

Reaction Pathways for Addition of H₂ to Amido-Ditetrylnes R₂N-EE-NR₂ (E = Si, Ge, Sn). A Theoretical Study

Markus Hermann^a, Catharina Goedecke^a, Cameron Jones^{*,b}, Gernot Frenking^{*,a}

M. Hermann, C. Goedecke, Prof. Dr. G. Frenking, Fachbereich Chemie, Philipps-Universität Marburg, 35032, Marburg, Germany. Email: frenking@chemie.uni-marburg.de. Fax: +49-6421-282-5566

Prof. C. Jones, School of Chemistry, Monash University, PO Box 23, Melbourne, VIC, 3800, Australia. Email: cameron.jones@monash.edu. Tel: +61-(0)3-9902-0391. Fax: +61-(0)3-9905-4597. Web: <http://monash.edu/science/jonesgroup>

Supporting Information

Table S1. Calculated coordinates [Å] and energies [Hartrees] of the molecules. (BP86/def2-TZVPP//BP86/def2-SVP)

1Si'

20

-848.2941911129

N -2.1778521 0.0253044 -0.2759709

Si -0.8975508 -1.0114968 -0.8380110

N 2.2219520 -0.1096485 -0.3219303

Si 0.9156787 0.6113954 -1.2184048

C	3.5738969	0.4464484	-0.4461774
H	3.5680427	1.2799688	-1.1582983
H	3.9418322	0.8123682	0.5275754
H	4.2791846	-0.3235326	-0.8033941
C	2.1961218	-1.2212727	0.6288364
H	2.9630221	-1.9714732	0.3702141
H	2.4078752	-0.8709843	1.6536746
H	1.2135248	-1.7086724	0.6249963
C	-2.1271332	1.4292796	0.1321663
H	-2.9062753	2.0131867	-0.3872201
H	-2.3032199	1.5331728	1.2166324
H	-1.1479480	1.8638070	-0.1033255
C	-3.5300834	-0.5211212	-0.1171286
H	-3.8641180	-0.4508384	0.9321510
H	-4.2507872	0.0397231	-0.7368140
H	-3.5429924	-1.5738265	-0.4229731

TS1-2Si'

22

-848.9500673925

N	-2.3274480	0.1409382	-0.0649346
Si	-0.9324450	-0.9282365	0.0661105
H	0.6161394	1.5893931	0.8582805
N	2.3907317	-0.1782734	-0.2357336
Si	0.8751983	0.6627993	-0.5547125
H	0.1456500	0.7696543	1.0931952
C	3.6411438	0.5678589	-0.2651507
H	3.4791950	1.5735362	-0.7051973
H	4.0764981	0.7136825	0.7543035
H	4.4110996	0.0433433	-0.8791935
C	2.5402086	-1.5422277	0.2472450
H	3.3392148	-2.0798893	-0.3150479
H	2.8172773	-1.5827908	1.3303825
H	1.5984977	-2.1145018	0.1236582
C	-2.3609830	1.5850865	-0.2609658

H	-3.1423159	1.8635759	-1.0043488
H	-2.5994051	2.1274357	0.6837549
H	-1.3857734	1.9579554	-0.6392716
C	-3.6604432	-0.4360968	0.1066416
H	-4.1830609	-0.0061598	0.9922951
H	-4.2997306	-0.2402907	-0.7851087
H	-3.5828466	-1.5325670	0.2489718

2Si'

22

-849.5101596928

N	-2.3519165	0.2778805	0.2849428
Si	-0.9503217	-0.7212081	0.6317638
H	1.0193679	1.8481962	-0.7509102
N	2.3948693	-0.2358715	-0.2661772
Si	0.8013807	0.3696613	-0.5305452
H	0.0497312	0.6013459	1.0628484
C	3.5422734	0.5982121	0.0697724
H	3.3129204	1.6539432	-0.1178539
H	3.8267352	0.4918776	1.1327684
H	4.4172291	0.3166926	-0.5410572
C	2.6625205	-1.6648982	-0.1436375
H	3.5232108	-1.9512464	-0.7723650
H	2.8964299	-1.9503711	0.8973812
H	1.7865204	-2.2431082	-0.4635756
C	-2.3671362	1.6160862	-0.2775901
H	-2.4100099	1.6069051	-1.3841501
H	-3.2434054	2.1801958	0.0850802
H	-1.4662176	2.1692020	0.0218657
C	-3.6579663	-0.3704846	0.2965938
H	-4.3837000	0.2186381	0.8845961
H	-4.0731450	-0.4966764	-0.7205474
H	-3.5789716	-1.3678941	0.7523764

TS2-3Si'

22

-849.5100732312

N	-2.3321181	0.2714180	0.1647598
Si	-0.9388464	-0.7861841	0.2593096
H	1.0806526	2.0953857	0.0159579
N	2.4528537	-0.0632213	-0.1182045
Si	0.8720520	0.6206588	-0.2164900
H	0.0471662	0.3138262	1.2634091
C	3.5681179	0.5855350	0.5597999
H	3.3482164	1.6475175	0.7240268
H	3.7777580	0.1231204	1.5421306
H	4.4855797	0.5105224	-0.0489407
C	2.7176651	-1.4525980	-0.4735810
H	3.6261802	-1.5230932	-1.0964100
H	2.8718457	-2.0854444	0.4188123
H	1.8729937	-1.8669153	-1.0383498
C	-2.3639201	1.7152294	0.0059989
H	-2.4951885	2.0183933	-1.0498956
H	-3.1980461	2.1505404	0.5831049
H	-1.4350388	2.1682155	0.3770748
C	-3.6478513	-0.3540493	0.0924559
H	-4.3194392	0.0420865	0.8751771
H	-4.1340110	-0.1843275	-0.8855233
H	-3.5572670	-1.4398693	0.2382541

IM3Si'

22

-849.5269462473

N	-2.2995991	0.2623909	-0.1389637
Si	-0.9149227	-0.6639698	-0.6298316
H	0.9531794	2.0495659	-0.1643891
N	2.3659350	-0.1185008	-0.0776253
Si	0.8633991	0.6501924	0.3809698
H	0.7131015	0.8493420	1.8802446
C	3.6226625	0.6158509	-0.0304297

H	3.4484998	1.6800951	-0.2363117
H	4.1323777	0.5374208	0.9509489
H	4.3194014	0.2300964	-0.7952650
C	2.5395332	-1.5539895	0.0926762
H	3.2382746	-1.9483815	-0.6653928
H	2.9420105	-1.8274794	1.0888301
H	1.5801418	-2.0764082	-0.0369103
C	-2.3945927	1.4674216	0.6834981
H	-2.8103938	2.3062125	0.1000592
H	-3.0647243	1.2966185	1.5429426
H	-1.4122745	1.7612479	1.0673472
C	-3.6240157	-0.1695722	-0.6003298
H	-4.2828483	-0.3895207	0.2563427
H	-4.1050335	0.6193367	-1.2024213
H	-3.5283893	-1.0730933	-1.2147840

TS2-4Si'

22

-849.5044221123

N	0.1194305	0.0197236	0.1401388
Si	0.2310688	-0.0252114	1.9029733
H	3.9611241	0.2087384	1.6716000
N	3.1173030	0.1367856	4.0002838
Si	2.6250382	-0.0303905	2.3657074
H	0.7599569	1.4352838	2.1355650
C	4.4476740	0.5218401	4.4632516
H	5.1338615	0.6058665	3.6134429
H	4.4168519	1.4911997	4.9891301
H	4.8434197	-0.2295937	5.1668014
C	2.1527277	-0.0223277	5.0901673
H	2.5237056	-0.7523245	5.8282199
H	1.9856971	0.9345052	5.6116244
H	1.1908581	-0.3762049	4.6958249
C	0.8387645	0.9112469	-0.7523290
H	1.7774089	0.4621520	-1.1381438

H	0.2182989	1.1675268	-1.6303285
H	1.0934710	1.8430590	-0.2329414
C	-0.4023220	-1.1589913	-0.5360654
H	-1.0740314	-0.8698851	-1.3642507
H	0.3974766	-1.7949262	-0.9669389
H	-0.9760816	-1.7765736	0.1694813

4Si'

22

-849.5101596624

N	-2.3519868	0.2777821	0.2855410
Si	-0.9500986	-0.7209964	0.6322201
H	1.0195135	1.8488371	-0.7497148
N	2.3947475	-0.2356154	-0.2662225
Si	0.8013390	0.3701511	-0.5304375
H	0.0494539	0.6014531	1.0633608
C	3.5423668	0.5981835	0.0696738
H	3.3129058	1.6540672	-0.1169278
H	3.8274647	0.4909476	1.1324049
H	4.4169627	0.3171657	-0.5419065
C	2.6623331	-1.6647206	-0.1445085
H	3.5226421	-1.9508810	-0.7738468
H	2.8968063	-1.9506585	0.8962520
H	1.7860924	-2.2427049	-0.4641888
C	-2.3672023	1.6161473	-0.2766355
H	-2.4089791	1.6072305	-1.3832432
H	-3.2440408	2.1798208	0.0853314
H	-1.4667904	2.1695305	0.0238617
C	-3.6578350	-0.3709594	0.2961890
H	-4.3840609	0.2176291	0.8841238
H	-4.0724525	-0.4967468	-0.7212362
H	-3.5787832	-1.3685853	0.7514896

TS4-5Si'

24

-850.6909614901

Si	0.3127378	0.9662851	1.5791302
Si	2.1490659	-0.4300103	1.8004189
N	-0.3631534	1.6379122	0.1288607
N	2.8237359	-1.5184722	0.6292994
C	0.4664372	2.3514904	-0.8328042
H	0.1417911	3.4012861	-0.9448642
H	1.5140580	2.3513057	-0.5029796
H	0.4200307	1.8787849	-1.8297431
C	-1.7789806	1.6361547	-0.2118948
H	-2.1727089	2.6642460	-0.3018915
H	-1.9547036	1.1279383	-1.1772011
H	-2.3538165	1.1119283	0.5606478
C	4.2391536	-1.6219369	0.3027261
H	4.8143424	-0.8830795	0.8730866
H	4.6338528	-2.6268152	0.5363242
H	4.4131293	-1.4390377	-0.7729975
C	1.9934646	-2.4956173	-0.0621642
H	0.9463100	-2.3936685	0.2531084
H	2.0378922	-2.3554225	-1.1566353
H	2.3189479	-3.5282447	0.1563731
H	-0.8659696	0.2881485	2.2191793
H	3.3280776	0.4135146	2.1968236
H	1.1020014	0.9688126	3.3191265
H	1.3619655	0.1088257	3.4560796

