
C	2.76389500	-7.61596700	-1.07876100
C	2.66823800	-7.43334100	-2.46300200
C	1.75023800	-6.52788800	-2.99866500
C	0.92907800	-5.80609500	-2.12911200
C	-0.09447600	-4.78991600	-2.39089500
C	-0.58789900	-4.26715500	-3.58635700
C	-1.57395000	-3.28508300	-3.54327800
C	-2.07003900	-2.77699300	-2.32482200
C	-1.56390900	-3.32471100	-1.12534500
C	-0.60810800	-4.32869000	-1.16308800
H	-1.90622800	2.95063200	0.16588100
H	-1.97992800	2.91817600	4.48014200
H	-0.22265200	4.62671200	4.54503800
H	1.68189000	6.38622900	4.07436000
H	3.31614800	7.99944700	3.12698000
H	3.48605100	8.32133500	0.67656900
H	2.01389500	7.04254800	-0.86779300
H	1.90622800	2.95063200	-0.16588100
H	1.97992800	2.91817600	-4.48014200
H	0.22265200	4.62671200	-4.54503800
H	-1.68189000	6.38622900	-4.07436000
H	-3.31614800	7.99944700	-3.12698000
H	-3.48605100	8.32133500	-0.67656900
H	-2.01389500	7.04254800	0.86779300
H	-7.86671300	-1.74129700	-0.91006000
H	-8.92088700	-3.50830000	0.49005600
H	-8.17096400	-3.87373000	2.82209200
H	-6.36399400	-2.47818200	3.79853800
H	-4.37080400	-0.78016800	4.30755200
H	-2.65272700	0.96501100	4.29297200
H	-3.80248700	2.12164800	0.29890700

H	-3.80248700	-2.12164800	-0.29890700
H	-2.65272700	-0.96501100	-4.29297200
H	-4.37080400	0.78016800	-4.30755200
H	-6.36399400	2.47818200	-3.79853800
H	-8.17096400	3.87373000	-2.82209200
H	-8.92088700	3.50830000	-0.49005600
H	-7.86671300	1.74129700	0.91006000
H	3.80248700	-2.12164800	0.29890700
H	2.65272700	-0.96501100	4.29297200
H	4.37080400	0.78016800	4.30755200
H	6.36399400	2.47818200	3.79853800
H	8.17096400	3.87373000	2.82209200
H	8.92088700	3.50830000	0.49005600
H	7.86671300	1.74129700	-0.91006000
H	7.86671300	-1.74129700	0.91006000
H	8.92088700	-3.50830000	-0.49005600
H	8.17096400	-3.87373000	-2.82209200
H	6.36399400	-2.47818200	-3.79853800
H	4.37080400	-0.78016800	-4.30755200
H	2.65272700	0.96501100	-4.29297200
H	3.80248700	2.12164800	-0.29890700
H	-2.01389500	-7.04254800	-0.86779300
H	-3.48605100	-8.32133500	0.67656900
H	-3.31614800	-7.99944700	3.12698000
H	-1.68189000	-6.38622900	4.07436000
H	0.22265200	-4.62671200	4.54503800
H	1.97992800	-2.91817600	4.48014200
H	1.90622800	-2.95063200	0.16588100
H	2.01389500	-7.04254800	0.86779300
H	3.48605100	-8.32133500	-0.67656900
H	3.31614800	-7.99944700	-3.12698000
H	1.68189000	-6.38622900	-4.07436000
H	-0.22265200	-4.62671200	-4.54503800
H	-1.97992800	-2.91817600	-4.48014200
H	-1.90622800	-2.95063200	-0.16588100

DSF1

C	4.43315500	-0.16287900	-0.00482800
C	3.00875500	-0.58613500	-0.38209000
C	1.85146000	0.17713600	-0.36768500
C	0.62451300	-0.40051800	-0.74982400
C	0.60919400	-1.75555900	-1.13615800
C	1.77066400	-2.52553700	-1.14842900
C	2.97983400	-1.93852600	-0.77073900

