Electronic Supplementary Information

A DFT study of conjugated dienes polymerisation catalyzed by [Cp*ScR]+: Insights into the propensity for *cis*-1,4 insertion

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Computational Details

Scandium was represented with a Stuttgart–Dresden pseudopotential in combination with its polarized adapted basis set.[r1] Carbon and hydrogen atoms have been described with an all electron 6–311G(d,p) triple–ζ basis set.[r2] Calculations were carried out at the DFT level of theory using the hybrid functional B3PW91.[r3] Geometry optimisations were carried out without any symmetry restrictions, the nature of the *extrema* (*minimum*) was verified with analytical frequency calculations (298 K, 1 atm). For all transition states, the intrinsic reaction coordinate has been followed according to the IRC technique. All these computations have been performed with the Gaussian 03[r4] suite of programs. Population analysis were carried out to the NBO formalism. [r5]

[r1] M. Dolg, U. Wedig, H. Stoll, H. Preuss, *J. Chem. Phys.* **1987**, *86*, 866. J.M.L. Martin, A. Sundermann, *J. Chem. Phys.* **2001**, *114*, 3408.

[r2] A. D. McLeann, G. S. Chandler, *J. Chem. Phys.* **1980**, *72*, 5639. K. Raghavachari, J. S. Binkley, R. Seeger, J. A. Pople, *J. Chem. Phys.*, **1980**, *72*, 650. R. D. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.* **1971**, *54*, 724.

[r3] J. P. Perdew, Y. Wang, *Phys. Rev. B* **1992**, *45*, 13244. A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648.

[r4] Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al- Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004. .

[r5] A. E. Reed, L. A. Curtiss, F. Weinhold, *Chem. Rev.* **1988** *88* 899.

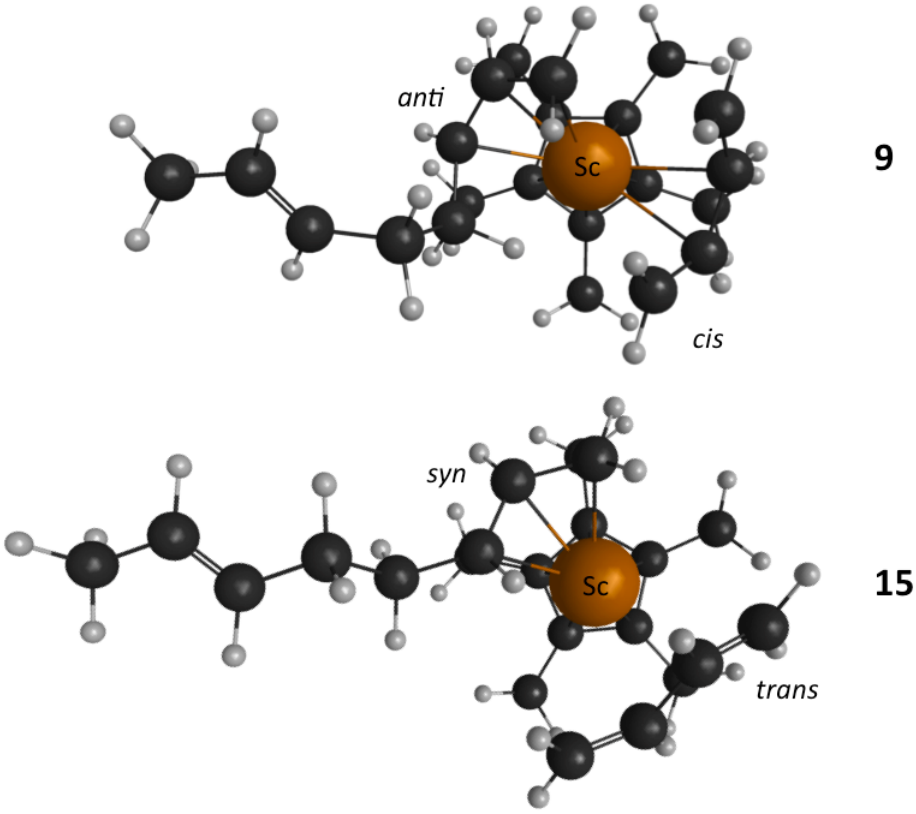

Figure S1: Structure of the adducts **9** and **15**

Cartesian coordinate (Å) and energy (Ha) of optimized stationary points

Monomers

trans-butadiene, C_4H_6

```
10
E : -155.971330
H : -155.880843
G : -155.912911
 C      0.008150      0.000000      0.074148
 C      0.022966      0.000000      1.410252
 C      1.232771      0.000000      2.214748
 C      1.247587      0.000000      3.550852
 H      0.929244      0.000000     -0.501947
 H     -0.920875      0.000000     -0.484772
 H     -0.920059      0.000000      1.954864
 H      2.175796      0.000000      1.670136
 H      0.326493      0.000000      4.126947
 H      2.176612      0.000000      4.109772
```

cis-butadiene, C_4H_6

```
10
E : -155.965833
H : -155.875400
G : -155.907720
 C     -0.112073     -0.117587      0.019784
 C      0.071045      0.095565      1.324190
 C      1.329143     -0.095548      2.050454
 C      2.550366      0.117586      1.556885
 H      0.686332     -0.493475     -0.612937
 H     -1.071949      0.063018     -0.451641
 H     -0.779155      0.416169      1.924603
 H      1.234351     -0.416134      3.086966
 H      2.699362      0.493523      0.549123
 H      3.438472     -0.063119      2.152573
```