5Si'

24

-850.7585999706

N	-0.9881588	-0.1026950	0.9269011
Si	0.1475666	-0.2316717	2.2388763
Si	2.3644604	-0.0056044	1.4357147
N	3.4727463	0.1259257	2.7701715
C	-2.3851664	0.2259121	1.1771966
C	-0.7833872	-0.8214622	-0.3226780

C	3.2925318	1.1358385	3.8042785
C	4.8476057	-0.3438980	2.6640484
H	0.0658220	-1.5135691	3.0318773
H	-0.2076490	0.8591816	3.2032666
H	2.7874370	-1.2242818	0.6742712
H	2.4128128	1.1385115	0.4522471
H	5.1855632	-0.7602028	3.6291516
H	4.9237278	-1.1370028	1.9094890
H	5.5538912	0.4629744	2.3855639
H	3.5994657	0.7404214	4.7881710
H	3.8875801	2.0503998	3.6135144
H	2.2374381	1.4322314	3.8778735
H	-1.1680742	-0.2319213	-1.1728904
H	0.2869136	-0.9988656	-0.4979787
H	-1.2934169	-1.8047433	-0.3421616
H	-2.7929660	0.8220839	0.3422465
H	-3.0248114	-0.6718745	1.2876074
H	-2.4783519	0.8228491	2.0938607

TS3-6-7Si'

24

-850.6864514889

C	3.0264948	0.7599020	0.9804015
N	2.0159053	0.0961967	0.1674142
C	2.0248990	-1.3493862	0.3157227
Si	1.2247515	0.9157889	-1.1510478
Si	-1.0681455	0.6244981	-1.6205732
N	-2.1209846	0.3483112	-0.2632649
C	-3.5275141	0.0430636	-0.4899241
C	-1.6968877	0.1534551	1.1149481
H	1.7661731	0.6552837	-2.5347457
H	1.4908709	2.3550172	-0.8332886
H	2.9514272	1.8488185	0.8693065
H	2.8890355	0.5133085	2.0482841
H	4.0545407	0.4591677	0.7013607

H	2.9662761	-1.8049305	-0.0467496
H	1.9043449	-1.6344018	1.3758470
H	1.1968789	-1.7975762	-0.2519701
H	-2.3149432	0.7547002	1.8049846
H	-1.7860614	-0.9055177	1.4266537
H	-0.6488100	0.4527368	1.2411071
H	-3.7603421	-1.0209002	-0.2931876
H	-4.1732217	0.6531295	0.1662256
H	-3.8025204	0.2584197	-1.5319382
H	-0.8935389	-0.7436031	-2.4028134
H	-0.0516835	-0.7733502	-1.6203383

6Si'

11

-424.7417545043

H	2.8566400	-0.6321573	-0.9554528
C	2.5955416	-0.2686162	0.0530734
H	2.3071130	0.7920368	-0.0435876
H	1.7395979	-0.8381761	0.4268922
C	4.9025328	0.3296646	0.5085419
H	5.7299849	0.1962807	1.2163212
H	5.2282903	-0.0205511	-0.4851118
H	4.6776949	1.4062598	0.4275935
N	3.7280389	-0.4158019	0.9654114
Si	3.8098817	-1.3256178	2.4371659
H	2.3528957	-1.8265541	2.3427806

7Si'

13

-425.9737361445

Si	2.9139635	-0.5742320	-1.0070791
H	2.5851776	-0.1182613	0.3762704
H	2.4825679	-2.0121767	-1.1135803
H	2.1407894	0.1931338	-2.0284085
N	4.5969601	-0.2665857	-1.2783013

C	5.5862761	-0.5510953	-0.2486771
H	5.1288606	-0.4903920	0.7480762
H	6.0421662	-1.5549768	-0.3541165
H	6.4041053	0.1891750	-0.2891206
C	5.1467761	-0.2435517	-2.6262974
H	5.9592402	0.5004988	-2.6953451
H	5.5645345	-1.2206675	-2.9385011
H	4.3711553	0.0395968	-3.3506362

1Ge'

20

-4423.834169006

N	-0.9564465	0.1436526	0.9020924
Ge	0.0557560	0.5627620	2.4092315
Ge	2.4383241	0.5625938	1.2555989
N	3.4505120	0.1438027	2.7627852
C	-2.4113041	0.1018731	1.0268740
C	-0.5277086	-0.2017634	-0.4484093
C	3.0217970	-0.2013501	4.1133286
C	4.9053431	0.1019889	2.6379663
H	-1.0131044	0.4553847	-1.1922236
H	0.5586551	-0.1019862	-0.5541752
H	-0.8069599	-1.2407091	-0.7005295
H	-2.8870702	0.8104359	0.3250232
H	-2.8033305	-0.9046667	0.7941658
H	-2.7078832	0.3664306	2.0493457
H	3.5072155	0.4559066	4.8570132
H	1.9354465	-0.1015341	4.2191198
H	3.3010210	-1.2402436	4.3656439
H	5.3811404	0.8106706	3.3396584
H	5.2973794	-0.9044950	2.8708548
H	5.2019153	0.3663468	1.6154480

TS1-2Ge'

-4424.9916646370

N	-2.403207	0.178946	0.095866
Ge	-0.885038	-0.837068	0.452608
H	0.773978	1.716150	0.552864
N	2.540919	-0.182242	-0.396420
Ge	0.953166	0.702985	-0.858607
H	0.188449	0.902200	0.850425
C	3.705140	0.554872	0.058344
H	3.634134	1.607388	-0.248655
H	3.817443	0.532772	1.161650
H	4.632250	0.134656	-0.373966
C	2.596128	-1.600581	-0.102161
H	3.516968	-2.051963	-0.514892
H	2.583183	-1.813020	0.986860
H	1.737297	-2.124073	-0.547269
C	-2.483679	1.538286	-0.414363
H	-3.161686	1.589447	-1.285386
H	-2.878000	2.232653	0.349502
H	-1.497206	1.898696	-0.731716
C	-3.713655	-0.391726	0.383090
H	-4.255439	0.204270	1.139190
H	-4.340766	-0.422690	-0.525985
H	-3.603974	-1.415733	0.764196

IM2Ge'

22

-4425.0287938320

N	-2.511826	0.310641	0.396796
Ge	-1.061023	-0.770419	0.877009
H	1.072047	1.772369	-0.913200
N	2.520609	-0.305124	-0.319577
Ge	0.800123	0.217156	-0.737046
H	-0.034246	0.566918	1.109829
C	3.635668	0.596993	-0.084026
H	3.367271	1.618798	-0.376017

H	3.930500	0.610293	0.982541
H	4.521796	0.287171	-0.667084
C	2.824833	-1.696284	-0.023611
H	3.689408	-2.045964	-0.615989
H	3.074762	-1.843387	1.043718
H	1.964212	-2.335293	-0.261208
C	-2.472304	1.689028	-0.050939
H	-2.492176	1.767677	-1.156322
H	-3.344622	2.249535	0.331383
H	-1.562428	2.184409	0.309915
C	-3.781245	-0.346913	0.128532
H	-4.610858	0.174227	0.639326
H	-4.020575	-0.369799	-0.952151
H	-3.759529	-1.384954	0.489702

TS2-3Ge'

22

-4425.0250780700

N	-2.461054	0.246293	-0.094556
Ge	-1.017695	-0.931890	0.114809
H	1.113741	2.138979	0.261558
N	2.590390	-0.033595	-0.124635
Ge	0.885626	0.664229	-0.225316
H	0.001021	0.104994	1.283289
C	3.650884	0.585070	0.652123
H	3.425125	1.643300	0.833556
H	3.793129	0.094281	1.634870
H	4.611675	0.525941	0.109953
C	2.851774	-1.417242	-0.483101
H	3.804193	-1.500327	-1.036515
H	2.925682	-2.077188	0.402939
H	2.049413	-1.804627	-1.125219
C	-2.428082	1.692041	-0.171475
H	-3.294838	2.068188	-0.743441
H	-2.451252	2.179786	0.822594

H	-1.516203	2.027988	-0.687370
C	-3.785454	-0.307205	0.146502
H	-4.219590	0.028234	1.107836
H	-4.486842	-0.014120	-0.655583
H	-3.742287	-1.406380	0.170059

IM3Ge'

22

-4425.0403773980

N	-2.430068	0.285554	-0.161822
Ge	-0.973291	-0.668515	-0.797332
H	1.049180	2.144359	-0.221536
N	2.486840	-0.152485	-0.262327
Ge	0.891442	0.680276	0.295072
H	0.868497	0.811302	1.869010
C	3.719580	0.593220	-0.045835
H	3.597239	1.634157	-0.374028
H	4.052935	0.606350	1.014332
H	4.536815	0.145798	-0.638931
C	2.626948	-1.554435	0.105925
H	3.437304	-2.019067	-0.482438
H	2.867158	-1.715861	1.179223
H	1.700752	-2.105979	-0.115934
C	-2.490501	1.440006	0.725516
H	-2.943357	2.306921	0.212919
H	-3.113130	1.219249	1.610371
H	-1.491481	1.723967	1.072014
C	-3.760797	-0.134918	-0.597315
H	-4.390639	-0.408237	0.267066
H	-4.274609	0.677518	-1.139902
H	-3.685096	-1.004300	-1.262842

TS2-4Ge'