C	4.33981700	-2.48365600	-0.68636400
C	4.83588800	-3.75938600	-0.96469100
C	6.20011100	-4.00437700	-0.79450100
C	7.05715400	-2.99023200	-0.35238100
C	6.56225500	-1.71161700	-0.07255500
C	5.20522000	-1.46538700	-0.24136900
C	4.55931500	0.37789500	1.42317300
C	4.23495300	-0.24975000	2.61980100
C	4.43609000	0.43961500	3.82061600
C	4.95574800	1.73886200	3.81718700
C	5.28215600	2.37134100	2.61561800
C	5.08177900	1.68521100	1.41595500
C	5.32810000	2.08515900	0.02346200
C	5.83312800	3.27096400	-0.51412900
C	5.96451100	3.38134600	-1.90019000
C	5.59697700	2.32222700	-2.73771400
C	5.09046900	1.13339600	-2.20112300
C	4.95853800	1.02192900	-0.82225500
C	-4.43315300	0.16287800	-0.00489500
C	-5.20521500	1.46538900	-0.24143800
C	-6.56225200	1.71161800	-0.07264200
C	-7.05714600	2.99023400	-0.35246700
C	-6.20009700	4.00438200	-0.79456900
C	-4.83587200	3.75939200	-0.96474100
C	-4.33980500	2.48366000	-0.68641400
C	-2.97982100	1.93853100	-0.77077300
C	-1.77064500	2.52554400	-1.14844100
C	-0.60917500	1.75556600	-1.13615800
C	-0.62450000	0.40052300	-0.74983100
C	-1.85145300	-0.17713300	-0.36771500
C	-3.00874800	0.58613700	-0.38213300
C	-4.55933600	-0.37790600	1.42310000
C	-4.23499100	0.24972800	2.61973800
C	-4.43614800	-0.43964500	3.82054500
C	-4.95580900	-1.73889100	3.81709700
C	-5.28220000	-2.37136000	2.61551900
C	-5.08180400	-1.68522100	1.41586400
C	-5.32810300	-2.08515800	0.02336400
C	-5.83312600	-3.27095700	-0.51424400
C	-5.96448700	-3.38132900	-1.90030800
C	-5.59693700	-2.32220400	-2.73781800
C	-5.09043400	-1.13337800	-2.20121000
C	-4.95852500	-1.02192300	-0.82233900
H	1.88297600	1.21186800	-0.03820100

H	-0.32733000	-2.20227900	-1.45716100
H	1.72888600	-3.56629100	-1.45956700
H	4.17445100	-4.55066000	-1.30835200
H	6.59995100	-4.99227500	-1.00740000
H	8.11636100	-3.19687300	-0.22502700
H	7.22946800	-0.92535200	0.27067100
H	3.83184300	-1.25900600	2.62479800
H	4.18632900	-0.03881200	4.76376800
H	5.10627000	2.26103500	4.75835400
H	5.68495600	3.38107900	2.61856200
H	6.12040200	4.09665300	0.13202300
H	6.35630100	4.29842300	-2.33219700
H	5.70563500	2.42323100	-3.81422800
H	4.80555900	0.31185800	-2.85312200
H	-7.22946900	0.92535100	0.27057000
H	-8.11635500	3.19687500	-0.22512700
H	-6.59993400	4.99228100	-1.00746800
H	-4.17443000	4.55066800	-1.30838700
H	-1.72886300	3.56629900	-1.45957200
H	0.32735300	2.20228800	-1.45714300
H	-1.88297400	-1.21186800	-0.03823700
H	-3.83187800	1.25898400	2.62474900
H	-4.18640000	0.03877400	4.76370400
H	-5.10634700	-2.26107000	4.75825800
H	-5.68500300	-3.38109700	2.61844800
H	-6.12041200	-4.09665100	0.13189700
H	-6.35627200	-4.29840100	-2.33232900
H	-5.70557700	-2.42320000	-3.81433400
H	-4.80551100	-0.31183600	-2.85319900

DSF2

C	3.89490000	-0.01350500	-0.02761100
C	2.86844600	-1.13476400	0.17047600
C	1.50866500	-1.11531800	-0.10035600
C	0.72833500	-2.26317300	0.14170900
C	1.36067900	-3.41088700	0.65995400
C	2.72730600	-3.43325600	0.93158200
C	3.48811600	-2.28877000	0.68566800
C	4.91915100	-2.01693300	0.86507900
C	5.95369600	-2.82437900	1.34348700
C	7.24567500	-2.29813300	1.40676600
C	7.50132200	-0.98435400	0.99809800
C	6.46632600	-0.17371900	0.51875800
C	5.17999600	-0.69513200	0.45473700

