

SUPPORTING INFORMATION

The regioselectivity of the Diels-Alder cycloaddition to C₆₀ in high spin states

Ouissam El Bakouri^a, Marc Garcia-Borràs^{a,b}, Rosa M. Girón^c, Salvatore Filippone^c,
Nazario Martín^{c,d*} and Miquel Solà^{a*}

^a *Institut de Química Computacional i Catàlisi (IQCC) and Departament de Química, Universitat de Girona, c/ Maria Aurèlia Capmany 6, 17003 Girona, Spain. E-mail: miquel.sola@udg.edu*

^b *Department of Chemistry and Biochemistry, University of California, Los Angeles 607 Charles E Young Drive East, Los Angeles (CA), 90095 (USA)*

^c *Departamento de Química Orgánica, Facultad de Química, Universidad Complutense, Avda. Complutense s/n E-28040 Madrid, Spain.*

^d *IMDEA–Nanociencia, C/ Faraday, 9, Campus de Cantoblanco, E-28049 Madrid, Spain.*

Table S1. MCI, I_{NB}, and HOMA results for the equivalent 5-MRs of ^{2S+1}C₆₀. The total summation was also computed for each aromaticity index. MCI and I_{NB} in electrons.

Table S2. MCI, I_{NB}, and HOMA results for the equivalent 6-MRs of ^{2S+1}C₆₀. The total summation was also computed for each aromaticity index. MCI and I_{NB} in electrons.

Table S3. MCI and I_{NB} results for the equivalent 5-MRs of ^{2S+1}C₇₀. The total summation was also computed for each aromaticity index. MCI and I_{NB} in electrons.

Table S4. MCI and I_{NB} results for the equivalent 6-MRs of ^{2S+1}C₇₀. The total summation was also computed for each aromaticity index. MCI and I_{NB} in electrons.

Table S5. Gibbs and electronic reaction energies and energy barriers (kcal/mol) for the reaction between ^{2S+1}C₆₀ (S = 1–6) and cyclopentadiene to get [5,6] and [6,6] additions.

Table S6. Reactant-complex Gibbs and electronic stabilization energies, reaction barriers for the formation of intermediate pro-int[6,6], and the sigma bond rotation barriers of the reaction between $^{2S+1}C_{60}$ and cyclopentadiene. Energies in kcal/mol.

Table S7. B3LYP-D3/6-31G(d) Gibbs and electronic reaction energies and energy barriers (kcal/mol) for the reaction between $^3C_{60}$ and isoindene.

Table S8. B3LYP-D3/6-31G(d) Gibbs and electronic energy barriers (kcal/mol) for the reaction between C_{60} and isoindene in open-shell singlet and triplet states.

Table S9. Gibbs and electronic stabilization energies of the reactant-complex and energy barriers for the formation of the diradical intermediate of the reaction between $^{2S+1}C_{60}$ and isoindene. Energies in kcal/mol.

Figure 1. Electronic energy profiles (Gibbs energies in gas-phase/toluene solution in parenthesis, kcal/mol) for the reaction between C_{60} and isoindene in the closed or open-shell (OS) singlet and triplet states at B3LYP-D3/6-31G(d) level ($\Delta E^{ISC}([5,6]) = E_{crossing}([5,6]) - E_{pro-int}([5,6]^{T1})$; $\Delta E^{ISC}([6,6]) = E_{crossing}([6,6]) - E_{pro-int}([6,6]^{T1})$). Values in italics correspond to biradical open-shell singlet species.

Table S10. a) Gibbs and electronic reaction energies and energy barriers and b) reactant-complex Gibbs and electronic stabilization energies and energy barriers for the formation of the diradical intermediate for the reaction between $^{2S+1}C_{60}$ and indene. Energies in kcal/mol.

Table S11. S^2 value of all the optimized stationary points for the DA between C_{60} and cyclopentadienyl (Cp) (S=1-6) at B3LYP-D3/6-31G(d).

Table S12. S^2 value of all the optimized stationary points for the DA between C_{60} and isoindene (OS- S_0 and T_1) at B3LYP-D3/6-31G(d).

Table S13. Cartesian xyz coordinates (in Å) of all the optimized stationary points at B3LYP-D3/6-31G(d).

Experimental Section.

Table S14. Reagents concentrations, type of irradiation and condition in the cycloaddition of indene and C_{60} .

Table S1. MCI, I_{NB} , and HOMA results for the equivalent 5-MRs of $2S+1C_{60}$. The total summation was also computed for each aromaticity index. MCI and I_{NB} in electrons.

5-MRs					
2S+1	Ring	MCI	I_{NB}	HOMA	Eq. rings
1	Ring 1	0.011061	0.032522	-0.153337	12
3	Ring 1	0.011842	0.032969	-0.096620	10
	Ring 2	0.012257	0.033197	-0.094534	2
5	Ring 1	0.013947	0.034066	0.049944	6
	Ring 2	0.012699	0.033433	-0.065059	5
	Ring 9	0.013944	0.034064	0.032837	1
7	Ring 1	0.015213	0.034663	0.062549	5
	Ring 3	0.016198	0.035101	0.154570	3
	Ring 4	0.015464	0.034777	0.107303	4
9	Ring 1	0.018260	0.035952	0.155851	5
	Ring 3	0.017437	0.035622	0.189038	3
	Ring 4	0.017838	0.035784	0.141094	4
11	Ring 1	0.020741	0.036880	0.246639	2
	Ring 2	0.020897	0.036935	0.247828	3
	Ring 3	0.019470	0.036417	0.221623	3
	Ring 4	0.023069	0.037673	0.283045	4
13	Ring 1	0.024438	0.038110	0.300976	12

2S+1	$\sum_{5-MRs} MCI$	$\sum_{5-MRs} I_{NB}$	$\sum_{5-MRs} HOMA$
1	0.132732	0.390264	-1.840044
3	0.142934	0.396084	-1.155268
5	0.161121	0.405625	0.007206
7	0.186515	0.417726	1.205667
9	0.214963	0.429762	1.910745
11	0.254859	0.444508	3.033811
13	0.293256	0.457320	3.611712

Table S2. MCI, I_{NB} , and HOMA results for the equivalent 6-MRs of $^{2S+1}C_{60}$. The total summation was also computed for each aromaticity index. MCI and I_{NB} in electrons.

6-MRs 2S+1	Ring	MCI	I_{NB}	HOMA	Eq. rings
1	Ring 13	0.017116	0.032335	0.416394	20
3	Ring 13	0.012390	0.030640	0.370529	9
	Ring 16	0.017332	0.030631	0.420038	11
5	Ring 13	0.011725	0.030359	0.446230	11
	Ring 16	0.014022	0.031278	0.424804	6
	Ring 17	0.013958	0.031254	0.403881	3
7	Ring 13	0.010043	0.029586	0.413583	3
	Ring 14	0.009998	0.029564	0.409440	3
	Ring 15	0.011262	0.030156	0.462366	8
	Ring 16	0.010739	0.029918	0.430032	5
	Ring 26	0.013383	0.031036	0.461007	1
9	Ring 13	0.010055	0.029592	0.416243	6
	Ring 15	0.009667	0.029398	0.392042	8
	Ring 16	0.009826	0.029478	0.414343	5
	Ring 26	0.010474	0.029794	0.392077	1
11	Ring 13	0.009051	0.029078	0.377516	14
	Ring 16	0.009234	0.029175	0.378601	5
	Ring 26	0.008756	0.028917	0.388812	1
13	Ring 13	0.008488	0.028768	0.402395	8
	Ring 14	0.007117	0.027936	0.235929	12

2S+1	$\sum_{6-MRs} MCI$	$\sum_{6-MRs} I_{NB}$	$\sum_{5-MRs} HOMA$
1	0.342320	0.646700	8.327880
3	0.303238	0.632564	7.955179
5	0.250837	0.613710	8.668997
7	0.218201	0.599744	8.779164
9	0.198197	0.590378	8.097586
11	0.182659	0.582417	7.567041
13	0.154120	0.565864	6.050308

Table S3. MCI and I_{NB} results for the equivalent 5-MRs of $^{2S+1}C_{70}$. The total summation was also computed for each aromaticity index. MCI and I_{NB} in electrons.

5-MRs				
2S+1	Ring	MCI	I_{NB}	Eq. Ring
1	Ring 1	0.0127890	0.0334800	12
3	Ring 1	0.0132300	0.0337080	1
	Ring 2	0.0128440	0.0335090	2
	Ring 3	0.0127000	0.0334340	2
	Ring 4	0.0126410	0.0334030	2
	Ring 5	0.0125100	0.0333330	2
	Ring 6	0.0133530	0.0337710	2
	Ring 10	0.0132350	0.0337110	1
5	Ring 1	0.0138050	0.0339960	4
	Ring 2	0.0124730	0.0333140	4
	Ring 3	0.0106990	0.0323070	2
	Ring 4	0.0150190	0.0345740	2
7	Ring 1	0.0150600	0.0345930	10
	Ring 3	0.0132700	0.0337280	2
9	Ring 1	0.0156440	0.0348570	4
	Ring 2	0.0170130	0.0354470	4
	Ring 3	0.0157790	0.0349170	2
	Ring 4	0.0180630	0.0358740	2
11	Ring 1	0.018512	0.036051	7
	Ring 3	0.017498	0.035647	1
	Ring 7	0.019122	0.036285	4
13	Ring 1	0.0197730	0.0365290	4
	Ring 2	0.0207890	0.0368970	4
	Ring 3	0.0236890	0.0378730	2
	Ring 4	0.0213770	0.0371030	2

2S+1	$\sum_{5-MR} MCI$	$\sum_{5-MR} I_{NB}$
1	0.153468	0.401760
3	0.154561	0.402319
5	0.156548	0.403002
7	0.177140	0.413386
9	0.198312	0.422798
11	0.223570	0.433144
13	0.252380	0.443656

Table S4. MCI and I_{NB} results for the equivalent 6-MRs of $^{2S+1}C_{70}$. The total summation was also computed for each aromaticity index. MCI and I_{NB} in electrons.

6-MRs				
2S+1	Ring	MCI	I_{NB}	Eq. Ring
1	Ring 13	0.016699	0.032202	10
	Ring 14	0.011907	0.030437	10
	Ring 15	0.020584	0.033345	5
3	Ring 13	0.013485	0.031075	2
	Ring 14	0.010502	0.029807	4
	Ring 15	0.015754	0.031891	3
	Ring 16	0.016908	0.032269	4
	Ring 17	0.012325	0.030613	2
	Ring 18	0.019630	0.033082	1
	Ring 19	0.014097	0.031306	3
	Ring 20	0.009957	0.029543	2
	Ring 21	0.021997	0.033716	1
	Ring 24	0.011874	0.030423	2
	Ring 27	0.024132	0.034240	1
	5	Ring 13	0.012655	0.030748
Ring 14		0.011507	0.030264	2
Ring 15		0.016790	0.032232	2
Ring 16		0.013760	0.031180	4
Ring 17		0.014662	0.031512	4
Ring 18		0.006891	0.027786	2
Ring 20		0.013521	0.031089	4
Ring 21		0.018021	0.032614	1
Ring 22		0.016950	0.032283	2
7	Ring 13	0.013090	0.030922	8
	Ring 14	0.012851	0.030827	12
	Ring 15	0.011685	0.030342	5
9	Ring 13	0.012185	0.030555	8
	Ring 14	0.012768	0.030794	8
	Ring 15	0.011091	0.030079	2
	Ring 16	0.009465	0.029295	4
	Ring 18	0.007482	0.028169	2
	Ring 21	0.005722	0.026938	1
11	Ring 13	0.010130	0.029629	4
	Ring 14	0.009700	0.029415	3
	Ring 15	0.007203	0.027992	4
	Ring 17	0.011832	0.030405	5
	Ring 21	0.005951	0.027115	1
	Ring 28	0.009026	0.029064	4
	Ring 29	0.012104	0.030521	2
	Ring 36	0.015731	0.031884	1
	Ring 37	0.008150	0.028574	1

13	Ring 13	0.006900	0.027792	5
	Ring 14	0.013162	0.030950	2
	Ring 15	0.006327	0.027393	2
	Ring 16	0.008535	0.028794	4
	Ring 17	0.011525	0.030272	4
	Ring 20	0.010070	0.029599	4
	Ring 22	0.005890	0.027068	2
	Ring 23	0.006642	0.027616	2

2S+1	$\sum_{6-MR} MCI$	$\sum_{6-MR} I_{NB}$	MCI_{6-MR}	I_{NB}_{6-MR}
1	0.38898	0.793115	0.015559	0.031725
3	0.360234	0.782241	0.014409	0.031290
5	0.340689	0.775860	0.013628	0.031034
7	0.317357	0.769010	0.012694	0.030760
9	0.280352	0.751406	0.011214	0.030056
11	0.247736	0.735625	0.009909	0.029425
13	0.219062	0.719674	0.008762	0.028787

Table S5. Gibbs and electronic reaction energies and energy barriers (kcal/mol) for the reaction between $^{2S+1}C_{60}$ ($S = 1-6$) and cyclopentadiene to get [5,6] and [6,6] additions.

S	$\Delta E_R[5,6]$	$\Delta E_R[6,6]$	$\Delta E^\ddagger [5,6]$	$\Delta E^\ddagger [6,6]$	$\Delta\Delta E_R ([6,6]-[5,6])$	$\Delta\Delta E^\ddagger ([6,6]-[5,6])$
0	-3.20	-23.07	23.81	10.26	-13.55	-19.87
1	-29.80	-25.68	9.57	19.13	9.56	4.13
2	-31.59	-26.85	9.31	19.02	9.71	4.74
3	-30.18	-21.70	11.33	21.79	10.47	8.48
4	-34.39	-21.67	11.63	26.75	15.13	12.72
5	-29.37	-16.27	14.35	28.92	14.57	13.10
6	-34.07	-13.73	16.87	33.98	17.11	20.33

S	$\Delta G_R[5,6]$	$\Delta G_R[6,6]$	$\Delta G^\ddagger [5,6]$	$\Delta G^\ddagger [6,6]$	$\Delta\Delta G_R ([6,6]-[5,6])$	$\Delta\Delta G^\ddagger ([6,6]-[5,6])$
0	14.46	-4.82	28.17	14.53	-13.64	-19.29
1	-10.11	-6.97	11.31	19.36	8.05	3.14
2	-10.92	-7.49	11.23	18.75	7.52	3.43
3	-9.29	-2.44	13.20	22.55	9.35	6.85
4	-13.03	-2.28	14.16	27.34	13.17	10.75
5	-8.98	2.81	16.73	29.49	12.77	11.79
6	-12.84	5.06	18.94	34.14	15.20	17.90

Table S6. For the reaction between $^{2S+1}C_{60}$ and cyclopentadiene, reactant-complex Gibbs and electronic stabilization energies, reaction barriers for the formation of intermediate pro-int[6,6], and C–C bond rotation energy barriers for the transformation of pro-int[6,5] to pro-int[5,6]. Energies in kcal/mol.

S	$\Delta E(\text{reactant-complex})$	$\Delta G(\text{reactant-complex})$	$\Delta E^{\ddagger}_{\text{pro-int}[6,6]}$	$\Delta G^{\ddagger}_{\text{pro-int}[6,6]}$	$\Delta E^{\ddagger}_{(\text{rot})}^a$	$\Delta G^{\ddagger}_{(\text{rot})}^a$
0	-6.52	3.85	-	-	-	-
1	-8.24	3.67	5.16	7.08	6.71	7.26
2	-8.57	3.57	4.05	5.49	6.50	7.26
3	-8.59	5.21	3.48	3.52	6.58	6.68
4	-9.48	3.94	0.97	1.75	6.22	6.91
5	-8.73	3.10	0.81	2.45	6.28	6.62
6	-19.94	-7.46	0.26	1.83	6.36	6.40

^a From pro-int[6,6] to the transition state that leads to pro-int[5,6]

Table S7. B3LYP-D3/6-31G(d) Gibbs and electronic reaction energies and energy barriers (kcal/mol) for the reaction between closed- and open-shell singlet and triplet C₆₀ and isoindene. ΔE^\ddagger and ΔG^\ddagger calculated as the difference between the TS_{adduct} and the pro-int[5,6] or pro-int[6,6].

S	$\Delta E_R[5,6]$	$\Delta E_R[6,6]$	$\Delta E^\ddagger [5,6]$	$\Delta E^\ddagger [6,6]$	$\Delta\Delta E_R ([6,6]-[5,6])$	$\Delta\Delta E^\ddagger ([6,6]-[5,6])$
0	-28.52	-48.72	12.44	2.10	-20.20	-10.34
OS-S ₀	-6.03	-26.22	1.54	-	-20.19	-
1	-55.19	-49.05	6.83	16.70	6.14	9.87

S	$\Delta G_R[5,6]$	$\Delta G_R[6,6]$	$\Delta G^\ddagger [5,6]$	$\Delta G^\ddagger [6,6]$	$\Delta\Delta G_R ([6,6]-[5,6])$	$\Delta\Delta G^\ddagger ([6,6]-[5,6])$
0	-10.18	-29.60	14.30	4.00	-19.43	-10.30
OS-S ₀	-10.18	-29.60	2.70	-	-19.42	-
1	-34.76	-30.06	7.89	16.63	4.70	8.74

Table S8. B3LYP-D3/6-31G(d) Gibbs and electronic energy barriers (kcal/mol) for the reaction between C₆₀ and isoindene in open-shell singlet and triplet states. ΔE^\ddagger and ΔG^\ddagger calculated as the difference between the TS_{biradical} and the reactant complex.

S	$\Delta E^\ddagger_{\text{pro-int}[5,6]}$	$\Delta E^\ddagger_{\text{pro-int}[6,6]}$
0 (OS-S)	13.11	13.11
1	0.98	2.00

S	$\Delta G^\ddagger_{\text{pro-int}[5,6]}$	$\Delta G^\ddagger_{\text{pro-int}[5,6]}$
0 (OS-S)	13.24	13.24
1	1.59	2.34

Table S9. Gibbs and electronic stabilization energies of the reactant-complex and energy barriers for the formation of the diradical intermediate of the reaction between $^{2S+1}C_{60}$ and isoindene. Energies in kcal/mol.

S	$\Delta E(\text{complex-reactants})$	$\Delta G(\text{complex-reactants})$	$\Delta E^{\#}_{(\text{rot})}^a$	$\Delta G^{\#}_{(\text{rot})}^a$
0	-11.66	1.09	-	-
OS-S	-11.66	1.09	-	-
1	-25.44	-9.85	7.07	8.07

^a From pro-int[6,6] to the rotation transition state.

Figure S1. Electronic energy profiles (Gibbs energies in gas-phase/toluene solution in parenthesis, kcal/mol) for the reaction between C_{60} and isoindene in the closed or open-shell (OS) singlet and triplet states at B3LYP-D3/6-31G(d) level ($\Delta E^{ISC}([5,6]) = E_{crossing}([5,6]) - E_{pro-int}([5,6]^{T1})$; $\Delta E^{ISC}([6,6]) = E_{crossing}([6,6]) - E_{pro-int}([6,6]^{T1})$). Values in italics correspond to biradical open-shell singlet species.

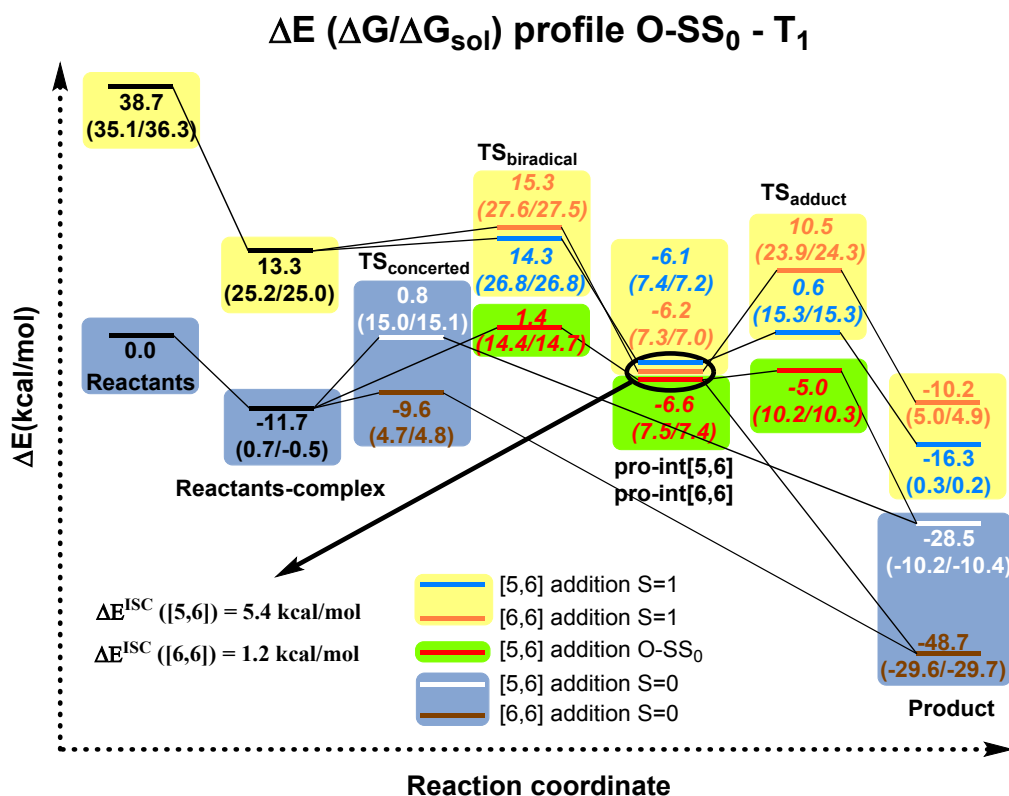


Table S10. a) Gibbs and electronic reaction energies and energy barriers and b) reactant-complex Gibbs and electronic stabilization energies and energy barriers for the formation of the diradical intermediate for the reaction between $^{2S+1}C_{60}$ and indene. Energies in kcal/mol.

a)

S	$\Delta E_R[5,6]$	$\Delta E_R[6,6]$	$\Delta E^\# [5,6]$	$\Delta E^\# [6,6]$	$\Delta \Delta E_R ([6,6]-[5,6])$	$\Delta \Delta E^\# ([6,6]-[5,6])$
0	22.59	3.22	39.54	22.88	-19.36	-16.66
1	-32.55	-26.13	20.72	27.12	6.42	6.40

b)

S	$\Delta E(\text{complex-reactants})$	$\Delta E^\#_{\text{pro-int}[6,6]}$
0	-10.84	-
1	-11.64	6.25

Table S11. S^2 value of all the optimized stationary points for the DA between C_{60} and cyclopentadienyl (Cp) (S=1-6) at B3LYP-D3/6-31G(d).

	S					
	1	2	3	4	5	6
${}^{2S+1}C_{60}$	2.00	6.01	12.00	20.01	30.01	42.03
Pre-react	2.01	6.01	12.01	20.02	30.02	42.06
TS _{bir} [5,6]	2.03	6.06	12.03	20.03	30.03	42.03
Proint[5,6]	2.07	6.06	12.06	20.05	30.05	42.06
TS _{bir} [6,6]	2.04	6.05	12.03	20.03	30.03	42.03
Proint[6,6]	2.07	6.07	12.06	20.05	30.05	42.06
TS[5,6]	2.06	6.03	12.05	20.04	30.06	42.06
Prod[5,6]	2.05	6.04	12.04	20.04	30.05	42.05
TS[6,6]	2.04	6.04	12.04	20.06	30.03	42.04
Prod[6,6]	2.01	6.01	12.02	20.02	30.02	42.04

Table S12. S^2 value of all the optimized stationary points for the DA between C_{60} and isoindene ($OS-S_0$ and T_1) at B3LYP-D3/6-31G(d).

	S	
	$OS-S_0$	T_1
Pre-react	0.00	2.02
TS _{bir} [5,6]	0.23	2.04
Proint[5,6]	0.98	2.07
TS _{bir} [6,6]	0.23	2.04
Proint[6,6]	-	2.07
TS[5,6]	0.65	2.06
Prod[5,6]	0.00	2.05
TS[6,6]	-	2.04
Prod[6,6]	0.00	2.01

Table S13. Cartesian xyz coordinates (in Å) of all the optimized stationary points at B3LYP-D3/6-31G(d).