22

-4425.0254645590

N	-0.015933	0.009566	0.020195
Ge	0.037732	-0.013698	1.897349
H	4.156545	0.010728	1.739497
N	3.205640	0.131339	4.118383
Ge	2.693499	-0.103725	2.373742
H	0.579546	1.517480	2.051594
C	4.558980	0.393283	4.589178
H	5.262295	0.376421	3.749505
H	4.622433	1.379289	5.082395
H	4.869917	-0.366916	5.327074
C	2.212212	0.125539	5.186913
H	2.475005	-0.616276	5.960537
H	2.149794	1.112377	5.677121
H	1.221271	-0.126711	4.788015
C	0.611912	0.997172	-0.836563
H	1.600489	0.662381	-1.215583
H	-0.017599	1.205458	-1.722022
H	0.755856	1.937294	-0.291380
C	-0.330665	-1.227131	-0.673716
H	-1.017016	-1.041804	-1.520385
H	0.570137	-1.725250	-1.088051
H	-0.820338	-1.935315	0.009430

IM4Ge'

22

-4424.974865996

N	-1.1469797	-0.2313446	0.7930308
Ge	0.2623004	-0.8180512	1.8421530
Ge	2.2271382	0.8193363	1.8282786
N	3.6392493	0.2316154	2.8730071
C	-2.4481161	0.1836864	1.2862130
C	-0.9676950	-0.0200283	-0.6327437
C	3.4634873	0.0179818	4.2988668
C	4.9387751	-0.1835740	2.3757153
H	-0.4606379	-0.7235745	3.2512868

H	2.9463309	0.7263983	0.4170953
H	-1.7482961	-0.5423215	-1.2148646
H	-1.0237089	1.0533922	-0.8950058
H	0.0108888	-0.3988736	-0.9561757
H	-3.2606450	-0.3309355	0.7416718
H	-2.5425456	-0.0464808	2.3533655
H	-2.6015401	1.2722215	1.1548070
H	5.7531160	0.3293289	2.9191682
H	5.0916349	-1.2725016	2.5045886
H	5.0306861	0.0485786	1.3087671
H	4.2460194	0.5386117	4.8798655
H	2.4860642	0.3970994	4.6254823
H	3.5192509	-1.0559510	4.5591599

TS4-5Ge'

24

-4426.1836241080

Ge	0.183010	0.910734	1.389163
Ge	2.278501	-0.435235	1.602560
N	-0.566753	1.916812	0.027816
N	3.027403	-1.814872	0.621096
C	0.207482	2.922061	-0.679852
H	-0.168326	3.944182	-0.485714
H	1.260413	2.883642	-0.369792
H	0.169470	2.758674	-1.772424
C	-1.981307	1.916033	-0.303935
H	-2.455455	2.891395	-0.085282
H	-2.135708	1.708960	-1.379253
H	-2.507905	1.143421	0.269364
C	4.441461	-1.916994	0.303406
H	4.968566	-1.004721	0.608170
H	4.916277	-2.776492	0.813042
H	4.594351	-2.053529	-0.783346
C	2.252690	-2.990116	0.261533
H	1.200139	-2.857305	0.545740

H	2.289244	-3.174107	-0.827831
H	2.629217	-3.901402	0.762929
H	-1.011914	-0.026799	1.785751
H	3.473492	0.579141	1.687204
H	0.956289	0.953093	3.041037
H	1.507034	0.037751	3.186633

IM5Ge'

24

-4426.2400015260

N	-1.046358	0.045536	0.739147
Ge	0.089423	-0.113579	2.217908
Ge	2.406837	0.100881	1.446547
N	3.541041	-0.046073	2.927743
C	-2.451024	0.302927	1.038099
C	-0.884428	-0.953066	-0.311251
C	3.379571	0.962392	3.968770
C	4.945599	-0.308825	2.633037
H	-0.111133	-1.462476	2.983672
H	-0.325953	1.039282	3.166109
H	2.825049	-1.058057	0.507042
H	2.605704	1.444792	0.671660
H	5.454085	-0.664480	3.545671
H	5.035997	-1.096114	1.872682
H	5.501133	0.582828	2.273145
H	3.874148	0.623097	4.894787
H	3.814646	1.949625	3.705481
H	2.315827	1.114754	4.199210
H	-1.381552	-0.606536	-1.233214
H	0.179262	-1.100696	-0.545092
H	-1.316589	-1.943753	-0.056259
H	-2.961504	0.665450	0.129290
H	-3.004334	-0.592852	1.391106
H	-2.541856	1.083479	1.805340

TS3-6-7Ge'

24

-4426.1822927420

C	3.570383	0.017177	0.230894
N	2.236107	-0.311632	-0.259841
C	1.591172	-1.322869	0.567322
Ge	1.178709	1.198598	-0.683220
Ge	-1.350815	1.300903	-1.700895
N	-2.405602	0.517947	-0.365200
C	-2.949338	-0.822755	-0.476096
C	-2.337076	1.014638	0.998707
H	2.063027	2.030135	-1.650920
H	0.986163	2.051116	0.622473
H	4.049580	0.753328	-0.428980
H	3.578486	0.425181	1.264748
H	4.199263	-0.890107	0.231773
H	2.190756	-2.249314	0.560007
H	1.466549	-1.022144	1.630274
H	0.597272	-1.569711	0.167000
H	-3.340891	1.031682	1.459071
H	-1.683352	0.395704	1.645751
H	-1.943106	2.040900	1.018009
H	-2.314687	-1.582877	0.024192
H	-3.951491	-0.876967	-0.014102
H	-3.049932	-1.110863	-1.531195
H	-0.761124	-0.179349	-2.396341
H	0.046894	0.023413	-1.741016

IM6Ge'

11

-2212.5066567120

H	2.854888	-0.624601	-0.966902
C	2.601965	-0.261054	0.045159
H	2.305391	0.798414	-0.055083
H	1.748624	-0.832471	0.422859

C	4.907763	0.341044	0.493737
H	5.738058	0.210582	1.199039
H	5.237665	-0.005185	-0.501424
H	4.687734	1.419761	0.409686
N	3.737031	-0.400729	0.947147
Ge	3.819780	-1.373643	2.518594
H	2.289321	-1.875350	2.380819

IM7Ge'

-2213.7081347350

Ge	2.867615	-0.594479	-1.001091
H	2.489273	-0.170875	0.434159
H	2.637994	-2.129555	-1.157725
H	2.028370	0.152432	-2.059552
N	4.637998	-0.078927	-1.261583
C	5.594977	-0.516775	-0.252802
H	5.184524	-0.365037	0.755123
H	5.888943	-1.583510	-0.346835
H	6.517287	0.083849	-0.331031
C	5.157690	-0.211139	-2.617183
H	6.074822	0.393038	-2.723407
H	5.416988	-1.253711	-2.898181
H	4.426109	0.165152	-3.345611

1Ge

150

-7631.439692030

C	2.6384781	1.8169166	17.1172252
C	1.7056303	2.7849514	16.6854797
C	0.8575634	3.3663829	17.6519719
C	0.9499771	3.0031571	19.0067005
C	1.8878763	2.0440107	19.4216095
C	2.7315706	1.4484854	18.4685250
C	1.6529605	3.1820142	15.2028245

C	0.2245093	3.5470382	14.7742652
C	-0.2044065	4.8788232	14.5967537
C	-1.5479100	5.1695621	14.3008764
C	-2.4850547	4.1331855	14.1668847
C	-2.0672400	2.7996929	14.3233520
C	-0.7269742	2.5122963	14.6228468
C	2.6910498	4.2477574	14.8301938
C	3.3063702	4.2405175	13.5404674
C	4.2153583	5.2901360	13.2061173
C	4.5034143	6.2866981	14.1578115
C	3.9206884	6.2962241	15.4373320
C	3.0130432	5.2666708	15.7456119
N	3.0201023	3.1887924	12.5966563
Si	4.0740884	1.7121808	12.6400310
C	5.3739044	1.9362988	14.0021835
C	4.8416255	5.3613958	11.8078763
C	6.2763570	5.9091346	11.8200490
C	6.5658458	7.2688432	11.5774495
C	7.8870962	7.7460305	11.6250125
C	8.9477472	6.8704377	11.9081296
C	8.6756678	5.5115370	12.1407885
C	7.3542927	5.0399662	12.0961226
C	4.2836433	7.3497266	16.4589864
C	4.9672321	1.4600667	10.9890134
C	3.0606667	0.1582774	13.0221642
Ge	1.5370913	3.6045601	11.4682499
Ge	1.4508648	1.3165167	9.9194409
N	-0.0334037	1.7313271	8.7923222
C	-0.3200436	0.6792729	7.8489904
C	-1.2287655	-0.3703163	8.1841229
C	-1.5172341	-1.3671597	7.2328414
C	-0.9352488	-1.3769630	5.9529920
C	-0.0278798	-0.3473978	5.6439148
C	0.2945841	0.6717232	6.5589267
C	-1.8544631	-0.4411401	9.5826418

C	-3.2893924	-0.9883628	9.5711369
C	-3.5790751	-2.3481545	9.8131146
C	-4.9004520	-2.8250084	9.7659792
C	-5.9610615	-1.9489754	9.4840327
C	-5.6887811	-0.5900277	9.2519276
C	-4.3672587	-0.1187940	9.2961085
C	-1.2987491	-2.4307354	4.9318092
C	1.3322447	1.7375795	6.1854309
C	1.2791942	2.1337450	4.7025470
C	2.1283617	1.5532792	3.7364576
C	2.0357989	1.9160166	2.3816001
C	1.0966378	2.8736933	1.9661728
C	0.2518311	3.4682757	2.9188694
C	0.3451792	3.1004457	4.2703079
Si	-1.0876918	3.2077207	8.7491385
C	-2.3881969	2.9829585	7.3877544
C	-1.9797517	3.4601121	10.4006775
C	-0.0749364	4.7617877	8.3657888
C	-0.9825554	-1.1859648	10.6035857
C	-0.0352536	-2.1628912	10.2327998
C	0.6699027	-2.8895178	11.2084705
C	0.4482726	-2.6452135	12.5727642
C	-0.4802480	-1.6613009	12.9563966
C	-1.1859115	-0.9406055	11.9810555
C	2.7608389	1.3733198	6.6141148
C	3.1907335	0.0416701	6.7903856
C	4.5343457	-0.2483511	7.0863657
C	5.4706808	0.7886104	7.2216501
C	5.0519224	2.1219260	7.0663285
C	3.7114991	2.4086230	6.7667926
C	3.9697791	6.1060523	10.7867969
C	3.0238169	7.0843745	11.1573812
C	2.3187923	7.8109162	10.1815881
C	2.5392171	7.5651738	8.8173387
C	3.4664156	6.5799516	8.4339266