C	3.97439300	0.50152500	-1.46855900
C	4.25319000	-0.21004600	-2.62906700
C	4.27420100	0.47135300	-3.85085800
C	4.01883100	1.84619400	-3.90331000
C	3.73832700	2.56295100	-2.73798700
C	3.71678900	1.88478600	-1.51741900
C	3.45793800	2.36300900	-0.15214900
C	3.15613000	3.63802800	0.33079000
C	2.95598500	3.81009400	1.70219600
C	3.05571000	2.72424400	2.57918400
C	3.35773600	1.44586100	2.09742600
C	3.55740700	1.27284600	0.73318800
C	-3.89489900	-0.01350600	0.02761100
C	-5.17999600	-0.69513200	-0.45473700
C	-6.46632600	-0.17372000	-0.51875800
C	-7.50132200	-0.98435400	-0.99809800
C	-7.24567500	-2.29813300	-1.40676600
C	-5.95369600	-2.82437900	-1.34348700
C	-4.91915000	-2.01693300	-0.86507900
C	-3.48811600	-2.28877000	-0.68566800
C	-2.72730500	-3.43325600	-0.93158200
C	-1.36067800	-3.41088700	-0.65995400
C	-0.72833500	-2.26317300	-0.14170900
C	-1.50866500	-1.11531800	0.10035600
C	-2.86844600	-1.13476400	-0.17047600
C	-3.55740700	1.27284600	-0.73318800
C	-3.35773600	1.44586100	-2.09742600
C	-3.05571000	2.72424400	-2.57918400
C	-2.95598600	3.81009400	-1.70219600
C	-3.15613100	3.63802800	-0.33079000
C	-3.45793900	2.36300900	0.15214900
C	-3.71678900	1.88478600	1.51741900
C	-3.73832800	2.56295100	2.73798700
C	-4.01883100	1.84619300	3.90331000
C	-4.27420100	0.47135300	3.85085800
C	-4.25318900	-0.21004700	2.62906700
C	-3.97439300	0.50152400	1.46855900
H	1.04701300	-0.22723300	-0.52291100
H	0.76175700	-4.29056500	0.87747900
H	3.18569700	-4.33086200	1.33899100
H	5.76040800	-3.84562200	1.66210200
H	8.06033200	-2.91498300	1.77686500
H	8.51222300	-0.58955400	1.05343800
H	6.66691500	0.84644000	0.20224600

H	4.45162800	-1.27787700	-2.59014300
H	4.49046300	-0.07233200	-4.76654300
H	4.03848900	2.36128000	-4.86010200
H	3.54021000	3.63081200	-2.78474700
H	3.07650000	4.48479100	-0.34620100
H	2.72000400	4.79681300	2.09188200
H	2.89659700	2.87431700	3.64360500
H	3.43418600	0.60345600	2.77981400
H	-6.66691500	0.84644000	-0.20224500
H	-8.51222300	-0.58955400	-1.05343700
H	-8.06033100	-2.91498300	-1.77686500
H	-5.76040800	-3.84562200	-1.66210200
H	-3.18569700	-4.33086200	-1.33899100
H	-0.76175600	-4.29056500	-0.87747900
H	-1.04701300	-0.22723300	0.52291100
H	-3.43418600	0.60345600	-2.77981400
H	-2.89659700	2.87431700	-3.64360500
H	-2.72000500	4.79681300	-2.09188200
H	-3.07650100	4.48479100	0.34620100
H	-3.54021000	3.63081200	2.78474700
H	-4.03849000	2.36128000	4.86010200
H	-4.49046300	-0.07233200	4.76654300
H	-4.45162700	-1.27787700	2.59014300

TS1

C	-0.11129500	5.15754700	0.29338000
C	-0.72978900	4.26819800	1.37664700
C	-1.70232100	3.28995100	1.24193000
C	-2.21589600	2.62786500	2.37963900
C	-1.70507500	3.00629900	3.63952200
C	-0.70360900	3.96357800	3.77771400
C	-0.20309100	4.59663700	2.64024900
C	0.83745100	5.61559300	2.47408400
C	1.67387700	6.23503500	3.40579400
C	2.60548200	7.17288500	2.95620000
C	2.69994500	7.48798200	1.59590000
C	1.85950600	6.87233700	0.66173200
C	0.93328400	5.93763300	1.10705700
C	0.46868000	4.46287900	-0.94201300
C	1.40756700	3.44399000	-1.00448100
C	1.86771200	2.97844800	-2.25526500
C	1.35035300	3.58170500	-3.41982100
C	0.38645600	4.58504500	-3.36286800
C	-0.06422100	5.02601000	-2.11827500

