Computational details

All computations were carried out using the TPSSTPSS functional as implemented in the GAUSSIAN 09 software package.[S1] All atoms were modeled at the 6-31G(d,p) level of theory.[S3] Geometry optimizations were performed with the account of the solvent effects (SMD, toluene) without applying any geometry constraints (C1 symmetry).

Starting geometries for the transition state search were located by QST3 procedure. The transition states were subsequently fully optimized as saddle points of first order, employing the Berny algorithm.S5 Geometries of the starting points and reaction products were optimized independently. Frequency calculations were carried out to confirm the nature of the stationary points, yielding zero imaginary frequencies for all minima and one imaginary frequency for all transition states, which represented the vector for the C−C bond formation.

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Cartesian coordinates

TS*R*(*d*)

$\nu = i244.52$

Sum of electronic and zero-point Energies= -10299.139735 a.u.

Sum of electronic and thermal Energies= -10299.035896 a. u.

Sum of electronic and thermal Enthalpies= -10299.034952 a. u.

Sum of electronic and thermal Free Energies= -10299.282925 a. u.

1 8 0 3.383314 -3.800761 -5.404935

2 14 0 1.641617 -7.877655 -8.085334

3 14 0 1.397854 -5.294745 -9.742746

4 14 0 4.659093 -4.498337 -6.187697

5 14 0 5.156555 -10.002215 -5.138589

6 14 0 4.494129 -7.507983 -6.761220

7 8 0 5.787702 -7.790660 -7.706131

8 8 0 3.152697 -7.349817 -7.684504

9 14 0 4.189549 -6.065140 -11.035605

10 14 0 4.698917 -11.375524 -10.058601

11 14 0 3.628328 -8.942475 -11.780240

12 8 0 4.282517 -12.904012 -10.523542

13 14 0 7.342467 -7.863431 -8.257222

14 14 0 9.114335 -12.138923 -7.188438

15 14 0 7.759478 -10.776629 -9.558712

16 8 0 9.586340 -13.716770 -6.967070

17 8 0 8.719665 -11.869166 -8.757421

18 8 0 6.292007 -11.502637 -9.688237

19 8 0 7.678956 -9.412510 -8.673840

20 8 0 4.714052 -6.131109 -5.887535

21 8 0 4.246310 -8.751759 -5.701927

22 8 0 0.627575 -7.910024 -6.784107

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24 8 0 4.405123 -10.306032 -11.259260

25 8 0 4.176980 -7.688993 -10.823296

26 8 0 1.997735 -9.112802 -11.646877

27 8 0 4.038425 -8.675262 -13.349394

28 8 0 2.724285 -5.391368 -10.696915

29 8 0 0.989704 -6.752683 -9.100637

30 8 0 1.836774 -4.178785 -8.578514

31 8 0 0.099350 -4.680383 -10.541757

32 8 0 7.313758 -4.617163 -3.175887

33 14 0 8.320264 -5.685695 -3.918951

34 14 0 7.630715 -8.836036 -3.749849

35 14 0 10.652879 -9.058520 -4.367814

36 14 0 11.740064 -11.456889 -5.751897

37 8 0 11.574203 -10.420226 -4.469303

38 8 0 10.425663 -11.251691 -6.757585

39 8 0 13.145124 -10.984175 -6.474559

40 8 0 9.130781 -9.489399 -3.875320

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42 8 0 7.671671 -7.215840 -3.843435

43 8 0 6.750224 -9.536550 -4.964753

44 8 0 7.811484 -11.812110 -6.202514

45 8 0 11.793695 -13.025870 -5.252432

46 8 0 1.710079 -9.325069 -8.875679

47 8 0 4.570600 -10.542733 -3.703859

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55 8 0 7.558459 -6.806504 -9.478041

56 8 0 10.653283 -8.213295 -5.765664

57 8 0 4.423782 -4.190756 -7.805714

58 8 0 3.868723 -10.860674 -8.705634

59 1 0 3.414655 -12.980644 -10.955329

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62 1 0 1.695292 -9.189869 -10.708680

63 1 0 4.298765 -7.742796 -13.497580

64 1 0 -0.439903 -5.330379 -11.024942

65 1 0 13.466094 -11.568750 -7.182237

66 1 0 6.915256 -4.337758 -5.866385

67 1 0 5.054423 -4.904549 -9.253048

68 1 0 8.294732 -6.705460 -6.519365

69 1 0 4.671468 -4.976139 -12.979131

70 1 0 10.311772 -6.464053 -3.137966

71 1 0 9.219761 -4.824016 -5.939619

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79 6 0 12.237645 -4.597818 -8.282256

80 6 0 12.761988 -3.353850 -7.882091

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87 1 0 11.030527 0.534585 -3.137198

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93 1 0 7.806857 0.228661 -5.107476

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96 1 0 8.565657 -2.233458 -2.307095

97 1 0 8.640760 -0.630926 -1.529395

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99 1 0 13.664355 -4.941549 -9.891962

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117 1 0 12.519215 -10.901999 -11.503539

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131 1 0 7.067700 -8.920133 -1.542094

132 1 0 7.827589 -10.948745 -5.731918

133 1 0 4.304877 -11.026446 -7.823828

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TS*S*(*d*)

$\boldsymbol{\nu}$ = *i*186.72

Sum of electronic and zero-point Energies= -10299.153760 a. u.

Sum of electronic and thermal Energies= -10299.051946 a. u.

Sum of electronic and thermal Enthalpies= -10299.051001 a. u.

Sum of electronic and thermal Free Energies= -10299.292518 a. u.

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2 14 0 3.326051 -4.626694 -9.654553

3 14 0 2.701230 -2.039153 -11.151302

4 14 0 6.131818 -1.079233 -7.737087

5 14 0 6.988723 -6.505496 -6.811851

6 14 0 6.184729 -4.085784 -8.485080

7 8 0 7.446759 -4.357106 -9.487279

8 8 0 4.797227 -3.943780 -9.345597

9 14 0 5.493399 -2.368515 -12.621201

10 14 0 6.672619 -7.684832 -11.708443

11 14 0 5.333704 -5.327357 -13.291206

12 8 0 6.280544 -9.100248 -12.459131

13 14 0 8.948139 -3.986423 -10.075608

14 14 0 10.471628 -8.643148 -8.416087

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16 8 0 11.539457 -9.413300 -9.434588

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34 14 0 9.333729 -5.110407 -5.462717

35 14 0 12.341414 -5.357016 -6.419992

36 14 0 12.862829 -8.305930 -6.528726

37 8 0 13.209866 -6.734357 -6.134356

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39 8 0 13.799048 -8.909994 -7.735038

40 8 0 10.927008 -5.448203 -5.569959

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42 8 0 9.087466 -3.492520 -5.520163

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45 8 0 13.101523 -9.230753 -5.184643

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59 1 0 6.248863 -9.883106 -11.883437

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61 1 0 10.921994 -7.563795 -12.494255

62 1 0 3.450284 -5.947492 -12.280569

63 1 0 5.261122 -5.398046 -15.557551

64 1 0 0.816224 -2.181958 -12.357856

65 1 0 13.267544 -9.170787 -8.520018

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76 6 0 12.671384 0.675047 -7.987062

77 7 0 12.233921 -0.617279 -7.954459

78 6 0 13.152281 -1.586856 -8.031940

79 6 0 14.528144 -1.319324 -8.130914

80 6 0 14.871807 0.047809 -8.158764

81 7 0 13.971805 1.038168 -8.094431

82 1 0 12.784232 -2.610185 -8.007544

83 6 0 11.687594 1.697025 -7.891660

84 6 0 10.828809 2.565405 -7.828730

85 6 0 9.792460 3.605013 -7.753665

86 6 0 8.644006 3.247648 -8.736095

87 1 0 9.009731 3.199714 -9.768829

88 1 0 7.868611 4.022939 -8.679707

89 1 0 8.191795 2.282725 -8.481157

90 6 0 9.241789 3.656966 -6.301587

91 1 0 8.457158 4.422633 -6.242495

92 1 0 10.033731 3.913941 -5.588034

93 1 0 8.809594 2.692748 -6.009853

94 6 0 10.408916 4.976493 -8.135526

95 1 0 10.810191 4.956447 -9.156003

96 1 0 11.219940 5.250217 -7.449962

97 1 0 9.632848 5.751438 -8.084226

98 6 0 15.523708 -2.405067 -8.099325

99 1 0 16.569885 -2.075834 -8.131082

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104 1 0 15.418649 -6.935655 -8.800437

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116 1 0 13.626501 -3.369539 -10.944839

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118 1 0 13.858232 -1.626343 -10.705682

119 6 0 16.702762 -1.679452 -10.636573

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122 1 0 17.672988 -1.921735 -10.181877

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125 1 0 8.310538 -0.457952 -5.447538

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128 1 0 2.694828 -5.446202 -7.655439

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131 1 0 8.856725 -5.258136 -3.243306

132 1 0 9.185665 -10.221760 -7.399327

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TS*R*(*l*)

$\nu = i186.73$

Sum of electronic and zero-point Energies= -10299.153681

Sum of electronic and thermal Energies= -10299.051895

Sum of electronic and thermal Enthalpies= -10299.050951

Sum of electronic and thermal Free Energies= -10299.292211

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2	14	3.326000000	-4.594400000	9.673900000
3	14	2.719700000	-2.003600000	11.172300000
4	14	6.142100000	-1.061600000	7.745700000
5	14	6.968600000	-6.492700000	6.819500000
6	14	6.183200000	-4.067900000	8.495100000
7	8	7.447300000	-4.344300000	9.493200000
8	8	4.799600000	-3.918900000	9.360700000
9	14	5.516600000	-2.346400000	12.632000000
10	14	6.663800000	-7.669200000	11.717600000
11	14	5.343900000	-5.303300000	13.304500000
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13	14	8.953100000	-3.982500000	10.075500000
14	14	10.445800000	-8.647900000	8.410600000
15	14	9.596700000	-6.927500000	10.744000000
16	8	11.513000000	-9.423600000	9.425500000
17	8	9.853500000	-7.315800000	9.165100000
18	8	8.265000000	-7.690400000	11.320400000
19	8	9.484600000	-5.310300000	10.914400000
20	8	6.427700000	-2.691400000	7.632600000
21	8	5.974900000	-5.336700000	7.460400000
22	8	2.405200000	-4.730000000	8.310700000
23	8	10.933600000	-7.557900000	11.513800000