Sc complexes

I

```
33
E : -515.872424
H : -515.569657
G : -515.634814
C      0.288353     -5.924889     -3.432653
C      1.049885     -7.129536     -3.558666
C      1.339111     -7.319073     -4.945068
C      0.767208     -6.228228     -5.672544
C      0.120343     -5.364747     -4.736712
C      1.587169     -7.949760     -2.423344
Sc    -1.034777     -7.449752     -4.707993
C      2.183194     -8.414952     -5.525115
C      0.906447     -5.985612     -7.147094
C     -0.544765     -4.058021     -5.056402
C     -0.158988     -5.305029     -2.141644
C     -2.759403     -8.702057     -4.839441
C     -2.015277     -9.572669     -3.847673
H     -2.946767     -9.203113     -5.792902
H     -3.704449     -8.317497     -4.447380
H     -2.503182     -9.674248     -2.875982
H     -1.758109    -10.567771     -4.216615
H     -0.979281     -9.167379     -3.542682
H      3.235009     -8.108861     -5.542087
H      2.129456     -9.334866     -4.938757
H      1.907917     -8.653847     -6.555179
H      1.819677     -5.414761     -7.347451
H      0.983378     -6.913964     -7.718221
H      0.075485     -5.405823     -7.555576
H      0.188871     -3.245375     -5.019846
H     -0.980679     -4.044897     -6.058246
H     -1.332211     -3.804886     -4.342658
H     -0.371397     -6.051693     -1.372731
H      0.630140     -4.657147     -1.744486
```

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H    -1.047952    -4.681726    -2.262751
H     0.918098    -7.956176    -1.560073
H     1.774464    -8.986008    -2.711709
H     2.542144    -7.533971    -2.083919
```

2

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43
E : -671.879011
H : -671.482917
G : -671.558671
Sc   -0.611437    -8.308485    -4.155095
C     1.437101    -7.237740    -3.401627
C     1.643487    -7.653786    -4.748321
C     0.760083    -6.900186    -5.581177
C    -0.006600    -6.038283    -4.750162
C     0.405115    -6.248986    -3.399992
C    -2.286649    -8.309343    -5.490602
H    -2.557217    -7.443090    -6.090320
H    -3.185479    -8.695145    -4.994330
C    -1.548328    -9.381199    -6.269224
H    -2.048606   -10.352031    -6.302801
H    -1.299931    -9.083902    -7.288744
H    -0.521639    -9.642388    -5.841759
C    -0.309509   -11.249646    -3.456269
H    -1.210256   -11.550696    -3.984915
H     0.607331   -11.766921    -3.716131
C    -0.342032   -10.331880    -2.472735
H     0.568688   -10.092584    -1.926534
C     2.268758    -7.651694    -2.224560
H     3.140164    -6.993899    -2.130837
H     1.727196    -7.584793    -1.277599
H     2.656593    -8.668740    -2.324168
C     2.696769    -8.612554    -5.221570
H     3.632191    -8.080977    -5.428815
H     2.926387    -9.377966    -4.475935
H     2.409903    -9.120844    -6.145091
C     0.737536    -6.916452    -7.077968
H     1.411866    -6.146414    -7.469080
H     1.073421    -7.870589    -7.489346
H    -0.255893    -6.703927    -7.479116
C    -0.970387    -4.988384    -5.209983
H    -1.784285    -4.833090    -4.498036
H    -0.455731    -4.027714    -5.325982
H    -1.416244    -5.235701    -6.174637
C    -0.031877    -5.415486    -2.230204
H    -1.105123    -5.207502    -2.239146
H     0.215844    -5.877243    -1.272480
H     0.476656    -4.445305    -2.253033
C    -1.550422    -9.596509    -2.103559
C    -1.543046    -8.514046    -1.304290
H    -2.493161    -9.945938    -2.525957
H    -2.457708    -7.981192    -1.068969
H    -0.631763    -8.168508    -0.826474
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3

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43
E : -671.868222
H : -671.472592
G : -671.545894
Sc   -0.728394    -8.093878    -3.870107
C     1.376148    -7.040848    -3.161111
C     1.598887    -7.620783    -4.442979
C     0.768808    -6.948518    -5.384922
C     0.014579    -5.960993    -4.679505
C     0.390268    -6.018905    -3.304758
C    -1.794856    -9.056056    -5.501454
H    -1.583783    -7.998785    -5.804042
H    -2.689326    -9.036149    -4.841342
C    -2.052033    -9.868863    -6.745831
H    -2.881006    -9.462446    -7.334351
H    -1.169299    -9.886810    -7.389729
H    -2.310258   -10.903137    -6.503123
C    -0.626196   -10.639032    -4.261241
H    -1.594657   -11.115712    -4.361095
H     0.104229   -10.917425    -5.012417
C    -0.215975   -10.168416    -3.021942
H     0.836583   -10.002352    -2.809635
C     2.182662    -7.323183    -1.929625
H     3.149367    -6.811475    -1.993224
H     1.697317    -6.958379    -1.021875
H     2.401502    -8.386301    -1.794678
C     2.644804    -8.641722    -4.772591
H     3.580496    -8.145773    -5.054262
H     2.876997    -9.290408    -3.924647
H     2.357090    -9.275512    -5.614780
C     0.809337    -7.134593    -6.871635
H     1.570590    -6.480818    -7.311349
H     1.066140    -8.158556    -7.151125
H    -0.138800    -6.882637    -7.352986
C    -0.916843    -4.956125    -5.293141
H    -1.727730    -4.668127    -4.618771
H    -0.372725    -4.038091    -5.541082
H    -1.366285    -5.318500    -6.220521
C    -0.085440    -5.089248    -2.227727
H    -1.101931    -4.730450    -2.407465
H    -0.065104    -5.551639    -1.238355
H     0.557625    -4.203408    -2.179898
C    -1.213227    -9.762926    -2.050245
C    -1.044739    -8.775231    -1.139278
H    -2.209549   -10.193773    -2.166441
H    -1.858730    -8.468820    -0.491961
H    -0.067435    -8.346145    -0.940607
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4

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43
E : -671.916261
H : -671.517661
G : -671.594426
Sc    0.084400    -8.131872    -3.814731
C     1.595582    -6.511180    -2.866992
C     2.163339    -6.990990    -4.087964
C     1.311061    -6.597972    -5.164075
C     0.200914    -5.895403    -4.609407
C     0.377073    -5.844856    -3.190793
C    -2.224791   -10.050515    -5.906504
H    -1.310180   -10.221473    -6.490611
H    -2.298243    -8.960484    -5.747367
C    -3.433982   -10.511175    -6.713621
H    -3.494969    -9.990690    -7.671923
H    -3.376047   -11.583381    -6.920439
H    -4.365456   -10.326048    -6.171485
C    -2.096406   -10.750504    -4.547800
H    -2.992810   -10.556798    -3.947973
H    -2.064523   -11.835247    -4.708287
C    -0.879449   -10.314505    -3.780439
H     0.087202   -10.639225    -4.203042
C     2.252828    -6.544339    -1.523012
H     2.931434    -5.690337    -1.419065
H     1.527887    -6.482455    -0.709953
H     2.847209    -7.447887    -1.373863
C     3.483644    -7.691028    -4.220248
H     4.290570    -6.956952    -4.321626
H     3.718277    -8.300559    -3.344533
H     3.529779    -8.334038    -5.102509
C     1.571139    -6.823397    -6.624700
H     2.141928    -5.984723    -7.038246
H     2.159248    -7.725469    -6.810220
H     0.649648    -6.894883    -7.207847
C    -0.906252    -5.241203    -5.383498
H    -1.841348    -5.195423    -4.819578
H    -0.634965    -4.208052    -5.626659
H    -1.108068    -5.745503    -6.331601
C    -0.521741    -5.141734    -2.218805
H    -1.559150    -5.105141    -2.560240
H    -0.506182    -5.610096    -1.232355
H    -0.196533    -4.103668    -2.087509
C    -0.863759    -9.871270    -2.469023
C     0.275505    -9.287395    -1.871478
H    -1.829135    -9.721218    -1.980761
H     0.225924    -8.917314    -0.854808
H     1.256019    -9.694963    -2.147220
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5

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37
E : -593.292201
H : -592.952928
G : -593.021616
C     0.757221    -1.219167    -1.740850
C     1.550169    -0.108677    -2.157820
C     2.404481     0.254110    -1.074739
C     2.152182    -0.647325     0.009037
C     1.133316    -1.552630    -0.402370
Sc    0.165537     0.639925    -0.370417
C     0.044824     1.236131     1.805266
C     0.542031     2.416271     1.208291
C    -0.023295     2.978180     0.076394
C     0.506152     4.175280    -0.658489
H     0.371704     4.091760    -1.741027
H     1.570324     4.319420    -0.458725
H    -0.015793     5.086555    -0.346729
H    -1.099145     2.772072    -0.079546
H    -1.048069     1.113761     1.831465
H     0.553062     0.807578     2.659836
H     1.542390     2.748505     1.486064
```