C	4.1719685	5.8593103	9.4094138
H	-2.2354868	-2.1581859	7.4991884
H	0.4384577	-0.3274609	4.6464246
H	-2.0960319	-2.0673440	4.2473109
H	-1.6783174	-3.3538893	5.4129154
H	-0.4311739	-2.7042927	4.2978625
H	-1.9212586	0.6031437	9.9478040
H	0.1507864	-2.3565101	9.1661272
H	1.4028100	-3.6494298	10.8958876
H	1.0002627	-3.2141619	13.3365092
H	-0.6596430	-1.4588028	14.0238717
H	-1.9228232	-0.1817226	12.2890278
H	-2.7590518	-3.0419227	10.0538630
H	-5.1013789	-3.8905327	9.9583609
H	-6.9965640	-2.3214850	9.4523846
H	-6.5114211	0.1104929	9.0395750
H	-4.1664476	0.9492937	9.1168639
H	1.0671624	2.6466527	6.7614031
H	2.4629563	-0.7774407	6.6940730
H	4.8481885	-1.2956154	7.2171216
H	6.5225194	0.5613632	7.4533520
H	5.7769679	2.9437552	7.1738771
H	3.3935606	3.4548052	6.6317197
H	2.8817853	0.8153518	4.0515185
H	2.7094680	1.4488872	1.6462843
H	1.0277991	3.1616209	0.9058063
H	-0.4824795	4.2282441	2.6093640
H	-0.3190871	3.5767577	5.0086751
H	-2.6335351	2.6039075	10.6638894
H	-2.6220546	4.3639865	10.3365476
H	-1.2746426	3.6230211	11.2420514
H	0.6919809	4.9698574	9.1406373
H	-0.7516848	5.6419389	8.3346412
H	0.4388036	4.7008339	7.3847862
H	-1.9291821	2.8540345	6.3873953

H	-3.0445355	3.8781018	7.3516608
H	-3.0288296	2.0957052	7.5629703
H	5.2218642	7.0777443	13.8920421
H	2.5460269	5.2466178	16.7427798
H	5.0801277	6.9859329	17.1441989
H	4.6640270	8.2727927	15.9783562
H	3.4155729	7.6235488	17.0921429
H	4.9089705	4.3172122	11.4425449
H	2.8386783	7.2790607	12.2240212
H	1.5869283	8.5719046	10.4939984
H	1.9872918	8.1340294	8.0534798
H	3.6448576	6.3763492	7.3665015
H	4.9078785	5.0993925	9.1015973
H	5.7458265	7.9622493	11.3356612
H	8.0878508	8.8115264	11.4322947
H	9.9831516	7.2431960	11.9400573
H	9.4983479	4.8113507	12.3540859
H	7.1536475	3.9719072	12.2757304
H	1.9178054	2.2732211	14.6262888
H	0.5239743	5.6974925	14.6922027
H	-1.8609756	6.2169341	14.1691259
H	-3.5367950	4.3609967	13.9352842
H	-2.7929450	1.9783022	14.2169063
H	-0.4097704	1.4659998	14.7587556
H	0.1052732	4.1056509	17.3373373
H	0.2771123	3.4709745	19.7423154
H	1.9564641	1.7555624	20.4818510
H	3.4650254	0.6875378	18.7776539
H	3.3018715	1.3398590	16.3785572
H	5.6223131	2.3157032	10.7271591
H	5.6084044	0.5553770	11.0530072
H	4.2626985	1.2987043	10.1468776
H	2.2950082	-0.0499168	12.2460876
H	3.7372899	-0.7219213	13.0545897
H	2.5452877	0.2194496	14.0022879

H	4.9144934	2.0651360	15.0023647
H	6.0300540	1.0410216	14.0383738
H	6.0147986	2.8234568	13.8274159

TS1-2Ge

152

-7632.600558895

C	3.6061106	2.4034133	6.4762615
C	2.6889957	1.3284993	6.4452520
C	3.1597467	0.0406152	6.7747460
C	4.5083660	-0.1691179	7.1146316
C	5.4089425	0.9070154	7.1376428
C	4.9507411	2.1981773	6.8192711
C	1.2443646	1.5942421	5.9978336
C	1.1666315	1.7876510	4.4767786
C	1.9896516	1.0675819	3.5841226
C	1.8788327	1.2453240	2.1944526
C	0.9477120	2.1551199	1.6677836
C	0.1307866	2.8887435	2.5445170
C	0.2425869	2.7052264	3.9318386
C	0.2474547	0.5585210	6.5368669
C	-0.3016099	0.6971678	7.8564663
C	-1.1635840	-0.3385293	8.3362657
C	-1.4791192	-1.4303247	7.5023953
C	-0.9654823	-1.5611198	6.2026615
C	-0.0965638	-0.5520357	5.7465957
N	0.0028756	1.8513591	8.6539041
Si	-1.0014302	3.3251095	8.5257468
C	0.0814190	4.8322976	8.1272473
C	-1.7390634	-0.3067752	9.7575557
C	-0.9530677	-1.1594735	10.7678756
C	0.0313975	-2.0959497	10.3948917
C	0.6989035	-2.8682684	11.3638585
C	0.3965628	-2.7165483	12.7253227
C	-0.5817696	-1.7825956	13.1129916

C	-1.2456364	-1.0161599	12.1441148
C	-1.3534233	-2.7183299	5.3108872
Ge	1.6572656	1.7224259	9.6639646
C	-3.2365179	-0.6540897	9.7799775
C	-3.7011120	-1.9534274	10.0783534
C	-5.0735781	-2.2553633	10.0537859
C	-6.0133786	-1.2609801	9.7380432
C	-5.5668369	0.0392491	9.4474290
C	-4.1945947	0.3349109	9.4681078
C	-2.2794992	3.0852647	7.1464625
C	-1.9288152	3.7067313	10.1367299
Ge	1.5875690	3.7233884	11.5568888
N	3.1076291	3.2914605	12.6327602
Si	4.2576503	1.8848668	12.6179074
C	3.3528152	0.2345007	12.8215760
C	3.3475284	4.3096097	13.6286449
C	2.7170887	4.2275524	14.9078470
C	3.0097360	5.1918639	15.8896600
C	3.8972183	6.2576268	15.6534153
C	4.4837803	6.3455901	14.3782862
C	4.2259940	5.4035905	13.3641929
C	1.6842877	3.1287197	15.1870481
C	0.2782464	3.5090996	14.7029259
C	-0.1841280	4.8427866	14.6932405
C	-1.5101661	5.1434120	14.3385491
C	-2.3969918	4.1166130	13.9773730
C	-1.9452281	2.7857656	13.9660532
C	-0.6214498	2.4861728	14.3241989
C	4.8509984	5.5825321	11.9756254
C	3.9423674	6.3445852	11.0018160
C	3.0062809	7.3092383	11.4291950
C	2.2573160	8.0486222	10.4972078
C	2.4253666	7.8312553	9.1206762
C	3.3444069	6.8621401	8.6813779
C	4.0932210	6.1276357	9.6133105

C	4.2342939	7.2512686	16.7414433
C	1.6731294	2.6594551	16.6486529
C	2.5935257	1.6743476	17.0688106
C	2.6322872	1.2367192	18.4018240
C	1.7440373	1.7769689	19.3474352
C	0.8169437	2.7508036	18.9429753
C	0.7797846	3.1843900	17.6062726
C	5.4639544	2.0865909	14.0660771
C	5.2575907	1.8248956	11.0092582
C	6.2619392	6.1877708	12.0275193
C	6.5066353	7.5581999	11.7991801
C	7.8081816	8.0833805	11.8820271
C	8.8929740	7.2464002	12.1879858
C	8.6653004	5.8772373	12.4093831
C	7.3641171	5.3576948	12.3292699
H	-2.1660001	-2.2023517	7.8836014
H	0.3187644	-0.6256789	4.7294410
H	-2.1282975	-2.4142179	4.5739241
H	-1.7691006	-3.5635573	5.8941151
H	-0.4881734	-3.0947677	4.7279279
H	-1.6427308	0.7435646	10.1027485
H	0.2839864	-2.2196153	9.3319125
H	1.4646386	-3.5930740	11.0461545
H	0.9184414	-3.3211378	13.4829508
H	-0.8318686	-1.6547281	14.1779492
H	-2.0196402	-0.2965574	12.4547493
H	-2.9778747	-2.7384877	10.3467041
H	-5.4096280	-3.2772428	10.2897622
H	-7.0888439	-1.4958893	9.7241046
H	-6.2918180	0.8321071	9.2057244
H	-3.8582179	1.3573373	9.2376026
H	0.9603413	2.5636886	6.4539241
H	2.4588710	-0.8074856	6.7683971
H	4.8541030	-1.1834832	7.3676289
H	6.4639522	0.7437647	7.4058979

H	5.6480163	3.0503272	6.8355413
H	3.2571865	3.4157837	6.2165960
H	2.7379378	0.3662159	3.9837286
H	2.5323656	0.6714566	1.5189068
H	0.8644952	2.2984874	0.5794221
H	-0.5960038	3.6142235	2.1469517
H	-0.3981722	3.2915674	4.6091419
H	-2.6471305	2.9082462	10.4125768
H	-2.5035249	4.6504780	10.0225800
H	-1.2419298	3.8485574	10.9967775
H	0.8607803	5.0128061	8.8970006
H	-0.5452690	5.7481043	8.0862745
H	0.5929149	4.7305661	7.1479405
H	-1.8064204	2.8816243	6.1656654
H	-2.8980764	4.0019074	7.0462639
H	-2.9599444	2.2355921	7.3559683
H	5.1813453	7.1707774	14.1653697
H	2.5351001	5.0988696	16.8790646
H	5.0970064	6.9007841	17.3491166
H	4.5130319	8.2389065	16.3230333
H	3.3861874	7.3986506	17.4396440
H	4.9616177	4.5658175	11.5491043
H	2.8604444	7.4808516	12.5060561
H	1.5326747	8.7974006	10.8530837
H	1.8378235	8.4088663	8.3907476
H	3.4789879	6.6779919	7.6043224
H	4.8192993	5.3774339	9.2613613
H	5.6678776	8.2228098	11.5422865
H	7.9738928	9.1566279	11.6992582
H	9.9127443	7.6569069	12.2476472
H	9.5074350	5.2069991	12.6420196
H	7.1984864	4.2828176	12.5037394
H	1.9879291	2.2523629	14.5801623
H	0.5061336	5.6554019	14.9644227
H	-1.8497552	6.1908099	14.3395171