24	8	6.377100000	-6.492800000	12.815600000
25	8	5.696100000	-3.974400000	12.397200000
26	8	3.772400000	-5.768600000	13.227600000
27	8	5.680700000	-4.836400000	14.866100000
28	8	3.997500000	-1.881500000	12.180200000
29	8	2.499500000	-3.550900000	10.644900000
30	8	3.078600000	-0.951100000	9.923600000
31	8	1.320000000	-1.477600000	11.857600000
32	8	8.955200000	-0.876100000	4.834800000
33	14	9.856100000	-2.024800000	5.591600000
34	14	9.316100000	-5.111000000	5.461100000
35	14	12.325900000	-5.371600000	6.409200000
36	14	12.832900000	-8.322600000	6.515800000
37	8	13.186600000	-6.752900000	6.119300000
38	8	11.228600000	-8.375900000	6.999600000
39	8	13.769900000	-8.930500000	7.719500000
40	8	10.908300000	-5.455000000	5.563800000
41	8	8.648700000	-5.740300000	4.069000000
42	8	9.076500000	-3.492000000	5.517600000
43	8	8.497400000	-5.890900000	6.653700000
44	8	9.051400000	-9.505000000	8.051800000
45	8	13.062700000	-9.249200000	5.171400000
46	8	3.490600000	-6.023300000	10.492600000
47	8	6.408200000	-7.007300000	5.360400000
48	8	7.540700000	-0.295300000	7.304200000
49	8	6.613600000	-1.537400000	11.692600000
50	8	10.051900000	-3.791400000	8.848600000
51	8	5.793400000	-1.993400000	14.213100000
52	8	11.327600000	-2.060200000	4.881900000

53	8	9.926900000	-1.675200000	7.245700000
54	8	13.100300000	-4.062900000	5.743000000
55	8	8.955800000	-2.654800000	11.014200000
56	8	12.138300000	-5.225500000	8.033000000
57	8	5.689100000	-0.628800000	9.282900000
58	8	5.764700000	-7.424500000	10.340200000
59	1	6.231100000	-9.865600000	11.894300000
60	1	11.499000000	-9.035500000	10.331300000
61	1	10.917900000	-7.568500000	12.486800000
62	1	3.453200000	-5.912600000	12.300600000
63	1	5.278700000	-5.372600000	15.571000000
64	1	0.839400000	-2.137100000	12.387100000
65	1	13.239300000	-9.189400000	8.505800000
66	1	8.388900000	-0.745900000	7.554100000
67	1	6.292900000	-1.157800000	10.827700000
68	1	9.934100000	-2.983200000	8.265500000
69	1	5.798400000	-2.806600000	14.763500000
70	1	11.966800000	-2.777300000	5.123600000
71	1	10.770300000	-1.144500000	7.537600000
72	1	13.915300000	-3.771900000	6.246700000
73	1	8.090500000	-2.288400000	11.347000000
74	1	11.328800000	-4.747500000	8.375700000
75	1	4.705300000	-0.666500000	9.447200000
76	6	12.686000000	0.662900000	7.980800000
77	7	12.242800000	-0.627300000	7.941700000
78	6	13.156900000	-1.601200000	8.014700000
79	6	14.533800000	-1.340300000	8.115500000
80	6	14.883800000	0.025100000	8.148400000
81	7	13.988100000	1.019700000	8.088700000

82	1	12.784800000	-2.622800000	7.985600000
83	6	11.706800000	1.689700000	7.891600000
84	6	10.852100000	2.562600000	7.835400000
85	6	9.820000000	3.607000000	7.769100000
86	6	8.675300000	3.251500000	8.756600000
87	1	9.046100000	3.199700000	9.787400000
88	1	7.902500000	4.029800000	8.706000000
89	1	8.218100000	2.288900000	8.501700000
90	6	9.261400000	3.666200000	6.320400000
91	1	8.480300000	4.435900000	6.268400000
92	1	10.050500000	3.921700000	5.603100000
93	1	8.822700000	2.705100000	6.028000000
94	6	10.444200000	4.974700000	8.151700000
95	1	10.850000000	4.950400000	9.170300000
96	1	11.253300000	5.246600000	7.463100000
97	1	9.671300000	5.753100000	8.105800000
98	6	15.523700000	-2.431100000	8.082100000
99	1	16.571600000	-2.107500000	8.114100000
100	8	15.252300000	-3.483500000	7.285100000
101	1	12.948400000	-8.775200000	4.330100000
102	30	15.506800000	-4.454200000	8.970600000
103	6	15.796800000	-6.300500000	9.558900000
104	1	15.400100000	-6.961700000	8.776300000
105	6	15.046100000	-6.605800000	10.865100000
106	1	15.263400000	-7.631100000	11.214200000
107	1	15.337700000	-5.930200000	11.685600000
108	1	13.956800000	-6.528500000	10.745600000
109	6	17.304200000	-6.569700000	9.709000000
110	1	17.846900000	-6.440400000	8.761600000

111	1	17.774400000	-5.907500000	10.453700000
112	1	17.488800000	-7.604000000	10.048000000
113	6	15.688700000	-2.828800000	10.450200000
114	1	16.126800000	-3.725100000	10.922500000
115	6	14.325700000	-2.563000000	11.075000000
116	1	13.620600000	-3.392700000	10.924700000
117	1	14.432300000	-2.428800000	12.164700000
118	1	13.857400000	-1.649800000	10.688000000
119	6	16.702400000	-1.711500000	10.622200000
120	1	16.357400000	-0.756400000	10.204400000
121	1	16.886200000	-1.532700000	11.694500000
122	1	17.672000000	-1.955700000	10.167300000
123	1	4.905300000	-0.981600000	5.869200000
124	1	2.391600000	-0.833400000	9.243900000
125	1	8.315400000	-0.452500000	5.447400000
126	8	6.927300000	-7.719400000	7.938700000
127	1	7.644300000	-8.404700000	7.898600000
128	1	2.685500000	-5.412600000	7.677200000
129	1	4.330100000	-6.551500000	10.346200000
130	1	6.962600000	-6.663200000	4.625400000
131	1	8.831100000	-5.258600000	3.243500000
132	1	9.149200000	-10.219900000	7.397200000
133	1	6.218600000	-7.534200000	9.452300000
134	1	15.930700000	0.328200000	8.193700000

TS*S*(*l*)

$\boldsymbol{\nu} = i244.56$

Sum of electronic and zero-point Energies= -10299.139728 a. u.

Sum of electronic and thermal Energies= -10299.035892 a. u.

Sum of electronic and thermal Enthalpies= -10299.034948 a. u.

Sum of electronic and thermal Free Energies= -10299.282907 a. u.