C	0.600144	-2.699718	0.402648
C	-0.242338	-1.953519	-2.586074
C	3.483743	1.293867	-1.108291
C	2.938110	-0.722525	1.280688
H	2.368319	-1.180698	2.090556
H	3.834547	-1.333889	1.128081
H	3.274817	0.259501	1.618828
H	3.669604	1.726624	-0.122917
H	4.425762	0.845857	-1.443373
H	3.254919	2.110001	-1.796489
C	1.531015	0.525419	-3.517300
H	1.866519	1.564402	-3.494087
H	2.207282	-0.011704	-4.191416
H	0.541329	0.499006	-3.981197
H	-1.035386	-2.415076	-1.992087
H	-0.709894	-1.309514	-3.335439
H	0.250868	-2.764176	-3.133725
H	-0.426043	-2.960089	0.131740
H	1.207962	-3.595033	0.231552
H	0.624724	-2.495954	1.475198

6

47
E : -749.295791
H : -748.862575
G : -748.938159

C	0.215555	0.404441	-0.225907
C	0.315389	-0.192024	1.061627
C	-0.968126	-0.111923	1.684272
C	-1.848799	0.557394	0.790313
C	-1.127357	0.846278	-0.408101
Sc	-0.165947	2.192172	1.435513
C	0.166918	3.760467	-0.530222
C	1.302109	4.068968	0.151796
C	1.498098	-0.969453	1.553963
C	-1.383121	-0.785418	2.954593
C	-3.320377	0.762936	1.001146
C	-1.749618	1.227836	-1.716235
C	1.291132	0.385610	-1.269874
C	0.848385	1.672913	3.534437
C	-0.274225	2.418016	3.873561
C	-0.506260	3.724101	3.440564
C	-1.175456	3.941474	-0.019355
C	-1.469325	4.629795	1.122908
C	0.938105	0.305545	4.008523
H	0.346699	4.369712	3.241774
H	-1.405010	4.234526	3.760082
H	-1.091420	1.886190	4.357377
H	-2.494704	4.700629	1.466239
H	-0.770677	5.326523	1.564560
H	-1.983485	3.495115	-0.585338
H	0.262108	3.268316	-1.491712
H	1.288624	4.683474	1.047577
H	2.276418	3.876256	-0.282473
H	-1.804902	-1.771213	2.727979
H	-0.548621	-0.949850	3.638379
H	-2.156550	-0.229545	3.490276
H	2.448144	-0.514481	1.262509
H	1.499034	-1.091227	2.638411
H	1.486863	-1.977131	1.123309
H	2.283548	0.576566	-0.852679
H	1.334544	-0.598779	-1.749697
H	1.114057	1.115181	-2.062211
H	-1.113287	1.863539	-2.337060
H	-1.946568	0.322419	-2.301093
H	-2.711915	1.728445	-1.590017
H	-3.885080	-0.098312	0.626568
H	-3.575463	0.874510	2.057538
H	-3.697894	1.643121	0.475169
H	1.584752	2.320827	3.061265
H	1.432043	0.289472	4.978929
H	-0.063125	-0.112029	4.103871
H	1.512781	-0.287747	3.298823