H	-3.4350960	4.3514738	13.6971095
H	-2.6311512	1.9745171	13.6772950
H	-0.2796403	1.4387939	14.3236440
H	0.0352401	3.9345273	17.2992434
H	0.1087783	3.1747767	19.6719559
H	1.7696300	1.4339181	20.3932069
H	3.3573597	0.4643168	18.7021099
H	3.2894408	1.2384813	16.3344507
H	5.9565319	2.6812206	10.9175244
H	5.8650177	0.8953305	10.9920979
H	4.6096686	1.8118749	10.1098359
H	2.7564341	-0.0469866	11.9302257
H	4.1101662	-0.5644921	12.9708376
H	2.6767464	0.2201478	13.7002829
H	4.9481409	2.0823282	15.0468994
H	6.1896158	1.2459531	14.0566030
H	6.0360944	3.0338522	14.0073854
H	1.0878203	0.6825671	10.9019785
H	0.9547146	1.6473415	11.3602495

IM2Ge

152

-7632.639125818

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C	2.8234569	1.3828874	6.7903573
C	3.2298587	0.0554842	7.0296029
C	4.5810566	-0.2530809	7.2764132
C	5.5498457	0.7608333	7.2911449
C	5.1552342	2.0928240	7.0689467
C	1.3773619	1.7788089	6.4467602
C	1.2794215	2.3326226	5.0155450
C	2.1160380	1.8725914	3.9754754
C	1.9807263	2.3646684	2.6660672
C	1.0108390	3.3360355	2.3697089
C	0.1785076	3.8120338	3.3966495

C	0.3137544	3.3134680	4.7022237
C	0.3571478	0.6634712	6.7035100
C	-0.4130202	0.6171357	7.9048192
C	-1.2848161	-0.5016457	8.1138917
C	-1.3991820	-1.4929567	7.1242860
C	-0.6711934	-1.4390700	5.9204140
C	0.2040597	-0.3558809	5.7418944
N	-0.3597461	1.6746225	8.8754199
Si	-1.5258775	3.0475935	8.7682753
C	-0.6222965	4.6893757	8.4869560
C	-2.0520811	-0.6465633	9.4351821
C	-1.1972582	-1.2754888	10.5435276
C	-0.2344814	-2.2729754	10.2798567
C	0.4667985	-2.8930668	11.3279921
C	0.2261369	-2.5197137	12.6603989
C	-0.7172694	-1.5154581	12.9366843
C	-1.4194789	-0.9000701	11.8876325
C	-0.8542717	-2.4912690	4.8509149
Ge	0.8330036	1.5157678	10.3429091
C	-3.4020616	-1.3633119	9.2860205
C	-3.5579024	-2.7465078	9.5163668
C	-4.8051812	-3.3721890	9.3453796
C	-5.9253600	-2.6252280	8.9475937
C	-5.7880882	-1.2442926	8.7258674
C	-4.5404509	-0.6244311	8.8952946
C	-2.6994865	2.7227454	7.3198619
C	-2.5162462	3.2051869	10.3767751
Ge	1.6582435	3.7041227	11.3975964
N	3.0886897	3.1833520	12.5892369
Si	4.0518680	1.6675047	12.6726823
C	2.9785810	0.1920431	13.1948191
C	3.4011541	4.2458683	13.5085923
C	2.7820633	4.3152149	14.7949718
C	3.1616991	5.3260924	15.6993581
C	4.1284444	6.2951154	15.3807557

C	4.7035430	6.2420372	14.0973519
C	4.3562252	5.2541890	13.1582026
C	1.6735306	3.3297098	15.1815840
C	0.2726166	3.8090432	14.7734794
C	-0.0390890	5.1647318	14.5448411
C	-1.3529988	5.5609090	14.2341101
C	-2.3780541	4.6073767	14.1440991
C	-2.0783997	3.2497904	14.3596502
C	-0.7678963	2.8582019	14.6683989
C	4.9615711	5.2922399	11.7489028
C	4.0847447	6.0602100	10.7487506
C	3.2267740	7.1106250	11.1367788
C	2.4887030	7.8300703	10.1802233
C	2.5917655	7.5089287	8.8177929
C	3.4386763	6.4598950	8.4180740
C	4.1754661	5.7450235	9.3741130
C	4.5590386	7.3393122	16.3853378
C	1.7260081	2.9272653	16.6626438
C	2.6487688	1.9461039	17.0873539
C	2.7431211	1.5718370	18.4367435
C	1.9123906	2.1758276	19.3961639
C	0.9873874	3.1504796	18.9891210
C	0.8933309	3.5194364	17.6358110
C	5.4223363	1.8867139	13.9637264
C	4.8459667	1.2729148	11.0000438
C	6.4134194	5.7899160	11.7233631
C	6.7454062	7.1381699	11.4714263
C	8.0838795	7.5674006	11.4825390
C	9.1195810	6.6541853	11.7376254
C	8.8048892	5.3059230	11.9785740
C	7.4666959	4.8823661	11.9698386
H	-2.0939338	-2.3306105	7.2933244
H	0.7842645	-0.2890849	4.8082969
H	-1.7685212	-2.2954106	4.2493146
H	-0.9694964	-3.5042520	5.2874097

H	0.0016899	-2.5143628	4.1481053
H	-2.2820609	0.3814677	9.7775579
H	-0.0300356	-2.5631503	9.2382230
H	1.2113773	-3.6714313	11.0994204
H	0.7765005	-3.0039197	13.4813966
H	-0.9094167	-1.2097801	13.9767779
H	-2.1658480	-0.1217991	12.1131595
H	-2.6937994	-3.3424036	9.8468371
H	-4.9008287	-4.4532986	9.5318405
H	-6.9031872	-3.1143895	8.8190013
H	-6.6597941	-0.6430213	8.4240002
H	-4.4468547	0.4596610	8.7245587
H	1.1121525	2.6079683	7.1343437
H	2.4819819	-0.7504869	7.0195220
H	4.8739437	-1.2990188	7.4578310
H	6.6069712	0.5188159	7.4799389
H	5.9048859	2.8995364	7.0811741
H	3.5094103	3.4409357	6.6425444
H	2.8956358	1.1278914	4.1973038
H	2.6455860	1.9888902	1.8726350
H	0.9082583	3.7255832	1.3451554
H	-0.5800152	4.5810143	3.1823472
H	-0.3429999	3.6971013	5.4978821
H	-3.1716689	2.3273903	10.5528269
H	-3.1663491	4.1042521	10.3302102
H	-1.8570325	3.3205535	11.2613311
H	0.0830614	4.9213941	9.3126296
H	-1.3596624	5.5189200	8.4438554
H	-0.0436428	4.7039622	7.5412474
H	-2.1598407	2.6458940	6.3549990
H	-3.4282541	3.5565516	7.2400487
H	-3.2688461	1.7807417	7.4465969
H	5.4614230	6.9911324	13.8191580
H	2.6914072	5.3469597	16.6950548
H	5.5185874	7.0556998	16.8700647

H	4.7218693	8.3263526	15.9067500
H	3.8099014	7.4663951	17.1915689
H	4.9802457	4.2432859	11.3913179
H	3.1302199	7.3637462	12.2031277
H	1.8239362	8.6450950	10.5063497
H	2.0124983	8.0701140	8.0686130
H	3.5250474	6.1977812	7.3520512
H	4.8366176	4.9247630	9.0527729
H	5.9450233	7.8608688	11.2506383
H	8.3176162	8.6247017	11.2819849
H	10.1682524	6.9893043	11.7410919
H	9.6071572	4.5761684	12.1694258
H	7.2325071	3.8217687	12.1530210
H	1.8594888	2.4088620	14.5929180
H	0.7565568	5.9214308	14.6105262
H	-1.5728589	6.6259407	14.0610545
H	-3.4062584	4.9165262	13.9012421
H	-2.8736569	2.4916555	14.2870696
H	-0.5421201	1.7941955	14.8426363
H	0.1530685	4.2734128	17.3279864
H	0.3264111	3.6271610	19.7298549
H	1.9819867	1.8828100	20.4550941
H	3.4685496	0.8008668	18.7399478
H	3.3055512	1.4662690	16.3447539
H	5.5623760	2.0609178	10.6898751
H	5.4094114	0.3188535	11.0733842
H	4.1075859	1.1573241	10.1820934
H	2.0634075	0.0821649	12.5789826
H	3.5586285	-0.7488869	13.0891416
H	2.6583237	0.2695895	14.2541278
H	5.0148726	2.0987732	14.9724043
H	6.0250070	0.9561305	14.0259298
H	6.1068963	2.7207838	13.7110574
H	1.6317430	0.2299873	9.9052671
H	2.1987501	2.7654459	9.9487923

Ts2-3Ge

152

-7632.638939184

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C	3.2654328	0.1479584	6.9521355
C	4.6187197	-0.1345116	7.2177066
C	5.5624273	0.9014853	7.2749432
C	5.1408677	2.2281601	7.0710085
C	1.3785353	1.8418023	6.3932155
C	1.2729656	2.4125233	4.9700604
C	2.1131482	1.9755694	3.9230256
C	1.9714567	2.4847240	2.6208375
C	0.9914735	3.4503982	2.3393289
C	0.1560405	3.9042047	3.3738459
C	0.2978787	3.3888502	4.6721506
C	0.3811613	0.7032428	6.6385554
C	-0.3725136	0.6216203	7.8502246
C	-1.2132700	-0.5211106	8.0533602
C	-1.3215364	-1.4966064	7.0463879
C	-0.6150774	-1.4052781	5.8326986
C	0.2359163	-0.3010364	5.6610020
N	-0.3284690	1.6680065	8.8321803
Si	-1.5250271	3.0093987	8.7772328
C	-0.6598473	4.6809058	8.5534165
C	-1.9532873	-0.7140729	9.3831469
C	-1.0923366	-1.4052254	10.4505308
C	-0.0642446	-2.3153072	10.1286915
C	0.6385836	-2.9961578	11.1389008
C	0.3303379	-2.7738427	12.4900502
C	-0.6815266	-1.8568156	12.8255696
C	-1.3822877	-1.1806071	11.8155159
C	-0.7936419	-2.4394567	4.7450298
Ge	0.9805914	1.5503861	10.2045008