C	-1.06026700	6.03844200	-1.75399100
C	-1.88033200	6.84704500	-2.54491900
C	-2.76524000	7.72677200	-1.91858800
C	-2.83011500	7.79834100	-0.52241800
C	-2.00675100	6.99219100	0.27124700
C	-1.12658200	6.11554500	-0.35045800
C	-5.65243500	-0.09505600	-0.31702100
C	-6.55173800	-1.18991000	0.25694600
C	-7.51476600	-1.95130800	-0.39331000
C	-8.21103200	-2.92442200	0.33262300
C	-7.93880700	-3.13046200	1.68961200
C	-6.97011800	-2.36798300	2.34583100
C	-6.27645000	-1.39330100	1.62481100
C	-5.23307300	-0.44712900	2.03710700
C	-4.57257800	-0.25190800	3.25116300
C	-3.59290100	0.73418400	3.34418100
C	-3.25882900	1.57154200	2.25675800
C	-3.94087600	1.35825500	1.04085100
C	-4.89039900	0.35596400	0.93613400
C	-4.66691200	-0.58925200	-1.38490100
C	-3.75504300	-1.62792500	-1.29106600
C	-2.85932700	-1.88000000	-2.34927600
C	-2.93559100	-1.05478200	-3.49148200
C	-3.87324300	-0.02979400	-3.60034300
C	-4.74863200	0.20906300	-2.53902000
C	-5.81050300	1.20469700	-2.34904800
C	-6.29820500	2.19948300	-3.19932700
C	-7.34146200	3.01477500	-2.75500400
C	-7.88988100	2.84038100	-1.47954900
C	-7.40088200	1.84646300	-0.62419300
C	-6.36388100	1.03279800	-1.06366900
C	5.65474700	0.08665900	-0.31778800
C	4.89935900	-0.36492000	0.93930300
C	3.93137700	-1.34942200	1.04226200
C	3.26869400	-1.57658000	2.26660900
C	3.64401600	-0.77017900	3.36422300
C	4.63644500	0.20290200	3.27030200
C	5.27492600	0.41320000	2.04717500
C	6.32097300	1.35438900	1.63080600
C	7.03617500	2.31207500	2.35358800
C	7.99819100	3.07733400	1.69088400
C	8.24279200	2.89059600	0.32583800
C	7.52569900	1.93382000	-0.40147800
C	6.56880600	1.16999800	0.25505000

C	6.35893700	-1.04634800	-1.06518900
C	7.39154100	-1.86602500	-0.62660900
C	7.87396700	-2.86259100	-1.48256700
C	7.32362700	-3.03349100	-2.75770200
C	6.28485300	-2.21200100	-3.20097600
C	5.80367700	-1.21467700	-2.34989600
C	4.74731500	-0.21315000	-2.53827600
C	3.87216000	0.02902600	-3.59882900
C	2.93938900	1.05810200	-3.48922300
C	2.86799400	1.88392000	-2.34715500
C	3.76323700	1.62833400	-1.28933400
C	4.67083600	0.58573400	-1.38388900
C	0.11028700	-5.15305700	0.30085600
C	-0.94894200	-5.91905200	1.10896400
C	-1.86731500	-6.86096000	0.66243600
C	-2.72980400	-7.45561300	1.59000000
C	-2.66589300	-7.11166300	2.94511100
C	-1.74266800	-6.16620100	3.39592500
C	-0.88340800	-5.56853100	2.47072100
C	0.15893400	-4.55206700	2.63975500
C	0.63476900	-3.89486800	3.77399500
C	1.64951700	-2.95122000	3.63976700
C	2.20538600	-2.61421700	2.38695100
C	1.71357500	-3.29900900	1.25283600
C	0.72124700	-4.25757300	1.38349200
C	1.12332400	-6.11520500	-0.33763600
C	1.99617300	-6.99597400	0.28857900
C	2.82057800	-7.80537500	-0.50073300
C	2.76406100	-7.73269900	-1.89718400
C	1.88665800	-6.84878600	-2.52826200
C	1.06547600	-6.03701400	-1.74180100
C	0.07503100	-5.02072100	-2.11155000
C	-0.36949300	-4.57786000	-3.35787600
C	-1.33262600	-3.57373400	-3.41856300
C	-1.85551600	-2.97138300	-2.25594800
C	-1.39941300	-3.43689500	-1.00376400
C	-0.46181900	-4.45648300	-0.93796500
H	-2.05272000	3.03339600	0.24824000
H	-2.10293100	2.55316800	4.54055800
H	-0.32927500	4.21486900	4.76690100
H	1.60651700	5.99017700	4.46282300
H	3.26519900	7.66077400	3.66886200
H	3.43299400	8.21693800	1.26111000
H	1.93343700	7.12047000	-0.39368200