Standart orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---

1 8 0 3.382789 -3.801570 5.406105

2 14 0 1.642033 -7.876377 8.087493

3 14 0 1.399106 -5.293129 9.744461

4 14 0 4.659286 -4.498375 6.188387

5 14 0 5.155343 -10.002385 5.140198

6 14 0 4.494324 -7.507954 6.762836

7 8 0 5.788112 -7.791386 7.707251

8 8 0 3.153247 -7.348958 7.686505

9 14 0 4.190929 -6.063866 11.036592

10 14 0 4.699349 -11.374159 10.060500

11 14 0 3.629294 -8.940988 11.781955

12 8 0 4.283140 -12.902630 10.525694

13 14 0 7.343144 -7.863347 8.257721

14 14 0 9.113499 -12.139539 7.188664

15 14 0 7.760177 -10.776362 9.559353

16 8 0 9.585450 -13.717426 6.967386

17 8 0 8.719271 -11.869608 8.757714

18 8 0 6.292218 -11.501276 9.689242

19 8 0 7.680889 -9.412094 8.674580

20 8 0 4.714804 -6.131258 5.889009

21 8 0 4.245531 -8.751659 5.703676

22 8 0 0.627867 -7.908356 6.786354

23 8 0 8.416428 -10.399677 11.017928

24 8 0 4.406056 -10.304774 11.261403

25 8 0 4.177780 -7.687760 10.824601

26 8 0 1.998692 -9.111391 11.648865

27 8 0 4.039588 -8.673325 13.350979

28 8 0 2.725770 -5.389627 10.698339

29 8 0 0.990662 -6.751263 9.102990

30 8 0 1.837901 -4.177610 8.579765

31 8 0 0.100882 -4.678360 10.543610

32 8 0 7.312690 -4.618241 3.175301

33 14 0 8.319407 -5.686440 3.918572

34 14 0 7.629199 -8.836762 3.750356

35 14 0 10.651424 -9.059593 4.367090

36 14 0 11.738895 -11.457690 5.751378

37 8 0 11.572758 -10.421298 4.468596

38 8 0 10.424661 -11.252339 6.757250

39 8 0 13.144065 -10.984772 6.473692

40 8 0 9.129127 -9.490603 3.875248

41 8 0 6.831008 -9.347221 2.385394

42 8 0 7.670778 -7.216617 3.844217

43 8 0 6.749011 -9.537085 4.965581

44 8 0 7.810298 -11.812866 6.203134

45 8 0 11.792479 -13.026775 5.252231

46 8 0 1.710095 -9.323861 8.877729

47 8 0 4.568685 -10.543088 3.705815

48 8 0 6.078293 -3.842400 5.653752

49 8 0 5.348720 -5.346233 10.100143

50 8 0 8.411595 -7.565343 7.019091

51 8 0 4.549993 -5.879889 12.646791

52 8 0 9.772343 -5.639538 3.169791

53 8 0 8.372611 -5.322846 5.561608

54 8 0 11.230306 -8.100342 3.126712

55 8 0 7.559252 -6.806173 9.478291

56 8 0 10.652383 -8.213962 5.764675

57 8 0 4.424701 -4.190123 7.806385

58 8 0 3.868636 -10.859438 8.707808

59 1 0 3.415928 -12.979040 10.958821

60 1 0 8.915596 -14.413777 7.078780

61 1 0 8.439783 -11.113665 11.677356

62 1 0 1.695994 -9.188498 10.710757

63 1 0 4.300219 -7.740884 13.498824

64 1 0 -0.438409 -5.328171 11.027003

65 1 0 13.465216 -11.569229 7.181385

66 1 0 6.915143 -4.337368 5.865728

67 1 0 5.055480 -4.903869 9.253482

68 1 0 8.294447 -6.705275 6.519269

69 1 0 4.673521 -4.974660 12.979842

70 1 0 10.310536 -6.465274 3.137051

71 1 0 9.219656 -4.824197 5.938725

72 1 0 12.196266 -7.982348 3.096606

73 1 0 6.765532 -6.287874 9.773270

74 1 0 9.823787 -8.141566 6.315451

75 1 0 3.460743 -4.091713 8.050383

76 6 0 11.063238 -3.042151 6.372205

77 7 0 10.473878 -4.233416 6.685516

78 6 0 11.050944 -4.984642 7.635080

79 6 0 12.238209 -4.598016 8.280635

80 6 0 12.762530 -3.354134 7.880168

81 7 0 12.196701 -2.576350 6.946350

82 1 0 10.548433 -5.912470 7.898036

83 6 0 10.424980 -2.221895 5.399033

84 6 0 9.879760 -1.486314 4.588359

85 6 0 9.210324 -0.596923 3.627381

86 6 0 10.013967 0.723953 3.502861

87 1 0 11.029385 0.533861 3.135051

88 1 0 9.508460 1.393350 2.794366

89 1 0 10.087747 1.234990 4.470338

90 6 0 7.776160 -0.295362 4.143252

91 1 0 7.257664 0.344618 3.417023

92 1 0 7.199029 -1.218160 4.272061

93 1 0 7.806475 0.227933 5.106519

94 6 0 9.134592 -1.301055 2.244921

95 1 0 10.137652 -1.532241 1.866627

96 1 0 8.564513 -2.234586 2.306297

97 1 0 8.639271 -0.632181 1.528301

98 6 0 12.825535 -5.419773 9.366558

99 1 0 13.665132 -4.941524 9.890202

100 8 0 11.976575 -6.139131 10.097001

101 1 0 11.083598 -13.573532 5.654828

102 30 0 12.973756 -7.649525 9.430703

103 6 0 14.471946 -6.574887 8.150534

104 1 0 14.838724 -7.590778 8.382469

105 6 0 15.584999 -5.618280 8.550644

106 1 0 16.503314 -5.832895 7.978417

107 1 0 15.330150 -4.568505 8.347158

108 1 0 15.840769 -5.702174 9.616063

109 6 0 14.110521 -6.535521 6.670455

110 1 0 13.278989 -7.208803 6.422810

111 1 0 13.833469 -5.526312 6.339680

112 1 0 14.975231 -6.847076 6.059184

113 6 0 13.060182 -9.557651 9.850888

114 1 0 12.436673 -10.081585 9.110463

115 6 0 12.467130 -9.828055 11.245888

116 1 0 11.412079 -9.530676 11.307385

117 1 0 12.520884 -10.901624 11.503039

118 1 0 13.008425 -9.286845 12.036531

119 6 0 14.496160 -10.096244 9.739748

120 1 0 15.177959 -9.601408 10.448442

121 1 0 14.543651 -11.176413 9.970009

122 1 0 14.919284 -9.959621 8.733602

123 1 0 3.203088 -4.143794 4.513703

124 1 0 1.161282 -3.939680 7.921519

125 1 0 6.713582 -4.168276 3.811525

126 8 0 5.117626 -11.181560 6.311085

127 1 0 5.968878 -11.683224 6.377888

128 1 0 0.671248 -8.712202 6.241100

129 1 0 2.528628 -9.891374 8.741330

130 1 0 5.116175 -10.237822 2.949968

131 1 0 7.065243 -8.920602 1.542822

132 1 0 7.826580 -10.949806 5.731988

133 1 0 4.304500 -11.025546 7.825910

134 1 0 13.661195 -2.953431 8.350817

TS*R*(*d*) — optimized starting point

Sum of electronic and zero-point Energies= -10299.169904 a.u.

Sum of electronic and thermal Energies= -10299.064266 a.u.

Sum of electronic and thermal Enthalpies= -10299.063322 a.u.

Sum of electronic and thermal Free Energies= -10299.319118 a.u.

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---

1 8 0 -3.774626 3.922026 2.479430

2 14 0 -6.048132 -0.447421 1.125722

3 14 0 -6.968744 1.835066 -0.718648

4 14 0 -2.776892 3.174470 1.397059

5 14 0 -1.714099 -2.052060 3.102074

6 14 0 -2.949286 0.091645 1.350004

7 8 0 -2.018888 -0.435379 0.121855

8 8 0 -4.520341 0.136094 0.892911

9 14 0 -4.696644 0.883097 -2.713885

10 14 0 -3.569694 -4.180520 -1.147881

11 14 0 -5.293469 -2.085899 -2.789201

12 8 0 -3.964687 -5.781254 -1.239418

13 14 0 -0.681543 -0.423160 -0.854312

14 14 0 1.537701 -4.430380 0.235207

15 14 0 -0.535291 -3.498070 -1.803335

16 8 0 2.153898 -5.943672 0.538209

17 8 0 0.677098 -4.433994 -1.160486

18 8 0 -1.936325 -4.173220 -1.280011

19 8 0 -0.352983 -1.973253 -1.267698

20 8 0 -2.483207 1.598907 1.815605

21 8 0 -2.820658 -0.914887 2.654801

22 8 0 -6.559153 -0.251776 2.682170

23 8 0 -0.419713 -3.468288 -3.442412

24 8 0 -4.313953 -3.336867 -2.333999

25 8 0 -4.548044 -0.685128 -2.269339

26 8 0 -6.789018 -2.239880 -2.121555

27 8 0 -5.410826 -2.083533 -4.429169

28 8 0 -6.009850 1.603307 -2.025511

29 8 0 -7.062743 0.493567 0.227477

30 8 0 -6.251827 3.125645 0.066439

31 8 0 -8.487926 2.301815 -1.138646

32 8 0 0.641611 3.614523 3.451553

33 14 0 1.434223 2.424641 2.640727

34 14 0 0.989555 -0.651542 3.479153

35 14 0 3.702454 -0.915182 2.014253

36 14 0 4.424607 -3.502325 0.690028

37 8 0 4.597693 -2.276681 1.790240

38 8 0 2.856667 -3.461338 0.119576

39 8 0 5.515855 -3.143830 -0.492504

40 8 0 2.423695 -1.289141 3.001719

41 8 0 0.670531 -0.948388 5.082564

42 8 0 0.891808 0.936345 3.143303

43 8 0 -0.169716 -1.551293 2.711278

44 8 0 0.565470 -3.958841 1.504432

45 8 0 4.711000 -4.968925 1.382526

46 8 0 -6.171444 -2.006463 0.599346

47 8 0 -1.819097 -2.348541 4.712853

48 8 0 -1.311647 3.938662 1.349200

49 8 0 -3.343308 1.746251 -2.315192

50 8 0 0.666819 0.044455 -0.007212

51 8 0 -4.881577 0.807638 -4.361774

52 8 0 3.037761 2.595761 2.912726

53 8 0 1.012190 2.516335 1.009066

54 8 0 4.597356 0.200471 2.872224

55 8 0 -0.909858 0.560136 -2.134769

56 8 0 3.217402 -0.221443 0.614372

57 8 0 -3.556904 3.277557 -0.068159

58 8 0 -3.991110 -3.490966 0.311588

59 1 0 -4.914063 -5.967082 -1.337693

60 1 0 1.527091 -6.665791 0.715775

61 1 0 -0.624798 -4.301982 -3.898758

62 1 0 -6.778803 -2.177452 -1.135155

63 1 0 -5.276404 -1.186390 -4.797540

64 1 0 -9.112070 1.577823 -1.320589

65 1 0 5.648638 -3.831388 -1.167039

66 1 0 -0.544500 3.427227 0.977389

67 1 0 -3.390339 2.336315 -1.509946

68 1 0 0.684844 0.986825 0.324536

69 1 0 -4.956385 1.647943 -4.845359

70 1 0 3.616772 1.796993 2.913426

71 1 0 1.711738 2.952797 0.381469

72 1 0 5.534752 0.283318 2.616994

73 1 0 -1.817233 0.940136 -2.268660

74 1 0 2.283975 -0.341708 0.284636

75 1 0 -4.551893 3.322623 0.013418

76 6 0 2.869121 4.727032 -1.238039

77 7 0 2.858086 3.489583 -0.650972

78 6 0 3.890727 2.675570 -0.897470

79 6 0 4.962355 3.072523 -1.723903

80 6 0 4.878017 4.366640 -2.277065

81 7 0 3.853605 5.192143 -2.049760

82 1 0 3.869411 1.688017 -0.433715

83 6 0 1.773871 5.594059 -0.989322

84 6 0 0.857301 6.388452 -0.823645

85 6 0 -0.239649 7.347306 -0.636698

86 6 0 0.142870 8.695311 -1.303170

87 1 0 1.048681 9.115802 -0.850080

88 1 0 -0.677945 9.411790 -1.168221

89 1 0 0.319830 8.567821 -2.377851

90 6 0 -1.524144 6.773989 -1.298423

91 1 0 -2.343755 7.492090 -1.163939

92 1 0 -1.813190 5.823327 -0.837716

93 1 0 -1.375394 6.614583 -2.373197

94 6 0 -0.481704 7.554208 0.883613

95 1 0 0.414663 7.952390 1.374298

96 1 0 -0.758917 6.610029 1.364594

97 1 0 -1.300625 8.272677 1.020211

98 6 0 6.103765 2.205499 -1.995707

99 1 0 6.884409 2.621397 -2.657915

100 8 0 6.215234 1.057928 -1.525206

101 1 0 3.948185 -5.581399 1.301403

102 30 0 7.940757 -0.219167 -1.536355

103 6 0 8.799874 0.458255 0.110788

104 1 0 9.675851 -0.190684 0.283247

105 6 0 9.319508 1.889945 -0.103545

106 1 0 9.830087 2.287258 0.793401

107 1 0 8.501521 2.595118 -0.327518

108 1 0 10.038742 1.952251 -0.934041

109 6 0 7.923919 0.387178 1.374581

110 1 0 7.582831 -0.638858 1.578388

111 1 0 7.033233 1.028906 1.264932

112 1 0 8.462354 0.738541 2.274384

113 6 0 7.859007 -1.175772 -3.255303

114 1 0 6.914656 -1.747562 -3.277201

115 6 0 7.829800 -0.209698 -4.453668

116 1 0 6.961435 0.465341 -4.420670

117 1 0 7.777157 -0.747185 -5.418866

118 1 0 8.733465 0.419592 -4.499693

119 6 0 9.011953 -2.185358 -3.403804

120 1 0 9.995818 -1.690885 -3.378562

121 1 0 8.962145 -2.737308 -4.361465

122 1 0 9.010527 -2.935069 -2.598622

123 1 0 -3.581412 3.757462 3.418304

124 1 0 -6.687466 3.437481 0.879570

125 1 0 -0.128944 3.959720 2.950177

126 8 0 -2.034248 -3.408733 2.196982

127 1 0 -1.211255 -3.881987 1.910320

128 1 0 -6.270839 -0.936358 3.309562

129 1 0 -5.325422 -2.548280 0.554135

130 1 0 -1.082205 -1.930809 5.209459

131 1 0 1.131372 -0.400301 5.741374

132 1 0 0.701281 -3.045559 1.842467

133 1 0 -3.288636 -3.498861 1.021249

134 1 0 5.669235 4.744699 -2.927263

TS*R*(*d*) — optimized product

Sum of electronic and zero-point Energies= -10299.207281 a.u.

Sum of electronic and thermal Energies= -10299.103393 a.u.

Sum of electronic and thermal Enthalpies= -10299.102449 a.u.

Sum of electronic and thermal Free Energies= -10299.352782 a.u.