7

47
E : -749.292636
H : -748.859561
G : -749.932986

C	0.285120	0.438143	-0.250378
C	0.312537	-0.259759	0.992230
C	-0.963948	-0.107731	1.610307
C	-1.766614	0.709737	0.764978
C	-1.008315	1.016786	-0.403252
Sc	0.058436	2.118994	1.516027
C	0.582028	3.804723	-0.193704
C	1.775875	3.803398	0.480656
C	1.420218	-1.158672	1.453795
C	-1.461192	-0.836094	2.820828
C	-3.213401	1.039929	0.987151
C	-1.564995	1.607104	-1.661149
C	1.368018	0.402335	-1.286606
C	0.790588	1.453338	3.729957
C	-0.209402	2.375220	3.924946
C	-0.137153	3.748800	3.524809
C	-0.677761	4.056271	0.422732
C	-0.795897	4.651202	1.699522
C	0.562969	0.090538	4.169804
H	0.863706	4.175377	3.510445
H	-0.860330	4.396720	4.003756
H	-1.155442	2.013509	4.323144
H	-1.805070	4.864135	2.032665
H	-0.072970	5.413524	1.969663
H	-1.580692	3.842408	-0.136595
H	0.569131	3.443831	-1.216727
H	1.890949	4.321915	1.428684
H	2.694114	3.535527	-0.028769
H	-2.110554	-1.662914	2.512669
H	-0.649939	-1.275856	3.403336
H	-2.055480	-0.204256	3.486835
H	2.406110	-0.788708	1.161786
H	1.420349	-1.300312	2.536747
H	1.310908	-2.152293	1.005043
H	2.367301	0.403434	-0.844204
H	1.286800	-0.510124	-1.888026
H	1.308828	1.244317	-1.978886
H	-0.812157	2.119086	-2.264257
H	-1.976133	0.808608	-2.289083
H	-2.383464	2.305735	-1.472550
H	-3.855089	0.273041	0.538516
H	-3.469371	1.084905	2.048435
H	-3.496939	1.993508	0.534925
H	1.672067	1.952910	3.330778
H	0.951022	-0.034590	5.179595
H	-0.505575	-0.119432	4.162942
H	1.072511	-0.597874	3.497214

8

47
E : -749.316756
H : -748.881624
G : -749.959832

C	0.590311	0.416179	-0.348995
C	-0.194882	-0.341013	0.567121
C	0.041588	0.167605	1.879709
C	0.984140	1.235073	1.772314
C	1.320026	1.392097	0.397215
Sc	2.112090	-0.779196	1.092308
C	3.103118	-1.950941	-0.652653
C	3.891053	-0.799470	-0.502984
C	4.449519	-0.309845	0.677203
C	5.111904	-1.085982	1.814626
C	4.442127	-2.330222	2.435000
C	3.101562	-2.061128	3.064333
C	1.999892	-2.841731	3.046644
H	1.881743	-3.819281	2.577325
C	-1.167285	-1.421867	0.198517
C	-0.686098	-0.235251	3.128395
C	1.461699	2.104226	2.897718
C	2.155390	2.491674	-0.183629
C	0.541601	0.315755	-1.843014
H	4.394267	-3.156095	1.722701
H	5.106561	-2.676444	3.237522
H	3.054104	-1.161813	3.689170
H	5.304378	-0.372937	2.623728
H	6.103172	-1.399876	1.462956
H	4.833464	0.704558	0.606432
H	3.809244	-0.068888	-1.307367
H	3.306114	-2.836917	-0.047509
H	2.655008	-2.160965	-1.616634
H	-1.565931	0.402117	3.270630
H	-1.049370	-1.264534	3.085270
H	-0.073141	-0.126170	4.026956
H	-0.838014	-1.992689	-0.673161
H	-1.339598	-2.125144	1.017015
H	-2.140980	-0.987629	-0.054154
H	0.260507	-0.683329	-2.180996
H	-0.203208	1.013259	-2.242457
H	1.496878	0.570028	-2.307669
H	2.656918	2.189721	-1.105554
H	1.522280	3.350680	-0.432891
H	2.917295	2.845959	0.513267
H	0.811585	2.979814	3.004005
H	1.449820	1.584711	3.859140

H	2.474006	2.479461	2.729447
C	0.836466	-2.471632	3.828928
H	0.053578	-3.215640	3.689432
H	1.107809	-2.423367	4.882477
H	0.474239	-1.497933	3.502398