H	1. 77032400	2. 98998700	-0. 08748600
H	1. 72444800	3. 27228700	-4. 39056800
H	0. 00406100	5. 02285600	-4. 28148100
H	-1. 83578500	6. 79211300	-3. 62973900
H	-3. 41131800	8. 36001000	-2. 52085900
H	-3. 52659400	8. 48546500	-0. 04955400
H	-2. 05834200	7. 05064100	1. 35512200
H	-7. 72649400	-1. 79353400	-1. 44755900
H	-8. 96919500	-3. 52523100	-0. 16239100
H	-8. 48751000	-3. 89094100	2. 23893700
H	-6. 76399400	-2. 53144800	3. 40053200
H	-4. 79953800	-0. 86930900	4. 11666300
H	-3. 06513900	0. 83630900	4. 28575000
H	-3. 73271800	1. 97545300	0. 17392400
H	-3. 74148800	-2. 25203700	-0. 40304200
H	-2. 22814300	-1. 19995100	-4. 30167000
H	-3. 90088500	0. 58537000	-4. 49623700
H	-5. 87686800	2. 33856500	-4. 19167900
H	-7. 73167300	3. 79198300	-3. 40678300
H	-8. 70208700	3. 48239600	-1. 14949600
H	-7. 82702000	1. 71357900	0. 36674100
H	3. 69164600	-1. 93810300	0. 16405700
H	3. 14294500	-0. 88704200	4. 31828300
H	4. 89204000	0. 79711800	4. 14401400
H	6. 85100500	2. 46088500	3. 41432200
H	8. 56304200	3. 82514200	2. 24123200
H	8. 99567200	3. 49375100	-0. 17435700
H	7. 71640800	1. 79076200	-1. 46182500
H	7. 81930900	-1. 73588000	0. 36397500
H	8. 68262000	-3. 50945800	-1. 15326000
H	7. 70882800	-3. 81278900	-3. 40996400
H	5. 86191000	-2. 34825700	-4. 19304300
H	3. 89601100	-0. 58686300	-4. 49432200
H	2. 23139000	1. 20599700	-4. 29839200
H	3. 75229000	2. 25249900	-0. 40121700
H	-1. 91804200	-7. 13098600	-0. 38897400
H	-3. 45620300	-8. 19070900	1. 25414800
H	-3. 34264200	-7. 58336200	3. 65269000
H	-1. 69839700	-5. 89955100	4. 44889700
H	0. 22949300	-4. 11520800	4. 75835600
H	2. 01814100	-2. 47449000	4. 54075000
H	2. 09845400	-3. 07975400	0. 26325200
H	2. 04131300	-7. 05503100	1. 37272800
H	3. 51129300	-8. 49583800	-0. 02429800

H	3.41085900	-8.36843100	-2.49605200
H	1.84868300	-6.79320600	-3.61329400
H	0.01626400	-5.01548600	-4.27518500
H	-1.70231000	-3.26383900	-4.39087500
H	-1.76537300	-2.98345000	-0.08783300

TS2

C	-4.36321000	4.28068500	1.03683100
C	-4.94149300	3.07718200	0.27925800
C	-4.92707100	1.74181200	0.65112100
C	-5.44384200	0.77020700	-0.22457800
C	-5.96033600	1.18065500	-1.46819800
C	-6.00143400	2.52758700	-1.83014400
C	-5.49674800	3.48477700	-0.94689900
C	-5.41581000	4.94950100	-1.03294400
C	-5.85471800	5.83570900	-2.01896100
C	-5.66195600	7.20606600	-1.82901000
C	-5.03825900	7.68536300	-0.67183300
C	-4.59238600	6.79926800	0.31543100
C	-4.78492600	5.43561700	0.13072700
C	-2.84332800	4.13217400	1.19213500
C	-1.87987600	4.10548600	0.19765100
C	-0.52559200	3.89035300	0.52603000
C	-0.20256900	3.69587000	1.88638800
C	-1.16536700	3.75874800	2.89167100
C	-2.49843800	3.99030300	2.54733200
C	-3.71184400	4.13920500	3.35983900
C	-3.89762300	4.12305700	4.74400300
C	-5.18225700	4.32206700	5.25491700
C	-6.26711600	4.53265600	4.39664500
C	-6.08507100	4.54292800	3.00885800
C	-4.80802100	4.34804900	2.49750200
C	-4.38951700	-4.20238400	-1.02965800
C	-4.83850700	-5.33998200	-0.10888400
C	-4.66272700	-6.70869300	-0.27128400
C	-5.13488500	-7.57336100	0.72249400
C	-5.76822700	-7.06823700	1.86354800
C	-5.94391400	-5.69275300	2.03019500
C	-5.47772800	-4.82811400	1.03731700
C	-5.53623500	-3.36478700	0.92712700
C	-6.05275800	-2.39379400	1.78704300
C	-5.99688300	-1.05348300	1.40670600
C	-5.45280500	-0.66312200	0.16834000
C	-4.92330200	-1.64904400	-0.68437400