1 8 0 -3.311314 4.695647 1.367096

2 14 0 -5.796957 0.292514 0.905480

3 14 0 -6.414465 2.123819 -1.493654

4 14 0 -2.284701 3.657363 0.594907

5 14 0 -1.732599 -1.109021 3.515061

6 14 0 -2.681828 0.674159 1.249953

7 8 0 -1.710159 -0.158357 0.242974

8 8 0 -4.212018 0.689853 0.668616

9 14 0 -4.115400 0.563446 -3.017283

10 14 0 -3.531082 -4.030864 -0.289935

11 14 0 -5.017593 -2.269904 -2.463956

12 8 0 -4.003653 -5.588065 -0.009335

13 14 0 -0.331853 -0.514304 -0.598042

14 14 0 1.426655 -4.347987 1.591266

15 14 0 -0.374823 -3.705664 -0.784627

16 8 0 1.890419 -5.789846 2.274855

17 8 0 0.627260 -4.610567 0.182811

18 8 0 -1.899862 -4.126151 -0.365909

19 8 0 -0.063870 -2.131834 -0.497278

20 8 0 -2.148932 2.220681 1.414050

21 8 0 -2.708256 -0.025963 2.747997

22 8 0 -6.383405 0.884847 2.329612

23 8 0 -0.057555 -4.005338 -2.370895

24 8 0 -4.208336 -3.471892 -1.668058

25 8 0 -4.149302 -0.865299 -2.217246

26 8 0 -6.552544 -2.124253 -1.890494

27 8 0 -5.053664 -2.633414 -4.067295

28 8 0 -5.400419 1.519361 -2.628335

29 8 0 -6.669422 1.065164 -0.261566

30 8 0 -5.645608 3.519916 -0.990598

31 8 0 -7.865547 2.563846 -2.128716

32 8 0 0.996950 4.300151 2.794122

33 14 0 1.756593 2.931631 2.281969

34 14 0 1.058354 0.138760 3.722507

35 14 0 3.802117 -0.670894 2.509997

36 14 0 4.365976 -3.546131 1.979904

37 8 0 4.614211 -2.089226 2.726890

38 8 0 2.832129 -3.545100 1.325600

39 8 0 5.523518 -3.611786 0.804936

40 8 0 2.459113 -0.677903 3.479861

41 8 0 0.658105 0.232028 5.333550

42 8 0 1.080802 1.606736 3.031020

43 8 0 -0.132245 -0.843368 3.117506

44 8 0 0.453205 -3.521911 2.661425

45 8 0 4.491178 -4.796381 3.047117

46 8 0 -6.026108 -1.334331 0.745847

47 8 0 -1.929256 -1.010543 5.141642

48 8 0 -0.771093 4.310470 0.505536

49 8 0 -2.716808 1.389647 -2.711116

50 8 0 0.999953 0.121924 0.162154

51 8 0 -4.196245 0.117062 -4.614582

52 8 0 3.344856 3.052506 2.657956

53 8 0 1.441845 2.713008 0.646799

54 8 0 4.726525 0.582948 3.119199

55 8 0 -0.450092 0.009245 -2.136758

56 8 0 3.459748 -0.416433 0.935371

57 8 0 -2.943571 3.422751 -0.914575

58 8 0 -3.957630 -2.988587 0.940046

59 1 0 -4.957966 -5.750068 -0.102101

60 1 0 1.193633 -6.388716 2.593801

61 1 0 -0.329946 -4.879118 -2.699275

62 1 0 -6.580488 -1.848089 -0.941913

63 1 0 -4.791813 -1.864462 -4.614430

64 1 0 -8.528739 1.854018 -2.184533

65 1 0 5.615705 -4.477043 0.370709

66 1 0 -0.015728 3.686663 0.324368

67 1 0 -2.760225 2.154855 -2.068620

68 1 0 1.048895 1.115018 0.288745

69 1 0 -4.152171 0.824152 -5.280769

70 1 0 3.851100 2.223451 2.827371

71 1 0 2.202866 2.980644 -0.053148

72 1 0 5.648629 0.614133 2.807792

73 1 0 -1.286518 0.478538 -2.394520

74 1 0 2.510275 -0.372775 0.625700

75 1 0 -3.931821 3.566009 -0.939233

76 6 0 3.675982 4.406649 -1.598095

77 7 0 3.236612 3.191369 -1.166526

78 6 0 3.719162 2.095520 -1.782021

79 6 0 4.650905 2.169269 -2.824980

80 6 0 5.016810 3.470477 -3.205565

81 7 0 4.551940 4.582488 -2.611896

82 1 0 3.341224 1.133761 -1.447916

83 6 0 3.165625 5.572021 -0.952118

84 6 0 2.745615 6.592137 -0.425755

85 6 0 2.231463 7.821235 0.198921

86 6 0 2.993353 9.045047 -0.374520

87 1 0 4.067110 8.974926 -0.162429

88 1 0 2.607753 9.964126 0.086587

89 1 0 2.859482 9.118868 -1.460512

90 6 0 0.716620 7.949935 -0.120170

91 1 0 0.319471 8.851702 0.364901

92 1 0 0.159479 7.079494 0.244257

93 1 0 0.550578 8.035858 -1.200912

94 6 0 2.443487 7.742554 1.734960

95 1 0 3.510023 7.665612 1.978987

96 1 0 1.930735 6.874134 2.163743

97 1 0 2.045667 8.653477 2.202203

98 6 0 5.159581 0.908016 -3.514002

99 1 0 5.306743 1.164639 -4.581760

100 8 0 4.174558 -0.093457 -3.387603

101 1 0 3.684664 -5.355185 3.066564

102 30 0 4.641268 -1.818847 -3.145791

103 6 0 6.561918 0.437150 -2.990676

104 1 0 6.758453 -0.488271 -3.566476

105 6 0 7.686242 1.432575 -3.315922

106 1 0 8.665183 0.998714 -3.073715

107 1 0 7.583613 2.356655 -2.730588

108 1 0 7.694073 1.700637 -4.381445

109 6 0 6.560252 0.070823 -1.498052

110 1 0 5.789557 -0.674966 -1.260847

111 1 0 6.373742 0.952140 -0.870110

112 1 0 7.529114 -0.354680 -1.206437

113 6 0 5.104518 -3.684621 -3.013114

114 1 0 5.953097 -3.741102 -2.310616

115 6 0 3.966024 -4.552421 -2.447495

116 1 0 3.657459 -4.228631 -1.445215

117 1 0 4.271716 -5.611985 -2.375912

118 1 0 3.070680 -4.525521 -3.084711

119 6 0 5.588100 -4.222994 -4.373788

120 1 0 4.794858 -4.182163 -5.134945

121 1 0 5.902068 -5.278815 -4.299122

122 1 0 6.446147 -3.657307 -4.765035

123 1 0 -3.223993 4.729725 2.335058

124 1 0 -6.096009 4.045910 -0.306118

125 1 0 0.288039 4.578524 2.173682

126 8 0 -2.136519 -2.612212 2.929398

127 1 0 -1.354471 -3.217538 2.866866

128 1 0 -6.193542 0.347742 3.117568

129 1 0 -5.224459 -1.927096 0.874231

130 1 0 -1.176167 -0.548604 5.570925

131 1 0 1.117155 0.902187 5.869302

132 1 0 0.619663 -2.554652 2.737967

133 1 0 -3.304908 -2.886798 1.687966

134 1 0 5.703455 3.633936 -4.037604

TS*S*(*d*) — optimized starting point

Sum of electronic and zero-point Energies= -10299.173444 a.u.

Sum of electronic and thermal Energies= -10299.068827 a.u.

Sum of electronic and thermal Enthalpies= -10299.067882 a.u.

Sum of electronic and thermal Free Energies= -10299.319574 a.u.