C₆₀ + CPD

C₅H₆

E=-194.1159158

G=-194.049579

C	0.000034000	-1.216860000	0.000348000
H	0.000058000	-1.880844000	-0.877641000
H	0.000046000	-1.880132000	0.878899000
C	1.181093000	-0.281739000	-0.000340000
H	2.213488000	-0.611153000	-0.000543000
C	0.734885000	0.991017000	0.000108000
H	1.346866000	1.886964000	0.000213000
C	-1.181078000	-0.281804000	-0.000363000
H	-2.213454000	-0.611275000	-0.000582000
C	-0.734940000	0.990976000	0.000144000
H	-1.346970000	1.886890000	0.000268000

S=0

¹C₆₀

E=-2286.490509

G=-2286.156523

C	-1.694489000	-0.065437000	3.120423000
C	-1.376577000	1.347887000	2.983997000
C	-2.020003000	2.116872000	2.014326000
C	-3.008692000	1.505346000	1.139162000
C	-3.313307000	0.150557000	1.270168000
C	-2.642663000	-0.651407000	2.281971000
C	-0.463816000	-0.775031000	3.434392000
C	0.614787000	0.199554000	3.491647000
C	0.050880000	1.511392000	3.213074000

C	0.776238000	2.437702000	2.464024000
C	-1.263075000	3.082250000	1.231955000
C	-2.863440000	2.093891000	-0.183562000
C	-3.029054000	1.302999000	-1.320653000
C	-3.346919000	-0.110179000	-1.183867000
C	-3.486141000	-0.674337000	0.084172000
C	-2.922367000	-1.986327000	0.363050000
C	-2.400791000	-1.972099000	1.721343000
C	-1.220877000	-2.652314000	2.022533000
C	-0.231889000	-2.041246000	2.897465000
C	1.881092000	-0.132035000	3.009931000
C	2.122919000	-1.452687000	2.449098000
C	1.088694000	-2.387043000	2.393927000
C	0.915882000	-3.212199000	1.208197000
C	-0.511558000	-3.375803000	0.978361000
C	-1.011301000	-3.389407000	-0.323747000
C	-2.242168000	-2.679911000	-0.637874000
C	-2.096797000	-2.091529000	-1.960577000
C	-2.637641000	-0.833891000	-2.227943000
C	-1.784382000	3.068249000	-0.126250000
C	0.463816000	0.775031000	-3.434392000
C	0.231890000	2.041246000	-2.897465000
C	1.220877000	2.652313000	-2.022533000
C	2.400791000	1.972099000	-1.721343000
C	2.642663000	0.651408000	-2.281971000
C	1.376577000	-1.347887000	-2.983997000
C	-0.050880000	-1.511392000	-3.213074000
C	-0.614787000	-0.199554000	-3.491647000
C	-1.881092000	0.132035000	-3.009931000
C	-2.122919000	1.452687000	-2.449098000
C	-1.088694000	2.387043000	-2.393926000
C	0.511558000	3.375803000	-0.978361000

C	1.011301000	3.389407000	0.323747000
C	2.242168000	2.679911000	0.637874000
C	2.922368000	1.986327000	-0.363050000
C	3.486141000	0.674338000	-0.084172000
C	3.313307000	-0.150557000	-1.270168000
C	3.008692000	-1.505346000	-1.139162000
C	2.020003000	-2.116872000	-2.014326000
C	-0.776238000	-2.437703000	-2.464024000
C	-0.105152000	-3.239706000	-1.452313000
C	1.263075000	-3.082250000	-1.231955000
C	1.784381000	-3.068249000	0.126250000
C	2.863440000	-2.093891000	0.183562000
C	3.029054000	-1.302999000	1.320653000
C	3.346919000	0.110180000	1.183867000
C	2.637641000	0.833891000	2.227943000
C	2.096797000	2.091529000	1.960576000
C	-0.915883000	3.212199000	-1.208197000
C	0.105152000	3.239706000	1.452313000
C	1.694489000	0.065437000	-3.120423000

pre-reactants

E=-2480.616821

G=-2480.199972

C	1.327518000	1.741065000	2.305783000
C	1.138889000	2.537852000	1.177335000
C	-0.207193000	2.859128000	0.727104000
C	-1.310062000	2.367219000	1.424705000
C	-1.113939000	1.534161000	2.601607000
C	0.176388000	1.228003000	3.033855000
C	-2.460441000	1.855311000	0.697818000
C	-2.460441000	1.855311000	-0.697818000
C	-1.310062000	2.367219000	-1.424705000

C	-0.207193000	2.859128000	-0.727104000
C	-2.975671000	0.704600000	-1.424654000
C	-2.144209000	0.506684000	-2.602237000
C	-1.113939000	1.534161000	-2.601607000
C	0.176388000	1.228003000	-3.033855000
C	0.492688000	-0.119110000	-3.482116000
C	-0.494662000	-1.104542000	-3.482431000
C	-1.840670000	-0.785026000	-3.032824000
C	1.839048000	-0.438838000	-3.032588000
C	2.142757000	-1.730517000	-2.602302000
C	1.112718000	-2.758400000	-2.602592000
C	-0.178128000	-2.451327000	-3.032592000
C	2.974472000	-1.927951000	-1.424921000
C	2.458823000	-3.077478000	-0.697411000
C	1.308109000	-3.590349000	-1.424987000
C	0.204880000	-4.082155000	-0.727444000
C	0.204880000	-4.082155000	0.727444000
C	1.308109000	-3.590349000	1.424987000
C	2.458823000	-3.077478000	0.697411000
C	2.974472000	-1.927951000	1.424921000
C	2.142757000	-1.730517000	2.602302000
C	1.112718000	-2.758400000	2.602592000
C	-0.178128000	-2.451327000	3.032592000
C	-0.494662000	-1.104542000	3.482431000
C	0.492688000	-0.119110000	3.482116000
C	1.839048000	-0.438838000	3.032588000
C	2.355305000	0.710603000	2.305411000
C	-2.144209000	0.506684000	2.602237000
C	-1.840670000	-0.785026000	3.032824000
C	3.153672000	0.521081000	1.177307000
C	3.469544000	-0.825954000	0.727562000
C	-1.141600000	-3.762713000	1.177044000

C	-1.329195000	-2.964728000	2.305506000
C	-2.356966000	-1.934602000	2.305810000
C	3.469544000	-0.825954000	-0.727562000
C	-1.329195000	-2.964728000	-2.305506000
C	-1.141600000	-3.762713000	-1.177044000
C	-1.973561000	-3.564774000	0.000000000
C	-2.356966000	-1.934602000	-2.305810000
C	-3.154149000	-1.744570000	-1.177045000
C	-2.958295000	-2.577067000	0.000000000
C	1.327518000	1.741065000	-2.305783000
C	2.355305000	0.710603000	-2.305411000
C	3.153672000	0.521081000	-1.177307000
C	-3.470716000	-0.397454000	-0.727501000
C	1.138889000	2.537852000	-1.177335000
C	-3.154149000	-1.744570000	1.177045000
C	-3.470716000	-0.397454000	0.727501000
C	-2.975671000	0.704600000	1.424654000
C	1.972049000	2.340087000	0.000000000
C	2.957803000	1.353491000	0.000000000
C	0.289843000	6.103006000	-1.180223000
C	0.289843000	6.103006000	1.180223000
C	-0.982479000	6.165227000	0.733932000
C	-0.982479000	6.165227000	-0.733932000
C	1.223740000	6.065369000	0.000000000
H	0.618383000	6.080424000	-2.212353000
H	-1.877170000	6.198883000	-1.346384000
H	-1.877170000	6.198883000	1.346384000
H	0.618383000	6.080424000	2.212353000
H	1.851673000	5.162734000	0.000000000
H	1.920642000	6.917261000	0.000000000

TS[5,6]

E=-2480.578872

G=-2480.155073

C	-3.173766000	0.691008000	-0.391612000
C	-3.013364000	-0.749703000	0.096545000
C	-2.554292000	-1.011987000	1.403930000
C	-2.184109000	0.043282000	2.296788000
C	-2.153899000	1.379054000	1.811527000
C	-2.534980000	1.687190000	0.492407000
C	-2.483581000	0.657007000	-1.757553000
C	-2.178275000	-0.706058000	-2.118212000
C	-2.458928000	-1.558180000	-0.979005000
C	-1.661398000	-2.671270000	-0.727570000
C	-1.703075000	-2.165560000	1.680646000
C	-1.078376000	-0.434025000	3.126766000
C	-0.027064000	0.413610000	3.473301000
C	-0.016210000	1.798497000	2.998377000
C	-1.048464000	2.269681000	2.200981000
C	-0.759681000	3.124726000	1.070068000
C	-1.673719000	2.740901000	0.003634000
C	-1.252577000	2.774045000	-1.320110000
C	-1.651612000	1.670745000	-2.204110000
C	-1.101735000	-1.008030000	-2.964098000
C	-0.254441000	0.057990000	-3.451420000
C	-0.521382000	1.372553000	-3.065564000
C	0.570732000	2.265735000	-2.714332000
C	0.119848000	3.124028000	-1.629273000
C	1.010329000	3.481349000	-0.610164000
C	0.556537000	3.477508000	0.770153000
C	1.640430000	2.983660000	1.602053000
C	1.358609000	2.161264000	2.695326000
C	-0.792361000	-1.809258000	2.751296000
C	3.559888000	-0.658801000	1.763747000

C	2.744624000	-1.689953000	2.228368000
C	2.351031000	-2.766189000	1.330242000
C	2.787225000	-2.764233000	0.006054000
C	3.639519000	-1.688254000	-0.480118000
C	4.023046000	0.718500000	-0.088722000
C	3.570441000	1.569780000	1.002183000
C	3.281412000	0.717622000	2.146135000
C	2.195756000	1.005430000	2.972524000
C	1.340014000	-0.070331000	3.453581000
C	1.614298000	-1.393111000	3.095648000
C	0.976919000	-3.129087000	1.644270000
C	0.097102000	-3.475629000	0.618645000
C	0.552171000	-3.471126000	-0.763077000
C	1.869321000	-3.124880000	-1.063883000
C	2.155220000	-2.273744000	-2.209478000
C	3.247338000	-1.385455000	-1.845632000
C	3.252356000	-0.062987000	-2.297705000
C	3.647837000	1.009821000	-1.400399000
C	2.768644000	2.678307000	0.735848000
C	2.375960000	2.982429000	-0.634194000
C	2.809272000	2.167355000	-1.679551000
C	1.885810000	1.801012000	-2.741965000
C	2.162938000	0.424193000	-3.127438000
C	1.116408000	-0.427771000	-3.479667000
C	1.111374000	-1.805691000	-3.009012000
C	-0.261881000	-2.164183000	-2.694276000
C	-0.535076000	-2.973525000	-1.592359000
C	0.523424000	-2.279659000	2.735250000
C	-1.271028000	-2.981044000	0.641041000
C	4.015679000	-0.656567000	0.381391000
C	-4.883166000	1.003753000	-0.556423000
C	-5.521118000	-1.176131000	-0.037789000

C	-5.769013000	-0.378310000	1.082416000
C	-5.471803000	0.942607000	0.772457000
H	-5.483083000	1.766887000	1.475432000
H	-6.046193000	-0.744203000	2.064522000
H	-5.597980000	-2.255224000	-0.083205000
H	-4.950980000	1.938242000	-1.111064000
C	-5.397268000	-0.279864000	-1.227740000
H	-6.400168000	-0.066308000	-1.628797000
H	-4.784829000	-0.663685000	-2.043762000

TS[6,6]

E=-2480.600470

G=-2480.176809

C	-2.530688000	1.423949000	1.043383000
C	-3.065775000	0.730513000	-0.153398000
C	-3.065689000	-0.730412000	-0.153463000
C	-2.530740000	-1.423958000	1.043290000
C	-2.159500000	-0.736406000	2.187270000
C	-2.159486000	0.736306000	2.187330000
C	-1.777475000	2.586041000	0.629126000
C	-1.715889000	2.586407000	-0.821948000
C	-2.432345000	1.422252000	-1.300130000
C	-1.958981000	0.734413000	-2.408333000
C	-2.432336000	-1.422079000	-1.300211000
C	-1.777543000	-2.586055000	0.628951000
C	-0.686945000	-3.035130000	1.378286000
C	-0.293588000	-2.313204000	2.570193000
C	-1.014657000	-1.178757000	2.959011000
C	-0.307319000	-0.000115000	3.436134000
C	-1.014633000	1.178577000	2.959096000
C	-0.293538000	2.313033000	2.570356000
C	-0.686879000	3.035061000	1.378507000

C	-0.564534000	3.033370000	-1.473892000
C	0.578957000	3.486926000	-0.693886000
C	0.519293000	3.487565000	0.699049000
C	1.662284000	3.037240000	1.477182000
C	1.158590000	2.309006000	2.633439000
C	1.834942000	1.177888000	3.091635000
C	1.085987000	-0.000132000	3.504283000
C	1.834913000	-1.178136000	3.091545000
C	1.158539000	-2.309212000	2.633275000
C	-1.715939000	-2.586308000	-0.822124000
C	2.881520000	-2.603648000	-0.625374000
C	1.784659000	-3.036558000	-1.371122000
C	1.383378000	-2.308186000	-2.566322000
C	2.097600000	-1.177432000	-2.964621000
C	3.241349000	-0.728135000	-2.188694000
C	4.022627000	-0.697605000	0.152604000
C	3.523694000	-1.425494000	1.308919000
C	2.819002000	-2.603903000	0.828734000
C	1.662218000	-3.037365000	1.476961000
C	0.519218000	-3.487611000	0.698795000
C	0.578886000	-3.486886000	-0.694139000
C	-0.068778000	-2.311321000	-2.628682000
C	-0.752562000	-1.178304000	-3.080335000
C	-0.006675000	0.000131000	-3.495070000
C	1.387472000	0.000113000	-3.441104000
C	2.097623000	1.177606000	-2.964532000
C	3.241362000	0.728231000	-2.188637000
C	3.625175000	1.425611000	-1.042707000
C	4.022649000	0.697519000	0.152654000
C	3.040558000	-0.728111000	2.416953000
C	3.040577000	0.727884000	2.417008000
C	3.523721000	1.425334000	1.309019000

C	2.819054000	2.603788000	0.828918000
C	2.881568000	2.603635000	-0.625189000
C	1.784721000	3.036619000	-1.370899000
C	1.383429000	2.308354000	-2.566160000
C	-0.068730000	2.311526000	-2.628520000
C	-0.752535000	1.178550000	-3.080243000
C	-0.564595000	-3.033242000	-1.474106000
C	-1.958996000	-0.734189000	-2.408396000
C	3.625145000	-1.425606000	-1.042807000
C	-5.192055000	1.157156000	-0.297479000
C	-5.192298000	-1.157047000	-0.297958000
C	-5.599554000	-0.698779000	0.971359000
C	-5.599462000	0.698413000	0.971648000
H	-5.742193000	1.324216000	1.844959000
H	-5.742342000	-1.324929000	1.844412000
H	-5.213303000	2.194941000	-0.610079000
H	-5.213422000	-2.194718000	-0.610932000
C	-5.372393000	0.000257000	-1.252933000
H	-6.414853000	0.000429000	-1.609979000
H	-4.719497000	0.000362000	-2.127372000

Prod[5,6]

E=-2480.611524

G=-2480.183054

C	3.267416000	0.820694000	0.217693000
C	3.267431000	-0.820742000	0.217676000
C	2.591213000	-1.438020000	-0.972743000
C	2.214679000	-0.722245000	-2.097221000
C	2.214687000	0.722308000	-2.097230000
C	2.591200000	1.438031000	-0.972725000
C	2.476447000	1.175301000	1.479888000
C	2.157048000	-0.000045000	2.241284000

C	2.476469000	-1.175377000	1.479858000
C	1.654772000	-2.283402000	1.574872000
C	1.720315000	-2.609134000	-0.865601000
C	1.111873000	-1.435329000	-2.776790000
C	0.085712000	-0.736491000	-3.387817000
C	0.085706000	0.736601000	-3.387804000
C	1.111865000	1.435420000	-2.776767000
C	0.816686000	2.619472000	-2.002213000
C	1.720308000	2.609142000	-0.865532000
C	1.274568000	3.044405000	0.369866000
C	1.654786000	2.283332000	1.574957000
C	1.069990000	-0.000049000	3.139261000
C	0.230820000	1.169750000	3.253371000
C	0.513796000	2.285790000	2.463816000
C	-0.567983000	3.025521000	1.830750000
C	-0.099526000	3.487513000	0.535071000
C	-0.974132000	3.500196000	-0.555549000
C	-0.504124000	3.052864000	-1.854309000
C	-1.579919000	2.318477000	-2.492946000
C	-1.286889000	1.180268000	-3.251049000
C	0.816699000	-2.619404000	-2.002286000
C	-3.528323000	-1.178234000	-1.496638000
C	-2.722776000	-2.311549000	-1.592719000
C	-2.346835000	-3.042818000	-0.389384000
C	-2.793961000	-2.607588000	0.856018000
C	-3.639858000	-1.425326000	0.957458000
C	-4.000330000	0.725897000	-0.195433000
C	-3.528329000	1.178296000	-1.496598000
C	-3.232580000	0.000040000	-2.298630000
C	-2.132797000	0.000053000	-3.155357000
C	-1.286881000	-1.180162000	-3.251090000
C	-1.579909000	-2.318395000	-2.493012000

C	-0.974147000	-3.500203000	-0.555665000
C	-0.099543000	-3.487541000	0.534962000
C	-0.567989000	-3.025571000	1.830640000
C	-1.886252000	-2.602472000	1.993495000
C	-2.179833000	-1.425717000	2.800942000
C	-3.260500000	-0.700246000	2.156301000
C	-3.260497000	0.700190000	2.156326000
C	-3.639860000	1.425310000	0.957510000
C	-2.722774000	2.311609000	-1.592639000
C	-2.346831000	3.042833000	-0.389280000
C	-2.793947000	2.607573000	0.856110000
C	-1.886243000	2.602418000	1.993584000
C	-2.179822000	1.425645000	2.801001000
C	-1.143619000	0.728288000	3.421934000
C	-1.143621000	-0.728380000	3.421910000
C	0.230814000	-1.169855000	3.253324000
C	0.513789000	-2.285867000	2.463725000
C	-0.504128000	-3.052807000	-1.854398000
C	1.274570000	-3.044462000	0.369773000
C	-4.000329000	-0.725875000	-0.195461000
C	4.822824000	1.127781000	0.318936000
C	4.822636000	-1.127773000	0.318905000
C	5.435113000	-0.669836000	-0.994399000
C	5.435159000	0.669915000	-0.994406000
H	5.704088000	1.327568000	-1.812744000
H	5.703772000	-1.327446000	-1.812855000
H	5.017599000	-2.157625000	0.621856000
H	5.017579000	2.157698000	0.621917000
C	5.296050000	-0.000016000	1.256478000
H	6.381796000	-0.000225000	1.380859000
H	4.813037000	0.000015000	2.236955000

Prod[6,6]

E=-2480.643181

G=-2480.213789

C	2.571783000	-1.440316000	1.007688000
C	3.247641000	-0.804871000	-0.203426000
C	3.247642000	0.804867000	-0.203434000
C	2.571784000	1.440325000	1.007674000
C	2.202664000	0.741110000	2.135789000
C	2.202663000	-0.741089000	2.135796000
C	1.799148000	-2.583676000	0.601042000
C	1.719367000	-2.582632000	-0.849578000
C	2.440956000	-1.436244000	-1.338324000
C	1.947534000	-0.740933000	-2.419797000
C	2.440957000	1.436228000	-1.338338000
C	1.799150000	2.583681000	0.601015000
C	0.716877000	3.038011000	1.361682000
C	0.340099000	2.314938000	2.554019000
C	1.066801000	1.177452000	2.922530000
C	0.366732000	0.000017000	3.408472000
C	1.066800000	-1.177422000	2.922542000
C	0.340097000	-2.314912000	2.554043000
C	0.716875000	-3.037998000	1.361713000
C	0.559477000	-3.036539000	-1.485971000
C	-0.574179000	-3.491190000	-0.693175000
C	-0.497378000	-3.491433000	0.698385000
C	-1.630129000	-3.040650000	1.490900000
C	-1.110633000	-2.311692000	2.639472000
C	-1.779651000	-1.178585000	3.104494000
C	-1.024324000	0.000018000	3.504969000
C	-1.779651000	1.178618000	3.104482000
C	-1.110631000	2.311720000	2.639448000
C	1.719368000	2.582622000	-0.849604000

C	-2.875014000	2.605610000	-0.596722000
C	-1.787710000	3.040451000	-1.355846000
C	-1.398888000	2.311348000	-2.554735000
C	-2.115659000	1.178251000	-2.942779000
C	-3.249230000	0.728681000	-2.155132000
C	-4.003043000	0.697599000	0.194767000
C	-3.490978000	1.426214000	1.345016000
C	-2.794719000	2.605715000	0.856857000
C	-1.630127000	3.040666000	1.490869000
C	-0.497376000	3.491440000	0.698349000
C	-0.574176000	3.491183000	-0.693211000
C	0.052239000	2.314724000	-2.630161000
C	0.733168000	1.177753000	-3.077904000
C	-0.016121000	-0.000018000	-3.483247000
C	-1.409430000	-0.000017000	-3.424613000
C	-2.115660000	-1.178280000	-2.942767000
C	-3.249230000	-0.728701000	-2.155125000
C	-3.621166000	-1.426477000	-1.004841000
C	-4.003043000	-0.697594000	0.194774000
C	-2.992678000	0.728571000	2.446569000
C	-2.992679000	-0.728544000	2.446576000
C	-3.490979000	-1.426199000	1.345031000
C	-2.794721000	-2.605704000	0.856883000
C	-2.875016000	-2.605614000	-0.596695000
C	-1.787712000	-3.040464000	-1.355815000
C	-1.398890000	-2.311373000	-2.554711000
C	0.052237000	-2.314751000	-2.630138000
C	0.733168000	-1.177786000	-3.077893000
C	0.559479000	3.036523000	-1.486002000
C	1.947534000	0.740906000	-2.419803000
C	-3.621166000	1.426469000	-1.004856000
C	4.802728000	-1.123818000	-0.311365000

C	4.802730000	1.123813000	-0.311380000
C	5.429827000	0.669843000	0.993438000
C	5.429816000	-0.669831000	0.993452000
H	5.702126000	-1.329420000	1.809335000
H	5.702146000	1.329444000	1.809308000
H	4.988602000	-2.155164000	-0.613991000
H	4.988603000	2.155155000	-0.614020000
C	5.255771000	-0.000009000	-1.261798000
H	6.336808000	-0.000010000	-1.423757000
H	4.734978000	-0.000013000	-2.224203000

S=1

${}^3C_{60}$

E=-2286.428559

G=-2286.100624

C	0.604226000	2.679813000	2.225513000
C	1.850038000	2.650138000	1.458005000
C	1.851802000	3.021914000	0.119408000
C	0.607306000	3.442766000	-0.525449000
C	-0.595192000	3.477763000	0.223938000
C	-0.596847000	3.096748000	1.599042000
C	0.601782000	1.563156000	3.113620000
C	1.846416000	0.819092000	2.914911000
C	2.624589000	1.502134000	1.895920000
C	3.367213000	0.763533000	0.969255000
C	2.628114000	2.263177000	-0.846089000
C	0.607464000	2.943933000	-1.862169000
C	-0.595211000	2.478200000	-2.449962000
C	-1.841213000	2.520155000	-1.683187000
C	-1.841535000	3.007197000	-0.381803000

C	-2.619601000	2.336991000	0.645745000
C	-1.843774000	2.381092000	1.873088000
C	-1.846285000	1.293699000	2.737903000
C	-0.601786000	0.862153000	3.375942000
C	1.844052000	-0.568933000	2.975394000
C	0.596861000	-1.288633000	3.237881000
C	-0.604325000	-0.563364000	3.437889000
C	-1.850266000	-1.044353000	2.839290000
C	-2.624611000	0.109822000	2.416826000
C	-3.367499000	0.059701000	1.233109000
C	-3.364928000	1.197037000	0.328556000
C	-3.364982000	0.688234000	-1.032685000
C	-2.619469000	1.340744000	-2.019706000
C	1.851978000	2.202991000	-2.072545000
C	-0.601782000	-1.563156000	-3.113620000
C	0.601786000	-0.862153000	-3.375942000
C	1.846285000	-1.293699000	-2.737903000
C	1.843774000	-2.381092000	-1.873088000
C	0.596847000	-3.096748000	-1.599042000
C	-1.850038000	-2.650138000	-1.458005000
C	-2.624589000	-1.502134000	-1.895920000
C	-1.846416000	-0.819092000	-2.914911000
C	-1.844052000	0.568933000	-2.975394000
C	-0.596861000	1.288633000	-3.237881000
C	0.604325000	0.563364000	-3.437889000
C	2.624611000	-0.109822000	-2.416826000
C	3.367499000	-0.059701000	-1.233109000
C	3.364928000	-1.197037000	-0.328556000
C	2.619601000	-2.336991000	-0.645745000
C	1.841535000	-3.007197000	0.381803000
C	0.595192000	-3.477763000	-0.223938000
C	-0.607306000	-3.442766000	0.525449000

C	-1.851802000	-3.021914000	-0.119408000
C	-3.367213000	-0.763533000	-0.969255000
C	-3.368969000	-1.152045000	0.430914000
C	-2.628114000	-2.263177000	0.846089000
C	-1.851978000	-2.202991000	2.072545000
C	-0.607464000	-2.943933000	1.862169000
C	0.595211000	-2.478200000	2.449962000
C	1.841213000	-2.520155000	1.683187000
C	2.619469000	-1.340744000	2.019706000
C	3.364982000	-0.688234000	1.032685000
C	1.850266000	1.044353000	-2.839290000
C	3.368969000	1.152045000	-0.430914000
C	-0.604226000	-2.679813000	-2.225513000

pre-reactants

E=-2480.557608

G=-2480.144360

C	1.606668000	1.577965000	-2.293453000
C	2.416314000	1.474092000	-1.169663000
C	2.871970000	0.158987000	-0.711396000
C	2.480823000	-1.005214000	-1.427940000
C	1.653363000	-0.897063000	-2.581267000
C	1.206618000	0.373617000	-3.024093000
C	2.092048000	-2.212498000	-0.694857000
C	2.091996000	-2.212434000	0.695231000
C	2.480717000	-1.005071000	1.428225000
C	2.871928000	0.159047000	0.711588000
C	1.011551000	-2.853766000	1.423135000
C	0.728989000	-2.032307000	2.588634000
C	1.653200000	-0.896814000	2.581490000
C	1.206433000	0.373915000	3.024172000
C	-0.140006000	0.549044000	3.466981000