C	-4.95263400	-2.98030800	-0.29459600
C	-2.86293700	-4.14062000	-1.19183700
C	-1.89942100	-4.08642700	-0.19815000
C	-0.52700300	-4.05575900	-0.52805500
C	-0.19463200	-4.05924500	-1.90092200
C	-1.16043300	-4.11769000	-2.90284200
C	-2.50983900	-4.17025600	-2.55151400
C	-3.73162300	-4.27877600	-3.35630800
C	-3.91715100	-4.35597800	-4.73862400
C	-5.21559700	-4.47239200	-5.23956200
C	-6.31402200	-4.51079600	-4.37337000
C	-6.13103600	-4.43115500	-2.98811100
C	-4.84035800	-4.31639000	-2.48644300
C	4.36318100	4.28070700	-1.03682500
C	4.94147300	3.07720700	-0.27925500
C	4.92705900	1.74183700	-0.65111800
C	5.44384200	0.77023600	0.22457700
C	5.96034100	1.18068700	1.46819500
C	6.00143000	2.52761800	1.83014200
C	5.49673200	3.48480600	0.94690000
C	5.41578300	4.94952900	1.03294800
C	5.85468800	5.83573900	2.01896400
C	5.66191400	7.20609400	1.82901500
C	5.03820800	7.68538800	0.67184300
C	4.59233800	6.79929100	-0.31542100
C	4.78489000	5.43564100	-0.13072100
C	4.80799300	4.34808000	-2.49749500
C	6.08504400	4.54296000	-3.00884900
C	6.26709000	4.53270200	-4.39663600
C	5.18223100	4.32212600	-5.25491000
C	3.89759700	4.12311500	-4.74400000
C	3.71181700	4.13924900	-3.35983500
C	2.49841000	3.99033900	-2.54733000
C	1.16533900	3.75879100	-2.89167200
C	0.20254100	3.69589900	-1.88639000
C	0.52556400	3.89036100	-0.52602900
C	1.87984800	4.10548900	-0.19764700
C	2.84330000	4.13219100	-1.19213100
C	4.38954100	-4.20236100	1.02965400
C	4.83854000	-5.33995700	0.10888100
C	4.66276600	-6.70866800	0.27128000
C	5.13493100	-7.57333500	-0.72249600
C	5.76827500	-7.06820700	-1.86354900
C	5.94395500	-5.69272200	-2.03019600

C	5.47776100	-4.82808500	-1.03731800
C	5.53626000	-3.36475800	-0.92712800
C	6.05278200	-2.39376200	-1.78704200
C	5.99689800	-1.05345200	-1.40670500
C	5.45281400	-0.66309300	-0.16834100
C	4.92331300	-1.64901800	0.68437000
C	4.95265300	-2.98028200	0.29459300
C	4.84038100	-4.31636500	2.48643900
C	6.13105900	-4.43112100	2.98810800
C	6.31404400	-4.51076300	4.37336800
C	5.21561700	-4.47236800	5.23955900
C	3.91717100	-4.35596400	4.73861800
C	3.73164500	-4.27876100	3.35630300
C	2.50986200	-4.17024900	2.55150700
C	1.16045500	-4.11769300	2.90283400
C	0.19465400	-4.05925100	1.90091300
C	0.52702700	-4.05575700	0.52804600
C	1.89944600	-4.08641500	0.19814200
C	2.86296000	-4.14060600	1.19183000
H	-4.49708900	1.43593200	1.60097800
H	-6.36464000	0.43086500	-2.14282600
H	-6.42958500	2.82052500	-2.78555200
H	-6.34254100	5.46940700	-2.91873200
H	-6.00132400	7.90700600	-2.58708200
H	-4.89788800	8.75460500	-0.53836800
H	-4.10482400	7.17308700	1.21191500
H	-2.17447700	4.27698900	-0.83240900
H	0.82251800	3.47976000	2.16794000
H	-0.87229800	3.61968500	3.92921700
H	-3.05802000	3.96393400	5.41589400
H	-5.34009000	4.31586600	6.33020700
H	-7.25955000	4.68988300	4.81045200
H	-6.92933900	4.70402700	2.34361600
H	-4.16804500	-7.10259000	-1.15515700
H	-5.00788900	-8.64634400	0.60674500
H	-6.12832900	-7.75295200	2.62686000
H	-6.43911500	-5.30583700	2.91723400
H	-6.50282400	-2.67168300	2.73681500
H	-6.41028200	-0.29157200	2.06182700
H	-4.47466500	-1.35821500	-1.63050600
H	-2.22257800	-4.08447200	0.83667800
H	0.84418900	-4.02470800	-2.20762000
H	-0.85288200	-4.13050000	-3.94546000
H	-3.06754500	-4.32851000	-5.41618700