9

57
E : -905.296670
H : -904.767668
G : -904.855881

C	2.604577	0.140283	-0.484843
C	1.970993	-1.108693	-0.217471
C	1.127327	-1.423231	-1.318299
C	1.211868	-0.347308	-2.256509
C	2.108160	0.623438	-1.733813
Sc	0.166915	0.573495	-0.243270
C	1.160155	2.502435	0.971130
C	0.089798	3.239455	0.554345
C	2.275338	-2.024048	0.930579
C	0.501473	-2.763094	-1.557748
C	0.613069	-0.320590	-3.628391
C	2.574795	1.855483	-2.450807
C	3.810235	0.665669	0.231257
C	-1.807502	-0.477653	-1.123023
C	-2.013717	-0.965334	0.273176
C	-3.453956	-0.817443	0.833606
C	-4.397734	-1.773917	0.167880
C	-5.474078	-1.474951	-0.562454
C	-1.910645	0.851098	-1.511939
C	-1.908261	1.947075	-0.641940
C	1.081273	1.451083	1.965353
C	-0.076816	0.941027	2.460324
H	-1.718723	-2.016030	0.335116
H	-1.355462	-0.440166	1.024037
H	-1.758605	-1.226931	-1.900912
H	-2.321815	1.833605	0.356249
H	-1.987354	2.942569	-1.058359
H	-1.798930	1.056350	-2.575186
H	0.214785	3.991045	-0.216457
H	-0.823347	3.296952	1.130490
H	2.131213	2.697129	0.534322
H	2.017244	0.996681	2.270260
H	-1.034826	1.429808	2.310895
H	-0.059832	0.126477	3.175276
H	1.307082	-0.770585	-4.347513
H	-0.319269	-0.885114	-3.691817
H	0.417279	0.696974	-3.974862
H	0.056310	-3.190862	-0.655961
H	-0.263832	-2.735627	-2.334544
H	1.267515	-3.470791	-1.894262
H	1.417251	-2.643280	1.203089
H	3.090513	-2.708319	0.668681
H	2.591229	-1.481277	1.824226
H	3.831825	0.392109	1.288317
H	4.711909	0.233844	-0.217724
H	3.921106	1.749696	0.155408
H	3.391825	1.610868	-3.138910
H	1.782918	2.312993	-3.049102
H	2.955333	2.615905	-1.765324
H	-3.420974	-1.030981	1.909225
H	-3.794739	0.213635	0.723137
H	-4.169235	-2.827424	0.324185
C	-6.241884	-2.592401	-1.076536
H	-5.737811	-0.433846	-0.742637
H	-7.087719	-2.217883	-1.651185
H	-5.608775	-3.203097	-1.718519
H	-6.605808	-3.195464	-0.245997

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57
E : -905.293512
H : -904.765119
G : -904.851413

C	2.663658	0.178947	-0.489238
C	2.029511	-1.055574	-0.168650
C	1.185782	-1.415683	-1.259702
C	1.281658	-0.386833	-2.245443
C	2.174292	0.606938	-1.759017
Sc	0.240340	0.618440	-0.268109
C	1.005562	2.575592	0.754059
C	-0.200718	3.178604	0.337589
C	2.316598	-1.911783	1.029138
C	0.535903	-2.754408	-1.438867
C	0.708486	-0.421025	-3.628316
C	2.653972	1.803056	-2.526540
C	3.826545	0.781461	0.235383
C	1.059041	1.632005	1.823494
C	-0.042345	0.997133	2.333638
C	-1.794839	-0.287931	-1.264419
C	-2.028249	-0.892965	0.083724
C	-3.499133	-0.825366	0.578855
C	-4.386544	-1.730699	-0.222515
C	-5.437723	-1.385404	-0.968980
C	-1.798170	1.058094	-1.536380
C	-1.835088	2.108332	-0.559743
H	-1.714154	-1.939240	0.067004
H	-1.416533	-0.408924	0.889555
H	-1.737342	-0.967191	-2.105259
H	-2.351739	1.875321	0.367515
H	-2.114273	3.076139	-0.956808
H	-1.655939	1.352409	-2.574627
H	-0.116464	3.936742	-0.432507
H	-0.944673	3.401040	1.095048
H	1.930703	2.886121	0.284413
H	2.041244	1.298605	2.141721
H	-1.041162	1.402791	2.202021
H	0.064876	0.232551	3.093865
H	1.455941	-0.806131	-4.331281
H	-0.162623	-1.073952	-3.706529
H	0.423625	0.571549	-3.987457
H	0.228968	-3.199138	-0.489368
H	-0.336133	-2.719479	-2.095045
H	1.246080	-3.452637	-1.896160
H	1.448282	-2.501067	1.333751
H	3.122577	-2.621180	0.810170
H	2.634006	-1.323135	1.892440
H	3.915413	0.411472	1.258428
H	4.755828	0.509957	-0.277528
H	3.800767	1.874139	0.269499
H	3.476065	1.523041	-3.195123
H	1.872184	2.238820	-3.154189
H	3.034319	2.589206	-1.870600
H	-3.510179	-1.140700	1.629176
H	-3.857361	0.205511	0.551706
H	-4.135981	-2.789012	-0.161235
C	-6.148266	-2.463516	-1.628755
H	-5.722417	-0.337979	-1.057139
H	-6.978485	-2.053701	-2.202087
H	-5.469312	-2.989429	-2.298351
H	-6.530643	-3.157117	-0.881342

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57
E : -905.320893
H : -904.790468
G : -904.880758