1 8 0 -4.029671 3.736265 2.286707

2 14 0 -5.731900 -0.993444 1.028973

3 14 0 -7.010392 1.039773 -0.872744

4 14 0 -3.019452 3.095433 1.148794

5 14 0 -1.291634 -1.787114 3.207408

6 14 0 -2.760318 0.001013 1.231578

7 8 0 -1.733809 -0.488092 0.056025

8 8 0 -4.315512 -0.188962 0.755266

9 14 0 -4.637377 0.457746 -2.891386

10 14 0 -2.637173 -4.324343 -0.946534

11 14 0 -4.587685 -2.572361 -2.692554

12 8 0 -3.003597 -5.912726 -1.191771

13 14 0 -0.489958 -0.186978 -0.994669

14 14 0 1.929891 -4.132623 1.261291

15 14 0 0.314663 -3.157583 -1.078321

16 8 0 2.755589 -5.115576 0.201336

17 8 0 1.022930 -3.057023 0.416655

18 8 0 -1.004468 -4.115388 -0.968150

19 8 0 -0.010322 -1.649374 -1.612243

20 8 0 -2.499383 1.584383 1.586889

21 8 0 -2.550752 -0.907198 2.593507

22 8 0 -6.270206 -0.783775 2.575684

23 8 0 1.357934 -3.966970 -2.088219

24 8 0 -3.338225 -3.518500 -2.182685

25 8 0 -4.199595 -1.020734 -2.293837

26 8 0 -6.032409 -3.071380 -2.094893

27 8 0 -4.678885 -2.549375 -4.353334

28 8 0 -6.050328 0.950452 -2.189922

29 8 0 -6.885069 -0.302040 0.077213

30 8 0 -6.499174 2.423021 -0.083006

31 8 0 -8.593690 1.264952 -1.258016

32 8 0 0.384039 4.259503 3.012350

33 14 0 1.248261 3.031982 2.339089

34 14 0 1.115720 0.064173 3.485643

35 14 0 3.810918 -0.335006 1.953325

36 14 0 4.692104 -3.176701 2.163536

37 8 0 4.902982 -1.534355 2.264875

38 8 0 3.048817 -3.480587 2.265127

39 8 0 5.277295 -3.810801 0.764701

40 8 0 2.675848 -0.299832 3.149677

41 8 0 0.805547 -0.091593 5.113987

42 8 0 0.764911 1.575687 2.970637

43 8 0 0.135916 -1.060674 2.801915

44 8 0 0.789002 -4.902911 2.215398

45 8 0 5.486942 -3.866586 3.432718

46 8 0 -5.601981 -2.584304 0.596522

47 8 0 -1.407569 -1.920939 4.843708

48 8 0 -1.665973 4.038465 0.996596

49 8 0 -3.458538 1.559683 -2.518403

50 8 0 0.846898 0.407409 -0.209482

51 8 0 -4.794677 0.361669 -4.524135

52 8 0 2.835341 3.324237 2.602285

53 8 0 0.849429 2.910352 0.702162

54 8 0 4.568952 1.145224 2.155149

55 8 0 -0.898412 0.855154 -2.174092

56 8 0 3.228078 -0.559474 0.445944

57 8 0 -3.881568 3.063433 -0.268299

58 8 0 -3.212574 -3.768605 0.514321

59 1 0 -2.721111 -6.521818 -0.488706

60 1 0 2.405815 -5.049166 -0.717354

61 1 0 1.991987 -3.416628 -2.586022

62 1 0 -6.094981 -2.982627 -1.110532

63 1 0 -5.105750 -3.313698 -4.776786

64 1 0 -9.097719 0.454217 -1.445019

65 1 0 4.629729 -4.416317 0.340778

66 1 0 -0.860569 3.599699 0.620553

67 1 0 -3.610886 2.155132 -1.733589

68 1 0 0.770985 1.346387 0.132448

69 1 0 -4.810208 -0.572722 -4.825575

70 1 0 3.471402 2.575803 2.490897

71 1 0 1.459551 3.390360 0.023923

72 1 0 5.327241 1.306367 1.563472

73 1 0 -1.859134 1.034962 -2.370852

74 1 0 2.303696 -0.261414 0.206550

75 1 0 -4.863322 2.923772 -0.148923

76 6 0 2.573274 5.171264 -1.641731

77 7 0 2.455034 3.883016 -1.190742

78 6 0 3.217028 2.952439 -1.772195

79 6 0 4.122004 3.270139 -2.804024

80 6 0 4.156621 4.621685 -3.203229

81 7 0 3.400239 5.569270 -2.641883

82 1 0 3.112829 1.928660 -1.416554

83 6 0 1.771282 6.158103 -1.014978

84 6 0 1.088883 7.023680 -0.482546

85 6 0 0.266265 8.055831 0.160433

86 6 0 0.585385 9.437965 -0.467607

87 1 0 1.640382 9.701474 -0.325714

88 1 0 -0.032689 10.206366 0.014697

89 1 0 0.367804 9.441814 -1.542316

90 6 0 -1.232882 7.706710 -0.057526

91 1 0 -1.850498 8.464995 0.441422

92 1 0 -1.476853 6.722993 0.358645

93 1 0 -1.482813 7.703846 -1.125229

94 6 0 0.589058 8.076667 1.680666

95 1 0 1.639921 8.337004 1.854919

96 1 0 0.393950 7.102494 2.142847

97 1 0 -0.041657 8.831028 2.168845

98 6 0 4.982239 2.260791 -3.423247

99 1 0 5.643142 2.613708 -4.236628

100 8 0 4.994369 1.069641 -3.072129

101 1 0 5.493322 -3.338742 4.249422

102 30 0 6.371742 -0.600688 -2.601213

103 6 0 7.645083 0.519572 -1.595591

104 1 0 7.810489 1.421112 -2.214800

105 6 0 7.165856 0.996956 -0.213843

106 1 0 7.919444 1.627424 0.292712

107 1 0 6.967845 0.143526 0.453715

108 1 0 6.244086 1.595465 -0.298694

109 6 0 8.992827 -0.214491 -1.468635

110 1 0 9.400435 -0.502140 -2.448985

111 1 0 8.898442 -1.136200 -0.874749

112 1 0 9.759478 0.407083 -0.969646

113 6 0 5.597171 -2.095564 -3.602868

114 1 0 5.523913 -1.775497 -4.658115

115 6 0 6.484079 -3.354943 -3.564664

116 1 0 7.494218 -3.159830 -3.954265

117 1 0 6.061181 -4.182050 -4.165107

118 1 0 6.602807 -3.737610 -2.539283

119 6 0 4.166426 -2.438010 -3.138817

120 1 0 4.162030 -2.760876 -2.086648

121 1 0 3.739241 -3.265194 -3.742732

122 1 0 3.490265 -1.574621 -3.224701

123 1 0 -3.782911 3.559146 3.210582

124 1 0 -7.011935 2.688548 0.700783

125 1 0 -0.456210 4.418859 2.527697

126 8 0 -1.439738 -3.272422 2.483010

127 1 0 -0.650441 -3.874239 2.486856

128 1 0 -5.791786 -1.283567 3.259163

129 1 0 -4.695089 -3.011276 0.651010

130 1 0 -0.780896 -1.315044 5.296518

131 1 0 1.132051 0.615832 5.696388

132 1 0 1.136005 -5.438366 2.951318

133 1 0 -2.538910 -3.583788 1.232604

134 1 0 4.822996 4.947033 -4.004046

TS*S*(*d*) — optimized product

Sum of electronic and zero-point Energies= -10299.219806 a.u.

Sum of electronic and thermal Energies= -10299.117123 a.u.

Sum of electronic and thermal Enthalpies= -10299.116179 a.u.

Sum of electronic and thermal Free Energies= -10299.363273 a.u.

---

1 8 0 -3.686104 3.509121 2.752557

2 14 0 -5.656517 -0.920705 1.367429

3 14 0 -7.184651 1.305160 0.028242

4 14 0 -2.846679 3.021035 1.416572

5 14 0 -1.315835 -2.115081 2.862571

6 14 0 -2.744887 -0.090613 1.106578

7 8 0 -1.805235 -0.584603 -0.132726

8 8 0 -4.335950 -0.168170 0.697316

9 14 0 -5.298577 1.056930 -2.590469

10 14 0 -3.140197 -3.902771 -1.394802

11 14 0 -5.211040 -2.128742 -2.906427

12 8 0 -3.583010 -5.382309 -1.975535

13 14 0 -0.685339 -0.152910 -1.282329

14 14 0 1.646524 -4.374236 0.522274

15 14 0 -0.068820 -3.118193 -1.628769

16 8 0 2.372986 -5.306419 -0.650560

17 8 0 0.735160 -3.215213 -0.195270

18 8 0 -1.505943 -3.893434 -1.540985

19 8 0 -0.250557 -1.552542 -2.057716

20 8 0 -2.358320 1.442594 1.542083

21 8 0 -2.558960 -1.106737 2.406120

22 8 0 -5.546038 -0.951185 3.012728

23 8 0 0.917632 -3.947557 -2.684846

24 8 0 -3.794640 -2.666221 -2.252249

25 8 0 -5.092999 -0.491648 -3.073295

26 8 0 -6.510231 -2.579087 -2.006385

27 8 0 -5.317680 -2.818850 -4.402921

28 8 0 -6.450704 1.119197 -1.411389

29 8 0 -6.990757 -0.029541 0.982103

30 8 0 -6.479951 2.669046 0.691962

31 8 0 -8.799231 1.598205 -0.104913

32 8 0 0.657685 3.802503 3.173892

33 14 0 1.399400 2.606079 2.320707

34 14 0 1.208805 -0.435516 3.111586

35 14 0 3.746542 -0.721043 1.285706

36 14 0 4.493078 -3.612361 1.334255

37 8 0 4.812300 -1.987478 1.428302

38 8 0 2.842810 -3.831219 1.501281

39 8 0 4.983320 -4.275868 -0.087700

40 8 0 2.717219 -0.770434 2.582281

41 8 0 1.053642 -0.782164 4.735254

42 8 0 0.823467 1.126357 2.816883

43 8 0 0.126335 -1.454898 2.408115

44 8 0 0.532026 -5.173097 1.482711

45 8 0 5.303998 -4.363372 2.559961

46 8 0 -5.862067 -2.403979 0.662714

47 8 0 -1.347589 -2.343112 4.491900

48 8 0 -1.477527 3.927662 1.226302

49 8 0 -3.851367 1.649661 -2.062937

50 8 0 0.718979 0.390371 -0.594351

51 8 0 -5.763086 2.000306 -3.862794

52 8 0 3.010997 2.745812 2.546810

53 8 0 0.936692 2.712314 0.697494

54 8 0 4.561777 0.709076 1.472443

55 8 0 -1.270100 0.959509 -2.315916

56 8 0 3.023585 -0.888826 -0.171902

57 8 0 -3.890203 3.227526 0.141762

58 8 0 -3.573302 -3.703897 0.200549

59 1 0 -4.537651 -5.562893 -2.006274

60 1 0 1.980372 -5.133109 -1.538592

61 1 0 0.528021 -4.186931 -3.544216

62 1 0 -6.419784 -2.467768 -1.025269

63 1 0 -6.089919 -2.551952 -4.928726

64 1 0 -9.364157 0.807439 -0.060638

65 1 0 4.252423 -4.762956 -0.531739

66 1 0 -0.707983 3.491302 0.774173

67 1 0 -3.855508 2.296183 -1.302305

68 1 0 0.703070 1.271404 -0.116446

69 1 0 -6.630664 1.789958 -4.247549

70 1 0 3.602839 2.023059 2.209241

71 1 0 1.627207 3.211490 0.095902

72 1 0 5.150453 0.955326 0.680112

73 1 0 -2.251408 1.126941 -2.323161

74 1 0 2.139215 -0.457293 -0.340666

75 1 0 -4.851325 3.118137 0.388228

76 6 0 3.234357 5.047665 -0.894395

77 7 0 2.899451 3.738888 -0.727724

78 6 0 3.849674 2.817342 -0.963609

79 6 0 5.154960 3.159787 -1.336727

80 6 0 5.395892 4.539018 -1.459657

81 7 0 4.461525 5.481919 -1.261971

82 1 0 3.561825 1.777895 -0.826402

83 6 0 2.218623 6.018251 -0.650698

84 6 0 1.340045 6.841348 -0.439485

85 6 0 0.283417 7.830711 -0.177290

86 6 0 0.656074 9.173752 -0.858658

87 1 0 1.606640 9.561249 -0.472576

88 1 0 -0.129270 9.914579 -0.658234

89 1 0 0.747680 9.051550 -1.944710

90 6 0 -1.062904 7.303807 -0.742776

91 1 0 -1.852108 8.041611 -0.545899

92 1 0 -1.345561 6.356601 -0.269322

93 1 0 -0.999209 7.146675 -1.826371

94 6 0 0.162867 8.035827 1.358097

95 1 0 1.101809 8.414037 1.779870

96 1 0 -0.089811 7.095454 1.861485

97 1 0 -0.631393 8.765820 1.563327

98 6 0 6.232756 2.115931 -1.559380

99 1 0 7.203272 2.601059 -1.349822

100 8 0 6.033259 1.019942 -0.656645

101 1 0 5.358595 -3.851634 3.385240

102 30 0 7.066722 -0.459960 -1.024793

103 6 0 8.363825 -1.822621 -1.448698

104 1 0 9.138700 -1.289696 -2.028083

105 6 0 9.042164 -2.392748 -0.188742

106 1 0 9.842412 -3.102057 -0.460218

107 1 0 8.332473 -2.941544 0.445928

108 1 0 9.500008 -1.607430 0.429829

109 6 0 7.802566 -2.944137 -2.341579

110 1 0 7.370880 -2.552781 -3.274200

111 1 0 7.020521 -3.519612 -1.828670

112 1 0 8.597989 -3.654872 -2.623793

113 6 0 6.297383 1.593840 -3.032402

114 1 0 7.084806 0.815721 -2.999609

115 6 0 4.990260 0.929557 -3.491649

116 1 0 4.633243 0.191616 -2.762268

117 1 0 5.139662 0.417026 -4.450651

118 1 0 4.196314 1.674135 -3.636209

119 6 0 6.760717 2.677809 -4.017395

120 1 0 6.010312 3.474420 -4.111397

121 1 0 6.909872 2.247643 -5.015860

122 1 0 7.709187 3.135381 -3.703871

123 1 0 -3.282210 3.290708 3.609877

124 1 0 -6.821621 2.947947 1.560217

125 1 0 -0.164905 4.104946 2.731561

126 8 0 -1.615253 -3.529439 2.051438

127 1 0 -0.857591 -4.161701 1.935497

128 1 0 -4.653573 -1.181691 3.334608

129 1 0 -5.016501 -2.940774 0.584403

130 1 0 -0.623016 -1.847258 4.934005

131 1 0 1.457135 -0.151060 5.356152

132 1 0 0.893983 -5.796704 2.137344

133 1 0 -2.842477 -3.700322 0.883653

134 1 0 6.390376 4.905348 -1.720112

TS*R*(*l*) — optimized starting point

Sum of electronic and zero-point Energies= -10299.169201 a.u.