C	-3.3134439	-1.4098785	9.2281375
C	-3.4733624	-2.8017757	9.3971205
C	-4.7272435	-3.4122595	9.2214353
C	-5.8503788	-2.6412965	8.8811816
C	-5.7088613	-1.2523857	8.7212526
C	-4.4541007	-0.6474826	8.8942419
C	-2.6927635	2.7087601	7.3190187
C	-2.5207440	3.0905835	10.3897838
Ge	1.4412663	3.5760665	11.6109765
N	2.9491219	3.0918834	12.7040339
Si	3.8769852	1.5520879	12.8120644
C	2.7478583	0.1134055	13.3109021
C	3.3430943	4.1880221	13.5521313
C	2.8016302	4.3104230	14.8717388
C	3.2501445	5.3400128	15.7180269
C	4.2139087	6.2809011	15.3090575
C	4.7078837	6.1763698	13.9975136
C	4.2889080	5.1643898	13.1114985
C	1.6962663	3.3561293	15.3410489
C	0.3019969	3.7942072	14.8720354
C	-0.0367703	5.1467807	14.6564881
C	-1.3467320	5.5141387	14.3005855
C	-2.3400902	4.5344498	14.1480458
C	-2.0130343	3.1813809	14.3486260
C	-0.7060099	2.8177087	14.7057951
C	4.8140806	5.1551287	11.6712890
C	3.9475985	5.9867637	10.7128447
C	3.1155120	7.0392888	11.1461365
C	2.3843964	7.8085508	10.2226287
C	2.4706335	7.5372752	8.8487765
C	3.2917505	6.4854736	8.4039552
C	4.0189218	5.7199056	9.3268211
C	4.7181931	7.3439470	16.2577822
C	1.7271183	3.0838474	16.8512429
C	2.6043936	2.1030310	17.3637547

C	2.6788701	1.8421058	18.7407482
C	1.8714327	2.5602654	19.6393902
C	0.9891833	3.5338970	19.1445450
C	0.9156352	3.7900642	17.7642112
C	5.2268310	1.7477624	14.1279603
C	4.7124857	1.1389715	11.1628606
C	6.2971926	5.5424526	11.5773417
C	6.7170961	6.8470075	11.2416127
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C	7.2894970	4.5757810	11.8514102
H	-1.9935842	-2.3533701	7.2109824
H	0.8020340	-0.2061079	4.7211700
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H	-0.9420524	-3.4549416	5.1646725
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H	0.1883429	-2.4929209	9.0726387
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H	-0.9274484	-1.6687624	13.8822217
H	-2.1821650	-0.4728962	12.0857829
H	-2.6059955	-3.4159689	9.6831103
H	-4.8262486	-4.5003655	9.3592440
H	-6.8335174	-3.1187391	8.7489882
H	-6.5826003	-0.6331133	8.4650385
H	-4.3569706	0.4427217	8.7718375
H	1.0953889	2.6571783	7.0901757
H	2.5370785	-0.6748504	6.9112154
H	4.9332059	-1.1772006	7.3807850
H	6.6211778	0.6803697	7.4797161
H	5.8712139	3.0514486	7.1135661
H	3.4709455	3.5462131	6.6430335
H	2.9005665	1.2358860	4.1340273

H	2.6391068	2.1269527	1.8214346
H	0.8840237	3.8535425	1.3205424
H	-0.6098435	4.6690421	3.1711757
H	-0.3601486	3.7557461	5.4748410
H	-3.1585666	2.1943258	10.5341448
H	-3.1875532	3.9784052	10.3760765
H	-1.8643960	3.1861406	11.2790899
H	0.0596247	4.8955486	9.3712164
H	-1.4133616	5.4968008	8.5588191
H	-0.1013949	4.7440989	7.5974753
H	-2.1519443	2.6820965	6.3521003
H	-3.4427165	3.5260108	7.2705340
H	-3.2372531	1.7481750	7.4104686
H	5.4591200	6.9026091	13.6494945
H	2.8393094	5.4019021	16.7379006
H	5.5221053	6.9445072	16.9138560
H	5.1419588	8.2113725	15.7141633
H	3.9134026	7.7132451	16.9249731
H	4.7356980	4.1067457	11.3186044
H	3.0345207	7.2585367	12.2209899
H	1.7402063	8.6249444	10.5847806
H	1.8982113	8.1382731	8.1256275
H	3.3642277	6.2610139	7.3282887
H	4.6583657	4.8969613	8.9705907
H	5.9639540	7.6129269	11.0016445
H	8.3855957	8.2023011	10.9298027
H	10.1270966	6.4634563	11.4335912
H	9.4073283	4.1257916	12.0156473
H	6.9853528	3.5482009	12.1056737
H	1.8894363	2.3858687	14.8417817
H	0.7367240	5.9215397	14.7667517
H	-1.5890959	6.5758957	14.1382181
H	-3.3652561	4.8210063	13.8678329
H	-2.7828046	2.4040056	14.2253021
H	-0.4588169	1.7565326	14.8677060

S

H	0.2072635	4.5439388	17.3885763
H	0.3449581	4.0977641	19.8371976
H	1.9252260	2.3561263	20.7198576
H	3.3687584	1.0689481	19.1133569
H	3.2391453	1.5310239	16.6684820
H	5.4808636	1.8919431	10.8928771
H	5.2227375	0.1558128	11.2435895
H	4.0054373	1.0724277	10.3125924
H	1.8482030	0.0291010	12.6689357
H	3.3011341	-0.8455760	13.2293635
H	2.4025897	0.2114898	14.3608916
H	4.8089510	1.9778337	15.1281631
H	5.8056339	0.8033468	14.2067491
H	5.9357065	2.5628119	13.8790963
H	1.8036883	0.3005172	9.7452231
H	2.0902642	2.8574667	9.8388450

IM3Ge

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-7632.648726485

C	2.0112879	1.1539048	17.0725607
C	1.3820848	2.3647037	16.7002381
C	0.5867360	3.0202651	17.6596508
C	0.4222611	2.4836566	18.9507369
C	1.0520702	1.2820113	19.3060559
C	1.8511685	0.6174046	18.3572526
C	1.5938694	2.8918053	15.2696972
C	1.0513616	1.8955818	14.2335109
C	-0.1257807	1.1488586	14.4615123
C	-0.6251762	0.2677483	13.4878898
C	0.0495199	0.1034327	12.2668244
C	1.2316562	0.8249957	12.0323252
C	1.7238571	1.7087927	13.0067237
C	1.0686920	4.3189521	15.0562302
C	1.9357005	5.4596226	15.1451331

C	1.3440496	6.7603315	15.0345232
C	-0.0356255	6.8856086	14.7812883
C	-0.8829344	5.7734848	14.6505208
C	-0.3036050	4.5019902	14.8048923
N	3.3537467	5.3116796	15.3013882
Si	4.4121533	5.1972426	13.8693202
C	5.4306096	3.5944759	13.9222245
C	2.1740019	8.0353953	15.2305632
C	2.0835049	8.6181354	16.6516107
C	1.1329103	8.2011292	17.6041530
C	1.0582949	8.8154918	18.8685284
C	1.9358644	9.8563344	19.2063000
C	2.8988736	10.2750532	18.2700507
C	2.9699444	9.6600108	17.0115994
C	-2.3509319	5.9311260	14.3268430
Ge	4.0372848	5.0200704	17.0751038
C	1.8573401	9.1091053	14.1770483
C	0.9196131	10.1378544	14.4156108
C	0.6170673	11.0872067	13.4248062
C	1.2537823	11.0352516	12.1741396
C	2.1978345	10.0250442	11.9255387
C	2.4927910	9.0752467	12.9168603
C	3.3414807	5.2300467	12.3083527
C	5.6646111	6.6230354	13.7882002
Ge	6.5834431	5.5751736	17.3544317
N	6.7651853	5.7062976	19.2387252
Si	5.5169379	5.7222747	20.5644666
C	4.3577324	7.2026676	20.3671364
C	8.1484419	5.8258359	19.6387381
C	8.7663755	7.1064795	19.7541076
C	10.0995750	7.1935447	20.1973512
C	10.8592006	6.0544669	20.5202610
C	10.2454018	4.7970556	20.3713147
C	8.9148901	4.6588089	19.9346715
C	8.0036894	8.3721334	19.3452168

C	8.0816843	8.6387480	17.8367363
C	9.2266272	8.3270534	17.0726406
C	9.2964121	8.6628481	15.7101513
C	8.2189149	9.3095242	15.0835308
C	7.0670396	9.6128881	15.8291271
C	6.9996973	9.2799036	17.1914318
C	8.3036005	3.2667159	19.7318132
C	8.3649546	2.8038276	18.2709702
C	9.4223200	3.1642108	17.4080867
C	9.4928492	2.6497179	16.1021746
C	8.5020370	1.7729895	15.6319051
C	7.4347570	1.4179993	16.4754614
C	7.3684592	1.9287089	17.7812336
C	12.2722080	6.1782445	21.0425321
C	8.3931862	9.6066126	20.1714384
C	7.8385955	9.7793151	21.4589505
C	8.1831748	10.8806197	22.2572965
C	9.0943433	11.8392398	21.7811387
C	9.6490893	11.6846791	20.5009559
C	9.2992236	10.5808698	19.7031525
C	6.4148989	5.8787548	22.2260893
C	4.5179454	4.1135867	20.5890695
C	8.8672571	2.2101954	20.6923884
C	9.8991636	1.3222755	20.3227768
C	10.4086741	0.3856497	21.2392011
C	9.8910954	0.3141802	22.5422389
C	8.8562941	1.1864899	22.9214507
C	8.3523799	2.1216499	22.0044806
H	-0.4620920	7.8949059	14.6705093
H	-0.9452892	3.6121083	14.7111501
H	-2.5398463	5.7820833	13.2413447
H	-2.7218039	6.9421482	14.5874806
H	-2.9720958	5.1868367	14.8653691
H	3.2322029	7.7359623	15.0865015
H	0.4368885	7.3880624	17.3523723