H	-5.37425800	-4.53485700	-6.31292900
H	-7.31779700	-4.60368900	-4.77918000
H	-6.98539500	-4.46060100	-2.31689500
H	4.49707400	1.43595500	-1.60097300
H	6.36465500	0.43089900	2.14282000
H	6.42958400	2.82055900	2.78554700
H	6.34251700	5.46943900	2.91873200
H	6.00127900	7.90703600	2.58708700
H	4.89782800	8.75462900	0.53837900
H	4.10476900	7.17310600	-1.21190200
H	6.92931200	4.70405000	-2.34360400
H	7.25952500	4.68993000	-4.81044000
H	5.34006500	4.31593600	-6.33020100
H	3.05799300	3.96400200	-5.41589300
H	0.87226900	3.61974400	-3.92922000
H	-0.82254700	3.47979500	-2.16794500
H	2.17445000	4.27697800	0.83241500
H	4.16808400	-7.10256900	1.15515100
H	5.00794000	-8.64631800	-0.60674800
H	6.12838200	-7.75292000	-2.62686000
H	6.43915600	-5.30580300	-2.91723300
H	6.50285200	-2.67164900	-2.73681300
H	6.41029500	-0.29153900	-2.06182500
H	4.47467100	-1.35819200	1.63050100
H	6.98541900	-4.46055900	2.31689400
H	7.31781900	-4.60364900	4.77917900
H	5.37427700	-4.53483300	6.31292500
H	3.06756400	-4.32850300	5.41618100
H	0.85290300	-4.13050900	3.94545200
H	-0.84416700	-4.02472300	2.20761000
H	2.22260300	-4.08445400	-0.83668600

TS3

C	-5.64541200	0.39510000	-0.65582000
C	-4.57143700	1.07175600	-1.51968200
C	-3.78692700	2.17446600	-1.22064700
C	-2.90923100	2.68426400	-2.19837700
C	-2.82647300	2.04207300	-3.44955700
C	-3.61611200	0.93270300	-3.75098400
C	-4.50372600	0.45387000	-2.78767000
C	-5.49881700	-0.63186300	-2.84386800
C	-5.82206300	-1.52386200	-3.86703300
C	-6.84237000	-2.45496000	-3.65033600
C	-7.52799900	-2.49264900	-2.43044000

C	-7.20387500	-1.59866800	-1.40169500
C	-6.19252400	-0.67289900	-1.61514000
C	-5.12731800	-0.21620900	0.65741200
C	-4.18360800	-1.21364700	0.83160900
C	-3.91103300	-1.71657800	2.12478600
C	-4.60887800	-1.14456500	3.21184200
C	-5.54585400	-0.12762200	3.04107200
C	-5.82012900	0.33464600	1.75548300
C	-6.78979500	1.32734600	1.26358600
C	-7.69374600	2.14080900	1.94826400
C	-8.51711400	2.99858700	1.21268600
C	-8.43786300	3.04159800	-0.18430500
C	-7.53088900	2.22584300	-0.87341300
C	-6.71278000	1.37312000	-0.14574400
C	0.09932400	5.70310100	0.70586000
C	0.64456700	7.07224100	0.25734900
C	1.46286800	7.95276200	0.95000000
C	1.83805400	9.15251500	0.33166200
C	1.39552200	9.45788000	-0.96105900
C	0.57018700	8.57182400	-1.65995500
C	0.19541500	7.37647000	-1.04451400
C	-0.64713000	6.26686000	-1.52311600
C	-1.30248500	6.07837300	-2.73909300
C	-2.03099200	4.90626300	-2.93808400
C	-2.11484300	3.91451600	-1.94119400
C	-1.45360700	4.11601600	-0.71234400
C	-0.73000700	5.28212100	-0.51238200
C	1.23900700	4.74087400	1.06751800
C	2.18955400	4.18005100	0.23456000
C	3.18117600	3.33371500	0.77398200
C	3.18219700	3.09432600	2.16356500
C	2.20530400	3.63631400	2.99952000
C	1.21790800	4.45370700	2.44871700
C	0.04007600	5.10589500	3.04975900
C	-0.44485700	5.09342100	4.35799900
C	-1.62946100	5.77987700	4.64358700
C	-2.31803900	6.46727100	3.63749200
C	-1.83029000	6.48622600	2.32387500
C	-0.65588700	5.80546900	2.03766900
C	-0.97533400	-5.61411200	0.42175900
C	0.19999900	-4.93643300	-0.30740100
C	1.33850400	-4.37106600	0.23728000
C	2.34493400	-3.87072800	-0.61428300
C	2.15062800	-3.93372700	-2.00846000