C	-1.038123000	-0.544106000	3.467414000
C	-0.580705000	-1.858670000	3.017888000
C	-0.600316000	1.863229000	3.018314000
C	-1.912148000	2.033043000	2.590166000
C	-2.833211000	0.899430000	2.586199000
C	-2.387311000	-0.367714000	3.025621000
C	-2.195922000	2.851983000	1.422532000
C	-3.277870000	2.210549000	0.695309000
C	-3.668037000	1.007384000	1.427423000
C	-4.052997000	-0.151073000	0.716546000
C	-4.052943000	-0.151143000	-0.716748000
C	-3.667941000	1.007242000	-1.427711000
C	-3.277819000	2.210481000	-0.695689000
C	-2.195834000	2.851846000	-1.422906000
C	-1.911987000	2.032791000	-2.590445000
C	-2.833047000	0.899179000	-2.586427000
C	-2.387128000	-0.368012000	-3.025707000
C	-1.037905000	-0.544446000	-3.467393000
C	-0.139786000	0.548703000	-3.467001000
C	-0.600125000	1.862944000	-3.018491000
C	0.488445000	2.505406000	-2.302412000
C	0.729152000	-2.032552000	-2.588358000
C	-0.580513000	-1.858959000	-3.017719000
C	0.220340000	3.289809000	-1.175597000
C	-1.150797000	3.465560000	-0.727035000
C	-3.601552000	-1.463430000	-1.171564000
C	-2.789179000	-1.569890000	-2.295776000
C	-1.672613000	-2.498551000	-2.302124000
C	-1.150849000	3.465633000	0.726668000
C	-2.789321000	-1.569669000	2.295781000
C	-3.601629000	-1.463315000	1.171515000
C	-3.330919000	-2.280019000	0.000019000

C	-1.672754000	-2.498326000	2.302291000
C	-1.406610000	-3.282497000	1.175788000
C	-2.253791000	-3.170272000	0.000098000
C	1.606527000	1.578180000	2.293436000
C	0.488305000	2.505631000	2.302236000
C	0.220266000	3.289922000	1.175339000
C	-0.036841000	-3.464551000	0.726404000
C	2.416252000	1.474196000	1.169710000
C	-1.406540000	-3.282611000	-1.175533000
C	-0.036786000	-3.464624000	-0.726041000
C	1.011639000	-2.853901000	-1.422761000
C	2.149015000	2.294159000	-0.000019000
C	1.066914000	3.181932000	-0.000103000
C	5.904707000	0.259643000	1.177649000
C	5.904925000	0.261413000	-1.177196000
C	5.915289000	-1.017966000	-0.730244000
C	5.915182000	-1.019066000	0.728776000
C	5.935882000	1.196066000	0.000932000
H	5.899473000	0.585104000	2.210703000
H	5.904516000	-1.912725000	1.342658000
H	5.904719000	-1.910706000	-1.345466000
H	5.899831000	0.588418000	-2.209762000
H	5.098727000	1.906612000	0.001354000
H	6.851138000	1.808363000	0.001488000

TS_{bir}[5,6]

E=-2480.549386

G=-2480.133081

C	-2.996102000	-0.235409000	-0.686940000
C	-2.557205000	1.049277000	-1.290496000
C	-1.769487000	1.081112000	-2.429024000
C	-1.273993000	-0.169493000	-3.016931000

C	-1.608079000	-1.408690000	-2.413149000
C	-2.421077000	-1.451250000	-1.249943000
C	-2.899164000	-0.053314000	0.750619000
C	-2.547329000	1.332085000	1.028041000
C	-2.355059000	2.016900000	-0.237997000
C	-1.357018000	2.997789000	-0.364821000
C	-0.735684000	2.087825000	-2.570064000
C	0.054239000	0.065042000	-3.499447000
C	1.041129000	-0.933164000	-3.383166000
C	0.703746000	-2.215150000	-2.765840000
C	-0.584300000	-2.449892000	-2.298561000
C	-0.785887000	-3.135014000	-1.035727000
C	-1.920397000	-2.502712000	-0.379705000
C	-1.909629000	-2.324587000	1.002161000
C	-2.409586000	-1.067475000	1.588111000
C	-1.752281000	1.651015000	2.129990000
C	-1.257569000	0.598313000	2.996622000
C	-1.586524000	-0.746255000	2.714920000
C	-0.567623000	-1.783662000	2.840616000
C	-0.779548000	-2.766404000	1.786924000
C	0.319643000	-3.369391000	1.158690000
C	0.313568000	-3.555061000	-0.282287000
C	1.660483000	-3.310960000	-0.771697000
C	1.850765000	-2.656848000	-1.990609000
C	0.399277000	1.458116000	-3.220805000
C	4.027062000	0.065197000	-0.749252000
C	3.543883000	1.080032000	-1.583893000
C	3.052888000	2.325894000	-1.000942000
C	3.063355000	2.500864000	0.382318000
C	3.560346000	1.441788000	1.247856000
C	3.698537000	-1.028631000	1.301145000
C	3.491679000	-2.005005000	0.241808000

C	3.688699000	-1.325530000	-1.028730000
C	2.885732000	-1.642563000	-2.121570000
C	2.379500000	-0.585303000	-2.988208000
C	2.710954000	0.755847000	-2.717541000
C	1.913417000	2.769794000	-1.782335000
C	0.823211000	3.373272000	-1.151945000
C	0.832051000	3.554351000	0.291995000
C	1.927934000	3.126447000	1.041512000
C	1.723539000	2.445957000	2.311369000
C	2.735469000	1.408492000	2.433809000
C	2.403250000	0.178811000	3.025028000
C	2.900657000	-1.063942000	2.444073000
C	2.498189000	-2.976900000	0.369752000
C	1.666326000	-3.013353000	1.562260000
C	1.866549000	-2.073220000	2.579021000
C	0.725011000	-1.447948000	3.229351000
C	1.065919000	-0.056337000	3.510442000
C	0.086315000	0.941018000	3.392198000
C	0.429179000	2.220346000	2.778202000
C	-0.712585000	2.663484000	1.998682000
C	-0.518701000	3.316395000	0.778855000
C	1.696776000	1.791889000	-2.840610000
C	-0.531303000	3.030371000	-1.552915000
C	4.034269000	0.245473000	0.685344000
C	-5.218853000	-0.384059000	-1.116488000
C	-5.867097000	-0.250774000	1.134244000
C	-5.950806000	0.997655000	0.571211000
C	-5.620943000	0.918349000	-0.814590000
H	-5.594004000	1.756866000	-1.499686000
H	-6.201556000	1.912508000	1.095616000
H	-6.044220000	-0.501317000	2.172751000
H	-5.079089000	-0.769275000	-2.118910000

C	-5.574405000	-1.262245000	0.061868000
H	-6.493039000	-1.824221000	-0.178803000
H	-4.819935000	-2.006510000	0.332168000

Print[5,6]

E=-2480.58283

G=-2480.16278

C	-3.213891000	0.050059000	-0.658371000
C	-2.891533000	-0.295520000	0.808838000
C	-2.460340000	0.641093000	1.728728000
C	-2.068316000	1.995296000	1.297065000
C	-2.099298000	2.311337000	-0.066626000
C	-2.545000000	1.359096000	-1.039229000
C	-2.516635000	-1.120911000	-1.381613000
C	-2.183473000	-2.153761000	-0.441183000
C	-2.412603000	-1.645201000	0.904397000
C	-1.577932000	-2.046967000	1.955852000
C	-1.573840000	0.254212000	2.807378000
C	-0.947664000	2.415253000	2.105375000
C	0.094674000	3.168522000	1.545434000
C	0.052834000	3.516561000	0.133744000
C	-1.019328000	3.102209000	-0.651694000
C	-0.791406000	2.598558000	-1.989794000
C	-1.734829000	1.503996000	-2.209923000
C	-1.341746000	0.390447000	-2.963963000
C	-1.735600000	-0.955675000	-2.509825000
C	-1.127075000	-3.042031000	-0.683335000
C	-0.325828000	-2.882158000	-1.874953000
C	-0.621255000	-1.846360000	-2.766169000
C	0.453745000	-1.069896000	-3.361707000
C	0.005237000	0.311231000	-3.478963000
C	0.915163000	1.356337000	-3.261836000

C	0.502018000	2.524127000	-2.498944000
C	1.626953000	2.954070000	-1.682177000
C	1.406880000	3.439894000	-0.392847000
C	-0.639641000	1.343262000	3.042194000
C	3.649807000	1.103462000	1.388892000
C	2.872055000	0.945137000	2.536402000
C	2.482659000	-0.389191000	2.973231000
C	2.887626000	-1.508682000	2.242804000
C	3.694405000	-1.341973000	1.045035000
C	4.020531000	0.284165000	-0.784892000
C	3.577280000	1.665825000	-0.896032000
C	3.348403000	2.173245000	0.448869000
C	2.284987000	3.040140000	0.695536000
C	1.470495000	2.872065000	1.891864000
C	1.762686000	1.845939000	2.794658000
C	1.131833000	-0.313319000	3.499205000
C	0.235545000	-1.359877000	3.277897000
C	0.656034000	-2.526039000	2.515001000
C	1.954697000	-2.598701000	2.009143000
C	2.184172000	-3.105260000	0.664206000
C	3.258286000	-2.327252000	0.069240000
C	3.209358000	-1.993685000	-1.285810000
C	3.599461000	-0.659543000	-1.722373000
C	2.734768000	2.047187000	-1.939193000
C	2.290967000	1.060549000	-2.915336000
C	2.719779000	-0.265604000	-2.808615000
C	1.779950000	-1.352009000	-3.039038000
C	2.087731000	-2.423122000	-2.100779000
C	1.057135000	-3.172959000	-1.532492000
C	1.106048000	-3.518743000	-0.119356000
C	-0.247054000	-3.436371000	0.406550000
C	-0.467122000	-2.950640000	1.694839000

C	0.683188000	1.068165000	3.383797000
C	-1.146648000	-1.071633000	2.930399000
C	4.065223000	-0.061864000	0.625910000
C	-4.764228000	0.122920000	-0.955913000
C	-6.367287000	-0.670157000	0.665262000
C	-6.277651000	0.711309000	0.779680000
C	-5.412786000	1.236549000	-0.171465000
H	-5.162956000	2.282071000	-0.301441000
H	-6.815247000	1.304515000	1.512944000
H	-6.974709000	-1.321806000	1.282396000
H	-4.844748000	0.279211000	-2.038642000
C	-5.542027000	-1.148122000	-0.499926000
H	-6.184501000	-1.515335000	-1.313610000
H	-4.881284000	-1.982603000	-0.239952000

TS_{bir}[6,6]

E=-2480.549386

G=-2480.133081

C	-2.961485000	-0.765198000	-0.128789000
C	-2.464529000	-1.460021000	1.058487000
C	-2.085217000	-0.761815000	2.203958000
C	-2.094702000	0.716071000	2.199100000
C	-2.496980000	1.410607000	1.048924000
C	-2.888447000	0.693294000	-0.130443000
C	-2.378271000	-1.464943000	-1.283004000
C	-1.655275000	-2.628986000	-0.810854000
C	-1.708140000	-2.625567000	0.642187000
C	-0.606412000	-3.052495000	1.388588000
C	-0.947148000	-1.191741000	2.972695000
C	-0.972578000	1.174960000	2.970782000
C	-0.263187000	2.323698000	2.570705000
C	-0.676693000	3.049206000	1.379282000

C	-1.772431000	2.610558000	0.636897000
C	-1.718348000	2.606565000	-0.811754000
C	-2.414846000	1.406429000	-1.276157000
C	-1.925186000	0.710587000	-2.394923000
C	-1.910810000	-0.765809000	-2.390711000
C	-0.499395000	-3.059195000	-1.471662000
C	-0.017025000	-2.332806000	-2.627146000
C	-0.718039000	-1.199105000	-3.075094000
C	0.012184000	-0.008288000	-3.488531000
C	-0.748272000	1.167141000	-3.077402000
C	-0.068644000	2.317297000	-2.628642000
C	-0.570370000	3.042396000	-1.469589000
C	0.572679000	3.508334000	-0.698962000
C	0.520974000	3.511477000	0.695001000
C	-0.247458000	-0.000223000	3.438667000
C	3.545128000	1.467136000	1.284288000
C	3.073150000	0.766959000	2.396848000
C	3.089567000	-0.694359000	2.399303000
C	3.581064000	-1.387303000	1.287098000
C	4.064119000	-0.659266000	0.132414000
C	3.634491000	1.465372000	-1.059613000
C	2.879070000	2.640166000	-0.642540000
C	2.825240000	2.642735000	0.810827000
C	1.671826000	3.067676000	1.467117000
C	1.179995000	2.335075000	2.625656000
C	1.875450000	1.204833000	3.079451000
C	1.903425000	-1.157618000	3.082734000
C	1.232841000	-2.302633000	2.631146000
C	1.740766000	-3.024599000	1.471820000
C	2.887453000	-2.577754000	0.815916000
C	2.942227000	-2.580097000	-0.636845000
C	3.667807000	-1.389660000	-1.055780000

C	3.262691000	-0.698250000	-2.201042000
C	3.246341000	0.763315000	-2.204576000
C	1.777083000	3.062271000	-1.383188000
C	1.372522000	2.328287000	-2.574977000
C	2.103473000	1.198036000	-2.975040000
C	1.402670000	0.008534000	-3.440991000
C	2.129959000	-1.163857000	-2.971767000
C	1.430008000	-2.308571000	-2.571457000
C	1.848917000	-3.029159000	-1.377421000
C	0.652614000	-3.493428000	-0.693688000
C	0.600555000	-3.491638000	0.700719000
C	1.142448000	0.015380000	3.494365000
C	-0.212087000	-2.325961000	2.578701000
C	4.045047000	0.747706000	0.129236000
C	-5.251808000	-1.137822000	-0.159934000
C	-6.240964000	0.831760000	0.687029000
C	-6.205039000	0.903504000	-0.674071000
C	-5.649040000	-0.310981000	-1.204830000
H	-5.517134000	-0.527920000	-2.258488000
H	-6.532328000	1.743182000	-1.276434000
H	-6.581150000	1.604405000	1.365674000
H	-5.034114000	-2.193387000	-0.252999000
C	-5.701507000	-0.499133000	1.134380000
H	-6.489103000	-1.111939000	1.600426000
H	-4.906859000	-0.408853000	1.884432000

Print[6,6]

E=-2480.583691

G=-2480.163730

C	-2.497962000	0.812055000	-1.602291000
C	-3.209113000	-0.164974000	-0.643635000
C	-2.896780000	0.204300000	0.795348000

C	-2.412449000	1.498502000	1.173528000
C	-2.009006000	2.433678000	0.212332000
C	-2.041428000	2.056154000	-1.212514000
C	-1.785355000	0.082607000	-2.612438000
C	-1.786451000	-1.328177000	-2.251899000
C	-2.501418000	-1.483220000	-1.016365000
C	-2.043068000	-2.386287000	-0.076351000
C	-2.410253000	-0.747457000	1.747680000
C	-1.650948000	1.366601000	2.414072000
C	-0.516641000	2.144583000	2.630484000
C	-0.089295000	3.100906000	1.621368000
C	-0.824339000	3.229224000	0.433997000
C	-0.123696000	3.362633000	-0.836262000
C	-0.877638000	2.640276000	-1.847534000
C	-0.207494000	1.951277000	-2.862836000
C	-0.672232000	0.640525000	-3.255945000
C	-0.673310000	-2.126698000	-2.548149000
C	0.489953000	-1.537818000	-3.194832000
C	0.490356000	-0.187120000	-3.540846000
C	1.678951000	0.620988000	-3.319346000
C	1.246240000	1.944836000	-2.896837000
C	1.969209000	2.634647000	-1.922648000
C	1.269436000	3.363715000	-0.873039000
C	2.029093000	3.221335000	0.359719000
C	1.359667000	3.089783000	1.579599000
C	-1.650557000	-0.035968000	2.773388000
C	2.947397000	-0.072668000	2.651758000
C	1.832903000	-0.633438000	3.273786000
C	1.358670000	-1.950699000	2.870086000
C	2.027881000	-2.652770000	1.863441000
C	3.189137000	-2.067073000	1.218075000
C	4.070370000	0.151665000	0.595198000

C	3.642499000	1.474440000	1.019030000
C	2.947649000	1.337284000	2.290564000
C	1.833652000	2.128623000	2.566879000
C	0.671639000	1.544098000	3.217749000
C	0.671493000	0.192684000	3.564222000
C	-0.090257000	-1.939407000	2.911196000
C	-0.825199000	-2.623264000	1.932024000
C	-0.125018000	-3.351216000	0.882205000
C	1.268102000	-3.369898000	0.850714000
C	1.967891000	-3.235247000	-0.419829000
C	3.153149000	-2.428818000	-0.192771000
C	3.571428000	-1.511809000	-1.159460000
C	4.038231000	-0.194974000	-0.757699000
C	3.190378000	2.397423000	0.075179000
C	3.153837000	2.035863000	-1.335770000
C	3.571656000	0.766909000	-1.742790000
C	2.817793000	0.045187000	-2.754626000
C	2.817312000	-1.364666000	-2.393601000
C	1.678335000	-2.140603000	-2.612440000
C	1.245065000	-3.098322000	-1.605701000
C	-0.208589000	-3.087169000	-1.573045000
C	-0.879025000	-3.203675000	-0.351929000
C	-0.516909000	-0.615277000	3.336714000
C	-2.008609000	-2.031104000	1.354473000
C	3.641585000	-0.804356000	1.602488000
C	-4.757997000	-0.217537000	-0.918663000
C	-6.443350000	-0.414552000	0.804501000
C	-6.360679000	0.917862000	0.423462000
C	-5.426207000	1.093921000	-0.589359000
H	-5.160038000	2.031753000	-1.061474000
H	-6.949574000	1.719441000	0.858666000
H	-4.862980000	-0.470345000	-1.982012000

H	-7.092389000	-0.817094000	1.573416000
C	-5.500822000	-1.252417000	-0.018036000
H	-6.039897000	-1.988972000	-0.629849000
H	-4.808291000	-1.830227000	0.606609000

TS[5,6]

E=-2480.567578

G=-2480.144754

C	-3.229507000	-0.010137000	-0.787328000
C	-3.068109000	-0.379114000	0.721359000
C	-2.551588000	0.578099000	1.641633000
C	-2.163597000	1.927448000	1.223383000
C	-2.167430000	2.266350000	-0.130156000
C	-2.570747000	1.307639000	-1.131604000
C	-2.476393000	-1.159291000	-1.479383000
C	-2.158520000	-2.193050000	-0.537753000
C	-2.450034000	-1.710648000	0.795287000
C	-1.635837000	-2.097241000	1.859228000
C	-1.698325000	0.200556000	2.727329000
C	-1.082987000	2.377913000	2.074420000
C	-0.040881000	3.156943000	1.551214000
C	-0.048384000	3.515895000	0.144928000
C	-1.093574000	3.082482000	-0.674808000
C	-0.814964000	2.588071000	-2.007670000
C	-1.733891000	1.479896000	-2.268879000
C	-1.294088000	0.376951000	-3.025320000
C	-1.671992000	-0.975424000	-2.587888000
C	-1.083324000	-3.069950000	-0.762041000
C	-0.250528000	-2.884856000	-1.928769000
C	-0.536460000	-1.847684000	-2.820105000
C	0.539477000	-1.046788000	-3.377732000
C	0.066449000	0.327627000	-3.496596000

C	0.950868000	1.388107000	-3.240567000
C	0.492699000	2.542462000	-2.479264000
C	1.585570000	2.989504000	-1.628869000
C	1.319449000	3.463903000	-0.342993000
C	-0.786140000	1.304635000	3.006724000
C	3.548622000	1.150131000	1.485033000
C	2.740409000	0.969429000	2.607121000
C	2.358164000	-0.375288000	3.021631000
C	2.808022000	-1.483254000	2.294752000
C	3.644977000	-1.291713000	1.125179000
C	3.998326000	0.354563000	-0.681365000
C	3.534207000	1.728746000	-0.795598000
C	3.257738000	2.223255000	0.545403000
C	2.174792000	3.072023000	0.767503000
C	1.329650000	2.882159000	1.938648000
C	1.610617000	1.851597000	2.839804000
C	0.995939000	-0.326251000	3.508113000
C	0.118361000	-1.386545000	3.246887000
C	0.585437000	-2.538558000	2.485502000
C	1.900608000	-2.585955000	2.022507000
C	2.182200000	-3.080841000	0.682388000
C	3.258563000	-2.278227000	0.127423000
C	3.246295000	-1.934878000	-1.225554000
C	3.624298000	-0.589925000	-1.640490000
C	2.714530000	2.103021000	-1.859195000
C	2.318620000	1.116317000	-2.856705000
C	2.771182000	-0.204031000	-2.747427000
C	1.860178000	-1.306225000	-3.016655000
C	2.159443000	-2.380071000	-2.078428000
C	1.127132000	-3.155090000	-1.548223000
C	1.138455000	-3.511921000	-0.137328000
C	-0.232465000	-3.458238000	0.346108000

C	-0.501647000	-2.978117000	1.628309000
C	0.527704000	1.048458000	3.388529000
C	-1.252038000	-1.124688000	2.867586000
C	4.007329000	-0.001691000	0.725778000
C	-4.790520000	-0.007633000	-1.145289000
C	-5.264511000	-0.589988000	1.027024000
C	-5.604228000	0.801098000	0.874762000
C	-5.402781000	1.164806000	-0.422222000
H	-5.493991000	2.160942000	-0.837660000
H	-5.873838000	1.464726000	1.688906000
H	-5.373535000	-1.150070000	1.948810000
H	-4.925161000	-0.030755000	-2.228248000
C	-5.360623000	-1.199451000	-0.350457000
H	-6.409275000	-1.378106000	-0.626118000
H	-4.805373000	-2.130667000	-0.478677000

Prod[5,6]

E=-2480.591971

G=-2480.166309

C	-3.251613000	0.212414000	0.809334000
C	-3.251612000	0.212408000	-0.809333000
C	-2.573178000	-0.975335000	-1.440110000
C	-2.171260000	-2.153029000	-0.697832000
C	-2.171260000	-2.153025000	0.697847000
C	-2.573176000	-0.975325000	1.440118000
C	-2.473213000	1.481229000	1.169926000
C	-2.158579000	2.248318000	-0.000006000
C	-2.473213000	1.481220000	-1.169933000
C	-1.663302000	1.584460000	-2.286939000
C	-1.729002000	-0.870052000	-2.575514000
C	-1.097645000	-2.815697000	-1.417575000
C	-0.055410000	-3.442300000	-0.725745000

C	-0.055409000	-3.442295000	0.725767000
C	-1.097645000	-2.815688000	1.417593000
C	-0.809450000	-2.008760000	2.585274000
C	-1.729000000	-0.870035000	2.575521000
C	-1.283459000	0.384413000	3.042379000
C	-1.663301000	1.584475000	2.286931000
C	-1.084522000	3.161931000	-0.000010000
C	-0.246477000	3.272723000	1.171178000
C	-0.526677000	2.485704000	2.290158000
C	0.553049000	1.846153000	3.020449000
C	0.079596000	0.543680000	3.475931000
C	0.963249000	-0.549473000	3.480388000
C	0.499534000	-1.854370000	3.026388000
C	1.587374000	-2.499279000	2.306495000
C	1.313215000	-3.276083000	1.177660000
C	-0.809451000	-2.008777000	-2.585260000
C	3.529957000	-1.484340000	-1.176302000
C	2.715806000	-1.584791000	-2.303377000
C	2.325981000	-0.381942000	-3.031516000
C	2.778892000	0.871271000	-2.599218000
C	3.623092000	0.972389000	-1.426571000
C	3.991083000	-0.180566000	0.724781000
C	3.529958000	-1.484332000	1.176310000
C	3.246147000	-2.293769000	0.000006000
C	2.163314000	-3.170988000	0.000010000
C	1.313214000	-3.276091000	-1.177640000
C	1.587373000	-2.499293000	-2.306479000
C	0.963247000	-0.549495000	-3.480385000
C	0.079593000	0.543658000	-3.475934000
C	0.553047000	1.846134000	-3.020461000
C	1.871214000	2.007975000	-2.598243000
C	2.164716000	2.819834000	-1.424138000

C	3.244259000	2.175809000	-0.698338000
C	3.244260000	2.175813000	0.698322000
C	3.623093000	0.972398000	1.426563000
C	2.715808000	-1.584776000	2.303386000
C	2.325983000	-0.381923000	3.031517000
C	2.778894000	0.871288000	2.599211000
C	1.871216000	2.007992000	2.598229000
C	2.164717000	2.819843000	1.424119000
C	1.128263000	3.442450000	0.727747000
C	1.128262000	3.442446000	-0.727770000
C	-0.246478000	3.272715000	-1.171198000
C	-0.526678000	2.485689000	-2.290174000
C	0.499532000	-1.854389000	-3.026377000
C	-1.283461000	0.384393000	-3.042379000
C	3.991082000	-0.180571000	-0.724782000
C	-4.808052000	0.304831000	1.128175000
C	-4.808055000	0.304826000	-1.128176000
C	-5.407509000	-1.015264000	-0.669757000
C	-5.407500000	-1.015266000	0.669762000
H	-5.668741000	-1.835345000	1.328695000
H	-5.668759000	-1.835343000	-1.328687000
H	-5.003462000	0.604823000	-2.158726000
H	-5.003461000	0.604830000	2.158724000
C	-5.290066000	1.239534000	-0.000002000
H	-6.376454000	1.359483000	-0.000001000
H	-4.813317000	2.222988000	-0.000006000

TS[6,6]

E=-2480.553205

G=-2480.132880

C	2.553020000	0.401816000	1.715452000
C	3.204469000	-0.480070000	0.649178000

C	3.034982000	0.086687000	-0.758045000
C	2.566904000	1.466478000	-0.945670000
C	2.206854000	2.270481000	0.128425000
C	2.201018000	1.720230000	1.496336000
C	1.781771000	-0.405825000	2.608760000
C	1.706881000	-1.758332000	2.064010000
C	2.421276000	-1.795847000	0.840191000
C	1.918739000	-2.544347000	-0.233620000
C	2.434604000	-0.690806000	-1.807062000
C	1.813108000	1.534649000	-2.178382000
C	0.732663000	2.408658000	-2.306208000
C	0.355276000	3.246465000	-1.184030000
C	1.079431000	3.176329000	0.011614000
C	0.376007000	3.187617000	1.283622000
C	1.067445000	2.293967000	2.194545000
C	0.333930000	1.515928000	3.099566000
C	0.702106000	0.136065000	3.316154000
C	0.528129000	-2.520138000	2.255518000
C	-0.590287000	-1.943960000	2.952122000
C	-0.515750000	-0.642709000	3.483868000
C	-1.640300000	0.254991000	3.366734000
C	-1.117082000	1.595249000	3.119669000
C	-1.779645000	2.452768000	2.243798000
C	-1.018790000	3.269198000	1.308907000
C	-1.766717000	3.333005000	0.065252000
C	-1.095832000	3.324106000	-1.157151000
C	1.728578000	0.183692000	-2.706185000
C	-2.862207000	0.431225000	-2.638156000
C	-1.778042000	-0.119225000	-3.315890000
C	-1.406710000	-1.507768000	-3.094100000
C	-2.144943000	-2.298818000	-2.198009000
C	-3.272712000	-1.720615000	-1.492546000