Sum of electronic and thermal Energies= -10299.063988 a.u.

Sum of electronic and thermal Enthalpies= -10299.063043 a.u.

Sum of electronic and thermal Free Energies = -10299.317105 a. u.

---

1 8 0 -4.053917 2.917353 -3.034739

2 14 0 -5.429944 -1.556567 -1.167890

3 14 0 -7.102332 0.593157 0.121651

4 14 0 -3.091427 2.636898 -1.722998

5 14 0 -1.062898 -2.364914 -2.878491

6 14 0 -2.617316 -0.407717 -1.181740

7 8 0 -1.548211 -0.704538 0.014810

8 8 0 -4.159941 -0.616595 -0.652792

9 14 0 -5.017857 0.763598 2.593597

10 14 0 -2.429269 -4.036163 1.591872

11 14 0 -4.571403 -2.359094 3.127747

12 8 0 -2.677939 -5.504816 2.300554

13 14 0 -0.408277 -0.077116 1.048902

14 14 0 2.270381 -4.182644 -0.540140

15 14 0 0.546292 -2.920134 1.588835

16 8 0 3.139467 -4.944945 0.655198

17 8 0 1.302637 -3.038312 0.129702

18 8 0 -0.800466 -3.847300 1.618983

19 8 0 0.204548 -1.354057 1.906699

20 8 0 -2.428809 1.119075 -1.753515

21 8 0 -2.405971 -1.493635 -2.420114

22 8 0 -5.425701 -1.699572 -2.810821

23 8 0 1.657932 -3.555554 2.650708

24 8 0 -3.160003 -2.811895 2.403910

25 8 0 -4.603095 -0.709130 3.169826

26 8 0 -5.881939 -2.992563 2.364973

27 8 0 -4.501694 -2.937908 4.672622

28 8 0 -6.247756 0.608839 1.505300

29 8 0 -6.826190 -0.786355 -0.743837

30 8 0 -6.609001 1.965053 -0.699265

31 8 0 -8.725319 0.722540 0.363628

32 8 0 0.299618 3.754259 -3.649797

33 14 0 1.184741 2.700973 -2.749593

34 14 0 1.227574 -0.415106 -3.406513

35 14 0 3.928410 -0.402249 -1.821022

36 14 0 4.974761 -3.197885 -1.565431

37 8 0 5.078498 -1.581051 -1.920774

38 8 0 3.355671 -3.618362 -1.630071

39 8 0 5.577481 -3.568087 -0.082790

40 8 0 2.796615 -0.632610 -2.999365

41 8 0 0.957268 -0.846653 -4.991783

42 8 0 0.789578 1.137118 -3.142136

43 8 0 0.287784 -1.467685 -2.565569

44 8 0 1.177123 -5.142765 -1.367517

45 8 0 5.832614 -4.020826 -2.708074

46 8 0 -5.420431 -2.994713 -0.349978

47 8 0 -1.141870 -2.734355 -4.479330

48 8 0 -1.826765 3.702152 -1.691979

49 8 0 -3.688973 1.465923 1.910025

50 8 0 0.890183 0.537953 0.222414

51 8 0 -5.493253 1.752110 3.826914

52 8 0 2.765458 3.029233 -3.003463

53 8 0 0.723034 2.833848 -1.130031

54 8 0 4.624530 1.049550 -2.285162

55 8 0 -1.035508 1.070182 2.018317

56 8 0 3.346229 -0.369954 -0.299762

57 8 0 -4.071826 2.840652 -0.399152

58 8 0 -2.975057 -4.003631 0.018522

59 1 0 -3.604366 -5.767544 2.432892

60 1 0 2.777413 -4.743794 1.549883

61 1 0 1.364820 -3.701726 3.567076

62 1 0 -5.861438 -2.967159 1.374003

63 1 0 -5.260409 -2.712611 5.236219

64 1 0 -9.199362 -0.124265 0.432149

65 1 0 4.957656 -4.130324 0.432669

66 1 0 -1.003060 3.397065 -1.228702

67 1 0 -3.824484 2.040715 1.105691

68 1 0 0.739374 1.390780 -0.280083

69 1 0 -6.288956 1.470999 4.309430

70 1 0 3.443109 2.341328 -2.792007

71 1 0 1.281882 3.448178 -0.515514

72 1 0 5.417887 1.314096 -1.783878

73 1 0 -2.026445 1.137408 2.086917

74 1 0 2.407644 -0.094730 -0.098015

75 1 0 -5.029003 2.606050 -0.561061

76 6 0 1.950745 5.341869 1.257435

77 7 0 2.214243 4.151909 0.631662

78 6 0 3.294252 3.472851 1.025709

79 6 0 4.145550 3.948043 2.042978

80 6 0 3.779681 5.177680 2.629576

81 7 0 2.704488 5.875196 2.253068

82 1 0 3.494056 2.521929 0.535584

83 6 0 0.806436 6.065711 0.835902

84 6 0 -0.176870 6.709302 0.493164

85 6 0 -1.358808 7.484131 0.093195

86 6 0 -1.251550 8.918411 0.675176

87 1 0 -0.360973 9.432907 0.294481

88 1 0 -2.138099 9.495419 0.381482

89 1 0 -1.198244 8.896151 1.770159

90 6 0 -2.627471 6.779040 0.651534

91 1 0 -3.512720 7.359073 0.359269

92 1 0 -2.725061 5.765625 0.247535

93 1 0 -2.596200 6.720476 1.745960

94 6 0 -1.431973 7.540886 -1.457022

95 1 0 -0.542211 8.025536 -1.876837

96 1 0 -1.517922 6.533901 -1.879702

97 1 0 -2.315836 8.121089 -1.752811

98 6 0 5.345636 3.221840 2.447366

99 1 0 5.932944 3.657121 3.274882

100 8 0 5.721888 2.174443 1.885727

101 1 0 5.823005 -3.622419 -3.595058

102 30 0 6.784359 0.346124 2.192917

103 6 0 8.295117 0.489609 0.934801

104 1 0 8.951952 1.286146 1.332516

105 6 0 7.882925 0.921136 -0.485749

106 1 0 8.753382 1.051924 -1.155239

107 1 0 7.243764 0.160772 -0.962251

108 1 0 7.337179 1.878563 -0.479205

109 6 0 9.130674 -0.803209 0.874833

110 1 0 9.511786 -1.093803 1.865139

111 1 0 8.540573 -1.651489 0.495876

112 1 0 10.007206 -0.702847 0.207424

113 6 0 5.764005 -0.403701 3.714622

114 1 0 6.477197 -1.137067 4.134386

115 6 0 4.491177 -1.166662 3.318971

116 1 0 4.692146 -1.948586 2.574067

117 1 0 4.024763 -1.658961 4.192790

118 1 0 3.730664 -0.500546 2.887047

119 6 0 5.475736 0.630777 4.809278

120 1 0 4.783655 1.416035 4.463540

121 1 0 4.996371 0.172646 5.694217

122 1 0 6.389201 1.131382 5.165845

123 1 0 -3.678301 2.676440 -3.898787

124 1 0 -7.047045 2.132239 -1.552853

125 1 0 -0.565889 3.954827 -3.232048

126 8 0 -1.130466 -3.731096 -1.945058

127 1 0 -0.306251 -4.274292 -1.833937

128 1 0 -4.537329 -1.865478 -3.180306

129 1 0 -4.517577 -3.433163 -0.302943

130 1 0 -0.537558 -2.168321 -5.008430

131 1 0 1.290418 -0.244694 -5.679469

132 1 0 1.552619 -5.804825 -1.975067

133 1 0 -2.286477 -3.961250 -0.704953

134 1 0 4.380567 5.612241 3.430086

TS*R*(*l*) — optimized product

Sum of electronic and zero-point Energies= -10299.219806 a.u.

Sum of electronic and thermal Energies= -10299.117125 a.u.

Sum of electronic and thermal Enthalpies= -10299.116181 a.u.

Sum of electronic and thermal Free Energies= -10299.363246 a.u.