H	0.3029357	8.4736655	19.5933390
H	1.8736918	10.3398666	20.1933038
H	3.5944882	11.0913814	18.5205198
H	3.7122359	10.0087449	16.2760891
H	0.4287058	10.2057118	15.3984922
H	-0.1192277	11.8783571	13.6365809
H	1.0210844	11.7822853	11.3996513
H	2.7130744	9.9763083	10.9535175
H	3.2358397	8.2906017	12.7089034
H	2.6922194	2.9442054	15.1216326
H	0.0923271	3.9667477	17.3973972
H	-0.2048640	3.0157369	19.6832294
H	0.9233490	0.8623827	20.3157729
H	2.3528811	-0.3265931	18.6221606
H	2.6338673	0.6230081	16.3347066
H	-0.6493141	1.2457547	15.4250629
H	-1.5459071	-0.3015660	13.6903272
H	-0.3386675	-0.5909114	11.5057446
H	1.7800310	0.6962479	11.0861036
H	2.6562847	2.2610873	12.8140248
H	5.1775290	7.6161680	13.7113574
H	6.3188923	6.4999505	12.8987329
H	6.3294138	6.6477059	14.6773288
H	6.0832022	3.5460246	14.8192284
H	6.0965917	3.5355384	13.0353236
H	4.7922410	2.6871886	13.9277930
H	2.6143597	4.3947668	12.2824193
H	3.9881097	5.1526963	11.4090613
H	2.7562724	6.1677155	12.2286247
H	10.8170820	3.8883237	20.6160458
H	10.5546980	8.1907301	20.3049747
H	12.2820522	6.2593872	22.1514646
H	12.8863361	5.2946689	20.7774426
H	12.7778792	7.0820238	20.6478829
H	7.2257881	3.3603808	19.9719321

H	10.1969098	3.8597780	17.7644396
H	10.3268395	2.9427644	15.4457907
H	8.5549290	1.3728817	14.6079346
H	6.6471846	0.7392162	16.1142763
H	6.5344940	1.6367588	18.4391799
H	10.3029572	1.3558350	19.2995239
H	11.2135368	-0.2978893	20.9268828
H	10.2866203	-0.4226801	23.2581397
H	8.4341950	1.1354217	23.9371685
H	7.5385345	2.7976839	22.3115073
H	6.9342514	8.1785284	19.5619689
H	10.0713233	7.8092418	17.5511576
H	10.1995708	8.4109330	15.1328642
H	8.2716637	9.5696035	14.0153930
H	6.2143833	10.1135129	15.3449564
H	6.0955034	9.5275793	17.7703228
H	9.7295679	10.4815201	18.6952593
H	10.3577476	12.4327663	20.1126287
H	9.3646096	12.7060878	22.4035889
H	7.7332237	10.9932497	23.2559714
H	7.1208228	9.0361949	21.8411285
H	5.1518388	3.2413875	20.8502636
H	3.7288588	4.1937813	21.3664107
H	4.0089462	3.8830761	19.6321909
H	3.8774010	7.2443763	19.3702926
H	3.5454720	7.1413492	21.1217098
H	4.8875892	8.1633532	20.5297372
H	7.0154399	6.8077427	22.2929750
H	5.6647460	5.8965301	23.0448031
H	7.1053162	5.0325294	22.4140909
H	2.8986581	5.6123424	17.9610739
H	3.9692904	3.4653869	17.3114945

TS2-4Ge

-7632.630586180

C	3.5508362	2.5684983	7.2793051
C	2.7040351	1.5677027	6.7532806
C	3.2221143	0.2631418	6.6070177
C	4.5510498	-0.0293184	6.9570071
C	5.3864003	0.9770545	7.4683680
C	4.8786231	2.2765094	7.6322836
C	1.2827720	1.9400633	6.3102044
C	1.2408005	2.4767631	4.8708112
C	2.2119926	2.1449680	3.9038281
C	2.1234320	2.6415476	2.5909359
C	1.0648592	3.4854434	2.2210148
C	0.0940960	3.8315620	3.1771048
C	0.1845710	3.3318848	4.4848448
C	0.2869667	0.7998131	6.5528694
C	-0.3651287	0.6545550	7.8132514
C	-1.1948343	-0.4860521	8.0377250
C	-1.3888691	-1.4134732	6.9980641
C	-0.7875471	-1.2625995	5.7344560
C	0.0525707	-0.1520180	5.5416774
N	-0.2322926	1.6673128	8.8305399
Si	-1.4555417	3.0261582	8.8409745
C	-0.6022056	4.6824773	8.5178837
C	-1.8247502	-0.7237924	9.4155380
C	-0.8622270	-1.4061742	10.3976360
C	0.1632560	-2.2776171	9.9741049
C	0.9542560	-2.9671842	10.9103669
C	0.7378849	-2.7920503	12.2859508
C	-0.2677781	-1.9111309	12.7217941
C	-1.0564183	-1.2246887	11.7864915
C	-1.0630768	-2.2434355	4.6180760
Ge	1.1518827	1.5211842	10.0755308
C	-3.1722743	-1.4568682	9.3516495
C	-3.2759309	-2.8574188	9.4886909
C	-4.5218047	-3.5016689	9.3974420

C	-5.6911242	-2.7566095	9.1752249
C	-5.6043694	-1.3598710	9.0483101
C	-4.3577181	-0.7207839	9.1367997
C	-2.7058923	2.6907623	7.4627158
C	-2.3429987	3.0944107	10.5084442
Ge	1.5240915	3.5303165	11.5523180
N	3.0029382	3.1822295	12.7909377
Si	3.9129297	1.6701991	13.0018069
C	2.7750462	0.2391478	13.5128012
C	3.3161305	4.3373170	13.5811340
C	2.7019557	4.5455223	14.8611378
C	3.0940131	5.6368355	15.6585163
C	4.0574831	6.5707112	15.2387732
C	4.6126246	6.3937476	13.9599401
C	4.2602028	5.3160597	13.1256427
C	1.5773967	3.6269688	15.3573982
C	0.1713145	4.1503374	15.0183607
C	-0.0843092	5.4707354	14.5998624
C	-1.3960386	5.8993206	14.3207013
C	-2.4753460	5.0137913	14.4540106
C	-2.2334340	3.6909706	14.8691327
C	-0.9262600	3.2681613	15.1464188
C	4.8634925	5.2383041	11.7178674
C	4.1010126	6.0792690	10.6792536
C	3.0788637	6.9881189	11.0172746
C	2.4198319	7.7382151	10.0253249
C	2.7684145	7.5914785	8.6746826
C	3.7875111	6.6877664	8.3216972
C	4.4431602	5.9447717	9.3140206
C	4.4989453	7.7021170	16.1384537
C	1.6980851	3.2890536	16.8504263
C	2.5190427	2.2199310	17.2700432
C	2.6707707	1.9082990	18.6307192
C	2.0001534	2.6640957	19.6070009
C	1.1728521	3.7257381	19.2058573

C	1.0202107	4.0306822	17.8425948
C	5.2378797	1.9221828	14.3342095
C	4.7831568	1.1490944	11.3937733
C	6.3663227	5.5508159	11.7027626
C	6.8599905	6.8457147	11.4317607
C	8.2387052	7.1160005	11.4616056
C	9.1559145	6.0936051	11.7548240
C	8.6806544	4.7973451	12.0155895
C	7.3018588	4.5331356	11.9892506
H	-2.0479741	-2.2768490	7.1781128
H	0.5365527	-0.0081002	4.5627329
H	-2.0121299	-1.9956026	4.0946340
H	-1.1675167	-3.2793740	4.9989147
H	-0.2585916	-2.2346167	3.8565108
H	-2.0352622	0.2769182	9.8430435
H	0.3418800	-2.4199315	8.8977179
H	1.7467178	-3.6457159	10.5582327
H	1.3562884	-3.3321404	13.0189523
H	-0.4374937	-1.7563074	13.7982458
H	-1.8507472	-0.5460576	12.1358629
H	-2.3699372	-3.4515511	9.6824023
H	-4.5776098	-4.5957849	9.5087299
H	-6.6675481	-3.2607418	9.1095505
H	-6.5142398	-0.7615792	8.8851657
H	-4.3031761	0.3753729	9.0429188
H	0.9702659	2.7784043	6.9639716
H	2.5736367	-0.5370824	6.2204216
H	4.9341059	-1.0542624	6.8328108
H	6.4265738	0.7489572	7.7465543
H	5.5212263	3.0706440	8.0415341
H	3.1673463	3.5934017	7.4091512
H	3.0566436	1.4974723	4.1829491
H	2.8951022	2.3687814	1.8542091
H	0.9984656	3.8778544	1.1946045
H	-0.7375930	4.4996081	2.9041079

H	-0.5807987	3.6117680	5.2257011
H	-2.9609697	2.1914679	10.6909475
H	-3.0199494	3.9741597	10.5302099
H	-1.6363294	3.1992877	11.3573859
H	0.2060331	4.8873448	9.2504142
H	-1.3462632	5.5023675	8.6038520
H	-0.1618593	4.7348619	7.5014108
H	-2.2273420	2.6568082	6.4638006
H	-3.4596617	3.5060703	7.4540004
H	-3.2407593	1.7303894	7.5995044
H	5.3608706	7.1170585	13.5997051
H	2.6326606	5.7570246	16.6513401
H	5.3453323	7.3890830	16.7882312
H	4.8453473	8.5787174	15.5553321
H	3.6822628	8.0346556	16.8101122
H	4.7465731	4.1814916	11.3988548
H	2.7920100	7.1109958	12.0715898
H	1.6245533	8.4419073	10.3168055
H	2.2527896	8.1779721	7.8986967
H	4.0763169	6.5654179	7.2659286
H	5.2523931	5.2533128	9.0305106
H	6.1538138	7.6515128	11.1793297
H	8.5980972	8.1347545	11.2474185
H	10.2364082	6.3039690	11.7730949
H	9.3880069	3.9830338	12.2374509
H	6.9416571	3.5128503	12.1929715
H	1.6890809	2.6766504	14.7965346
H	0.7530098	6.1748689	14.4878585
H	-1.5701560	6.9368242	13.9947919
H	-3.5012506	5.3488740	14.2361667
H	-3.0711787	2.9840756	14.9757231
H	-0.7465486	2.2317664	15.4740777
H	0.3505832	4.8506728	17.5410668
H	0.6337721	4.3203570	19.9599988
H	2.1156270	2.4214080	20.6746452