C	2.861066	0.092406	-0.678260
C	2.162081	-0.941573	0.015740
C	1.156376	-1.451425	-0.857354
C	1.232958	-0.735343	-2.089473
C	2.282426	0.224896	-1.972345
Sc	0.569570	0.825835	-0.381930
C	1.149907	3.053971	0.348942
C	-0.038766	3.864266	-0.165397
C	-1.423905	3.214306	-0.375311
C	-1.428087	2.091053	-1.376535
C	-2.050651	0.895070	-1.292307
C	-2.931559	0.386737	-0.193516
C	-4.294541	-0.095160	-0.750357
C	-4.176091	-1.311482	-1.618920
C	-4.526139	-1.434354	-2.902563
C	2.519938	-1.496443	1.361263
C	0.242255	-2.604831	-0.565446
C	0.455047	-1.032975	-3.337159
C	2.759531	1.142865	-3.057957
C	4.082013	0.810599	-0.191145
C	1.211734	2.208796	1.457488
C	0.235158	1.295170	1.878963
H	-2.455151	-0.472569	0.301111
H	-3.096014	1.146610	0.573664
H	-1.977408	0.234109	-2.156667
H	-1.869721	2.909724	0.573008
H	-2.079901	4.000087	-0.771791
H	-0.912605	2.310967	-2.317674
H	0.264294	4.315167	-1.116560
H	-0.184362	4.706916	0.522848
H	2.096677	3.517553	0.084007
H	2.216170	2.030879	1.840302
H	-0.825053	1.526865	1.761015
H	0.458318	0.626760	2.702170
H	1.024859	-1.713260	-3.979960
H	-0.498286	-1.522425	-3.126691
H	0.252913	-0.137272	-3.930779

H	0.011307	-2.690430	0.499124
H	-0.701762	-2.534943	-1.111710
H	0.713075	-3.548063	-0.864204
H	1.655888	-1.923528	1.874367
H	3.261760	-2.295991	1.256185
H	2.954709	-0.739891	2.017659
H	4.128250	0.854638	0.898757
H	4.984161	0.286590	-0.526100
H	4.142833	1.831905	-0.573363
H	3.543000	0.656956	-3.650404
H	1.961627	1.414452	-3.753756
H	3.187792	2.064932	-2.658529
H	-4.927359	-0.329340	0.113449
H	-4.780516	0.730800	-1.275285
H	-3.785145	-2.196828	-1.117429
C	-4.346158	-2.739552	-3.508009
H	-4.921569	-0.576010	-3.443676
H	-4.667000	-2.704603	-4.548086
H	-3.294730	-3.019327	-3.461680
H	-4.941571	-3.474973	-2.968973

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47
E : -749.292986
H : -748.860664
G : -748.942111

Sc	-0.342417	1.060541	-0.926360
H	0.328854	-1.226784	1.978513
C	-0.678691	-1.461352	1.621354
C	-1.279766	-0.342170	0.820874
C	-2.082004	-0.507961	-0.294607
C	-2.579277	0.574091	-1.047963
H	-0.618680	-2.378078	1.030820
H	-1.285191	-1.681296	2.507173
H	-1.403891	0.608040	1.359499
H	-2.882084	1.472487	-0.500094
H	-3.158671	0.383183	-1.942590
H	-2.119147	-1.502094	-0.739338
C	-0.853436	3.999116	-0.886144
C	-0.567854	3.409739	0.289545
C	0.774679	2.986519	0.677456
C	1.035059	2.249008	1.769981
H	-1.866965	4.288184	-1.140637
H	-0.072602	4.256276	-1.595013
H	-1.371178	3.224956	1.002870
H	1.592920	3.300289	0.033516
H	0.253174	1.957914	2.465186
H	2.047565	1.954547	2.021602
C	1.438351	1.536014	-2.533077
C	1.797834	0.359612	-1.811270
C	0.852854	-0.658417	-2.129837
C	-0.096711	-0.108708	-3.043764
C	0.254988	1.249008	-3.279548
C	3.030067	0.171670	-0.976898
H	3.418163	1.117035	-0.591347
H	2.858998	-0.493877	-0.126601
H	3.829794	-0.279559	-1.574836
C	2.279284	2.770297	-2.665705
H	1.692321	3.667956	-2.874413
H	2.894217	2.961206	-1.783091
H	2.973056	2.653536	-3.505939
C	-0.424490	2.163621	-4.254761
H	-0.187749	3.213919	-4.072176
H	-0.100526	1.938718	-5.276995
H	-1.512066	2.056530	-4.234499
C	-1.162149	-0.871476	-3.767492
H	-0.744853	-1.330257	-4.671137
H	-1.578934	-1.680896	-3.164427
H	-1.985431	-0.228442	-4.083475
C	0.953763	-2.098238	-1.726112
H	1.407048	-2.224578	-0.740529
H	-0.018489	-2.594498	-1.716260
H	1.581572	-2.643415	-2.440156

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47
E : -749.267082
H : -748.834952
G : -748.910874

Sc	-0.046525	1.180893	-0.771857
H	0.032872	-1.002940	2.341633
C	-0.842237	-1.345769	1.778487
C	-1.533130	-0.225185	1.072414
C	-1.905207	-0.236865	-0.239951
C	-2.581804	0.860441	-0.912237
H	-0.533951	-2.137947	1.093738
H	-1.519595	-1.787749	2.518572
H	-1.883117	0.594460	1.698709
H	-3.436814	1.219795	-0.353904
H	-2.828293	0.689121	-1.955354
H	-1.602784	-1.090821	-0.844776
C	-1.952576	2.925529	-0.662993
C	-0.976405	3.062444	0.343344
C	0.388910	3.366688	0.046689
C	1.454950	2.780977	0.666909
H	-2.988240	3.132483	-0.438300
H	-1.680140	3.225637	-1.677222
H	-1.241089	2.859051	1.378011
H	0.588481	3.962090	-0.846676
H	1.315333	2.180660	1.568018
H	2.473145	3.047330	0.415375
C	1.767172	1.403220	-2.390131
C	1.938554	0.150946	-1.734384
C	0.840687	-0.685932	-2.094056
C	-0.021964	0.055973	-2.951853
C	0.540087	1.356658	-3.115483
C	3.131154	-0.277385	-0.932190
H	3.622369	0.564073	-0.439678
H	2.870546	-1.008826	-0.162889
H	3.877247	-0.752071	-1.579386
C	2.775425	2.507534	-2.467534
H	2.323476	3.502894	-2.447256
H	3.511925	2.451897	-1.664742
H	3.327328	2.435503	-3.411412
C	0.030398	2.430065	-4.032079
H	0.299257	3.432842	-3.689611
H	0.462407	2.314025	-5.032395
H	-1.055037	2.394645	-4.149875
C	-1.182585	-0.499677	-3.718082
H	-0.820491	-1.056931	-4.589104
H	-1.791133	-1.195029	-3.132965
H	-1.840045	0.285378	-4.096231
C	0.733557	-2.149602	-1.788364
H	1.101806	-2.399521	-0.790356
H	-0.289039	-2.523458	-1.878149
H	1.338919	-2.722757	-2.499697