1 8 0 3.686015 3.508735 2.753432

2 14 0 5.656521 -0.922520 1.366742

3 14 0 7.184503 1.303910 0.028616

4 14 0 2.846860 3.020341 1.417372

5 14 0 1.315166 -2.115891 2.861794

6 14 0 2.744923 -0.091182 1.106969

7 8 0 1.805360 -0.584438 -0.132668

8 8 0 4.336039 -0.168715 0.697910

9 14 0 5.298534 1.057249 -2.590385

10 14 0 3.139080 -3.902816 -1.396398

11 14 0 5.209522 -2.128521 -2.907492

12 8 0 3.582486 -5.381717 -1.978248

13 14 0 0.685318 -0.152696 -1.282129

14 14 0 -1.647535 -4.373879 0.521480

15 14 0 0.068030 -3.117866 -1.629500

16 8 0 -2.374600 -5.305226 -0.651648

17 8 0 -0.735561 -3.215161 -0.195810

18 8 0 1.504774 -3.893948 -1.542330

19 8 0 0.250588 -1.552155 -2.057843

20 8 0 2.358643 1.441874 1.543319

21 8 0 2.558755 -1.107811 2.406053

22 8 0 5.546798 -0.954029 3.012085

23 8 0 -0.919053 -3.946259 -2.685728

24 8 0 3.792968 -2.665290 -2.252972

25 8 0 5.092723 -0.491262 -3.073297

26 8 0 6.508683 -2.580458 -2.008157

27 8 0 5.315111 -2.817852 -4.404407

28 8 0 6.450566 1.119115 -1.411177

29 8 0 6.990981 -0.031752 0.981174

30 8 0 6.479495 2.667036 0.693586

31 8 0 8.798980 1.597554 -0.104324

32 8 0 -0.657161 3.802841 3.174585

33 14 0 -1.399132 2.606070 2.322090

34 14 0 -1.208853 -0.435659 3.112186

35 14 0 -3.746536 -0.720521 1.285945

36 14 0 -4.493755 -3.611540 1.334699

37 8 0 -4.812728 -1.986581 1.428784

38 8 0 -2.843481 -3.830904 1.500901

39 8 0 -4.984563 -4.275186 -0.087023

40 8 0 -2.717357 -0.769848 2.582632

41 8 0 -1.053782 -0.783830 4.735554

42 8 0 -0.823482 1.126624 2.819552

43 8 0 -0.126701 -1.454676 2.407702

44 8 0 -0.533282 -5.173518 1.481570

45 8 0 -5.304048 -4.361900 2.561202

46 8 0 5.861192 -2.405429 0.661097

47 8 0 1.346632 -2.345077 4.490951

48 8 0 1.477646 3.926824 1.226735

49 8 0 3.851388 1.650308 -2.063033

50 8 0 -0.719014 0.390351 -0.594040

51 8 0 5.763368 2.000583 -3.862608

52 8 0 -3.010734 2.746252 2.548067

53 8 0 -0.936549 2.711296 0.698774

54 8 0 -4.561292 0.709912 1.472292

55 8 0 1.269958 0.960003 -2.315460

56 8 0 -3.023524 -0.889256 -0.171527

57 8 0 3.890476 3.226825 0.142655

58 8 0 3.572193 -3.705059 0.199094

59 1 0 4.537216 -5.561737 -2.009602

60 1 0 -1.981945 -5.132003 -1.539661

61 1 0 -0.529792 -4.185312 -3.545342

62 1 0 6.418675 -2.469185 -1.026995

63 1 0 6.086671 -2.550289 -4.930867

64 1 0 9.364212 0.806967 -0.060800

65 1 0 -4.253655 -4.761692 -0.531723

66 1 0 0.708172 3.490196 0.774811

67 1 0 3.855546 2.296475 -1.302100

68 1 0 -0.703015 1.271044 -0.115467

69 1 0 6.630733 1.789779 -4.247593

70 1 0 -3.602636 2.023696 2.210160

71 1 0 -1.626624 3.210890 0.096929

72 1 0 -5.149851 0.956274 0.679924

73 1 0 2.251260 1.127383 -2.322911

74 1 0 -2.139322 -0.457458 -0.340518

75 1 0 4.851512 3.116463 0.389186

76 6 0 -3.232402 5.047896 -0.894021

77 7 0 -2.897829 3.739008 -0.727581

78 6 0 -3.848250 2.817709 -0.963688

79 6 0 -5.153444 3.160509 -1.336707

80 6 0 -5.394093 4.539857 -1.459207

81 7 0 -4.459515 5.482512 -1.261383

82 1 0 -3.560586 1.778184 -0.826686

83 6 0 -2.216367 6.018140 -0.650215

84 6 0 -1.337555 6.840954 -0.438862

85 6 0 -0.280887 7.830141 -0.176140

86 6 0 -0.652245 9.172812 -0.858948

87 1 0 -1.603159 9.560933 -0.474354

88 1 0 0.133115 9.913501 -0.658075

89 1 0 -0.742501 9.049834 -1.945024

90 6 0 1.065965 7.302424 -0.739591

91 1 0 1.855157 8.040093 -0.542163

92 1 0 1.347720 6.355390 -0.265268

93 1 0 1.003570 7.144701 -1.823180

94 6 0 -0.162195 8.036301 1.359254

95 1 0 -1.101553 8.415071 1.779601

96 1 0 0.089583 7.096197 1.863616

97 1 0 0.632023 8.766199 1.564984

98 6 0 -6.231676 2.117117 -1.559517

99 1 0 -7.201946 2.602711 -1.349964

100 8 0 -6.032714 1.021055 -0.656754

101 1 0 -5.363550 -3.847015 3.384169

102 30 0 -7.066557 -0.458602 -1.024752

103 6 0 -8.363600 -1.821347 -1.448392

104 1 0 -9.138875 -1.288431 -2.027252

105 6 0 -9.041582 -2.392830 -0.188849

106 1 0 -9.841415 -3.102357 -0.460947

107 1 0 -8.331586 -2.941709 0.445388

108 1 0 -9.499883 -1.608237 0.430294

109 6 0 -7.801871 -2.941927 -2.342218

110 1 0 -7.370383 -2.549736 -3.274568

111 1 0 -7.019591 -3.517428 -1.829692

112 1 0 -8.596978 -3.652829 -2.624928

113 6 0 -6.296579 1.595126 -3.032574

114 1 0 -7.084428 0.817428 -2.999787

115 6 0 -4.989787 0.930161 -3.491807

116 1 0 -4.633176 0.192108 -2.762338

117 1 0 -5.139484 0.417558 -4.450727

118 1 0 -4.195476 1.674310 -3.636494

119 6 0 -6.759375 2.679394 -4.017476

120 1 0 -6.008655 3.475738 -4.111244

121 1 0 -6.908554 2.249447 -5.016029

122 1 0 -7.707694 3.137285 -3.703966

123 1 0 3.282501 3.289315 3.610678

124 1 0 6.820774 2.945133 1.562245

125 1 0 0.165303 4.105119 2.731919

126 8 0 1.614047 -3.529794 2.049699

127 1 0 0.856395 -4.162080 1.933902

128 1 0 4.654197 -1.183624 3.334227

129 1 0 5.015506 -2.942079 0.582860

130 1 0 0.622105 -1.849349 4.933307

131 1 0 -1.455978 -0.152411 5.356970

132 1 0 -0.895680 -5.796295 2.136763

133 1 0 2.841347 -3.700977 0.882163

134 1 0 -6.388549 4.906448 -1.719404

TS*S*(*l*) — optimized starting point

Sum of electronic and zero-point Energies= -10299.169903 a.u.

Sum of electronic and thermal Energies= -10299.064265 a.u.

Sum of electronic and thermal Enthalpies= -10299.063321 a.u.

Sum of electronic and thermal Free Energies= -10299.319120 a.u.