H	3.3141614	1.0657650	18.9288400
H	3.0462309	1.6170534	16.5146864
H	5.5517053	1.8866189	11.0838951
H	5.2939597	0.1733014	11.5381890
H	4.0876701	1.0261046	10.5388863
H	1.9318484	0.1017582	12.8047804
H	3.3420437	-0.7151700	13.5374503
H	2.3353636	0.3970892	14.5191363
H	4.8009217	2.2019074	15.3132382
H	5.8175818	0.9850862	14.4714615
H	5.9490273	2.7266487	14.0587837
H	1.9553257	0.3219778	9.4457521
H	0.2803127	2.8881662	12.3634727

IM4Ge

152

-7632.644209768

C	3.1105262	1.5362512	16.9124813
C	1.9916770	2.2796488	16.4729036
C	0.9791816	2.5779164	17.4096541
C	1.0729893	2.1330509	18.7389543
C	2.1868147	1.3878113	19.1605922
C	3.2078520	1.0923950	18.2420155
C	1.8881424	2.6868245	14.9975460
C	1.2666344	1.5814240	14.1319767
C	0.3434257	0.6430399	14.6381805
C	-0.2191894	-0.3396274	13.8042812
C	0.1357172	-0.4075696	12.4479761
C	1.0616968	0.5154605	11.9316100
C	1.6187385	1.4957675	12.7665395
C	1.2129592	4.0532262	14.8203365
C	1.9682969	5.2580730	14.9992959
C	1.2794302	6.5071090	14.9425657
C	-0.0995869	6.5237959	14.6502609
C	-0.8424650	5.3525346	14.4322019

C	-0.1616543	4.1245783	14.5374824
N	3.3892296	5.1921620	15.1924255
Si	4.4790629	5.1520039	13.7520114
C	5.4954766	3.5528663	13.7138897
C	1.9932195	7.8313950	15.2395230
C	1.7529873	8.3486563	16.6690508
C	0.8193844	7.7783393	17.5558822
C	0.6100923	8.3257810	18.8358114
C	1.3330303	9.4525308	19.2530913
C	2.2808225	10.0224474	18.3830086
C	2.4883844	9.4729033	17.1102377
C	-2.3092714	5.4026272	14.0706591
Ge	4.1011351	4.8950151	16.9327815
C	1.6708453	8.9148474	14.1982686
C	0.6089519	9.8287925	14.3761528
C	0.3054569	10.7866732	13.3942784
C	1.0654028	10.8596706	12.2152742
C	2.1347092	9.9677446	12.0306150
C	2.4308230	9.0082889	13.0126289
C	3.4160167	5.2644661	12.1909771
C	5.7070001	6.5938221	13.8128626
Ge	5.8696384	6.5527021	17.7044116
N	6.5819992	6.2555953	19.4446198
Si	5.4926768	6.2966054	20.8853896
C	4.4774234	7.8964885	20.9242023
C	8.0029998	6.1895317	19.6372083
C	8.7586421	7.3940801	19.8156178
C	10.1335886	7.3223989	20.0975307
C	10.8141563	6.0944469	20.2023669
C	10.0708060	4.9232183	19.9847155
C	8.6917226	4.9402115	19.6935032
C	8.0838456	8.7607059	19.6387461
C	7.9800597	9.1682971	18.1635153
C	8.9919525	8.8695426	17.2262684
C	8.8978862	9.3148039	15.8971117

C	7.7844235	10.0609506	15.4761289
C	6.7639942	10.3568915	16.3952233
C	6.8615752	9.9126302	17.7245966
C	7.9774192	3.6160860	19.3969410
C	8.2174608	3.0982059	17.9675929
C	9.1494355	3.6694589	17.0796507
C	9.3585058	3.1216130	15.7998557
C	8.6369437	1.9935321	15.3837958
C	7.6907416	1.4226577	16.2549832
C	7.4834247	1.9725841	17.5276267
C	12.2807429	6.0428050	20.5645447
C	8.7058879	9.8657573	20.5043921
C	8.3542688	9.9511877	21.8699663
C	8.9118126	10.9311870	22.7049231
C	9.8378291	11.8541183	22.1884487
C	10.1922726	11.7863882	20.8320103
C	9.6291526	10.8040338	19.9980852
C	6.5561242	6.1829538	22.4460591
C	4.2634956	4.8558680	20.8246303
C	8.2993971	2.5329293	20.4386146
C	9.3615131	1.6190875	20.2614499
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C	8.9042325	0.5886683	22.4223688
C	7.8346662	1.4804250	22.6062817
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H	1.1653468	9.8845210	20.2515943
H	2.8596912	10.9042544	18.6994206

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-7633.791323302

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C	1.1673773	2.4131364	9.4055012
C	1.7259822	3.6853632	9.6156899
C	2.1285783	4.0738777	10.9031051
C	1.3280786	4.4899038	14.1286251
C	1.6923273	5.5034587	15.0787292
C	0.6476346	6.1836026	15.7763863
C	-0.6969495	5.8703153	15.4885324
C	-1.0649012	4.8974815	14.5479412
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C	0.9360922	7.2304198	16.8602667
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C	0.3302554	5.3858149	18.5827296
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C	0.3670352	5.8419320	20.9779324
C	0.7736811	7.1604836	20.7049341
C	0.9549600	7.5831957	19.3800402
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Ge	4.0867598	4.7928956	16.5478160
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C	-1.8397573	9.9298836	16.8984961
C	-1.2857384	10.9221163	16.0727220
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C	11.0913915	6.3922091	20.1053881
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C	8.8889243	5.3585284	20.4909975
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C	8.8742611	7.8117387	16.4184942
C	9.6039444	6.6539828	16.0822801
C	9.8841929	6.3382309	14.7398316
C	9.4398926	7.1750800	13.7057378
C	8.7037395	8.3301034	14.0256913
C	8.4233198	8.6401832	15.3643973
C	8.0601773	4.2608399	21.1720955
C	7.8432626	3.0273524	20.2841592
C	8.6936340	2.7025208	19.2075429
C	8.4865801	1.5327319	18.4535984
C	7.4246428	0.6699769	18.7632624
C	6.5678475	0.9832185	19.8346400
C	6.7774491	2.1479587	20.5849917
C	12.5672235	6.4768903	20.4199103
C	8.9569678	9.6599814	18.1662574
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C	9.7253338	12.3214530	18.8073191
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H	1.2463992	2.3493984	15.5816132
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H	5.7082976	0.4471458	14.3429294
H	4.7876291	2.3918694	13.0822194
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H	0.8530828	2.1042105	8.3966413
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H	10.4583364	5.4281736	14.5057439
H	9.6644479	6.9313269	12.6559271
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Si	4.4115133	5.2642670	13.8835537
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Si	5.4925864	6.0557639	20.7575857
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H	9.9282079	2.8242882	15.2474608
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H	6.9701309	3.0963713	22.0956254
H	7.1420608	8.4091002	19.5718869
H	9.8191929	7.4668216	17.3193291
H	10.0395903	8.3400125	14.9933906
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TS3-6-7Ge

154

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C	7.9724682	3.4422673	19.3840345
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IM6Ge

76

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78

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1Sn'

20

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TS1-2Sn'

22

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22

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C 3.1949779 -1.7479638 -0.0284602
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C -2.6846696 1.6997231 -0.0371960
H -2.8091450 1.8084653 -1.1328908
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C -4.1332641 -0.2283140 0.1394773
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H -4.1957029 -1.2733656 0.4765296

TS2-3Sn'

22

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H	4.8241776	0.6058442	-0.1399162
C	3.2422439	-1.5470976	-0.4083417
H	4.1806306	-1.6353554	-0.9888604
H	3.4173062	-2.0463730	0.5652450
H	2.4641032	-2.1125169	-0.9399461
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H	-1.7340196	1.9821709	0.8841550
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3Sn'

22

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H	4.2521850	0.5322809	1.0952619
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C	2.7640894	-1.5599272	0.1584306
H	3.5909774	-2.1153824	-0.3221376

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H	1.8257518	-2.0647704	-0.1206505
C	-2.7170843	1.3115444	0.8150684
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H	-4.6023916	-0.5244018	0.2770023
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TS2-4Sn'

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N	3.3246480	0.0520778	4.3843918
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H	5.0694508	0.6381916	5.4366262
C	2.6187620	-0.4550883	5.5468893
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C	1.0377308	0.5104395	-1.0076667
H	1.6496936	-0.3024804	-1.4464057
H	0.6533895	1.1145869	-1.8515095
H	1.6964509	1.1476503	-0.4052819
C	-1.0122665	-0.7718898	-0.9818510
H	-1.4648362	-0.1515100	-1.7782848
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4Sn'

22

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H -0.2766563 -0.3731914 -1.1217632

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TS4-5Sn'

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5Sn'

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H	-1.3298920	-0.2681208	-0.7332051
H	-2.3957392	1.5240958	1.5479307
H	-2.9701068	-0.1372372	1.2627706
H	-2.2830695	0.3196439	2.8491496

TS3-6-7

24

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N	2.7098188	-0.4265168	-0.3924404
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H	0.9216169	1.5860086	1.1671185
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6Sn'

11

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7Sn'

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H	1.8468518	0.2572211	-2.1727315
N	4.7032775	-0.0621153	-1.2693899
C	5.6559319	-0.5181432	-0.2647358
H	5.2524213	-0.3686430	0.7469286
H	5.9447575	-1.5863571	-0.3639809
H	6.5855858	0.0745535	-0.3396304
C	5.2273502	-0.2041406	-2.6221683
H	6.1517896	0.3922924	-2.7258780
H	5.4829981	-1.2481320	-2.9033186
H	4.5060932	0.1783303	-3.3584534