C	-4.001938000	0.456893000	-0.586803000
C	-3.479975000	1.794414000	-0.832395000
C	-2.783288000	1.782971000	-2.100994000
C	-1.610907000	2.535339000	-2.269072000
C	-0.482979000	1.970686000	-2.972692000
C	-0.554857000	0.660551000	-3.484453000
C	0.035081000	-1.581583000	-3.104255000
C	0.705067000	-2.439256000	-2.231962000
C	-0.055701000	-3.263926000	-1.308429000
C	-1.453896000	-3.192870000	-1.290478000
C	-2.157209000	-3.176187000	-0.017892000
C	-3.281497000	-2.263111000	-0.140231000
C	-3.645648000	-1.452630000	0.935211000
C	-4.013663000	-0.062290000	0.709841000
C	-2.990359000	2.556260000	0.235282000
C	-2.997377000	2.017386000	1.575865000
C	-3.501526000	0.726121000	1.815186000
C	-2.811644000	-0.163755000	2.721600000
C	-2.895660000	-1.514632000	2.178451000
C	-1.815356000	-2.387075000	2.295758000
C	-1.439606000	-3.235980000	1.178211000
C	0.014034000	-3.311081000	1.153046000
C	0.687920000	-3.318317000	-0.065304000
C	0.562356000	-0.233681000	-3.361345000
C	1.926794000	-2.012715000	-1.567399000
C	-3.628480000	-0.387037000	-1.706819000
C	4.777307000	-0.696079000	0.933157000
C	5.293934000	0.059640000	-1.179079000
C	5.643145000	1.098521000	-0.266935000
C	5.421894000	0.655374000	1.009538000
H	5.517870000	1.235810000	1.918889000
H	5.931399000	2.104039000	-0.551689000

H	4.901977000	-1.337720000	1.806826000
H	5.358194000	0.130772000	-2.258234000
C	5.314312000	-1.233914000	-0.408111000
H	6.346445000	-1.591774000	-0.286041000
H	4.713409000	-2.036210000	-0.840739000

Prod[6,6]

E=-2480.585391

G=-2480.161313

C	2.547496000	-1.027572000	-1.439985000
C	3.247777000	0.167789000	-0.799537000
C	3.247764000	0.167282000	0.799508000
C	2.547606000	-1.028474000	1.439343000
C	2.152582000	-2.170624000	0.718149000
C	2.152510000	-2.170126000	-0.719478000
C	1.799237000	-0.618158000	-2.562405000
C	1.739163000	0.839406000	-2.568520000
C	2.472580000	1.322247000	-1.432434000
C	2.001893000	2.418396000	-0.738929000
C	2.472616000	1.321369000	1.433138000
C	1.799387000	-0.619747000	2.562009000
C	0.682857000	-1.371288000	3.024613000
C	0.283353000	-2.566115000	2.296161000
C	0.997344000	-2.951896000	1.166313000
C	0.294606000	-3.445686000	-0.001039000
C	0.997305000	-2.951121000	-1.168113000
C	0.283274000	-2.564662000	-2.297714000
C	0.682766000	-1.369431000	-3.025447000
C	0.592597000	1.494444000	-3.023067000
C	-0.562058000	0.714914000	-3.466385000
C	-0.497811000	-0.697930000	-3.461619000
C	-1.656877000	-1.478017000	-3.023392000

C	-1.167758000	-2.641113000	-2.306988000
C	-1.849334000	-3.105882000	-1.176065000
C	-1.105825000	-3.522631000	-0.001068000
C	-1.849313000	-3.106609000	1.174205000
C	-1.167674000	-2.642535000	2.305376000
C	1.739252000	0.837834000	2.568945000
C	-2.864588000	0.634894000	2.591864000
C	-1.751043000	1.384312000	3.035157000
C	-1.345357000	2.580294000	2.303425000
C	-2.050885000	2.977214000	1.171764000
C	-3.204604000	2.201496000	0.718017000
C	-4.004379000	-0.145094000	0.696226000
C	-3.521704000	-1.307790000	1.422995000
C	-2.806159000	-0.824240000	2.593170000
C	-1.656761000	-1.479865000	3.022518000
C	-0.497686000	-0.700068000	3.461138000
C	-0.561973000	0.712817000	3.466846000
C	0.108152000	2.646741000	2.311220000
C	0.797947000	3.096484000	1.176201000
C	0.057652000	3.512564000	0.001069000
C	-1.342674000	3.463371000	0.001071000
C	-2.050928000	2.977929000	-1.169895000
C	-3.204610000	2.201922000	-0.716574000
C	-3.596211000	1.048973000	-1.428149000
C	-4.004408000	-0.144673000	-0.696200000
C	-3.050022000	-2.423203000	0.727498000
C	-3.050044000	-2.422764000	-0.728900000
C	-3.521759000	-1.306919000	-1.423692000
C	-2.806255000	-0.822651000	-2.593590000
C	-2.864653000	0.636471000	-2.591380000
C	-1.751157000	1.386176000	-3.034269000
C	-1.345469000	2.581698000	-2.301838000

C	0.108077000	2.648155000	-2.309618000
C	0.797896000	3.097172000	-1.174370000
C	0.592697000	1.492583000	3.023890000
C	2.001918000	2.417966000	0.740330000
C	-3.596157000	1.048092000	1.428886000
C	4.806895000	0.235991000	-1.123755000
C	4.806976000	0.235423000	1.123796000
C	5.400691000	-1.084456000	0.669556000
C	5.400292000	-1.084271000	-0.670227000
H	5.651571000	-1.906447000	-1.330496000
H	5.652270000	-1.906842000	1.329438000
H	4.996836000	0.533415000	-2.155680000
H	4.996920000	0.532358000	2.155857000
C	5.283953000	1.174631000	0.000256000
H	6.368765000	1.309043000	0.000270000
H	4.787804000	2.149839000	0.000552000

S=2

⁵C₆₀

E=-2286.365448

G=-2286.043413

C	-0.424571000	3.478982000	0.591775000
C	1.030221000	3.355436000	0.577796000
C	1.694215000	3.077281000	-0.607479000
C	0.939432000	2.909752000	-1.845567000
C	-0.471008000	3.033792000	-1.830519000
C	-1.152669000	3.314646000	-0.605776000
C	-0.897568000	2.890316000	1.808049000
C	0.247347000	2.409285000	2.562276000
C	1.434813000	2.696778000	1.816878000
C	2.504368000	1.776229000	1.803532000
C	2.801036000	2.126069000	-0.618440000

C	1.561587000	1.860315000	-2.594859000
C	0.772067000	0.950113000	-3.325664000
C	-0.682899000	1.078847000	-3.320358000
C	-1.291280000	2.091949000	-2.590229000
C	-2.499527000	1.817146000	-1.826418000
C	-2.411185000	2.558404000	-0.597698000
C	-2.878236000	2.000548000	0.600586000
C	-2.115260000	2.151680000	1.815053000
C	0.150251000	1.198824000	3.306615000
C	-1.087616000	0.449877000	3.312419000
C	-2.212131000	0.922814000	2.572558000
C	-3.029765000	-0.000502000	1.838577000
C	-3.443807000	0.657296000	0.601698000
C	-3.523095000	-0.067135000	-0.581024000
C	-3.046943000	0.515218000	-1.827106000
C	-2.407538000	-0.531914000	-2.576926000
C	-1.248727000	-0.264830000	-3.319034000
C	2.716023000	1.374407000	-1.833644000
C	0.897568000	-2.890316000	-1.808049000
C	2.115260000	-2.151680000	-1.815053000
C	2.878236000	-2.000548000	-0.600586000
C	2.411185000	-2.558404000	0.597698000
C	1.152669000	-3.314646000	0.605776000
C	-1.030221000	-3.355436000	-0.577796000
C	-1.434813000	-2.696778000	-1.816878000
C	-0.247347000	-2.409285000	-2.562276000
C	-0.150251000	-1.198824000	-3.306615000
C	1.087616000	-0.449877000	-3.312419000
C	2.212131000	-0.922814000	-2.572558000
C	3.443807000	-0.657296000	-0.601698000
C	3.523095000	0.067135000	0.581024000
C	3.046943000	-0.515218000	1.827106000

C	2.499527000	-1.817146000	1.826418000
C	1.291280000	-2.091949000	2.590229000
C	0.471008000	-3.033792000	1.830519000
C	-0.939432000	-2.909752000	1.845567000
C	-1.694215000	-3.077281000	0.607479000
C	-2.504368000	-1.776229000	-1.803532000
C	-3.194814000	-1.491636000	-0.584688000
C	-2.801036000	-2.126069000	0.618440000
C	-2.716023000	-1.374407000	1.833644000
C	-1.561587000	-1.860315000	2.594859000
C	-0.772067000	-0.950113000	3.325664000
C	0.682899000	-1.078847000	3.320358000
C	1.248727000	0.264830000	3.319034000
C	2.407538000	0.531914000	2.576926000
C	3.029765000	0.000502000	-1.838577000
C	3.194814000	1.491636000	0.584688000
C	0.424571000	-3.478982000	-0.591775000

Pre-reactants

E=-2480.495019

G=-2480.087303

C	1.346936000	-2.095839000	2.142966000
C	2.140532000	-2.048127000	1.005690000
C	2.810746000	-0.805065000	0.634333000
C	2.653598000	0.342853000	1.439861000
C	1.847349000	0.293086000	2.617998000
C	1.189867000	-0.909158000	2.976381000
C	2.466063000	1.659663000	0.806781000
C	2.442880000	1.760042000	-0.593668000
C	2.581297000	0.579835000	-1.405408000
C	2.774801000	-0.699631000	-0.790871000
C	1.463132000	2.624527000	-1.240111000

C	1.022796000	1.961060000	-2.465536000
C	1.712366000	0.706077000	-2.554013000
C	1.043582000	-0.441382000	-3.072560000
C	-0.323063000	-0.342493000	-3.509472000
C	-1.009562000	0.880595000	-3.409497000
C	-0.323492000	2.059293000	-2.874528000
C	-0.996430000	-1.585137000	-3.147601000
C	-2.312868000	-1.560444000	-2.700319000
C	-3.023183000	-0.290456000	-2.597282000
C	-2.371053000	0.907943000	-2.953823000
C	-2.719027000	-2.402705000	-1.583425000
C	-3.652908000	-1.649029000	-0.786857000
C	-3.840674000	-0.341738000	-1.416265000
C	-3.999824000	0.803715000	-0.616204000
C	-3.956024000	0.695334000	0.818043000
C	-3.769332000	-0.567072000	1.425990000
C	-3.628518000	-1.749814000	0.612076000
C	-2.648883000	-2.613100000	1.258025000
C	-2.207158000	-1.950213000	2.484258000
C	-2.894261000	-0.697245000	2.577348000
C	-2.222303000	0.448244000	3.096449000
C	-0.853001000	0.347225000	3.532055000
C	-0.168954000	-0.876388000	3.430026000
C	-0.861478000	-2.053339000	2.892147000
C	0.071099000	-2.805567000	2.111575000
C	1.134227000	1.564766000	2.719350000
C	-0.179330000	1.589995000	3.170138000
C	-0.350188000	-3.443060000	0.918259000
C	-1.744963000	-3.338884000	0.493822000
C	-3.268965000	1.862594000	1.343922000
C	-2.409855000	1.735392000	2.475180000
C	-1.158926000	2.452319000	2.519766000

C	-1.773084000	-3.239364000	-0.958890000
C	-2.533024000	2.094723000	-2.122013000
C	-3.326656000	2.042891000	-0.984682000
C	-2.885668000	2.696158000	0.246287000
C	-1.258667000	2.806370000	-2.090907000
C	-0.838282000	3.446134000	-0.898368000
C	-1.653674000	3.383950000	0.272885000
C	1.232513000	-1.735129000	-2.450024000
C	-0.018799000	-2.449281000	-2.497597000
C	-0.409911000	-3.257944000	-1.419920000
C	0.557686000	3.346933000	-0.473647000
C	2.087986000	-1.865772000	-1.321167000
C	-0.771199000	3.259679000	1.440675000
C	0.588660000	3.249724000	0.978099000
C	1.540913000	2.411141000	1.603175000
C	1.702731000	-2.702913000	-0.224536000
C	0.467674000	-3.387146000	-0.253211000
C	5.923752000	-0.681300000	-1.119574000
C	5.963729000	0.111961000	1.097797000
C	5.793291000	1.156916000	0.253738000
C	5.768791000	0.665640000	-1.121588000
C	6.088538000	-1.157077000	0.297800000
H	5.946725000	-1.332389000	-1.984849000
H	5.634193000	1.293225000	-1.995064000
H	5.675245000	2.196755000	0.535345000
H	6.017117000	0.153861000	2.178745000
H	5.333612000	-1.903401000	0.578980000
H	7.067031000	-1.637835000	0.450848000

TS_{bir}[5,6]

E=-2480.488566

G=-2480.078562

C	-2.969823000	-0.347166000	-0.656526000
C	-2.900145000	-0.161503000	0.785608000
C	-2.561925000	1.074624000	1.348870000
C	-2.204593000	2.209432000	0.473085000
C	-2.203705000	2.035222000	-0.922027000
C	-2.534508000	0.763699000	-1.495535000
C	-2.383926000	-1.669078000	-0.935533000
C	-2.082520000	-2.316189000	0.297967000
C	-2.388292000	-1.383054000	1.379447000
C	-1.581890000	-1.331369000	2.513559000
C	-1.730437000	1.135967000	2.515253000
C	-1.157920000	2.951902000	1.110158000
C	-0.112239000	3.508751000	0.336888000
C	-0.105944000	3.321573000	-1.104614000
C	-1.125872000	2.609783000	-1.720878000
C	-0.819345000	1.670051000	-2.795360000
C	-1.685208000	0.536922000	-2.640324000
C	-1.204752000	-0.770606000	-2.927881000
C	-1.555749000	-1.878904000	-2.065276000
C	-0.956430000	-3.174363000	0.403816000
C	-0.108758000	-3.398353000	-0.762445000
C	-0.411768000	-2.760745000	-1.972736000
C	0.657120000	-2.189940000	-2.778352000
C	0.157919000	-0.956057000	-3.371174000
C	1.011266000	0.146315000	-3.514216000
C	0.518642000	1.490068000	-3.217255000
C	1.570722000	2.223662000	-2.586884000
C	1.279543000	3.131783000	-1.538813000
C	-0.844915000	2.284563000	2.367640000
C	3.529001000	1.676258000	0.965849000
C	2.691435000	1.890339000	2.100295000
C	2.345940000	0.791531000	2.955578000

C	2.832843000	-0.510394000	2.672262000
C	3.690589000	-0.729834000	1.509451000
C	4.047722000	0.167672000	-0.760549000
C	3.544289000	1.395205000	-1.356207000
C	3.232382000	2.325210000	-0.271631000
C	2.108415000	3.176699000	-0.378766000
C	1.249000000	3.406772000	0.790523000
C	1.546262000	2.775157000	2.002470000
C	0.975522000	0.973280000	3.399829000
C	0.130581000	-0.130275000	3.540638000
C	0.634365000	-1.471402000	3.239718000
C	1.974361000	-1.641520000	2.816459000
C	2.282080000	-2.582232000	1.737622000
C	3.356991000	-2.015431000	0.938050000
C	3.355316000	-2.187657000	-0.453406000
C	3.708286000	-1.069596000	-1.321682000
C	2.732904000	1.343164000	-2.482530000
C	2.382121000	0.059747000	-3.070605000
C	2.864976000	-1.127298000	-2.494307000
C	1.981101000	-2.274232000	-2.348972000
C	2.294596000	-2.934229000	-1.089814000
C	1.261923000	-3.486447000	-0.315383000
C	1.262469000	-3.300215000	1.128078000
C	-0.122395000	-3.114326000	1.562211000
C	-0.414754000	-2.209465000	2.612076000
C	0.474652000	2.206411000	2.806549000
C	-1.243094000	-0.053759000	3.102335000
C	4.032461000	0.343107000	0.677349000
C	-5.230380000	-0.519031000	-1.148087000
C	-6.035108000	-0.190339000	1.034060000
C	-6.020940000	1.010942000	0.379307000
C	-5.590201000	0.813635000	-0.971871000

H	-5.485462000	1.594851000	-1.714693000
H	-6.277067000	1.971588000	0.810983000
H	-6.303848000	-0.355936000	2.070086000
H	-5.027914000	-0.986354000	-2.103413000
C	-5.667114000	-1.288208000	0.074926000
H	-6.559046000	-1.887244000	-0.175300000
H	-4.925535000	-1.994278000	0.462639000

Print[5,6]

E=-2480.522011

G=-2480.106774

C	-3.245429000	0.040916000	-0.644606000
C	-2.917984000	-0.257375000	0.831897000
C	-2.470197000	0.710967000	1.714196000
C	-2.062334000	2.037584000	1.231323000
C	-2.097101000	2.307405000	-0.137904000
C	-2.561768000	1.328474000	-1.072206000
C	-2.559685000	-1.161509000	-1.326641000
C	-2.233125000	-2.160454000	-0.352517000
C	-2.450980000	-1.604971000	0.970713000
C	-1.602846000	-1.970884000	2.034697000
C	-1.566972000	0.358494000	2.792060000
C	-0.921010000	2.470687000	2.022106000
C	0.132577000	3.204109000	1.415916000
C	0.085428000	3.501872000	0.018950000
C	-1.007410000	3.065165000	-0.760816000
C	-0.793325000	2.521615000	-2.061122000
C	-1.749963000	1.425283000	-2.245185000
C	-1.370460000	0.284206000	-2.956341000
C	-1.778287000	-1.037862000	-2.463389000
C	-1.171864000	-3.062029000	-0.569884000
C	-0.369912000	-2.934468000	-1.756827000

C	-0.660542000	-1.935248000	-2.684811000
C	0.417166000	-1.183053000	-3.311987000
C	-0.013575000	0.171737000	-3.468417000
C	0.909718000	1.234635000	-3.286737000
C	0.514998000	2.413218000	-2.581156000
C	1.652906000	2.868688000	-1.782289000
C	1.443717000	3.399211000	-0.515086000
C	-0.623058000	1.451427000	2.979637000
C	3.702143000	1.138316000	1.332733000
C	2.923484000	1.020730000	2.487250000
C	2.519666000	-0.291428000	2.962266000
C	2.910979000	-1.434961000	2.273700000
C	3.724050000	-1.317447000	1.075014000
C	4.056172000	0.240488000	-0.811486000
C	3.620968000	1.618101000	-0.966983000
C	3.402889000	2.172682000	0.356615000
C	2.333828000	3.048859000	0.578937000
C	1.520597000	2.915562000	1.773226000
C	1.808984000	1.926411000	2.710263000
C	1.158010000	-0.182009000	3.485056000
C	0.247447000	-1.248385000	3.297900000
C	0.648565000	-2.423764000	2.594367000
C	1.965332000	-2.530012000	2.074632000
C	2.180255000	-3.074406000	0.773453000
C	3.263728000	-2.328525000	0.138580000
C	3.211228000	-2.043144000	-1.221452000
C	3.617798000	-0.736250000	-1.709444000
C	2.763370000	1.961069000	-2.019199000
C	2.299854000	0.941298000	-2.941541000
C	2.719273000	-0.378700000	-2.794361000
C	1.770334000	-1.470673000	-2.977044000
C	2.068030000	-2.486102000	-2.018705000

C	1.025057000	-3.216942000	-1.402481000
C	1.079169000	-3.512634000	-0.007325000
C	-0.278807000	-3.404111000	0.525669000
C	-0.488001000	-2.873798000	1.791868000
C	0.726969000	1.170869000	3.331548000
C	-1.149191000	-0.962169000	2.953730000
C	4.107427000	-0.056365000	0.610491000
C	-4.794964000	0.121266000	-0.942542000
C	-6.417059000	-0.597592000	0.694421000
C	-6.310514000	0.785719000	0.763757000
C	-5.432041000	1.268222000	-0.197265000
H	-5.168141000	2.305720000	-0.359940000
H	-6.845894000	1.409488000	1.472923000
H	-7.036881000	-1.220498000	1.328671000
H	-4.874895000	0.241851000	-2.029964000
C	-5.586559000	-1.125355000	-0.445010000
H	-6.224627000	-1.519943000	-1.249289000
H	-4.932471000	-1.952551000	-0.147674000

TS_{bir}[6,6]

E=-2480.488566

G=-2480.078562

C	2.958712000	0.207112000	-0.739071000
C	2.475495000	1.578246000	-0.928178000
C	2.098031000	2.374710000	0.154736000
C	2.105185000	1.805909000	1.516530000
C	2.506041000	0.463709000	1.713021000
C	2.877468000	-0.346234000	0.604148000
C	2.368787000	-0.589281000	-1.825671000
C	1.659829000	0.274485000	-2.707103000
C	1.713510000	1.627443000	-2.156762000
C	0.612517000	2.476227000	-2.270226000

C	0.960489000	3.248894000	0.047769000
C	0.986924000	2.336137000	2.230438000
C	0.268476000	1.514341000	3.133208000
C	0.677600000	0.128719000	3.335562000
C	1.768980000	-0.382416000	2.650963000
C	1.721037000	-1.728666000	2.089764000
C	2.402571000	-1.693501000	0.827501000
C	1.919038000	-2.468776000	-0.261750000
C	1.900284000	-1.909138000	-1.596088000
C	0.487094000	-0.174488000	-3.367403000
C	0.008524000	-1.534371000	-3.139071000
C	0.710834000	-2.381181000	-2.269354000
C	-0.018345000	-3.232886000	-1.341249000
C	0.738298000	-3.287047000	-0.097319000
C	0.062027000	-3.315492000	1.129115000
C	0.558378000	-2.515794000	2.249451000
C	-0.567649000	-1.993347000	2.958809000
C	-0.524099000	-0.684697000	3.501520000
C	0.258917000	3.217456000	1.323827000
C	-3.531822000	0.604828000	1.837851000
C	-3.054394000	1.930612000	1.608281000
C	-3.076487000	2.485158000	0.282797000
C	-3.563547000	1.711673000	-0.799557000
C	-4.051119000	0.353337000	-0.564604000
C	-3.640462000	-1.562788000	0.939287000
C	-2.880067000	-1.617494000	2.178134000
C	-2.825172000	-0.264866000	2.729249000
C	-1.654345000	0.180614000	3.377932000
C	-1.165131000	1.547157000	3.148688000
C	-1.863740000	2.399581000	2.282896000
C	-1.891290000	3.306285000	0.112713000
C	-1.222130000	3.330172000	-1.112605000

C	-1.723963000	2.524242000	-2.226341000
C	-2.884895000	1.734804000	-2.056096000
C	-2.935461000	0.383384000	-2.617960000
C	-3.672426000	-0.463409000	-1.691692000
C	-3.271958000	-1.795514000	-1.494857000
C	-3.256956000	-2.356514000	-0.147796000
C	-1.778944000	-2.458781000	2.286335000
C	-1.381031000	-3.288148000	1.159618000
C	-2.113103000	-3.234184000	-0.038622000
C	-1.411805000	-3.206649000	-1.312944000
C	-2.139444000	-2.324390000	-2.214990000
C	-1.432515000	-1.506314000	-3.112860000
C	-1.846415000	-0.123595000	-3.311865000
C	-0.643370000	0.690560000	-3.476195000
C	-0.599991000	2.001635000	-2.936940000
C	-1.132310000	3.251868000	1.355294000
C	0.223326000	3.308833000	-1.153331000
C	-4.037373000	-0.184759000	0.731344000
C	5.232407000	0.292854000	-1.117774000
C	6.223627000	0.151694000	1.019866000
C	6.161724000	-1.097904000	0.475803000
C	5.608657000	-1.018757000	-0.847309000
H	5.458542000	-1.861839000	-1.511597000
H	6.470797000	-2.018127000	0.958202000
H	6.569270000	0.406308000	2.014297000
H	5.018436000	0.684003000	-2.103583000
C	5.708887000	1.157676000	0.027434000
H	6.516322000	1.822375000	-0.318253000
H	4.935140000	1.813442000	0.443135000

Print[6,6]

E=-2480.522793

G=-2480.107692

C	2.540983000	0.527548000	-1.705430000
C	3.245334000	0.538819000	-0.332583000
C	2.904066000	-0.728758000	0.431210000
C	2.400337000	-1.906328000	-0.207456000
C	2.006089000	-1.889531000	-1.546818000
C	2.068847000	-0.629571000	-2.300006000
C	1.849144000	1.764548000	-1.914989000
C	1.853044000	2.514116000	-0.672778000
C	2.548311000	1.749468000	0.320041000
C	2.078250000	1.734262000	1.622040000
C	2.403002000	-0.714074000	1.770680000
C	1.617976000	-2.670159000	0.770541000
C	0.459711000	-3.367740000	0.361949000
C	0.045911000	-3.330421000	-1.005358000
C	0.799520000	-2.591671000	-1.954524000
C	0.128748000	-1.803598000	-2.941656000
C	0.899021000	-0.586979000	-3.155442000
C	0.248502000	0.623309000	-3.392231000
C	0.730888000	1.827246000	-2.770457000
C	0.737188000	3.301912000	-0.324363000
C	-0.426836000	3.332157000	-1.196580000
C	-0.429701000	2.615109000	-2.385848000
C	-1.631761000	1.893311000	-2.802458000
C	-1.217291000	0.670375000	-3.410731000
C	-1.960558000	-0.515907000	-3.208034000
C	-1.293146000	-1.756902000	-2.977223000
C	-2.067028000	-2.517089000	-2.003003000
C	-1.415257000	-3.282567000	-1.038842000
C	1.620171000	-1.934538000	1.991674000
C	-3.014955000	-1.786861000	1.929301000
C	-1.894810000	-1.829973000	2.767943000