1 8 0 3.774896 3.921994 2.479033

2 14 0 6.048094 -0.447256 1.125744

3 14 0 6.968700 1.835089 -0.718776

4 14 0 2.776942 3.174559 1.396786

5 14 0 1.714136 -2.051791 3.102184

6 14 0 2.949248 0.091726 1.349832

7 8 0 2.018851 -0.435418 0.121730

8 8 0 4.520286 0.136115 0.892678

9 14 0 4.696638 0.882818 -2.713988

10 14 0 3.569799 -4.180589 -1.147527

11 14 0 5.293557 -2.086122 -2.789140

12 8 0 3.964440 -5.781416 -1.238974

13 14 0 0.681457 -0.423157 -0.854372

14 14 0 -1.537607 -4.430350 0.235387

15 14 0 0.535351 -3.498089 -1.803140

16 8 0 -2.153768 -5.943624 0.538526

17 8 0 -0.676976 -4.434094 -1.160292

18 8 0 1.936434 -4.172942 -1.279592

19 8 0 0.352758 -1.973251 -1.267651

20 8 0 2.483109 1.599010 1.815298

21 8 0 2.820690 -0.914679 2.654733

22 8 0 6.558852 -0.251551 2.682272

23 8 0 0.419909 -3.468493 -3.442230

24 8 0 4.314333 -3.337211 -2.333663

25 8 0 4.547944 -0.685395 -2.269425

26 8 0 6.789195 -2.239725 -2.121606

27 8 0 5.410744 -2.083980 -4.429121

28 8 0 6.009854 1.603010 -2.025610

29 8 0 7.062765 0.493813 0.227665

30 8 0 6.251709 3.125782 0.066063

31 8 0 8.487862 2.301827 -1.138853

32 8 0 -0.641645 3.614834 3.451500

33 14 0 -1.434216 2.424870 2.640758

34 14 0 -0.989491 -0.651259 3.479235

35 14 0 -3.702416 -0.915024 2.014368

36 14 0 -4.424528 -3.502262 0.690155

37 8 0 -4.597534 -2.276597 1.790351

38 8 0 -2.856620 -3.461387 0.119624

39 8 0 -5.515816 -3.143751 -0.492335

40 8 0 -2.423666 -1.288857 3.001894

41 8 0 -0.670437 -0.948069 5.082647

42 8 0 -0.891692 0.936611 3.143330

43 8 0 0.169751 -1.551042 2.711343

44 8 0 -0.565401 -3.958651 1.504570

45 8 0 -4.710929 -4.968831 1.382728

46 8 0 6.171592 -2.006290 0.599359

47 8 0 1.819190 -2.348030 4.713001

48 8 0 1.311746 3.938844 1.349149

49 8 0 3.343320 1.746029 -2.315349

50 8 0 -0.666834 0.044592 -0.007242

51 8 0 4.881619 0.807323 -4.361871

52 8 0 -3.037734 2.595966 2.912874

53 8 0 -1.012221 2.516499 1.009092

54 8 0 -4.597436 0.200594 2.872251

55 8 0 0.909761 0.560005 -2.134930

56 8 0 -3.217346 -0.221261 0.614507

57 8 0 3.556823 3.277585 -0.068512

58 8 0 3.991337 -3.491021 0.311903

59 1 0 4.913780 -5.967443 -1.337235

60 1 0 -1.526972 -6.665761 0.716052

61 1 0 0.625033 -4.302234 -3.898474

62 1 0 6.779015 -2.177360 -1.135202

63 1 0 5.276388 -1.186863 -4.797578

64 1 0 9.112032 1.577835 -1.320703

65 1 0 -5.648739 -3.831333 -1.166817

66 1 0 0.544554 3.427495 0.977334

67 1 0 3.390310 2.336086 -1.510092

68 1 0 -0.684802 0.986950 0.324536

69 1 0 4.956577 1.647619 -4.845448

70 1 0 -3.616750 1.797207 2.913546

71 1 0 -1.711753 2.952882 0.381509

72 1 0 -5.534852 0.283295 2.617076

73 1 0 1.817115 0.940064 -2.268818

74 1 0 -2.283949 -0.341555 0.284685

75 1 0 4.551812 3.322776 0.012949

76 6 0 -2.869287 4.726938 -1.238330

77 7 0 -2.858247 3.489566 -0.651114

78 6 0 -3.890828 2.675481 -0.897606

79 6 0 -4.962382 3.072250 -1.724218

80 6 0 -4.878013 4.366284 -2.277596

81 7 0 -3.853678 5.191879 -2.050276

82 1 0 -3.869548 1.688019 -0.433661

83 6 0 -1.774144 5.594083 -0.989553

84 6 0 -0.857651 6.388534 -0.823726

85 6 0 0.239174 7.347523 -0.636723

86 6 0 -0.143636 8.695607 -1.302859

87 1 0 -1.049428 9.115891 -0.849539

88 1 0 0.677103 9.412173 -1.167903

89 1 0 -0.320757 8.568311 -2.377537

90 6 0 1.523656 6.774538 -1.298772

91 1 0 2.343192 7.492707 -1.164200

92 1 0 1.812876 5.823788 -0.838352

93 1 0 1.374781 6.615402 -2.373568

94 6 0 0.481428 7.554136 0.883591

95 1 0 -0.414938 7.952039 1.374505

96 1 0 0.758888 6.609904 1.364326

97 1 0 1.300237 8.272728 1.020232

98 6 0 -6.103697 2.205119 -1.996051

99 1 0 -6.884241 2.620823 -2.658498

100 8 0 -6.215149 1.057616 -1.525354

101 1 0 -3.948131 -5.581322 1.301541

102 30 0 -7.940614 -0.219415 -1.536380

103 6 0 -8.799848 0.458266 0.110645

104 1 0 -9.675871 -0.190621 0.283060

105 6 0 -9.319433 1.889899 -0.104166

106 1 0 -9.830199 2.287464 0.792564

107 1 0 -8.501404 2.595031 -0.328130

108 1 0 -10.038498 1.952000 -0.934827

109 6 0 -7.924089 0.387462 1.374576

110 1 0 -7.583087 -0.638543 1.578663

111 1 0 -7.033343 1.029096 1.264967

112 1 0 -8.462667 0.739038 2.274215

113 6 0 -7.858839 -1.176398 -3.255111

114 1 0 -6.914256 -1.747822 -3.276924

115 6 0 -7.830112 -0.210688 -4.453775

116 1 0 -6.962048 0.464752 -4.421014

117 1 0 -7.777267 -0.748449 -5.418810

118 1 0 -8.734053 0.418190 -4.499955

119 6 0 -9.011384 -2.186502 -3.403190

120 1 0 -9.995450 -1.692428 -3.378008

121 1 0 -8.961445 -2.738733 -4.360684

122 1 0 -9.009576 -2.935960 -2.597772

123 1 0 3.581746 3.757548 3.417941

124 1 0 6.687235 3.437621 0.879257

125 1 0 0.129089 3.959804 2.950246

126 8 0 2.034264 -3.408584 2.197266

127 1 0 1.211275 -3.881830 1.910584

128 1 0 6.270348 -0.936048 3.309669

129 1 0 5.325620 -2.548185 0.554221

130 1 0 1.082215 -1.930375 5.209551

131 1 0 -1.131243 -0.399949 5.741454

132 1 0 -0.701148 -3.045324 1.842508

133 1 0 3.288841 -3.498892 1.021537

134 1 0 -5.669157 4.744204 -2.927962

TS*S*(*l*) — optimized product

Sum of electronic and zero-point Energies= -10299.207761 a.u.

Sum of electronic and thermal Energies= -10299.103819 a.u.

Sum of electronic and thermal Enthalpies= -10299.102875 a.u.

Sum of electronic and thermal Free Energies= -10299.353611 a.u.

---

1 8 0 3.330809 4.678044 1.409311

2 14 0 5.773756 0.253203 0.947821

3 14 0 6.420961 2.084076 -1.444502

4 14 0 2.295524 3.655579 0.627683

5 14 0 1.675799 -1.108780 3.534261

6 14 0 2.659908 0.666281 1.278723

7 8 0 1.689268 -0.159079 0.264174

8 8 0 4.194290 0.670179 0.708915

9 14 0 4.113330 0.552909 -2.982573

10 14 0 3.466576 -4.043895 -0.269043

11 14 0 4.981300 -2.292433 -2.431057

12 8 0 3.929372 -5.603907 0.011801

13 14 0 0.311515 -0.497129 -0.584366

14 14 0 -1.503629 -4.317417 1.589434

15 14 0 0.317416 -3.690233 -0.777068

16 8 0 -1.977689 -5.756808 2.271249

17 8 0 -0.700632 -4.583277 0.183553

18 8 0 1.834855 -4.131605 -0.353322

19 8 0 0.025890 -2.112392 -0.493511

20 8 0 2.137163 2.216436 1.439008

21 8 0 2.668970 -0.035138 2.776361

22 8 0 6.364845 0.836082 2.373889

23 8 0 0.002619 -3.984015 -2.366100

24 8 0 4.150853 -3.485923 -1.643976

25 8 0 4.130493 -0.877246 -2.184524

26 8 0 6.514578 -2.169582 -1.847951

27 8 0 5.021696 -2.651419 -4.035245

28 8 0 5.405845 1.495901 -2.586954

29 8 0 6.657863 1.016730 -0.216327

30 8 0 5.665010 3.486145 -0.938914

31 8 0 7.879891 2.510515 -2.070796

32 8 0 -1.005367 4.326413 2.803435

33 14 0 -1.768874 2.963860 2.280895

34 14 0 -1.106927 0.162870 3.728441

35 14 0 -3.847190 -0.621823 2.495219

36 14 0 -4.436027 -3.497745 1.973584

37 8 0 -4.677008 -2.031245 2.703041

38 8 0 -2.902971 -3.506380 1.318260

39 8 0 -5.595024 -3.578391 0.799982

40 8 0 -2.511039 -0.645255 3.474796

41 8 0 -0.715492 0.248111 5.341975

42 8 0 -1.117790 1.633549 3.042540

43 8 0 0.081192 -0.824484 3.126943

44 8 0 -0.528717 -3.498610 2.663948

45 8 0 -4.565632 -4.737513 3.052564

46 8 0 5.983189 -1.376202 0.786566

47 8 0 1.862779 -1.016075 5.162332

48 8 0 0.789864 4.325519 0.532062

49 8 0 2.721444 1.391795 -2.680302

50 8 0 -1.017274 0.148538 0.173147

51 8 0 4.196091 0.108161 -4.580221

52 8 0 -3.361830 3.098382 2.631253

53 8 0 -1.427877 2.741351 0.651998

54 8 0 -4.763222 0.640448 3.099538

55 8 0 0.438753 0.032275 -2.120359

56 8 0 -3.490343 -0.369547 0.923916

57 8 0 2.961208 3.418349 -0.878578

58 8 0 3.892851 -3.005464 0.964138

59 1 0 4.883187 -5.771268 -0.076483

60 1 0 -1.285234 -6.354488 2.601738

61 1 0 0.260758 -4.862266 -2.694179

62 1 0 6.540766 -1.893884 -0.899201

63 1 0 4.771130 -1.878085 -4.581514

64 1 0 8.535828 1.793843 -2.124993

65 1 0 -5.748184 -4.469169 0.441037

66 1 0 0.031016 3.705902 0.348615

67 1 0 2.769716 2.155588 -2.036326

68 1 0 -1.053072 1.142005 0.305917

69 1 0 4.160825 0.816570 -5.245538

70 1 0 -3.874417 2.273677 2.802771

71 1 0 -2.171328 3.006268 -0.071530

72 1 0 -5.682405 0.681234 2.780547

73 1 0 1.280560 0.493994 -2.374458

74 1 0 -2.538206 -0.331119 0.623004

75 1 0 3.950904 3.551425 -0.897148

76 6 0 -3.620525 4.397889 -1.663769

77 7 0 -3.154138 3.195975 -1.223059

78 6 0 -3.561896 2.088984 -1.871220

79 6 0 -4.446506 2.136723 -2.955521

80 6 0 -4.851557 3.426001 -3.337161

81 7 0 -4.458802 4.549238 -2.712545

82 1 0 -3.158663 1.139439 -1.532346

83 6 0 -3.176360 5.573873 -0.988901

84 6 0 -2.799479 6.596765 -0.436002

85 6 0 -2.332224 7.828668 0.219181

86 6 0 -3.110001 9.042275 -0.354440

87 1 0 -4.186326 8.943398 -0.168419

88 1 0 -2.757471 9.963364 0.128585

89 1 0 -2.953014 9.135295 -1.435856

90 6 0 -0.813748 7.998222 -0.061813

91 1 0 -0.449687 8.901439 0.445945

92 1 0 -0.244421 7.135812 0.303206

93 1 0 -0.624224 8.104456 -1.136858

94 6 0 -2.577482 7.721378 1.748496

95 1 0 -3.646729 7.610904 1.966318

96 1 0 -2.049783 6.861742 2.176913

97 1 0 -2.216704 8.636200 2.237692

98 6 0 -4.863873 0.861728 -3.679124

99 1 0 -4.959664 1.119772 -4.752394

100 8 0 -3.849389 -0.102300 -3.499612

101 1 0 -3.764494 -5.304246 3.069836

102 30 0 -4.284838 -1.847701 -3.338493

103 6 0 -6.272508 0.329224 -3.237912

104 1 0 -6.396160 -0.598331 -3.829829

105 6 0 -7.420657 1.277143 -3.615364

106 1 0 -8.390762 0.797036 -3.431776

107 1 0 -7.392522 2.197639 -3.016162

108 1 0 -7.382332 1.557346 -4.677129

109 6 0 -6.328170 -0.051830 -1.750652

110 1 0 -5.521017 -0.745472 -1.479197

111 1 0 -6.231203 0.832542 -1.107097

112 1 0 -7.280587 -0.542065 -1.512373

113 6 0 -4.764452 -3.713987 -3.435308

114 1 0 -4.627176 -4.005035 -4.490882

115 6 0 -6.258920 -3.889006 -3.095804

116 1 0 -6.911683 -3.296629 -3.753602

117 1 0 -6.572352 -4.942786 -3.199157

118 1 0 -6.478690 -3.589161 -2.060910

119 6 0 -3.891897 -4.646024 -2.577548

120 1 0 -3.970076 -4.404632 -1.508112

121 1 0 -4.201593 -5.699675 -2.696627

122 1 0 -2.828221 -4.585061 -2.842866

123 1 0 3.233157 4.716558 2.376106

124 1 0 6.117865 4.004458 -0.250213

125 1 0 -0.286536 4.600738 2.192827

126 8 0 2.067221 -2.614818 2.947079

127 1 0 1.279141 -3.211751 2.879613

128 1 0 6.165698 0.300887 3.160860

129 1 0 5.173322 -1.958762 0.908992

130 1 0 1.110447 -0.549886 5.588289

131 1 0 -1.174058 0.918477 5.877860

132 1 0 -0.688460 -2.530361 2.741220

133 1 0 3.237937 -2.899461 1.709506

134 1 0 -5.508556 3.571466 -4.195982