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47
E : -749.308649
H : -748.873738
G : -749.949443

Sc	0.342820	0.965893	-0.541858
H	-0.568670	-1.801034	0.898162
C	-1.566108	-1.619462	0.479159
C	-2.011945	-0.196212	0.614954
C	-2.537301	0.579249	-0.355064
C	-3.177121	1.920655	-0.106976
H	-1.588836	-1.965969	-0.553851
H	-2.241128	-2.257126	1.061483
H	-2.041931	0.188679	1.636601
H	-3.458446	1.985926	0.948862
H	-4.103847	1.987115	-0.684344
H	-2.582601	0.183476	-1.370875
C	-2.257552	3.113760	-0.441919
C	-0.928285	2.876571	0.209364
C	0.325847	3.330822	-0.135931
C	1.478155	2.719133	0.409379
H	-2.733118	4.032932	-0.079251
H	-2.147813	3.227774	-1.525532
H	-0.990457	2.403708	1.198307
H	0.438314	3.953450	-1.023691
H	1.398062	2.348848	1.440024
H	2.463307	3.080622	0.146260
C	1.930946	1.333876	-2.362725
C	2.334976	0.157495	-1.672044
C	1.324013	-0.834431	-1.859499
C	0.279416	-0.258735	-2.638289
C	0.646371	1.092906	-2.929159
C	3.649184	-0.055871	-0.982463
H	4.030695	0.861961	-0.530333
H	3.585748	-0.813433	-0.197292
H	4.403890	-0.403795	-1.696772
C	2.775518	2.544025	-2.604562
H	2.197650	3.471235	-2.611851
H	3.570830	2.646068	-1.865170
H	3.257501	2.464070	-3.585418
C	-0.101934	2.024718	-3.835976
H	0.149536	3.070542	-3.647711
H	0.148266	1.820656	-4.883227
H	-1.186140	1.919064	-3.743890
C	-0.865056	-0.990115	-3.273472
H	-0.554598	-1.379287	-4.249810
H	-1.202881	-1.847931	-2.688915

H	-1.726080	-0.343020	-3.457033
C	1.446219	-2.272178	-1.448792
H	1.865760	-2.394695	-0.445884
H	0.491207	-2.797704	-1.481593
H	2.122528	-2.795785	-2.133611

15

57
E : -905.298380
H : -904.771136
G : -904.865249

C	0.236787	1.199855	-3.286747
C	1.430996	1.465452	-2.549121
C	1.757475	0.292802	-1.806037
C	0.780656	-0.701834	-2.101510
C	-0.155115	-0.141292	-3.023087
Sc	-0.355427	1.075062	-0.924798
C	0.808556	3.035919	0.617598
C	1.056853	2.326168	1.731007
C	2.308284	2.670917	-2.708723
C	2.985206	0.085290	-0.969641
C	0.835984	-2.136222	-1.670419
C	-1.244425	-0.887637	-3.727928
C	-0.415192	2.114082	-4.280952
C	-2.120947	-0.434699	-0.236567
C	-2.603125	0.629043	-1.024374
C	-0.527860	3.464245	0.214295
C	-0.803746	4.020199	-0.979973
C	-1.307941	-0.244860	0.868526
C	-0.729489	-1.348666	1.709454
H	0.281686	-1.086813	2.046751
H	-0.625709	-2.254475	1.103836
C	-1.590935	-1.673861	2.948029
H	-1.417712	0.723892	1.379141
H	-2.885056	1.551903	-0.506753
H	-3.188895	0.419504	-1.910664
H	-2.173285	-1.442426	-0.648405
H	-1.812660	4.315040	-1.245852
H	-0.017918	4.243044	-1.694806
H	-1.334367	3.312878	0.931887
H	1.632308	3.323075	-0.031650
H	0.269074	2.061915	2.430137
H	2.065018	2.026818	1.993981
H	3.405811	1.027164	-0.610758
H	2.794016	-0.550409	-0.101080
H	3.767321	-0.408693	-1.556953
H	1.747969	3.580541	-2.938128
H	2.927730	2.863686	-1.829583
H	2.998748	2.514939	-3.545286
H	-0.156382	3.161704	-4.113400
H	-0.089162	1.865877	-5.297166
H	-1.504938	2.031560	-4.266957
H	-0.842290	-1.381621	-4.619853
H	-1.685352	-1.668448	-3.104738
H	-2.047330	-0.227015	-4.059644
H	1.327614	-2.261475	-0.703521
H	-0.155712	-2.588528	-1.604122
H	1.406020	-2.723742	-2.399252
C	-0.986530	-2.746317	3.802413
H	-1.720040	-0.755986	3.538495
H	-2.591335	-1.974122	2.618729
C	-1.536622	-3.938523	4.026310
H	-0.025297	-2.514368	4.263679
C	-0.950664	-5.016680	4.878035
H	-2.501077	-4.159342	3.566920
H	-0.804116	-5.936976	4.301959
H	0.011967	-4.720944	5.301568
H	-1.623534	-5.270650	5.704361