C	-1.404717000	-0.614283000	3.389750000
C	-2.054574000	0.597282000	3.166990000
C	-3.223258000	0.644344000	2.304542000
C	-4.113677000	-0.490703000	0.304156000
C	-3.696781000	-1.735938000	-0.319148000
C	-3.017863000	-2.536051000	0.686322000
C	-1.900737000	-3.300591000	0.328337000
C	-0.738706000	-3.339684000	1.200911000
C	-0.736131000	-2.622262000	2.390841000
C	0.056387000	-0.669263000	3.411591000
C	0.811121000	0.514044000	3.200437000
C	0.142705000	1.756353000	2.966992000
C	-1.279199000	1.812815000	2.947873000
C	-1.948594000	2.597777000	1.960751000
C	-3.156718000	1.883730000	1.549400000
C	-3.564605000	1.915289000	0.220005000
C	-4.056075000	0.705076000	-0.416433000
C	-3.232268000	-1.729922000	-1.637045000
C	-3.166016000	-0.483381000	-2.380457000
C	-3.569908000	0.707363000	-1.785739000
C	-2.793995000	1.928110000	-1.988898000
C	-2.791229000	2.664787000	-0.766670000
C	-1.625841000	3.365608000	-0.359556000
C	-1.206768000	3.330275000	1.004392000
C	0.259161000	3.289451000	1.032396000
C	0.911498000	2.512350000	1.988904000
C	0.465231000	-1.896101000	2.803047000
C	2.014497000	0.479489000	2.384332000
C	-3.692396000	-0.522689000	1.695062000
C	4.797941000	0.744147000	-0.481658000
C	6.461641000	-0.327180000	0.909201000
C	6.377910000	-1.024012000	-0.288660000

C	5.456097000	-0.438662000	-1.147459000
H	5.192643000	-0.785415000	-2.139296000
H	6.957923000	-1.910602000	-0.526014000
H	4.919278000	1.661314000	-1.072727000
H	7.103441000	-0.576154000	1.746237000
C	5.533357000	0.858230000	0.889357000
H	6.083807000	1.806597000	0.961075000
H	4.835772000	0.852396000	1.736118000

TS[5,6]

E=-2480.507171

G=-2480.088876

C	3.259873000	0.015782000	-0.780397000
C	3.095517000	0.343571000	0.736848000
C	2.564889000	-0.636304000	1.625723000
C	2.162940000	-1.965491000	1.167642000
C	2.167367000	-2.265224000	-0.190378000
C	2.586015000	-1.285039000	-1.161201000
C	2.517277000	1.192907000	-1.438106000
C	2.210896000	2.199605000	-0.470532000
C	2.489701000	1.677644000	0.844032000
C	1.668882000	2.035806000	1.921419000
C	1.702362000	-0.286130000	2.713224000
C	1.064442000	-2.423008000	2.005671000
C	0.007238000	-3.184325000	1.443663000
C	0.016340000	-3.500004000	0.051837000
C	1.078687000	-3.051492000	-0.767003000
C	0.813549000	-2.526231000	-2.066919000
C	1.743492000	-1.418199000	-2.299053000
C	1.315832000	-0.288645000	-3.017653000
C	1.709336000	1.041551000	-2.554147000
C	1.128521000	3.089900000	-0.672996000

C	0.290928000	2.925901000	-1.832008000
C	0.568780000	1.918847000	-2.753534000
C	-0.512401000	1.138968000	-3.336783000
C	-0.058168000	-0.210907000	-3.482896000
C	-0.954311000	-1.288650000	-3.254987000
C	-0.514580000	-2.451134000	-2.546872000
C	-1.616445000	-2.917292000	-1.709324000
C	-1.359716000	-3.426514000	-0.440970000
C	0.779992000	-1.391755000	2.952981000
C	-3.596847000	-1.177154000	1.443243000
C	-2.782991000	-1.027697000	2.570148000
C	-2.385852000	0.297373000	3.011837000
C	-2.823123000	1.426703000	2.321090000
C	-3.671575000	1.274870000	1.152571000
C	-4.035444000	-0.316268000	-0.699421000
C	-3.579884000	-1.688836000	-0.848969000
C	-3.312477000	-2.221170000	0.474535000
C	-2.221950000	-3.077928000	0.674622000
C	-1.374428000	-2.913452000	1.840863000
C	-1.647858000	-1.913267000	2.770144000
C	-1.008824000	0.219780000	3.490800000
C	-0.118803000	1.298629000	3.256833000
C	-0.567067000	2.458246000	2.550060000
C	-1.905747000	2.532578000	2.075340000
C	-2.173630000	3.055029000	0.774038000
C	-3.264726000	2.281205000	0.185757000
C	-3.252001000	1.978041000	-1.170621000
C	-3.647402000	0.654486000	-1.626605000
C	-2.750273000	-2.030876000	-1.922557000
C	-2.337874000	-1.017675000	-2.875143000
C	-2.779378000	0.298518000	-2.734270000
C	-1.860318000	1.405265000	-2.964158000

C	-2.146238000	2.430632000	-2.011626000
C	-1.098010000	3.190492000	-1.440645000
C	-1.110988000	3.502997000	-0.047996000
C	0.268911000	3.429893000	0.440243000
C	0.528870000	2.916454000	1.705703000
C	-0.559194000	-1.129131000	3.344332000
C	1.267003000	1.037239000	2.882821000
C	-4.046608000	0.000145000	0.718356000
C	4.820853000	0.006160000	-1.133467000
C	5.296507000	0.517877000	1.056602000
C	5.619932000	-0.872089000	0.863950000
C	5.418208000	-1.194563000	-0.443764000
H	5.499606000	-2.178897000	-0.888449000
H	5.879397000	-1.562681000	1.658747000
H	5.408323000	1.048916000	1.995059000
H	4.960124000	0.060096000	-2.214758000
C	5.402407000	1.167201000	-0.301646000
H	6.453631000	1.342572000	-0.569433000
H	4.856440000	2.106929000	-0.402828000

Prod[5,6]

E=-2480.531706

G=-2480.110393

C	3.280601000	-0.194202000	0.808840000
C	3.280604000	-0.194033000	-0.808867000
C	2.586909000	0.987422000	-1.436321000
C	2.171951000	2.158929000	-0.695219000
C	2.171948000	2.158787000	0.695668000
C	2.586898000	0.987124000	1.436535000
C	2.513075000	-1.471303000	1.165596000
C	2.211111000	-2.239756000	-0.000224000
C	2.513080000	-1.471059000	-1.165891000

C	1.698636000	-1.575661000	-2.286206000
C	1.736509000	0.877088000	-2.566020000
C	1.081766000	2.804798000	-1.419807000
C	0.023130000	3.425039000	-0.713241000
C	0.023127000	3.424885000	0.713941000
C	1.081757000	2.804501000	1.420383000
C	0.806792000	2.008069000	2.571426000
C	1.736494000	0.876557000	2.566201000
C	1.302590000	-0.383129000	3.025030000
C	1.698621000	-1.576132000	2.285890000
C	1.129146000	-3.161390000	-0.000326000
C	0.284591000	-3.257034000	1.161541000
C	0.556328000	-2.473949000	2.279644000
C	-0.530274000	-1.840154000	3.011573000
C	-0.075709000	-0.555391000	3.449520000
C	-0.970716000	0.548587000	3.454331000
C	-0.525424000	1.835660000	3.017306000
C	-1.620655000	2.476030000	2.295924000
C	-1.355482000	3.249992000	1.169853000
C	0.806804000	2.008606000	-2.571014000
C	-3.576896000	1.467659000	-1.173888000
C	-2.754622000	1.566424000	-2.300716000
C	-2.349538000	0.369008000	-3.015112000
C	-2.790592000	-0.884952000	-2.588519000
C	-3.648479000	-0.990178000	-1.423847000
C	-4.029281000	0.159968000	0.725558000
C	-3.576899000	1.467416000	1.174181000
C	-3.300972000	2.275737000	0.000227000
C	-2.210130000	3.155591000	0.000323000
C	-1.355473000	3.250237000	-1.169194000
C	-1.620645000	2.476504000	-2.295416000
C	-0.970697000	0.549305000	-3.454224000

C	-0.075688000	-0.554676000	-3.449636000
C	-0.530250000	-1.839529000	-3.011951000
C	-1.874629000	-2.017469000	-2.581088000
C	-2.154132000	-2.812661000	-1.427501000
C	-3.251142000	-2.184759000	-0.695459000
C	-3.251145000	-2.184906000	0.694999000
C	-3.648486000	-0.990472000	1.423631000
C	-2.754634000	1.565950000	2.301029000
C	-2.349550000	0.368380000	3.015183000
C	-2.790609000	-0.885487000	2.588333000
C	-1.874640000	-2.018007000	2.580668000
C	-2.154143000	-2.812962000	1.426915000
C	-1.100576000	-3.432490000	0.713410000
C	-1.100571000	-3.432336000	-0.714119000
C	0.284603000	-3.256790000	-1.162207000
C	0.556342000	-2.473477000	-2.280156000
C	-0.525404000	1.836285000	-3.016939000
C	1.302603000	-0.382495000	-3.025105000
C	-4.029274000	0.160120000	-0.725537000
C	4.837626000	-0.267814000	1.128299000
C	4.837642000	-0.267585000	-1.128334000
C	5.421465000	1.059890000	-0.669561000
C	5.421443000	1.059763000	0.669801000
H	5.673044000	1.882766000	1.328902000
H	5.673092000	1.883019000	-1.328494000
H	5.037063000	-0.565179000	-2.158809000
H	5.037046000	-0.565615000	2.158715000
C	5.331907000	-1.196189000	-0.000110000
H	6.419846000	-1.301234000	-0.000115000
H	4.867433000	-2.185073000	-0.000215000

TS[6,6]

E=-2480.492480

G=-2480.077808

C	-2.538694000	0.901749000	-1.528685000
C	-3.211486000	-0.242219000	-0.761006000
C	-3.040849000	-0.106460000	0.745946000
C	-2.554518000	1.145384000	1.326528000
C	-2.173916000	2.244044000	0.510218000
C	-2.164870000	2.116220000	-0.917945000
C	-1.780999000	0.385066000	-2.595417000
C	-1.719484000	-1.068285000	-2.468480000
C	-2.445825000	-1.457524000	-1.319248000
C	-1.961811000	-2.500197000	-0.509015000
C	-2.460032000	-1.169890000	1.526457000
C	-1.815212000	0.850690000	2.510410000
C	-0.709102000	1.637855000	2.891778000
C	-0.311407000	2.769653000	2.053715000
C	-1.025552000	3.064982000	0.895281000
C	-0.318167000	3.455766000	-0.309243000
C	-1.009714000	2.858058000	-1.428826000
C	-0.283980000	2.360319000	-2.512085000
C	-0.667481000	1.098380000	-3.120203000
C	-0.545613000	-1.755432000	-2.865284000
C	0.590164000	-1.014766000	-3.375448000
C	0.524408000	0.393644000	-3.503065000
C	1.665836000	1.205521000	-3.128124000
C	1.164035000	2.432234000	-2.513635000
C	1.836830000	3.002020000	-1.431643000
C	1.086608000	3.527891000	-0.306259000
C	1.821602000	3.212455000	0.898677000
C	1.135952000	2.844443000	2.061526000
C	-1.747303000	-0.597860000	2.633805000
C	2.861854000	-0.379043000	2.644385000

C	1.743704000	-1.092971000	3.129501000
C	1.362343000	-2.361069000	2.516400000
C	2.093132000	-2.869011000	1.434102000
C	3.235810000	-2.116672000	0.921135000
C	4.008974000	0.229370000	0.699098000
C	3.508447000	1.444827000	1.319662000
C	2.798257000	1.065491000	2.522269000
C	1.624787000	1.748269000	2.883865000
C	0.481415000	1.018643000	3.400924000
C	0.544658000	-0.391385000	3.520141000
C	-0.077867000	-2.427901000	2.508681000
C	-0.755240000	-2.997478000	1.429716000
C	-0.003102000	-3.530098000	0.310062000
C	1.402931000	-3.464649000	0.314932000
C	2.109082000	-3.074096000	-0.892774000
C	3.250008000	-2.245715000	-0.506661000
C	3.629894000	-1.151800000	-1.313853000
C	4.022024000	0.107193000	-0.691280000
C	3.035188000	2.494918000	0.517240000
C	3.043955000	2.367949000	-0.917326000
C	3.530336000	1.189462000	-1.518667000
C	2.831939000	0.603434000	-2.642177000
C	2.899457000	-0.845443000	-2.512484000
C	1.789428000	-1.634708000	-2.878110000
C	1.398397000	-2.774028000	-2.050789000
C	-0.053820000	-2.846995000	-2.053654000
C	-0.737787000	-3.209953000	-0.891525000
C	-0.587314000	-1.199453000	3.137034000
C	-1.970681000	-2.378535000	0.916833000
C	3.608694000	-0.895418000	1.527039000
C	-4.784404000	-0.345854000	-1.104202000
C	-5.317573000	-0.223976000	1.132006000

C	-5.638794000	1.039863000	0.555378000
C	-5.411522000	0.979890000	-0.793403000
H	-5.489088000	1.799031000	-1.497767000
H	-5.916982000	1.925033000	1.116220000
H	-4.905299000	-0.705782000	-2.127197000
H	-5.394735000	-0.465311000	2.185376000
C	-5.342781000	-1.239785000	0.019840000
H	-6.377412000	-1.533870000	-0.208295000
H	-4.755987000	-2.141188000	0.207241000

Prod[6,6]

E=-2480.524155

G=-2480.104933

C	-2.579984000	1.006504000	-1.436387000
C	-3.250130000	-0.206287000	-0.796778000
C	-3.250195000	-0.206364000	0.796577000
C	-2.580091000	1.006359000	1.436349000
C	-2.209679000	2.160291000	0.718602000
C	-2.209617000	2.160350000	-0.718495000
C	-1.817213000	0.602031000	-2.549858000
C	-1.735360000	-0.855070000	-2.548191000
C	-2.446161000	-1.341992000	-1.432291000
C	-1.947093000	-2.448701000	-0.718565000
C	-2.446272000	-1.342128000	1.432038000
C	-1.817422000	0.601800000	2.549887000
C	-0.712803000	1.368817000	3.008422000
C	-0.340427000	2.574029000	2.292013000
C	-1.065630000	2.959818000	1.164709000
C	-0.374139000	3.465204000	0.000146000
C	-1.065512000	2.959939000	-1.164452000
C	-0.340232000	2.574252000	-2.291795000
C	-0.712499000	1.369127000	-3.008229000

C	-0.551467000	-1.493414000	-3.007145000
C	0.567705000	-0.708069000	-3.448223000
C	0.487869000	0.714114000	-3.448665000
C	1.617642000	1.498925000	-3.013085000
C	1.109696000	2.660530000	-2.294660000
C	1.779024000	3.135011000	-1.166805000
C	1.032880000	3.555795000	0.000217000
C	1.778906000	3.134896000	1.167185000
C	1.109504000	2.660291000	2.295001000
C	-1.735572000	-0.855340000	2.548088000
C	2.882793000	-0.594328000	2.583577000
C	1.778666000	-1.361724000	3.013103000
C	1.404888000	-2.572628000	2.294584000
C	2.123723000	-2.968433000	1.166523000
C	3.262325000	-2.167333000	0.715666000
C	4.008560000	0.198811000	0.695981000
C	3.495772000	1.349404000	1.425755000
C	2.800905000	0.860391000	2.583609000
C	1.617339000	1.498645000	3.013243000
C	0.487516000	0.713780000	3.448761000
C	0.567351000	-0.708416000	3.448182000
C	-0.045494000	-2.649948000	2.291936000
C	-0.722195000	-3.116060000	1.164913000
C	0.021583000	-3.539913000	-0.000181000
C	1.429923000	-3.470970000	-0.000111000
C	2.123840000	-2.968316000	-1.166713000
C	3.262404000	-2.167288000	-0.715710000
C	3.628954000	-1.001873000	-1.426010000
C	4.008605000	0.198878000	-0.695746000
C	2.999660000	2.466120000	0.715661000
C	2.999736000	2.466218000	-0.715270000
C	3.495878000	1.349547000	-1.425435000

C	2.801109000	0.860681000	-2.583427000
C	2.883001000	-0.594110000	-2.583530000
C	1.778965000	-1.361408000	-3.013213000
C	1.405079000	-2.572415000	-2.294730000
C	-0.045301000	-2.649721000	-2.292206000
C	-0.722076000	-3.115952000	-1.165221000
C	-0.551770000	-1.493696000	3.007069000
C	-1.947155000	-2.448783000	0.718245000
C	3.628849000	-1.002010000	1.426111000
C	-4.806849000	-0.317308000	-1.123782000
C	-4.806939000	-0.317411000	1.123444000
C	-5.436754000	0.986050000	0.669615000
C	-5.436699000	0.986112000	-0.669887000
H	-5.710525000	1.800616000	-1.330616000
H	-5.710633000	1.800496000	1.330395000
H	-4.986470000	-0.618722000	-2.156266000
H	-4.986641000	-0.618917000	2.155887000
C	-5.259631000	-1.268861000	-0.000230000
H	-6.340619000	-1.430939000	-0.000280000
H	-4.738833000	-2.231227000	-0.000251000

S=3

${}^7C_{60}$

E=-2286.301217

G=-2285.984095

C	-0.441703000	3.490128000	0.614251000
C	1.012267000	3.359380000	0.601621000
C	1.686617000	3.071041000	-0.601039000
C	0.935581000	2.888329000	-1.811942000
C	-0.484100000	3.013372000	-1.802213000
C	-1.176735000	3.326830000	-0.580567000
C	-0.926085000	2.917309000	1.838865000

C	0.225110000	2.428690000	2.592060000
C	1.410285000	2.702161000	1.820467000
C	2.490369000	1.766928000	1.810634000
C	2.790156000	2.114813000	-0.610709000
C	1.562099000	1.831483000	-2.572884000
C	0.766038000	0.919489000	-3.313125000
C	-0.673482000	1.044860000	-3.309409000
C	-1.295921000	2.083142000	-2.557381000
C	-2.494406000	1.817353000	-1.806707000
C	-2.426118000	2.583702000	-0.573416000
C	-2.899151000	2.025877000	0.621402000
C	-2.137767000	2.191739000	1.848437000
C	0.131779000	1.232704000	3.330750000
C	-1.096200000	0.486958000	3.325232000
C	-2.221338000	0.960925000	2.589761000
C	-3.032097000	0.030941000	1.833490000
C	-3.454293000	0.682612000	0.621831000
C	-3.523672000	-0.057897000	-0.578858000
C	-3.039954000	0.514396000	-1.803961000
C	-2.398133000	-0.547884000	-2.572831000
C	-1.235695000	-0.277111000	-3.321143000
C	2.704598000	1.356033000	-1.827404000
C	0.926085000	-2.917309000	-1.838865000
C	2.137767000	-2.191739000	-1.848437000
C	2.899151000	-2.025877000	-0.621402000
C	2.426118000	-2.583702000	0.573416000
C	1.176735000	-3.326830000	0.580567000
C	-1.012267000	-3.359380000	-0.601621000
C	-1.410285000	-2.702161000	-1.820467000
C	-0.225110000	-2.428690000	-2.592060000
C	-0.131779000	-1.232704000	-3.330750000
C	1.096200000	-0.486958000	-3.325232000

C	2.221338000	-0.960925000	-2.589761000
C	3.454293000	-0.682612000	-0.621831000
C	3.523672000	0.057897000	0.578858000
C	3.039954000	-0.514396000	1.803961000
C	2.494406000	-1.817353000	1.806707000
C	1.295921000	-2.083142000	2.557381000
C	0.484100000	-3.013372000	1.802213000
C	-0.935581000	-2.888329000	1.811942000
C	-1.686617000	-3.071041000	0.601039000
C	-2.490369000	-1.766928000	-1.810634000
C	-3.185233000	-1.478212000	-0.582456000
C	-2.790156000	-2.114813000	0.610709000
C	-2.704598000	-1.356033000	1.827404000
C	-1.562099000	-1.831483000	2.572884000
C	-0.766038000	-0.919489000	3.313125000
C	0.673482000	-1.044860000	3.309409000
C	1.235695000	0.277111000	3.321143000
C	2.398133000	0.547884000	2.572831000
C	3.032097000	-0.030941000	-1.833490000
C	3.185233000	1.478212000	0.582456000
C	0.441703000	-3.490128000	-0.614251000

Pre-reactants

E=-2480.430826

G=-2480.025378

C	1.675617000	1.563352000	2.313977000
C	1.605331000	2.390237000	1.173757000
C	0.321646000	2.869031000	0.720922000
C	-0.866807000	2.521372000	1.434449000
C	-0.792853000	1.695371000	2.601605000
C	0.458344000	1.210462000	3.037715000
C	-2.069689000	2.170961000	0.708905000

C	-2.069689000	2.170961000	-0.708905000
C	-0.866807000	2.521372000	-1.434449000
C	0.321646000	2.869031000	-0.720922000
C	-2.739676000	1.116103000	-1.433484000
C	-1.958555000	0.815232000	-2.601426000
C	-0.792853000	1.695371000	-2.601605000
C	0.458344000	1.210462000	-3.037715000
C	0.581146000	-0.157890000	-3.475486000
C	-0.559313000	-1.015238000	-3.476869000
C	-1.836590000	-0.519232000	-3.037608000
C	1.857409000	-0.656958000	-3.037026000
C	1.976448000	-1.995342000	-2.603262000
C	0.809994000	-2.870984000	-2.605614000
C	-0.435247000	-2.386603000	-3.040040000
C	2.750704000	-2.296359000	-1.434652000
C	2.078996000	-3.353616000	-0.710200000
C	0.883121000	-3.708719000	-1.434587000
C	-0.297433000	-4.048672000	-0.727360000
C	-0.297433000	-4.048672000	0.727360000
C	0.883121000	-3.708719000	1.434587000
C	2.078996000	-3.353616000	0.710200000
C	2.750704000	-2.296359000	1.434652000
C	1.976448000	-1.995342000	2.603262000
C	0.809994000	-2.870984000	2.605614000
C	-0.435247000	-2.386603000	3.040040000
C	-0.559313000	-1.015238000	3.476869000
C	0.581146000	-0.157890000	3.475486000
C	1.857409000	-0.656958000	3.037026000
C	2.537562000	0.412752000	2.314112000
C	-1.958555000	0.815232000	2.601426000
C	-1.836590000	-0.519232000	3.037608000
C	3.312092000	0.112326000	1.173539000

C	3.410044000	-1.253015000	0.722947000
C	-1.576649000	-3.569677000	1.176431000
C	-1.650284000	-2.740665000	2.316749000
C	-2.514067000	-1.591683000	2.314879000
C	3.410044000	-1.253015000	-0.722947000
C	-1.650284000	-2.740665000	-2.316749000
C	-1.576649000	-3.569677000	-1.176431000
C	-2.376257000	-3.264011000	0.000000000
C	-2.514067000	-1.591683000	-2.314879000
C	-3.288946000	-1.293073000	-1.175085000
C	-3.217355000	-2.146707000	0.000000000
C	1.675617000	1.563352000	-2.313977000
C	2.537562000	0.412752000	-2.314112000
C	3.312092000	0.112326000	-1.173539000
C	-3.396125000	0.069841000	-0.723162000
C	1.605331000	2.390237000	-1.173757000
C	-3.288946000	-1.293073000	1.175085000
C	-3.396125000	0.069841000	0.723162000
C	-2.739676000	1.116103000	1.433484000
C	2.408883000	2.090231000	0.000000000
C	3.248551000	0.965752000	0.000000000
C	0.181929000	5.903324000	-1.177154000
C	0.181929000	5.903324000	1.177154000
C	-1.095825000	5.830714000	0.729514000
C	-1.095825000	5.830714000	-0.729514000
C	1.114182000	5.991291000	0.000000000
H	0.507314000	5.918638000	-2.210065000
H	-1.986337000	5.763540000	-1.344167000
H	-1.986337000	5.763540000	1.344167000
H	0.507314000	5.918638000	2.210065000
H	1.870417000	5.195313000	0.000000000
H	1.671733000	6.940765000	0.000000000

TS_{bir}[5,6]

E=-2480.425275

G=-2480.019773

C	-2.993257000	-0.438735000	-0.577813000
C	-2.915477000	-0.044796000	0.821840000
C	-2.560711000	1.266998000	1.185537000
C	-2.201756000	2.244848000	0.154966000
C	-2.208731000	1.871709000	-1.201788000
C	-2.555344000	0.529868000	-1.574452000
C	-2.424649000	-1.792995000	-0.662176000
C	-2.115483000	-2.243921000	0.657017000
C	-2.415912000	-1.163481000	1.586058000
C	-1.586566000	-0.944974000	2.701923000
C	-1.705929000	1.492326000	2.319303000
C	-1.124648000	3.058125000	0.670678000
C	-0.077004000	3.492942000	-0.192950000
C	-0.082816000	3.111280000	-1.576323000
C	-1.130385000	2.307103000	-2.077976000
C	-0.834161000	1.226292000	-2.987235000
C	-1.716320000	0.128596000	-2.674821000
C	-1.247855000	-1.205492000	-2.768977000
C	-1.602997000	-2.172427000	-1.750034000
C	-0.987187000	-3.084019000	0.876782000
C	-0.154069000	-3.476414000	-0.241235000
C	-0.459316000	-3.030161000	-1.534263000
C	0.605637000	-2.580413000	-2.416749000
C	0.117412000	-1.463181000	-3.176155000
C	0.983658000	-0.383637000	-3.485479000
C	0.507971000	0.971355000	-3.387126000
C	1.580269000	1.793442000	-2.884055000
C	1.293464000	2.853651000	-1.985767000