C	0.99398500	-4.49039200	-2.55725400
C	0.01643100	-5.00454300	-1.70379100
C	-1.26330800	-5.68389200	-1.97962100
C	-1.89721200	-5.98461500	-3.18551200
C	-3.12670600	-6.65036900	-3.15261100
C	-3.71290200	-7.01002200	-1.93378500
C	-3.07808000	-6.71053400	-0.72103500
C	-1.85753500	-6.05022400	-0.74980800
C	-0.45369900	-6.75297700	1.31261100
C	0.18340000	-7.92855700	0.94254800
C	0.61550600	-8.80624300	1.94590200
C	0.41521000	-8.49935900	3.29695900
C	-0.22559800	-7.31448800	3.67233000
C	-0.66224900	-6.44197500	2.67438400
C	-1.39696100	-5.16854700	2.75816000
C	-1.88024600	-4.45312600	3.85173200
C	-2.64790900	-3.31124700	3.63115100
C	-2.97409900	-2.86351400	2.33188500
C	-2.43335600	-3.57613100	1.23596500
C	-1.65061300	-4.69698800	1.45243000
C	6.29565600	-0.55702700	-0.50791900
C	7.36340200	-0.51576900	0.60194900
C	8.42454200	0.36431800	0.75466100
C	9.28674600	0.19738200	1.84600100
C	9.08269400	-0.84011900	2.76366900
C	8.01367000	-1.72824600	2.61056300
C	7.15255600	-1.56165300	1.52451800
C	5.95262300	-2.31300800	1.11696200
C	5.31955000	-3.40918300	1.70066700
C	4.15615700	-3.90843300	1.11672500
C	3.60159300	-3.32258000	-0.03919100
C	4.25758100	-2.22157200	-0.62916300
C	5.42273300	-1.73340400	-0.05819800
C	6.95947100	-0.72097200	-1.88425500
C	7.69966200	-1.78668200	-2.37498500
C	8.25008500	-1.69066000	-3.66021700
C	8.06226300	-0.53827600	-4.43218500
C	7.31715700	0.53757900	-3.93919000
C	6.76361100	0.44196800	-2.66175900
C	5.91477000	1.37867900	-1.90366900
C	5.41655800	2.64034100	-2.22785700
C	4.56229800	3.28238000	-1.33145900
C	4.17201700	2.67669600	-0.11918000
C	4.70585500	1.41205300	0.20864300

C	5.57667700	0.78763100	-0.66676200
H	-3.87781900	2.67143300	-0.26204900
H	-2.12450300	2.41716000	-4.18492900
H	-3.54098700	0.45734400	-4.72239800
H	-5.29335800	-1.49823400	-4.81311900
H	-7.10525100	-3.15546000	-4.43454000
H	-8.31623300	-3.22091700	-2.27961800
H	-7.73138900	-1.62816900	-0.45585500
H	-3.67737300	-1.61118400	-0.03755400
H	-4.44160800	-1.51468400	4.21366200
H	-6.06807300	0.27657500	3.90085400
H	-7.75740800	2.11153800	3.03008200
H	-9.22399100	3.63792100	1.72886000
H	-9.08347000	3.71306400	-0.73819300
H	-7.46690200	2.25958900	-1.95442500
H	1.80407100	7.71415800	1.95014100
H	2.47700500	9.85085100	0.85944700
H	1.69559800	10.39103400	-1.42367700
H	0.22835200	8.81202600	-2.66037900
H	-1.25622300	6.83134100	-3.51767600
H	-2.56799100	4.75902800	-3.86756400
H	-1.49010200	3.35143700	0.05474700
H	2.14636600	4.36193800	-0.83180000
H	3.96288900	2.47888400	2.59366100
H	2.21851400	3.41932300	4.06156500
H	0.08104900	4.55684200	5.13952400
H	-2.02097800	5.77650000	5.65431900
H	-3.23731500	6.98927500	3.87595600
H	-2.36017400	7.02003200	1.54401000
H	1.45386800	-4.30781800	1.31229700
H	2.93259500	-3.57275100	-2.66604500
H	0.87334900	-4.54070300	-3.63344200
H	-1.44858300	-5.70630100	-4.13236200
H	-3.63244400	-6.88909500	-4.08110300
H	-4.66717600	-7.52349100	-1.92738000
H	-3.53161400	-6.98711500	0.22332700
H	0.34150100	-8.16232600	-0.10347900
H	1.10923900	-9.73155200	1.67291400
H	0.75703800	-9.18969500	4.05950300
H	-0.38466500	-7.08400800	4.71969600
H	-1.67833600	-4.78171700	4.86497300
H	-3.00913100	-2.76921300	4.49405300
H	-2.64686100	-3.27626000	0.21906400
H	8.58080100	1.16520300	0.04200500

H	10.11930500	0.87787500	1.98097800
H	9.76018000	-0.95490500	3.60193900
H	7.85825300	-2.52921100	3.32456600
H	5.72380000	-3.87419300	2.59257300
H	3.67378400	-4.77739800	1.54775600
H	3.83513000	-1.74211300	-1.50418000
H	7.84742200	-2.67604600	-1.77405700
H	8.82689400	-2.51663600	-4.05967500
H	8.49660400	-0.48083700	-5.42361100
H	7.16983600	1.42612000	-4.54264600
H	5.68449300	3.12023300	-3.16229400
H	4.19310100	4.27220000	-1.57001700
H	4.40708700	0.91282600	1.12180700

TS4

C	-4.47612600	-3.79656500	-0.56399400
C	-3.10096800	-3.72135400	0.11881400
C	-1.85157200	-3.64133600	-0.47519400
C	-0.67829000	-3.66200400	0.31114900
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