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57
E : -905.272855
H : -904.745822
G : -904.835487

C	0.518613	1.262231	-3.120208
C	1.753796	1.298808	-2.408524
C	1.886834	0.074287	-1.694012
C	0.756004	-0.738561	-2.003758
C	-0.088559	-0.007556	-2.888025
Sc	-0.048789	1.219888	-0.761758
C	0.462692	3.434553	-0.079245
C	1.507351	2.845669	0.574134
C	2.800557	2.361112	-2.543868
C	3.072225	-0.358444	-0.883316
C	0.600074	-2.181285	-1.627704
C	-1.275807	-0.556444	-3.616989
C	0.040025	2.304376	-4.088071
C	-1.946586	-0.096768	-0.137929
C	-2.601180	0.976247	-0.865964
C	-0.912020	3.199218	0.234979
C	-1.894510	3.034589	-0.760651
C	-1.549929	-0.012079	1.165913
C	-0.876728	-1.103342	1.935384
H	0.023667	-0.718651	2.434107
H	-0.556662	-1.907016	1.265414
C	-1.804482	-1.693681	3.024937
H	-1.878762	0.850257	1.746463
H	-3.430161	1.402905	-0.315792
H	-2.871080	0.753911	-1.893346
H	-1.668386	-0.990990	-0.695015
H	-2.922436	3.289167	-0.549750
H	-1.613721	3.259969	-1.791722
H	-1.180542	3.065323	1.279879
H	0.681978	3.966977	-1.006856
H	1.346160	2.304567	1.508556
H	2.534381	3.058973	0.308556
H	3.594602	0.486494	-0.430179
H	2.795233	-1.048180	-0.082021
H	3.797101	-0.883269	-1.515789
H	2.384052	3.371604	-2.575488
H	3.535490	2.321270	-1.738672
H	3.348591	2.220595	-3.482292
H	0.369207	3.309883	-3.813432
H	0.438898	2.105986	-5.089257
H	-1.048638	2.319457	-4.178971
H	-0.942900	-1.159538	-4.469001
H	-1.896830	-1.208319	-2.996293
H	-1.913637	0.233141	-4.018677
H	0.968101	-2.396934	-0.621780
H	-0.436091	-2.521744	-1.690348
H	1.177206	-2.808797	-2.316328
C	-1.118746	-2.745999	3.841412
H	-2.143173	-0.876622	3.675380
H	-2.697669	-2.108682	2.547189
C	-1.483060	-4.026543	3.884670
H	-0.268446	-2.416170	4.439771
C	-0.824551	-5.085384	4.706469
H	-2.340832	-4.342869	3.289545
H	-0.470756	-5.909108	4.076839
H	0.025985	-4.692884	5.268382
H	-1.532886	-5.521150	5.419432

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57
E : -905.315285
H : -904.785592
G : -904.875581

C	0.481016	0.635288	-2.678761
C	1.789524	1.064372	-2.317168
C	2.318219	0.130162	-1.382785
C	1.354766	-0.906842	-1.202955
C	0.216850	-0.597737	-2.004932
Sc	0.376795	1.141294	-0.311628
C	0.406735	3.530144	-0.546016
C	1.563472	3.051663	0.118326
C	2.540774	2.195405	-2.944492
C	3.696671	0.152673	-0.794686
C	1.591311	-2.179121	-0.444348
C	-0.920130	-1.524576	-2.317127
C	-0.392122	1.263286	-3.724599
C	-2.432187	0.909429	0.039542
C	-3.109985	2.247385	-0.096238
C	-0.846006	3.246606	-0.052792
C	-2.185654	3.320085	-0.721827
C	-1.834465	0.489384	1.172361
C	-1.208690	-0.849200	1.425177
H	-0.141675	-0.742993	1.702031
H	-1.246970	-1.473025	0.529956
C	-1.891941	-1.594430	2.596904
H	-1.883403	1.148710	2.042015
H	-3.416116	2.588202	0.897769
H	-4.021217	2.144726	-0.691497
H	-2.453347	0.241117	-0.822914
H	-2.655748	4.301884	-0.589072
H	-2.089705	3.164289	-1.801057
H	-0.888938	3.073981	1.028637
H	0.505021	3.870936	-1.576414
H	1.508884	2.989822	1.213259
H	2.546364	3.304212	-0.257258
H	4.081496	1.168878	-0.691867
H	3.735064	-0.319493	0.190313
H	4.395304	-0.396092	-1.436408
H	1.888732	3.017641	-3.247282
H	3.313699	2.598157	-2.288224

H	3.043295	1.842743	-3.852337
H	-0.239172	2.342340	-3.797688
H	-0.168984	0.842943	-4.711783
H	-1.455227	1.088657	-3.540130
H	-0.647720	-2.168104	-3.161485
H	-1.171767	-2.189321	-1.488073
H	-1.827824	-0.993452	-2.613651
H	2.176999	-2.022418	0.465537
H	0.664651	-2.682769	-0.165071
H	2.161470	-2.879036	-1.065744
C	-1.230379	-2.902238	2.907034
H	-1.876197	-0.944300	3.480972
H	-2.943467	-1.752532	2.338126
C	-1.808065	-4.093732	2.757672
H	-0.212180	-2.851667	3.295029
C	-1.179172	-5.407185	3.086322
H	-2.832100	-4.130432	2.383778
H	-1.159681	-6.064205	2.210053
H	-0.156633	-5.289234	3.451938
H	-1.757820	-5.931580	3.854313