C	-0.814577000	2.600173000	1.995978000
C	3.575237000	1.793413000	0.688035000
C	2.746014000	2.175857000	1.781118000
C	2.397619000	1.216122000	2.789331000
C	2.872038000	-0.109380000	2.696072000
C	3.723489000	-0.505425000	1.577681000
C	4.072551000	0.042072000	-0.804384000
C	3.573313000	1.162075000	-1.567220000
C	3.266493000	2.243196000	-0.632941000
C	2.140483000	3.073354000	-0.853634000
C	1.296247000	3.473536000	0.269038000
C	1.597215000	3.032749000	1.559920000
C	1.020773000	1.468759000	3.197739000
C	0.165399000	0.386139000	3.503441000
C	0.651988000	-0.963799000	3.404992000
C	1.998875000	-1.209157000	2.998610000
C	2.294513000	-2.286813000	2.087540000
C	3.368100000	-1.860418000	1.208869000
C	3.358017000	-2.232896000	-0.142295000
C	3.715819000	-1.272096000	-1.165097000
C	2.739247000	0.945865000	-2.671652000
C	2.368083000	-0.407505000	-3.041230000
C	2.846391000	-1.494706000	-2.301128000
C	1.955487000	-2.603890000	-1.978692000
C	2.265844000	-3.050773000	-0.655371000
C	1.229381000	-3.480693000	0.212497000
C	1.244021000	-3.099827000	1.593489000
C	-0.132411000	-2.844552000	2.003927000
C	-0.418906000	-1.788349000	2.901636000
C	0.530727000	2.585636000	2.443223000
C	-1.224518000	0.400760000	3.068405000
C	4.068009000	0.426949000	0.594833000

C	-5.283524000	-0.647421000	-1.034603000
C	-6.058369000	0.067496000	1.063811000
C	-6.019613000	1.139306000	0.215451000
C	-5.604215000	0.703861000	-1.085095000
H	-5.486913000	1.345024000	-1.950133000
H	-6.248203000	2.165602000	0.478422000
H	-6.322390000	0.086732000	2.114006000
H	-5.090425000	-1.274887000	-1.895187000
C	-5.720380000	-1.185835000	0.305192000
H	-6.623762000	-1.804246000	0.170421000
H	-4.984500000	-1.824252000	0.805163000

Proint[5,6]

E=-2480.459329

G=-2480.049066

C	-3.239712000	-0.477596000	-0.441140000
C	-2.905533000	0.459545000	0.738098000
C	-2.450917000	1.779648000	0.561304000
C	-2.060179000	2.268369000	-0.744636000
C	-2.086716000	1.383262000	-1.843447000
C	-2.545633000	0.022826000	-1.690488000
C	-2.566152000	-1.783795000	0.034106000
C	-2.226160000	-1.676182000	1.411712000
C	-2.434515000	-0.292957000	1.837318000
C	-1.576528000	0.283933000	2.810467000
C	-1.558188000	2.383868000	1.536077000
C	-0.920475000	3.157523000	-0.572332000
C	0.129695000	3.168120000	-1.519873000
C	0.088636000	2.274191000	-2.643196000
C	-1.016808000	1.391116000	-2.803905000
C	-0.802244000	0.028995000	-3.234456000
C	-1.754946000	-0.813868000	-2.534879000

C	-1.382652000	-2.108734000	-2.124116000
C	-1.784894000	-2.580594000	-0.803811000
C	-1.162918000	-2.420208000	1.964144000
C	-0.368461000	-3.257737000	1.099564000
C	-0.667281000	-3.329007000	-0.259712000
C	0.410699000	-3.326555000	-1.240926000
C	-0.025727000	-2.566559000	-2.372886000
C	0.898399000	-1.742269000	-3.070003000
C	0.507922000	-0.432159000	-3.500842000
C	1.641345000	0.466844000	-3.338273000
C	1.428413000	1.809501000	-2.912191000
C	-0.618446000	3.239259000	0.826470000
C	3.703148000	1.768325000	-0.016307000
C	2.926593000	2.584418000	0.832816000
C	2.528322000	2.100973000	2.131542000
C	2.915172000	0.824861000	2.560512000
C	3.709060000	-0.018864000	1.683199000
C	4.039105000	-0.459584000	-0.720808000
C	3.600455000	0.297276000	-1.849866000
C	3.389913000	1.683483000	-1.419254000
C	2.320476000	2.416456000	-1.949476000
C	1.515923000	3.256136000	-1.073635000
C	1.811735000	3.336325000	0.284313000
C	1.164133000	2.566052000	2.391028000
C	0.254029000	1.735239000	3.086477000
C	0.652789000	0.430531000	3.517381000
C	1.971946000	-0.029617000	3.250036000
C	2.186284000	-1.389598000	2.818599000
C	3.255233000	-1.398396000	1.858034000
C	3.206134000	-2.265557000	0.752432000
C	3.596802000	-1.799502000	-0.545626000
C	2.731996000	-0.284398000	-2.800503000

C	2.279108000	-1.663739000	-2.622012000
C	2.704598000	-2.401992000	-1.523165000
C	1.760278000	-3.253085000	-0.810096000
C	2.063497000	-3.167061000	0.586063000
C	1.025578000	-3.167802000	1.539253000
C	1.076254000	-2.275059000	2.659441000
C	-0.267194000	-1.803060000	2.918149000
C	-0.478992000	-0.469228000	3.341062000
C	0.728430000	3.328261000	1.263999000
C	-1.133403000	1.652653000	2.641082000
C	4.093589000	0.439339000	0.426255000
C	-4.790247000	-0.631284000	-0.699182000
C	-6.392153000	0.170113000	0.919131000
C	-6.273358000	1.122154000	-0.085262000
C	-5.407726000	0.691353000	-1.082425000
H	-5.138911000	1.239544000	-1.976876000
H	-6.791887000	2.075912000	-0.094156000
H	-7.007552000	0.255832000	1.807055000
H	-4.880005000	-1.376941000	-1.498527000
C	-5.585492000	-1.052835000	0.572594000
H	-6.240485000	-1.907506000	0.348756000
H	-4.933376000	-1.379248000	1.390181000

TS_{bir}[6,6]

E=-2480.425275

G=-2480.019773

C	2.986743000	0.246314000	-0.701611000
C	2.522382000	1.639372000	-0.748106000
C	2.139797000	2.309488000	0.424048000
C	2.118777000	1.591849000	1.697661000
C	2.503296000	0.229081000	1.758336000
C	2.882298000	-0.452282000	0.568166000

C	2.406162000	-0.416689000	-1.876509000
C	1.713443000	0.553760000	-2.658168000
C	1.783924000	1.834343000	-1.966035000
C	0.676371000	2.706702000	-1.990234000
C	0.998189000	3.192113000	0.405146000
C	0.975863000	2.047249000	2.451666000
C	0.239633000	1.130289000	3.259958000
C	0.629628000	-0.253989000	3.323625000
C	1.744295000	-0.704201000	2.583635000
C	1.678908000	-1.959878000	1.881376000
C	2.389460000	-1.807615000	0.634322000
C	1.910504000	-2.449666000	-0.533373000
C	1.915311000	-1.745871000	-1.797577000
C	0.536968000	0.188246000	-3.371704000
C	0.042885000	-1.173594000	-3.296103000
C	0.724303000	-2.124733000	-2.522696000
C	-0.024033000	-3.056785000	-1.692725000
C	0.708140000	-3.257241000	-0.473611000
C	0.012227000	-3.409614000	0.752408000
C	0.496813000	-2.752011000	1.938200000
C	-0.639646000	-2.302033000	2.703067000
C	-0.578381000	-1.064299000	3.389308000
C	0.282142000	3.026572000	1.664289000
C	-3.573341000	0.431835000	1.876596000
C	-3.077519000	1.766245000	1.797310000
C	-3.076170000	2.461367000	0.540284000
C	-3.555994000	1.819966000	-0.618288000
C	-4.065904000	0.452966000	-0.541372000
C	-3.694513000	-1.625376000	0.745981000
C	-2.952138000	-1.824805000	1.971186000
C	-2.880800000	-0.543495000	2.665467000
C	-1.706529000	-0.179782000	3.363979000

C	-1.203751000	1.190099000	3.288376000
C	-1.882084000	2.143906000	2.520590000
C	-1.866153000	3.273942000	0.475450000
C	-1.178898000	3.420559000	-0.750636000
C	-1.669052000	2.760420000	-1.929427000
C	-2.851347000	1.961832000	-1.862944000
C	-2.915439000	0.703996000	-2.562803000
C	-3.674219000	-0.232869000	-1.750544000
C	-3.290406000	-1.582069000	-1.692815000
C	-3.303992000	-2.291641000	-0.429051000
C	-1.846115000	-2.684805000	1.990634000
C	-1.441645000	-3.369856000	0.777664000
C	-2.157044000	-3.176312000	-0.409446000
C	-1.441030000	-3.013400000	-1.669708000
C	-2.135320000	-2.035436000	-2.452031000
C	-1.407710000	-1.119150000	-3.256657000
C	-1.801936000	0.259201000	-3.313772000
C	-0.591353000	1.071108000	-3.378456000
C	-0.531264000	2.308959000	-2.693467000
C	-1.134771000	3.079332000	1.692566000
C	0.279384000	3.390677000	-0.786203000
C	-4.074834000	-0.225565000	0.684311000
C	5.282889000	0.383425000	-1.023759000
C	6.224957000	0.056722000	1.115344000
C	6.182869000	-1.139558000	0.461434000
C	5.657589000	-0.944890000	-0.861830000
H	5.526976000	-1.726053000	-1.601698000
H	6.486987000	-2.097843000	0.866673000
H	6.548364000	0.223733000	2.135506000
H	5.077279000	0.860133000	-1.972883000
C	5.725282000	1.144503000	0.204993000
H	6.534915000	1.842512000	-0.060701000

H 4.936874000 1.755956000 0.658813000

Proint[6,6]

E=-2480.460005

G=-2480.050064

C -2.518255000 1.041213000 -1.468883000
C -3.236503000 -0.057682000 -0.657143000
C -2.890769000 0.094410000 0.808728000
C -2.390814000 1.326023000 1.373045000
C -1.994501000 2.398313000 0.545860000
C -2.039579000 2.230573000 -0.892090000
C -1.823132000 0.465124000 -2.556476000
C -1.841327000 -0.989304000 -2.412465000
C -2.553162000 -1.319672000 -1.226109000
C -2.094079000 -2.359837000 -0.417069000
C -2.420797000 -0.987775000 1.616095000
C -1.628571000 1.005526000 2.548950000
C -0.460681000 1.750771000 2.877906000
C -0.045558000 2.835788000 2.034437000
C -0.789949000 3.148345000 0.873098000
C -0.106904000 3.463975000 -0.347294000
C -0.871534000 2.893849000 -1.446536000
C -0.212776000 2.344113000 -2.542172000
C -0.690658000 1.105859000 -3.123154000
C -0.722584000 -1.743009000 -2.826867000
C 0.443465000 -1.073419000 -3.357368000
C 0.454498000 0.334292000 -3.509157000
C 1.652554000 1.095168000 -3.183417000
C 1.246065000 2.330169000 -2.587289000
C 1.985047000 2.882436000 -1.515443000
C 1.311191000 3.459792000 -0.395345000
C 2.078203000 3.133834000 0.803540000

C	1.412811000	2.827673000	1.987111000
C	-1.640503000	-0.431379000	2.703952000
C	2.981324000	-0.474250000	2.584745000
C	1.845239000	-1.113147000	3.128290000
C	1.360505000	-2.359209000	2.535326000
C	2.018762000	-2.916465000	1.444325000
C	3.187934000	-2.255450000	0.887581000
C	4.094065000	0.046533000	0.601460000
C	3.692952000	1.302388000	1.216797000
C	2.998152000	0.985437000	2.436267000
C	1.879666000	1.733801000	2.827329000
C	0.715477000	1.071783000	3.368558000
C	0.704591000	-0.346023000	3.522322000
C	-0.092496000	-2.342455000	2.585879000
C	-0.843858000	-2.885436000	1.510103000
C	-0.167471000	-3.459599000	0.386047000
C	1.249842000	-3.481038000	0.341550000
C	1.932913000	-3.161739000	-0.875325000
C	3.139310000	-2.401804000	-0.537841000
C	3.555475000	-1.348700000	-1.370425000
C	4.041428000	-0.101402000	-0.781107000
C	3.243344000	2.363354000	0.402579000
C	3.187279000	2.201303000	-1.028438000
C	3.584846000	0.994788000	-1.620167000
C	2.809858000	0.423098000	-2.698722000
C	2.796813000	-1.011365000	-2.543419000
C	1.625436000	-1.757869000	-2.875804000
C	1.202510000	-2.839672000	-2.036901000
C	-0.261390000	-2.831130000	-1.998552000
C	-0.928421000	-3.128705000	-0.812098000
C	-0.490939000	-1.103213000	3.184587000
C	-2.041559000	-2.213125000	1.033490000

C	3.659764000	-1.045223000	1.464883000
C	-4.790242000	-0.041689000	-0.905836000
C	-6.408543000	-0.474586000	0.837913000
C	-6.312393000	0.899295000	0.661773000
C	-5.423180000	1.213759000	-0.358480000
H	-5.157398000	2.209278000	-0.692976000
H	-6.861260000	1.633779000	1.243148000
H	-4.916842000	-0.125537000	-1.992739000
H	-7.030783000	-0.980204000	1.567041000
C	-5.534791000	-1.190044000	-0.158208000
H	-6.131292000	-1.789214000	-0.860475000
H	-4.842831000	-1.892326000	0.322460000

TS[5,6]

E=-2480.441276

G=-2480.028028

C	3.245931000	-0.769496000	-0.226490000
C	3.090731000	0.786749000	-0.286583000
C	2.585845000	1.492589000	0.848699000
C	2.234841000	0.827541000	2.096122000
C	2.236887000	-0.576511000	2.159085000
C	2.603301000	-1.357873000	1.005875000
C	2.458326000	-1.216719000	-1.468303000
C	2.108218000	-0.094387000	-2.261267000
C	2.428355000	1.111268000	-1.551208000
C	1.583145000	2.244948000	-1.699274000
C	1.714111000	2.635411000	0.712064000
C	1.168131000	1.571730000	2.721367000
C	0.133429000	0.895376000	3.393910000
C	0.140904000	-0.548695000	3.467280000
C	1.181765000	-1.272417000	2.864241000
C	0.883695000	-2.480456000	2.114709000

C	1.756568000	-2.514891000	0.970510000
C	1.293620000	-3.044974000	-0.263394000
C	1.632899000	-2.353533000	-1.484204000
C	0.984514000	-0.139983000	-3.144263000
C	0.162421000	-1.314674000	-3.184983000
C	0.474446000	-2.414385000	-2.363659000
C	-0.574186000	-3.122503000	-1.685070000
C	-0.076233000	-3.507088000	-0.376591000
C	-0.928680000	-3.465735000	0.733362000
C	-0.449960000	-2.945721000	2.001968000
C	-1.515566000	-2.200017000	2.606624000
C	-1.228666000	-1.010806000	3.327124000
C	0.849129000	2.695392000	1.858802000
C	-3.533025000	1.220959000	1.478877000
C	-2.706411000	2.382293000	1.505803000
C	-2.362063000	3.043939000	0.283501000
C	-2.834417000	2.546533000	-0.950252000
C	-3.683749000	1.350806000	-0.977761000
C	-4.017700000	-0.744866000	0.284041000
C	-3.513898000	-1.114559000	1.581705000
C	-3.211500000	0.096651000	2.307883000
C	-2.077603000	0.144609000	3.170100000
C	-1.243976000	1.324152000	3.209675000
C	-1.547305000	2.427452000	2.384558000
C	-0.985897000	3.516914000	0.397441000
C	-0.142136000	3.470935000	-0.713278000
C	-0.632772000	2.953959000	-1.979731000
C	-1.971383000	2.500165000	-2.089041000
C	-2.273306000	1.277927000	-2.835285000
C	-3.338516000	0.579669000	-2.155651000
C	-3.327684000	-0.830981000	-2.086283000
C	-3.661903000	-1.490811000	-0.847741000

C	-2.668202000	-2.253385000	1.725146000
C	-2.309478000	-3.025930000	0.569983000
C	-2.786121000	-2.656671000	-0.702770000
C	-1.921787000	-2.711481000	-1.844021000
C	-2.242831000	-1.572875000	-2.699462000
C	-1.222039000	-0.893248000	-3.365069000
C	-1.234732000	0.557538000	-3.437177000
C	0.134889000	1.015180000	-3.294174000
C	0.428285000	2.199606000	-2.582431000
C	-0.492917000	3.128990000	1.705928000
C	1.239335000	3.035634000	-0.559341000
C	-4.024851000	0.712543000	0.212898000
C	4.804795000	-1.122075000	-0.322161000
C	5.261730000	1.125009000	-0.461578000
C	5.633493000	0.695988000	0.863158000
C	5.439779000	-0.648514000	0.961383000
H	5.549964000	-1.255723000	1.851518000
H	5.915587000	1.360258000	1.672525000
H	5.368771000	2.140194000	-0.827135000
H	4.937652000	-2.177776000	-0.565917000
C	5.355041000	-0.101311000	-1.338599000
H	6.401632000	-0.328379000	-1.584022000
H	4.783980000	-0.043875000	-2.267341000

Prod[5,6]

E=-2480.46523

G=-2480.04848

C	-3.269693000	0.810100000	-0.266030000
C	-3.269697000	-0.810132000	-0.265924000
C	-2.605693000	-1.432970000	0.931689000
C	-2.234154000	-0.701763000	2.120231000
C	-2.234154000	0.702039000	2.120141000

C	-2.605692000	1.433092000	0.931503000
C	-2.455429000	1.164611000	-1.512946000
C	-2.111774000	-0.000144000	-2.249408000
C	-2.455428000	-1.164805000	-1.512794000
C	-1.619554000	-2.293505000	-1.593189000
C	-1.746823000	-2.573491000	0.844772000
C	-1.177553000	-1.423416000	2.795961000
C	-0.139230000	-0.723215000	3.434290000
C	-0.139230000	0.723661000	3.434197000
C	-1.177553000	1.423779000	2.795778000
C	-0.872153000	2.589376000	1.991380000
C	-1.746822000	2.573602000	0.844440000
C	-1.278330000	3.045751000	-0.411947000
C	-1.619552000	2.293300000	-1.593486000
C	-0.989507000	-0.000203000	-3.141662000
C	-0.156702000	1.164229000	-3.242350000
C	-0.461763000	2.305512000	-2.474218000
C	0.590277000	3.041216000	-1.834726000
C	0.094123000	3.492525000	-0.545774000
C	0.945332000	3.497475000	0.566165000
C	0.461538000	3.041069000	1.856858000
C	1.525617000	2.318187000	2.498556000
C	1.232315000	1.170462000	3.273861000
C	-0.872153000	-2.589116000	1.991713000
C	3.518292000	-1.169490000	1.530901000
C	2.678108000	-2.324422000	1.617962000
C	2.321966000	-3.038561000	0.427065000
C	2.795646000	-2.603671000	-0.829214000
C	3.660626000	-1.421865000	-0.916598000
C	4.010419000	0.729681000	0.247470000
C	3.518293000	1.169685000	1.530752000
C	3.205181000	0.000149000	2.308309000

C	2.073729000	0.000205000	3.172112000
C	1.232315000	-1.170038000	3.274012000
C	1.525617000	-2.317865000	2.498853000
C	0.945331000	-3.497402000	0.566615000
C	0.094121000	-3.492595000	-0.545324000
C	0.590275000	-3.041454000	-1.834335000
C	1.934987000	-2.611030000	-1.970867000
C	2.247814000	-1.427867000	-2.771657000
C	3.323561000	-0.707740000	-2.125017000
C	3.323561000	0.707464000	-2.125107000
C	3.660626000	1.421744000	-0.916779000
C	2.678109000	2.324630000	1.617664000
C	2.321967000	3.038614000	0.426675000
C	2.795647000	2.603562000	-0.829548000
C	1.934988000	2.610773000	-1.971201000
C	2.247816000	1.427508000	-2.771839000
C	1.220826000	0.726323000	-3.408723000
C	1.220826000	-0.726763000	-3.408629000
C	-0.156704000	-1.164648000	-3.242200000
C	-0.461764000	-2.305832000	-2.473920000
C	0.461538000	-3.040827000	1.857249000
C	-1.278331000	-3.045803000	-0.411554000
C	4.010420000	-0.729652000	0.247564000
C	-4.822532000	1.128700000	-0.389170000
C	-4.822535000	-1.128749000	-0.389030000
C	-5.448518000	-0.669654000	0.918779000
C	-5.448488000	0.669770000	0.918708000
H	-5.725401000	1.328347000	1.733887000
H	-5.725453000	-1.328132000	1.734030000
H	-5.013505000	-2.158981000	-0.693095000
H	-5.013497000	2.158895000	-0.693361000
C	-5.285317000	-0.000084000	-1.333593000

H	-6.368931000	-0.000094000	-1.476149000
H	-4.787079000	-0.000148000	-2.306127000

TS[6,6]

E=-2480.425275

G=-2480.014124

C	2.590586000	-0.969648000	-1.446235000
C	3.244664000	0.211880000	-0.724166000
C	3.073267000	0.145819000	0.800228000
C	2.540420000	-1.065667000	1.415752000
C	2.167074000	-2.208031000	0.646091000
C	2.199723000	-2.153709000	-0.784821000
C	1.859168000	-0.511138000	-2.561860000
C	1.788036000	0.946730000	-2.503067000
C	2.476719000	1.385873000	-1.349943000
C	1.967046000	2.466844000	-0.601316000
C	2.426919000	1.245284000	1.505823000
C	1.754528000	-0.710259000	2.566592000
C	0.643473000	-1.487946000	2.971330000
C	0.261368000	-2.652691000	2.191217000
C	1.012822000	-3.004072000	1.042988000
C	0.336272000	-3.447946000	-0.138996000
C	1.058458000	-2.916743000	-1.283715000
C	0.357224000	-2.474077000	-2.402903000
C	0.761882000	-1.249577000	-3.072323000
C	0.619565000	1.609228000	-2.956457000
C	-0.498521000	0.843765000	-3.442017000
C	-0.428489000	-0.564016000	-3.498739000
C	-1.575235000	-1.362952000	-3.098372000
C	-1.093853000	-2.536083000	-2.428640000
C	-1.798388000	-3.058357000	-1.307593000
C	-1.079737000	-3.518286000	-0.160983000

C	-1.847263000	-3.162581000	1.026888000
C	-1.175214000	-2.738449000	2.185224000
C	1.683463000	0.723063000	2.623513000
C	-2.928255000	0.501466000	2.600892000
C	-1.828956000	1.242284000	3.066086000
C	-1.433773000	2.474583000	2.393041000
C	-2.150139000	2.921984000	1.269356000
C	-3.270885000	2.148847000	0.777720000
C	-4.044920000	-0.203314000	0.660425000
C	-3.542676000	-1.375148000	1.338695000
C	-2.856545000	-0.945415000	2.543030000
C	-1.687809000	-1.608539000	2.952297000
C	-0.558076000	-0.849409000	3.443719000
C	-0.627713000	0.561815000	3.499668000
C	0.002867000	2.532067000	2.398051000
C	0.710709000	3.047782000	1.283850000
C	-0.011665000	3.513768000	0.137671000
C	-1.427367000	3.444535000	0.116518000
C	-2.102485000	3.007986000	-1.066184000
C	-3.245953000	2.200622000	-0.663063000
C	-3.607865000	1.065342000	-1.413099000
C	-4.030393000	-0.145843000	-0.753054000
C	-3.041336000	-2.469181000	0.594216000
C	-3.015691000	-2.402171000	-0.845645000
C	-3.490815000	-1.253678000	-1.504546000
C	-2.766805000	-0.721690000	-2.655519000
C	-2.837302000	0.700249000	-2.598333000
C	-1.717260000	1.489842000	-2.983814000
C	-1.352766000	2.649757000	-2.222469000
C	0.097145000	2.731104000	-2.196928000
C	0.755597000	3.150833000	-1.042930000
C	0.503318000	1.351504000	3.084166000

C	1.93560000	2.40652500	0.82909100
C	-3.65711200	0.95498200	1.43122300
C	4.82201400	0.31743000	-1.04417700
C	5.21320900	0.28861400	1.21351300
C	5.61263100	-0.99335800	0.69847400
C	5.45275900	-0.98871400	-0.65574400
H	5.58040300	-1.83019600	-1.32581700
H	5.88278500	-1.84894400	1.30738500
H	4.96935400	0.63852000	-2.07624000
H	5.27390400	0.57415300	2.25745800
C	5.33081600	1.25995900	0.06331800
H	6.38076800	1.52963000	-0.11519000
H	4.74432400	2.17477200	0.17431200

Prod[6,6]

E=-2480.451707

G=-2480.037565

C	2.61387500	-0.94745000	-1.45669400
C	3.27548900	0.23514300	-0.75450800
C	3.24769300	0.16740800	0.84170200
C	2.56181700	-1.06714900	1.41673800
C	2.19096700	-2.18493200	0.64489700
C	2.21879200	-2.12952900	-0.78997100
C	1.87012500	-0.49612800	-2.56496500
C	1.79020900	0.96231300	-2.50286100
C	2.48386800	1.39844700	-1.35521100
C	1.96176100	2.47204500	-0.59863400
C	2.43102500	1.27377000	1.50982400
C	1.77368200	-0.70624100	2.53659700
C	0.66299200	-1.49108200	2.95863400
C	0.28624800	-2.65161400	2.18426100
C	1.03474800	-2.99330900	1.03965100

C	0.363352000	-3.438379000	-0.143037000
C	1.083886000	-2.900844000	-1.285548000
C	0.377028000	-2.466059000	-2.406137000
C	0.772840000	-1.238104000	-3.071749000
C	0.615334000	1.618627000	-2.951369000
C	-0.497112000	0.852941000	-3.438166000
C	-0.419388000	-0.561547000	-3.497765000
C	-1.559707000	-1.366307000	-3.101436000
C	-1.072371000	-2.538106000	-2.433345000
C	-1.778027000	-3.066323000	-1.312944000
C	-1.053244000	-3.520515000	-0.162635000
C	-1.820547000	-3.175116000	1.022491000
C	-1.156502000	-2.753085000	2.188205000
C	1.693970000	0.737790000	2.594674000
C	-2.926923000	0.482053000	2.597494000
C	-1.827493000	1.238844000	3.066018000
C	-1.445495000	2.471955000	2.405611000
C	-2.157661000	2.913895000	1.275726000
C	-3.272547000	2.131717000	0.778843000
C	-4.051877000	-0.223996000	0.660511000
C	-3.527783000	-1.388997000	1.332748000
C	-2.847546000	-0.960455000	2.537618000
C	-1.668949000	-1.628040000	2.946674000
C	-0.540891000	-0.856762000	3.420760000
C	-0.618763000	0.559437000	3.479450000
C	-0.000705000	2.530580000	2.400148000
C	0.699844000	3.047394000	1.291331000
C	-0.021659000	3.511563000	0.146005000
C	-1.438674000	3.438611000	0.126833000
C	-2.114470000	3.003933000	-1.060294000
C	-3.249761000	2.189069000	-0.659608000
C	-3.607982000	1.049148000	-1.412612000

C	-4.026997000	-0.163594000	-0.757938000
C	-3.016353000	-2.481287000	0.586739000
C	-2.994144000	-2.416650000	-0.850876000
C	-3.479471000	-1.264706000	-1.508410000
C	-2.754223000	-0.729418000	-2.657298000
C	-2.832704000	0.693433000	-2.598202000
C	-1.717527000	1.492239000	-2.982365000
C	-1.359329000	2.651351000	-2.217557000
C	0.089130000	2.737176000	-2.189876000
C	0.748615000	3.153301000	-1.034085000
C	0.505990000	1.358140000	3.076296000
C	1.934519000	2.405489000	0.835583000
C	-3.655956000	0.931715000	1.429330000
C	4.837755000	0.355570000	-1.046252000
C	4.798630000	0.262409000	1.198485000
C	5.435626000	-1.021829000	0.702327000
C	5.458075000	-0.966576000	-0.635802000
H	5.743244000	-1.753469000	-1.324600000
H	5.698334000	-1.863102000	1.333364000
H	5.036277000	0.698989000	-2.061972000
H	4.960770000	0.520835000	2.245467000
C	5.271279000	1.259205000	0.123389000
H	6.352148000	1.419833000	0.149286000
H	4.750927000	2.221410000	0.153814000

S=4

⁹C₆₀

E=-2286.219938

G=-2285.906558

C	-0.439915000	3.503573000	0.631805000
C	1.014615000	3.361214000	0.617247000
C	1.683988000	3.062136000	-0.593605000

C	0.933850000	2.885730000	-1.808506000
C	-0.485178000	3.011870000	-1.799105000
C	-1.177083000	3.326064000	-0.580097000
C	-0.918972000	2.937967000	1.842998000
C	0.235137000	2.440226000	2.590264000
C	1.423321000	2.730514000	1.840057000
C	2.516875000	1.783704000	1.830126000
C	2.782188000	2.110677000	-0.603314000
C	1.558673000	1.827165000	-2.567536000
C	0.764025000	0.916751000	-3.306863000
C	-0.675060000	1.042645000	-3.306553000
C	-1.297944000	2.081017000	-2.555420000
C	-2.494920000	1.816966000	-1.807142000
C	-2.422542000	2.579803000	-0.572715000
C	-2.895220000	2.022799000	0.621066000
C	-2.137944000	2.192305000	1.849482000
C	0.136294000	1.233585000	3.322245000
C	-1.094662000	0.489191000	3.322608000
C	-2.220165000	0.963567000	2.588212000
C	-3.031531000	0.032403000	1.830724000
C	-3.454294000	0.683057000	0.621887000
C	-3.537284000	-0.061547000	-0.595935000
C	-3.059345000	0.504236000	-1.807509000
C	-2.407908000	-0.559644000	-2.570660000
C	-1.235440000	-0.282100000	-3.312517000
C	2.702763000	1.353734000	-1.824011000
C	0.918972000	-2.937967000	-1.842998000
C	2.137944000	-2.192305000	-1.849482000
C	2.895220000	-2.022799000	-0.621066000
C	2.422542000	-2.579803000	0.572715000
C	1.177083000	-3.326064000	0.580097000
C	-1.014615000	-3.361214000	-0.617247000

C	-1.423321000	-2.730514000	-1.840057000
C	-0.235137000	-2.440226000	-2.590264000
C	-0.136294000	-1.233585000	-3.322245000
C	1.094662000	-0.489191000	-3.322608000
C	2.220165000	-0.963567000	-2.588212000
C	3.454294000	-0.683057000	-0.621887000
C	3.537284000	0.061547000	0.595935000
C	3.059345000	-0.504236000	1.807509000
C	2.494920000	-1.816966000	1.807142000
C	1.297944000	-2.081017000	2.555420000
C	0.485178000	-3.011870000	1.799105000
C	-0.933850000	-2.885730000	1.808506000
C	-1.683988000	-3.062136000	0.593605000
C	-2.516875000	-1.783704000	-1.830126000
C	-3.187189000	-1.480650000	-0.597809000
C	-2.782188000	-2.110677000	0.603314000
C	-2.702763000	-1.353734000	1.824011000
C	-1.558673000	-1.827165000	2.567536000
C	-0.764025000	-0.916751000	3.306863000
C	0.675060000	-1.042645000	3.306553000
C	1.235440000	0.282100000	3.312517000
C	2.407908000	0.559644000	2.570660000
C	3.031531000	-0.032403000	-1.830724000
C	3.187189000	1.480650000	0.597809000
C	0.439915000	-3.503573000	-0.631805000

Pre-reactants

E=-2480.350960

G=-2479.949863

C	-2.239787000	-1.081920000	-1.840631000
C	-2.875888000	-0.204448000	-0.877701000
C	-2.630287000	1.219274000	-0.943352000

C	-1.768923000	1.751840000	-1.971934000
C	-1.163640000	0.880377000	-2.914135000
C	-1.399311000	-0.542913000	-2.847504000
C	-1.874540000	-2.310837000	-1.172782000
C	-2.249417000	-2.186604000	0.203113000
C	-2.865176000	-0.868025000	0.384336000
C	-2.622905000	-0.133719000	1.571683000
C	-2.397643000	1.969261000	0.256394000
C	-1.016494000	2.854308000	-1.415862000
C	0.348089000	3.058367000	-1.816250000
C	0.956045000	2.158720000	-2.769586000
C	0.208555000	1.087964000	-3.314576000
C	0.822213000	-0.207132000	-3.491127000
C	-0.171874000	-1.215156000	-3.203956000
C	0.199842000	-2.414575000	-2.549773000
C	-0.652680000	-2.978848000	-1.528802000
C	-1.411343000	-2.715443000	1.213363000
C	-0.166983000	-3.393826000	0.848178000
C	0.193900000	-3.520803000	-0.508302000
C	1.588732000	-3.312760000	-0.916778000
C	1.581445000	-2.638772000	-2.174308000
C	2.570435000	-1.636724000	-2.463612000
C	2.176327000	-0.412172000	-3.122858000
C	2.952488000	0.674642000	-2.578444000
C	2.343556000	1.961010000	-2.397444000
C	-1.390361000	2.989637000	-0.039152000
C	3.054713000	2.301449000	1.173780000
C	1.829553000	2.970331000	1.535213000
C	0.981555000	2.409501000	2.557731000
C	1.353524000	1.208453000	3.213813000
C	2.581493000	0.533381000	2.854400000
C	4.060485000	0.191979000	0.890642000

C	4.049739000	0.860594000	-0.379279000
C	3.425996000	2.178817000	-0.195016000
C	2.587012000	2.708974000	-1.206698000
C	1.340725000	3.391505000	-0.839103000
C	0.981488000	3.517810000	0.518125000
C	-0.401720000	2.638293000	2.187788000
C	-1.386435000	1.638375000	2.475324000
C	-0.993892000	0.412526000	3.136991000
C	0.361544000	0.204050000	3.506771000
C	0.970128000	-1.090249000	3.327636000
C	2.346195000	-0.885314000	2.924845000
C	2.949344000	-1.750431000	1.982766000
C	3.822500000	-1.216827000	0.956825000
C	3.809695000	0.132331000	-1.558755000
C	3.572060000	-1.308190000	-1.490239000
C	3.579544000	-1.960702000	-0.242025000
C	2.565565000	-2.985314000	0.054416000
C	2.195860000	-2.855091000	1.425041000
C	0.827108000	-3.056936000	1.826832000
C	0.220834000	-2.161361000	2.779835000
C	-1.165150000	-1.961577000	2.405571000
C	-1.769755000	-0.674753000	2.584688000
C	-0.411377000	3.315742000	0.928859000
C	-2.390261000	1.313383000	1.505699000
C	3.420669000	1.067021000	1.843093000
C	-5.858564000	0.021414000	-1.261148000
C	-5.973600000	-0.546254000	1.019777000
C	-5.839538000	0.797420000	0.900866000
C	-5.773025000	1.150645000	-0.511598000
H	-5.654437000	2.160072000	-0.887664000
H	-5.771169000	1.509285000	1.715300000
H	-5.840901000	-0.040737000	-2.342199000

H	-6.044174000	-1.111007000	1.941242000
C	-6.036914000	-1.162954000	-0.351584000
H	-7.006849000	-1.655269000	-0.524389000
H	-5.271319000	-1.934929000	-0.502756000

TS_{bir}[5,6]

E=-2480.349422

G=-2479.947076

C	-2.410023000	-0.807681000	-1.740602000
C	-2.995462000	0.053929000	-0.713831000
C	-2.615657000	1.466544000	-0.711982000
C	-1.772566000	1.995406000	-1.756602000
C	-1.272872000	1.141097000	-2.774616000
C	-1.592898000	-0.267938000	-2.764427000
C	-2.079076000	-2.075985000	-1.150960000
C	-2.377219000	-2.002604000	0.252447000
C	-2.908733000	-0.675942000	0.530776000
C	-2.558697000	-0.022920000	1.726283000
C	-2.267557000	2.129279000	0.510140000
C	-0.919985000	3.012980000	-1.186531000
C	0.429689000	3.155798000	-1.648662000
C	0.930074000	2.278414000	-2.677677000
C	0.090755000	1.285650000	-3.232933000
C	0.612553000	-0.031759000	-3.503100000
C	-0.426659000	-0.992346000	-3.214673000
C	-0.097578000	-2.242406000	-2.641721000
C	-0.928656000	-2.802136000	-1.604472000
C	-1.526882000	-2.647005000	1.190241000
C	-0.349296000	-3.369952000	0.723057000
C	-0.064467000	-3.444874000	-0.654345000
C	1.314675000	-3.305251000	-1.127125000
C	1.286762000	-2.565913000	-2.345053000

C	2.316765000	-1.613918000	-2.635494000
C	1.969145000	-0.337766000	-3.213701000
C	2.835943000	0.668896000	-2.656571000
C	2.323524000	1.975435000	-2.384612000
C	-1.215132000	3.099231000	0.214083000
C	3.240354000	2.080266000	1.151721000
C	2.077466000	2.797887000	1.613830000
C	1.255066000	2.240150000	2.651281000
C	1.584710000	0.986056000	3.229233000
C	2.748569000	0.257853000	2.771230000
C	4.107725000	-0.066748000	0.718061000
C	4.065870000	0.668752000	-0.518199000
C	3.532694000	2.009673000	-0.235181000
C	2.673903000	2.645130000	-1.178430000
C	1.492513000	3.374795000	-0.709141000
C	1.209590000	3.448825000	0.668504000
C	-0.132391000	2.564649000	2.361322000
C	-1.154660000	1.614394000	2.646971000
C	-0.808834000	0.338064000	3.229848000
C	0.548510000	0.028735000	3.522646000
C	1.064458000	-1.288281000	3.254166000
C	2.431438000	-1.144686000	2.787652000
C	2.928526000	-1.989507000	1.772025000
C	3.784521000	-1.456359000	0.727452000
C	3.718096000	0.021005000	-1.711393000
C	3.392846000	-1.399177000	-1.699969000
C	3.426712000	-2.116926000	-0.492190000
C	2.364027000	-3.091266000	-0.191809000
C	2.073930000	-3.011379000	1.199083000
C	0.717526000	-3.150443000	1.667197000
C	0.222646000	-2.281848000	2.694662000
C	-1.170504000	-1.971048000	2.397943000

C	-1.675066000	-0.668880000	2.662539000
C	-0.165394000	3.312702000	1.142149000
C	-2.235081000	1.405443000	1.719359000
C	3.567929000	0.791476000	1.741011000
C	-5.397453000	0.165399000	-1.209835000
C	-6.013144000	-0.708803000	0.878558000
C	-5.987125000	0.653948000	0.956490000
C	-5.655510000	1.200771000	-0.331512000
H	-5.561781000	2.256224000	-0.555484000
H	-6.166741000	1.243160000	1.848284000
H	-5.218613000	0.266889000	-2.272469000
H	-6.225726000	-1.396540000	1.687769000
C	-5.756490000	-1.135025000	-0.540889000
H	-6.678683000	-1.540012000	-0.990993000
H	-4.999131000	-1.920874000	-0.639444000

Print[5,6]

E=-2480.386645

G=-2479.980078

C	-3.260690000	-0.044505000	-0.627541000
C	-2.900865000	-0.168221000	0.868230000
C	-2.426457000	0.917083000	1.638587000
C	-2.055470000	2.165588000	1.022129000
C	-2.111054000	2.280879000	-0.387703000
C	-2.580484000	1.182256000	-1.203237000
C	-2.584410000	-1.318649000	-1.183896000
C	-2.217880000	-2.177192000	-0.105124000
C	-2.413241000	-1.468824000	1.144820000
C	-1.539741000	-1.720297000	2.242875000
C	-1.512902000	0.686543000	2.744098000
C	-0.902791000	2.696240000	1.737105000
C	0.129697000	3.358171000	1.045559000

C	0.060157000	3.493684000	-0.386300000
C	-1.056676000	2.953951000	-1.094870000
C	-0.851891000	2.260426000	-2.340414000
C	-1.798136000	1.157537000	-2.395945000
C	-1.413362000	-0.068336000	-2.977750000
C	-1.800651000	-1.315866000	-2.336076000
C	-1.147720000	-3.105656000	-0.218740000
C	-0.361807000	-3.122333000	-1.417884000
C	-0.669603000	-2.227024000	-2.452705000
C	0.393436000	-1.552949000	-3.161488000
C	-0.055762000	-0.220938000	-3.469477000
C	0.857048000	0.858833000	-3.424186000
C	0.456218000	2.114606000	-2.857817000
C	1.589820000	2.653013000	-2.127043000
C	1.388307000	3.338401000	-0.908575000
C	-0.579479000	1.786817000	2.804136000
C	3.721150000	1.283858000	1.166677000
C	2.953584000	1.300838000	2.337149000
C	2.566422000	0.052724000	2.968774000
C	2.961363000	-1.170362000	2.404817000
C	3.751083000	-1.190102000	1.204538000
C	4.029101000	0.162938000	-0.841171000
C	3.585644000	1.511170000	-1.153327000
C	3.387577000	2.200313000	0.073645000
C	2.296046000	3.116428000	0.215967000
C	1.527979000	3.131266000	1.411361000
C	1.838165000	2.227336000	2.466080000
C	1.222359000	0.214804000	3.483067000
C	0.296331000	-0.869146000	3.430541000
C	0.686637000	-2.114679000	2.854471000
C	2.001803000	-2.277111000	2.335661000
C	2.205501000	-2.964650000	1.099000000

C	3.276304000	-2.294102000	0.387142000
C	3.208403000	-2.167444000	-1.012993000
C	3.582382000	-0.923613000	-1.635154000
C	2.691676000	1.727158000	-2.259820000
C	2.249405000	0.623140000	-3.053858000
C	2.684531000	-0.693087000	-2.749699000
C	1.752942000	-1.790343000	-2.804188000
C	2.073129000	-2.708360000	-1.743848000
C	1.030331000	-3.371979000	-1.047480000
C	1.088916000	-3.496112000	0.373524000
C	-0.250931000	-3.329505000	0.895558000
C	-0.451311000	-2.646606000	2.113844000
C	0.778475000	1.550682000	3.162576000
C	-1.082355000	-0.615081000	3.049738000
C	4.140810000	0.030306000	0.589339000
C	-4.813706000	0.006201000	-0.891749000
C	-6.427131000	-0.569762000	0.812467000
C	-6.315118000	0.813940000	0.766947000
C	-5.437623000	1.212963000	-0.232949000
H	-5.171160000	2.233059000	-0.480438000
H	-6.847659000	1.496088000	1.422568000
H	-7.050826000	-1.135170000	1.495075000
H	-4.923271000	0.032518000	-1.983252000
C	-5.588562000	-1.195222000	-0.270270000
H	-6.217176000	-1.684102000	-1.028490000
H	-4.919460000	-1.974622000	0.111661000

TS_{bir}[6,6]

E=-2480.345797

G=-2479.943207

C	-2.346315000	-1.115314000	-1.657031000
C	-2.968622000	-0.719615000	-0.394829000

C	-2.922507000	0.697528000	-0.038188000
C	-2.397766000	1.673305000	-0.964921000
C	-1.864207000	1.258442000	-2.212013000
C	-1.836855000	-0.144980000	-2.557370000
C	-1.637728000	-2.347038000	-1.460158000
C	-1.739779000	-2.706048000	-0.070053000
C	-2.521260000	-1.688220000	0.598279000
C	-2.173791000	-1.280325000	1.893161000
C	-2.574402000	1.107629000	1.279398000
C	-1.736810000	2.709968000	-0.207763000
C	-0.537574000	3.312481000	-0.716845000
C	0.000174000	2.881419000	-1.979584000
C	-0.651964000	1.866171000	-2.716410000
C	0.122012000	0.839715000	-3.371467000
C	-0.608484000	-0.401735000	-3.276164000
C	0.086132000	-1.619325000	-3.092120000
C	-0.427649000	-2.610190000	-2.183075000
C	-0.633156000	-3.315295000	0.588774000
C	0.599365000	-3.554833000	-0.146601000
C	0.691773000	-3.209177000	-1.512670000
C	1.914818000	-2.604632000	-2.037051000
C	1.537624000	-1.625708000	-3.001760000
C	2.257359000	-0.395905000	-3.097623000
C	1.540217000	0.842897000	-3.279580000
C	2.215674000	1.876045000	-2.536514000
C	1.456854000	2.895323000	-1.885353000
C	-1.833907000	2.365219000	1.180650000
C	2.821633000	2.368837000	1.467821000
C	1.602466000	2.614602000	2.193591000
C	1.095239000	1.625864000	3.100901000
C	1.792895000	0.404244000	3.291793000
C	3.017911000	0.147386000	2.565452000

C	4.103301000	0.705379000	0.402270000
C	3.709957000	1.681014000	-0.581240000
C	2.919410000	2.717928000	0.094193000
C	1.808532000	3.318192000	-0.574901000
C	0.568406000	3.566319000	0.162813000
C	0.476615000	3.219741000	1.527249000
C	-0.356415000	1.626864000	3.012413000
C	-1.069564000	0.398887000	3.105347000
C	-0.352455000	-0.840199000	3.295900000
C	1.066372000	-0.837228000	3.390427000
C	1.837149000	-1.863328000	2.738318000
C	3.048615000	-1.250665000	2.223855000
C	3.579540000	-1.657957000	0.981562000
C	4.123687000	-0.678360000	0.058271000
C	3.355276000	1.274963000	-1.873074000
C	3.377427000	-0.137376000	-2.222321000
C	3.757914000	-1.092544000	-1.264969000
C	3.009773000	-2.352681000	-1.159841000
C	2.913622000	-2.695498000	0.219328000
C	1.712331000	-3.301521000	0.736628000
C	1.182580000	-2.878967000	1.995692000
C	-0.276329000	-2.888766000	1.903956000
C	-1.028925000	-1.874943000	2.547516000
C	-0.741534000	2.615518000	2.048645000
C	-2.191059000	0.140398000	2.240906000
C	3.528569000	1.113199000	1.658883000
C	-5.398470000	-1.029874000	-0.560429000
C	-6.313151000	0.613641000	0.864464000
C	-6.235273000	1.113835000	-0.398056000
C	-5.708878000	0.102757000	-1.284528000
H	-5.554190000	0.230870000	-2.349772000
H	-6.511964000	2.115548000	-0.706500000

H	-5.153400000	-1.999441000	-0.971789000
H	-6.646782000	1.141062000	1.749742000
C	-5.826722000	-0.810425000	0.869458000
H	-6.630520000	-1.511837000	1.142455000
H	-5.021190000	-0.978430000	1.595400000

Print[6,6]

E=-2480.387187

G=-2479.980888

C	2.516204000	-0.209895000	-1.791015000
C	3.248281000	0.379537000	-0.566450000
C	2.920499000	-0.450298000	0.658716000
C	2.424464000	-1.807392000	0.582423000
C	2.004966000	-2.359275000	-0.651675000
C	2.028631000	-1.534534000	-1.832961000
C	1.799647000	0.808532000	-2.466373000
C	1.818792000	2.013219000	-1.660860000
C	2.554575000	1.757283000	-0.466079000
C	2.085821000	2.278336000	0.737907000
C	2.454492000	0.115418000	1.883575000
C	1.681908000	-2.088744000	1.779662000
C	0.513219000	-2.909379000	1.732517000
C	0.074819000	-3.455784000	0.474265000
C	0.800061000	-3.176440000	-0.699374000
C	0.097955000	-2.871012000	-1.917684000
C	0.849637000	-1.856239000	-2.617836000
C	0.176944000	-0.850583000	-3.330747000
C	0.656163000	0.508543000	-3.263019000
C	0.685805000	2.872865000	-1.668953000
C	-0.479543000	2.542032000	-2.460911000
C	-0.489063000	1.373841000	-3.252563000

C	-1.685582000	0.544283000	-3.324637000
C	-1.275227000	-0.820340000	-3.375473000
C	-2.020768000	-1.817566000	-2.679254000
C	-1.326001000	-2.846468000	-1.942442000
C	-2.073898000	-3.135395000	-0.749110000
C	-1.387987000	-3.442245000	0.459399000
C	1.692245000	-0.898625000	2.592722000
C	-2.962770000	-0.843311000	2.511986000
C	-1.802174000	-0.508973000	3.294934000
C	-1.341010000	0.842744000	3.357534000
C	-2.021009000	1.861544000	2.640873000
C	-3.188043000	1.535326000	1.844547000
C	-4.134152000	-0.348716000	0.531713000
C	-3.695529000	-1.721409000	0.475307000
C	-2.974882000	-2.020610000	1.714615000
C	-1.832206000	-2.882923000	1.687844000
C	-0.653756000	-2.546357000	2.484853000
C	-0.645778000	-1.375542000	3.276725000
C	0.119002000	0.823880000	3.380784000
C	0.850379000	1.812786000	2.682922000
C	0.153313000	2.844659000	1.960052000
C	-1.271787000	2.870564000	1.937379000
C	-1.970499000	3.186053000	0.719430000
C	-3.160718000	2.352631000	0.659335000
C	-3.589776000	1.814986000	-0.568482000
C	-4.086664000	0.451720000	-0.641246000
C	-3.243499000	-2.269087000	-0.731692000
C	-3.206146000	-1.452141000	-1.930223000
C	-3.620747000	-0.112771000	-1.878604000
C	-2.843798000	0.912102000	-2.581931000
C	-2.832860000	2.091806000	-1.774620000
C	-1.660282000	2.913610000	-1.709410000

C	-1.237257000	3.464585000	-0.462430000
C	0.224270000	3.433839000	-0.432631000
C	0.900845000	3.125750000	0.756564000
C	0.543416000	-0.545703000	3.338913000
C	2.051830000	1.465892000	1.945524000
C	-3.657124000	0.199371000	1.776956000
C	4.795780000	0.494375000	-0.812440000
C	6.455723000	0.051434000	0.889495000
C	6.353723000	-1.069195000	0.075698000
C	5.437924000	-0.864423000	-0.948533000
H	5.164969000	-1.578574000	-1.716109000
H	6.917949000	-1.985778000	0.218292000
H	4.908434000	1.092226000	-1.726329000
H	7.098874000	0.151341000	1.756037000
C	5.552277000	1.145896000	0.386144000
H	6.125277000	2.023892000	0.056666000
H	4.866035000	1.508481000	1.161502000

TS[5,6]

E=-2480.368118

G=-2479.95751

C	-3.274052000	0.011430000	-0.796207000
C	-3.121771000	-0.478640000	0.687309000
C	-2.586188000	0.413296000	1.672062000
C	-2.224876000	1.788513000	1.375054000
C	-2.233090000	2.238600000	0.044296000
C	-2.612492000	1.350716000	-1.021797000
C	-2.500383000	-1.068139000	-1.569797000
C	-2.153167000	-2.141287000	-0.710279000
C	-2.470485000	-1.791480000	0.646376000
C	-1.615398000	-2.253369000	1.687990000
C	-1.705709000	-0.041419000	2.722874000

C	-1.137252000	2.170363000	2.249999000
C	-0.098436000	3.014159000	1.786444000
C	-0.1111142000	3.480431000	0.431796000
C	-1.163469000	3.092050000	-0.432996000
C	-0.873094000	2.709328000	-1.790750000
C	-1.758728000	1.627701000	-2.143086000
C	-1.301852000	0.584219000	-2.987701000
C	-1.657823000	-0.773895000	-2.665125000
C	-1.047457000	-2.994548000	-1.001992000
C	-0.210257000	-2.707238000	-2.135751000
C	-0.508331000	-1.606942000	-2.954010000
C	0.560701000	-0.759775000	-3.441488000
C	0.078568000	0.591933000	-3.453298000
C	0.946797000	1.647884000	-3.105254000
C	0.472744000	2.724070000	-2.265331000
C	1.540155000	3.107147000	-1.390162000
C	1.262375000	3.481399000	-0.050591000
C	-0.822183000	1.039151000	3.085574000
C	3.561952000	1.065273000	1.557341000
C	2.735404000	0.774540000	2.674915000
C	2.385262000	-0.583655000	2.981593000
C	2.853208000	-1.631530000	2.157254000
C	3.707880000	-1.345615000	1.021234000
C	4.055736000	0.454616000	-0.633242000
C	3.541105000	1.818961000	-0.631674000
C	3.265925000	2.198520000	0.719177000
C	2.113649000	3.026823000	1.015462000
C	1.286967000	2.729683000	2.147551000
C	1.585776000	1.615691000	2.974153000
C	1.012900000	-0.592704000	3.461924000
C	0.145055000	-1.652084000	3.114555000
C	0.612833000	-2.712879000	2.276889000

C	1.958099000	-2.711274000	1.793698000
C	2.247193000	-3.097716000	0.447002000
C	3.326974000	-2.241360000	-0.042939000
C	3.310741000	-1.789192000	-1.368276000
C	3.676335000	-0.422628000	-1.671222000
C	2.693606000	2.264960000	-1.688388000
C	2.331088000	1.374262000	-2.745744000
C	2.805494000	0.038349000	-2.735307000
C	1.910121000	-1.042450000	-3.084249000
C	2.222532000	-2.174623000	-2.258788000
C	1.168784000	-3.015194000	-1.777406000
C	1.178913000	-3.472605000	-0.432619000
C	-0.192171000	-3.454047000	0.059445000
C	-0.470585000	-3.085532000	1.387666000
C	0.529838000	0.768389000	3.449406000
C	-1.243248000	-1.373676000	2.753593000
C	4.074802000	-0.008095000	0.726934000
C	-4.830970000	0.037968000	-1.151577000
C	-5.264073000	-0.685814000	0.982960000
C	-5.622831000	0.712465000	0.924768000
C	-5.440823000	1.161269000	-0.346683000
H	-5.544498000	2.181030000	-0.696655000
H	-5.887201000	1.319204000	1.783902000
H	-5.383724000	-1.306091000	1.864553000
H	-4.973593000	0.085167000	-2.232851000
C	-5.394225000	-1.203607000	-0.431655000
H	-6.447981000	-1.362855000	-0.697911000
H	-4.840730000	-2.123333000	-0.632490000

Prod[5,6]

E=-2480.390661

G=-2479.976904

C	3.294578000	-0.239899000	0.810568000
C	3.294546000	-0.235573000	-0.811775000
C	2.608492000	0.953670000	-1.429489000
C	2.222509000	2.134140000	-0.695865000
C	2.222465000	2.130379000	0.707225000
C	2.608394000	0.946021000	1.434579000
C	2.499773000	-1.500859000	1.161250000
C	2.163995000	-2.238683000	-0.005917000
C	2.499801000	-1.494636000	-1.169156000
C	1.651438000	-1.579640000	-2.292944000
C	1.740930000	0.857725000	-2.564163000
C	1.147466000	2.792288000	-1.410726000
C	0.099433000	3.435894000	-0.707353000
C	0.099403000	3.432022000	0.725617000
C	1.147456000	2.784716000	1.425582000
C	0.848245000	1.981379000	2.579374000
C	1.740780000	0.843982000	2.568638000
C	1.284907000	-0.415822000	3.032379000
C	1.651404000	-1.591879000	2.284565000
C	1.062692000	-3.152154000	-0.008359000
C	0.217888000	-3.252785000	1.148282000
C	0.505126000	-2.477514000	2.281038000
C	-0.570287000	-1.840712000	3.013442000
C	-0.096546000	-0.565393000	3.464123000
C	-0.970460000	0.546378000	3.469338000
C	-0.497257000	1.837263000	3.023035000
C	-1.563776000	2.484227000	2.314889000
C	-1.278706000	3.276424000	1.170892000
C	0.848345000	1.995162000	-2.568819000
C	-3.550702000	1.511164000	-1.153360000
C	-2.709247000	1.599763000	-2.302917000
C	-2.346743000	0.415907000	-3.022803000

C	-2.814813000	-0.847046000	-2.583650000
C	-3.679542000	-0.947252000	-1.425176000
C	-4.057192000	0.216319000	0.718379000
C	-3.550815000	1.504997000	1.161363000
C	-3.268461000	2.306838000	0.006094000
C	-2.117311000	3.190205000	0.008432000
C	-1.278677000	3.282724000	-1.153541000
C	-1.563685000	2.496584000	-2.301711000
C	-0.970396000	0.564930000	-3.466507000
C	-0.096495000	-0.546852000	-3.466972000
C	-0.570221000	-1.824537000	-3.023087000
C	-1.918722000	-1.984279000	-2.582702000
C	-2.219978000	-2.790953000	-1.438017000
C	-3.305029000	-2.141356000	-0.706728000
C	-3.305071000	-2.145120000	0.695271000
C	-3.679630000	-0.954879000	1.420065000
C	-2.709351000	1.587439000	2.311354000
C	-2.346810000	0.399729000	3.024889000
C	-2.814952000	-0.860863000	2.579130000
C	-1.918779000	-1.998067000	2.572084000
C	-2.219968000	-2.798589000	1.423103000
C	-1.158633000	-3.435090000	0.700026000
C	-1.158621000	-3.431269000	-0.718310000
C	0.217901000	-3.246551000	-1.165518000
C	0.505162000	-2.465297000	-2.294160000
C	-0.497157000	1.853461000	-3.013346000
C	1.284940000	-0.399606000	-3.034452000
C	-4.057105000	0.220142000	-0.717266000
C	4.848940000	-0.335645000	1.127937000
C	4.849052000	-0.329657000	-1.129618000
C	5.452093000	0.987927000	-0.667045000
C	5.452045000	0.984405000	0.672348000

H	5.714762000	1.802787000	1.332829000
H	5.714852000	1.809782000	-1.323182000
H	5.046496000	-0.628079000	-2.160343000
H	5.046480000	-0.639513000	2.157056000
C	5.327541000	-1.269204000	-0.003314000
H	6.413265000	-1.394820000	-0.003585000
H	4.844553000	-2.249409000	-0.005919000

TS[6,6]

E=-2480.344554

G=-2479.937325

C	-2.558295000	0.032849000	-1.744018000
C	-3.253429000	-0.604918000	-0.540151000
C	-3.124873000	0.248563000	0.738714000
C	-2.578066000	1.615861000	0.634073000
C	-2.195261000	2.183563000	-0.593948000
C	-2.183363000	1.381962000	-1.791952000
C	-1.797804000	-0.935835000	-2.448307000
C	-1.730399000	-2.135346000	-1.643819000
C	-2.470473000	-1.931115000	-0.443692000
C	-1.957559000	-2.441389000	0.764352000
C	-2.506705000	-0.307746000	1.925802000
C	-1.840694000	1.936261000	1.823589000
C	-0.723694000	2.826737000	1.765189000
C	-0.333473000	3.406124000	0.506805000
C	-1.053610000	3.088193000	-0.659947000
C	-0.354517000	2.847477000	-1.894657000
C	-1.036145000	1.795348000	-2.589200000
C	-0.303554000	0.836034000	-3.323896000
C	-0.686333000	-0.554032000	-3.252852000
C	-0.550451000	-2.927451000	-1.675965000
C	0.582263000	-2.527346000	-2.486157000

C	0.509123000	-1.349180000	-3.264945000
C	1.646925000	-0.446493000	-3.333888000
C	1.145486000	0.896196000	-3.366454000
C	1.832136000	1.933481000	-2.677193000
C	1.079869000	2.929557000	-1.938939000
C	1.813864000	3.239365000	-0.752758000
C	1.127045000	3.492593000	0.474436000
C	-1.756314000	0.736126000	2.598806000
C	2.875488000	0.968480000	2.482469000
C	1.755794000	0.560013000	3.262458000
C	1.380617000	-0.827530000	3.322464000
C	2.132395000	-1.803392000	2.611957000
C	3.273091000	-1.398949000	1.803734000
C	4.053715000	0.562334000	0.491048000
C	3.527289000	1.908829000	0.451267000
C	2.811720000	2.158673000	1.698593000
C	1.619812000	2.948047000	1.690755000
C	0.472864000	2.534310000	2.501219000
C	0.544682000	1.356301000	3.267682000
C	-0.059779000	-0.904007000	3.363229000
C	-0.741236000	-1.933612000	2.675881000
C	0.015209000	-2.920794000	1.948153000
C	1.442307000	-2.854893000	1.910273000
C	2.144319000	-3.105863000	0.685190000
C	3.285924000	-2.201049000	0.623874000
C	3.659260000	-1.619071000	-0.621506000
C	4.061448000	-0.227503000	-0.688496000
C	3.036289000	2.442488000	-0.754017000
C	3.044597000	1.643952000	-1.950840000
C	3.556395000	0.314134000	-1.916593000
C	2.837336000	-0.746608000	-2.613255000
C	2.913481000	-1.935867000	-1.819763000

C	1.786965000	-2.825363000	-1.749410000
C	1.412504000	-3.413655000	-0.494813000
C	-0.038857000	-3.473422000	-0.445539000
C	-0.722698000	-3.232934000	0.756425000
C	-0.581082000	0.453984000	3.325731000
C	-1.973904000	-1.665710000	1.959873000
C	3.638773000	-0.024705000	1.734470000
C	-4.813531000	-0.850035000	-0.805038000
C	-5.218258000	0.388041000	1.076701000
C	-5.599211000	1.200778000	-0.053589000
C	-5.422157000	0.474591000	-1.191132000
H	-5.531455000	0.825878000	-2.209991000
H	-5.864877000	2.250833000	-0.000203000
H	-4.953773000	-1.670999000	-1.510248000
H	-5.320425000	0.702210000	2.109470000
C	-5.368780000	-1.046933000	0.619496000
H	-6.425397000	-1.344654000	0.588285000
H	-4.810968000	-1.774267000	1.214808000

Prod[6,6]

E=-2480.370383

G=-2479.959775

C	-2.602027000	1.007535000	-1.440131000
C	-3.276517000	-0.202080000	-0.799832000
C	-3.276624000	-0.200300000	0.800096000
C	-2.602275000	1.010801000	1.437790000
C	-2.222178000	2.161932000	0.713617000
C	-2.222029000	2.160247000	-0.718539000
C	-1.830595000	0.597810000	-2.547973000
C	-1.751621000	-0.853069000	-2.542244000
C	-2.477357000	-1.341974000	-1.434988000
C	-1.969050000	-2.448408000	-0.711151000

C	-2.477559000	-1.338766000	1.437919000
C	-1.830951000	0.603580000	2.546561000
C	-0.718667000	1.368823000	3.007820000
C	-0.333397000	2.552207000	2.287890000
C	-1.063182000	2.945239000	1.151607000
C	-0.378028000	3.449660000	-0.003867000
C	-1.063022000	2.942627000	-1.158226000
C	-0.333136000	2.546990000	-2.293603000
C	-0.718352000	1.362014000	-3.010874000
C	-0.563879000	-1.492426000	-3.005575000
C	0.558741000	-0.708251000	-3.448643000
C	0.482589000	0.703571000	-3.451799000
C	1.619443000	1.495502000	-3.020576000
C	1.121081000	2.630454000	-2.307288000
C	1.807157000	3.117890000	-1.159937000
C	1.067521000	3.536739000	-0.003883000
C	1.807019000	3.120583000	1.153119000
C	1.120847000	2.635784000	2.301530000
C	-1.751896000	-0.847343000	2.544024000
C	2.894215000	-0.584195000	2.589996000
C	1.773946000	-1.363939000	3.019039000
C	1.402344000	-2.547750000	2.305678000
C	2.139408000	-2.959004000	1.159725000
C	3.286495000	-2.176153000	0.712519000
C	4.054934000	0.195364000	0.709193000
C	3.531127000	1.333167000	1.422931000
C	2.817042000	0.847690000	2.589203000
C	1.619115000	1.502380000	3.017297000
C	0.482205000	0.711390000	3.450240000
C	0.558381000	-0.700452000	3.450247000
C	-0.050324000	-2.623032000	2.291821000
C	-0.732463000	-3.098415000	1.158390000

C	0.004844000	-3.527259000	0.003920000
C	1.449156000	-3.454268000	0.003909000
C	2.139528000	-2.961601000	-1.153001000
C	3.286622000	-2.177806000	-0.707491000
C	3.657300000	-0.994590000	-1.423218000
C	4.055060000	0.193788000	-0.709368000
C	3.032172000	2.466798000	0.707952000
C	3.032257000	2.465232000	-0.713219000
C	3.531356000	1.329905000	-1.425652000
C	2.817366000	0.841792000	-2.590913000
C	2.894556000	-0.590074000	-2.588512000
C	1.774269000	-1.370797000	-3.015931000
C	1.402598000	-2.552975000	-2.299896000
C	-0.050137000	-2.628255000	-2.285984000
C	-0.732330000	-3.101019000	-1.151496000
C	-0.564185000	-1.485615000	3.008913000
C	-1.969146000	-2.446914000	0.716547000
C	3.657049000	-0.991290000	1.425583000
C	-4.833803000	-0.306433000	-1.123326000
C	-4.833960000	-0.303997000	1.123588000
C	-5.460501000	1.000481000	0.668351000
C	-5.460446000	0.999017000	-0.670986000
H	-5.732178000	1.813629000	-1.332462000
H	-5.732286000	1.816527000	1.328034000
H	-5.015129000	-0.608631000	-2.155302000
H	-5.015417000	-0.603974000	2.156188000
C	-5.288887000	-1.255755000	0.001128000
H	-6.370290000	-1.415057000	0.001227000
H	-4.770004000	-2.219217000	0.002188000

S=5

¹¹C₆₀

E=-2286.141067

G=-2285.829039

C	-0.433031000	3.485008000	0.616890000
C	1.008795000	3.351445000	0.603277000
C	1.683247000	3.060684000	-0.616219000
C	0.944304000	2.903399000	-1.835755000
C	-0.485659000	3.030176000	-1.830265000
C	-1.175140000	3.321689000	-0.597170000
C	-0.916706000	2.913285000	1.839576000
C	0.225292000	2.425335000	2.584235000
C	1.415766000	2.714349000	1.828367000
C	2.502458000	1.773728000	1.818610000
C	2.781566000	2.110166000	-0.625992000
C	1.567417000	1.837800000	-2.587954000
C	0.772424000	0.926702000	-3.327422000
C	-0.667542000	1.056885000	-3.335108000
C	-1.292359000	2.105692000	-2.580508000
C	-2.480994000	1.826343000	-1.812051000
C	-2.411754000	2.583446000	-0.589155000
C	-2.897120000	2.011012000	0.636868000
C	-2.145005000	2.176676000	1.854038000
C	0.122877000	1.216467000	3.328841000
C	-1.107396000	0.479031000	3.351545000
C	-2.243543000	0.954092000	2.613410000
C	-3.048912000	0.029751000	1.861429000
C	-3.449781000	0.681469000	0.638398000
C	-3.518687000	-0.066076000	-0.581663000
C	-3.035545000	0.505358000	-1.805097000
C	-2.395656000	-0.547688000	-2.565271000
C	-1.221169000	-0.266060000	-3.319659000
C	2.718282000	1.366636000	-1.850614000
C	0.916706000	-2.913285000	-1.839576000

C	2.145005000	-2.176676000	-1.854038000
C	2.897120000	-2.011012000	-0.636868000
C	2.411754000	-2.583446000	0.589155000
C	1.175140000	-3.321689000	0.597170000
C	-1.008795000	-3.351445000	-0.603277000
C	-1.415766000	-2.714349000	-1.828367000
C	-0.225292000	-2.425335000	-2.584235000
C	-0.122877000	-1.216467000	-3.328841000
C	1.107396000	-0.479031000	-3.351545000
C	2.243543000	-0.954092000	-2.613410000
C	3.449781000	-0.681469000	-0.638398000
C	3.518687000	0.066076000	0.581663000
C	3.035545000	-0.505358000	1.805097000
C	2.480994000	-1.826343000	1.812051000
C	1.292359000	-2.105692000	2.580508000
C	0.485659000	-3.030176000	1.830265000
C	-0.944304000	-2.903399000	1.835755000
C	-1.683247000	-3.060684000	0.616219000
C	-2.502458000	-1.773728000	-1.818610000
C	-3.179349000	-1.473638000	-0.584180000
C	-2.781566000	-2.110166000	0.625992000
C	-2.718282000	-1.366636000	1.850614000
C	-1.567417000	-1.837800000	2.587954000
C	-0.772424000	-0.926702000	3.327422000
C	0.667542000	-1.056885000	3.335108000
C	1.221169000	0.266060000	3.319659000
C	2.395656000	0.547688000	2.565271000
C	3.048912000	-0.029751000	-1.861429000
C	3.179349000	1.473638000	0.584180000
C	0.433031000	-3.485008000	-0.616890000

Pre-reactants

E=-2480.270893

G=-2479.873677

C	-2.367155000	1.166355000	-1.643477000
C	-2.904060000	0.703452000	-0.384311000
C	-2.591173000	1.411200000	0.830226000
C	-1.744037000	2.574945000	0.783903000
C	-1.220034000	3.026672000	-0.463451000
C	-1.530207000	2.326567000	-1.677137000
C	-2.034157000	0.011435000	-2.438491000
C	-2.355062000	-1.162927000	-1.667197000
C	-2.895510000	-0.731101000	-0.398473000
C	-2.575167000	-1.459282000	0.800194000
C	-2.272577000	0.678708000	2.029938000
C	-0.910976000	2.574498000	1.961238000
C	0.448521000	3.026128000	1.874560000
C	0.976073000	3.472665000	0.616178000
C	0.157991000	3.479143000	-0.545329000
C	0.692756000	3.064184000	-1.810648000
C	-0.341107000	2.330711000	-2.501436000
C	-0.012193000	1.191161000	-3.278821000
C	-0.858015000	0.026107000	-3.260242000
C	-1.505233000	-2.313412000	-1.724427000
C	-0.316007000	-2.287788000	-2.547815000
C	0.001086000	-1.129846000	-3.301939000
C	1.375383000	-0.677204000	-3.393073000
C	1.367498000	0.754339000	-3.377189000
C	2.393706000	1.475687000	-2.688975000
C	2.061043000	2.631779000	-1.906069000
C	2.892330000	2.620369000	-0.729923000
C	2.362284000	3.038884000	0.523833000
C	-1.231540000	1.398083000	2.727122000
C	3.212727000	-0.010981000	2.423831000

C	2.034328000	-0.025844000	3.251675000
C	1.190481000	-1.190066000	3.275465000
C	1.516595000	-2.331918000	2.498103000
C	2.705489000	-2.331064000	1.668693000
C	4.086353000	-0.709977000	0.377043000
C	4.077622000	0.737399000	0.391724000
C	3.533886000	1.162824000	1.654688000
C	2.680384000	2.317891000	1.716224000
C	1.491676000	2.289186000	2.544645000
C	1.177371000	1.129589000	3.298804000
C	-0.189794000	-0.754428000	3.383543000
C	-1.215122000	-1.470994000	2.696644000
C	-0.882782000	-2.628876000	1.908011000
C	0.481722000	-3.064903000	1.812841000
C	1.014128000	-3.480638000	0.545642000
C	2.395954000	-3.031925000	0.462665000
C	2.921889000	-2.581540000	-0.782742000
C	3.777796000	-1.412497000	-0.827482000
C	3.761212000	1.461111000	-0.798671000
C	3.445907000	0.752950000	-2.002105000
C	3.453604000	-0.682391000	-2.017001000
C	2.410312000	-1.401968000	-2.718812000
C	2.089513000	-2.576389000	-1.958743000
C	0.725964000	-3.025158000	-1.872079000
C	0.195999000	-3.471262000	-0.616103000
C	-1.186786000	-3.033656000	-0.525051000
C	-1.715023000	-2.613060000	0.730394000
C	-0.197685000	0.678137000	3.399548000
C	-2.264902000	-0.748573000	2.014831000
C	3.546417000	-1.166166000	1.630428000
C	-5.879349000	1.165364000	-0.319708000
C	-5.896802000	-1.186034000	-0.242559000

C	-5.846304000	-0.697237000	1.022236000
C	-5.836024000	0.759113000	0.974704000
H	-5.779262000	1.402637000	1.845103000
H	-5.797441000	-1.283156000	1.932894000
H	-5.882329000	2.187432000	-0.677882000
H	-5.914130000	-2.229137000	-0.533460000
C	-5.969759000	-0.040170000	-1.214377000
H	-6.920596000	-0.050934000	-1.770358000
H	-5.174954000	-0.071033000	-1.970609000

TS_{bir}[5,6]

E=-2480.269605

G=-2479.869766

C	2.450493000	-1.520499000	-1.167104000
C	3.001858000	-0.716852000	-0.078538000
C	2.598096000	-1.048207000	1.283689000
C	1.772990000	-2.195311000	1.544919000
C	1.298311000	-2.997557000	0.463975000
C	1.636304000	-2.660152000	-0.891309000
C	2.112013000	-0.646222000	-2.248954000
C	2.393514000	0.711205000	-1.834761000
C	2.904557000	0.671951000	-0.495501000
C	2.542487000	1.693084000	0.431667000
C	2.226345000	-0.010909000	2.211271000
C	0.897536000	-1.876783000	2.646885000
C	-0.447188000	-2.362268000	2.654995000
C	-0.927084000	-3.162748000	1.564406000
C	-0.072132000	-3.480783000	0.476783000
C	-0.573195000	-3.454499000	-0.867384000
C	0.470572000	-2.923701000	-1.710594000
C	0.147489000	-2.062091000	-2.786300000
C	0.971384000	-0.918241000	-3.070201000

C	1.533258000	1.780330000	-2.250616000
C	0.372847000	1.491393000	-3.058430000
C	0.095949000	0.160806000	-3.460410000
C	-1.265419000	-0.331567000	-3.461622000
C	-1.236941000	-1.698820000	-3.037768000
C	-2.269615000	-2.218363000	-2.202919000
C	-1.945645000	-3.098493000	-1.117264000
C	-2.810676000	-2.769643000	-0.016296000
C	-2.315053000	-2.799687000	1.314783000
C	1.178033000	-0.524419000	3.058847000
C	-3.275123000	0.638590000	2.249701000
C	-2.122859000	0.918699000	3.067530000
C	-1.301536000	2.059887000	2.784841000
C	-1.620113000	2.930996000	1.706111000
C	-2.784506000	2.667854000	0.879378000
C	-4.105826000	0.717083000	0.067404000
C	-4.063957000	-0.667115000	0.493942000
C	-3.555464000	-0.706379000	1.841602000
C	-2.684449000	-1.778967000	2.248891000
C	-1.524549000	-1.488786000	3.062856000
C	-1.249817000	-0.159325000	3.466632000
C	0.083131000	1.700161000	3.043051000
C	1.114030000	2.210447000	2.206125000
C	0.792741000	3.094254000	1.116850000
C	-0.577285000	3.460670000	0.868707000
C	-1.076832000	3.492867000	-0.476389000
C	-2.452429000	3.008272000	-0.463615000
C	-2.930102000	2.206269000	-1.538675000
C	-3.767108000	1.052974000	-1.270222000
C	-3.696642000	-1.694853000	-0.436801000
C	-3.359107000	-1.352730000	-1.776088000
C	-3.385560000	0.017081000	-2.195806000

C	-2.334471000	0.531999000	-3.044349000
C	-2.054856000	1.880522000	-2.638344000
C	-0.703083000	2.370214000	-2.648350000
C	-0.222637000	3.170477000	-1.565988000
C	1.165668000	2.801921000	-1.314770000
C	1.658268000	2.761830000	0.014151000
C	0.112194000	0.331703000	3.472111000
C	2.200964000	1.350296000	1.789886000
C	-3.606751000	1.517569000	1.150064000
C	5.396032000	-1.169394000	-0.033789000
C	6.004289000	1.037483000	-0.551987000
C	5.976876000	0.890263000	0.805123000
C	5.652423000	-0.472188000	1.132132000
H	5.558434000	-0.866992000	2.136367000
H	6.152533000	1.673770000	1.533164000
H	5.230084000	-2.236233000	-0.108524000
H	6.212205000	1.950115000	-1.096908000
C	5.752913000	-0.293118000	-1.206023000
H	6.676740000	-0.667834000	-1.678286000
H	4.996674000	-0.263692000	-1.998648000

Proint[5,6]

E=-2480.306458

G=-2479.902786

C	-3.262913000	-0.480884000	-0.409595000
C	-2.926178000	0.467845000	0.763751000
C	-2.465849000	1.798136000	0.571495000
C	-2.091355000	2.270447000	-0.729663000
C	-2.129533000	1.372041000	-1.833258000
C	-2.575937000	0.017987000	-1.662776000
C	-2.568987000	-1.778503000	0.064720000
C	-2.197372000	-1.651446000	1.422192000

C	-2.417017000	-0.277655000	1.849388000
C	-1.542072000	0.303390000	2.814083000
C	-1.544814000	2.398225000	1.526172000
C	-0.942702000	3.157251000	-0.576484000
C	0.094896000	3.156640000	-1.541098000
C	0.033178000	2.263726000	-2.665582000
C	-1.071410000	1.379819000	-2.809571000
C	-0.853910000	0.016713000	-3.233233000
C	-1.779720000	-0.819374000	-2.514098000
C	-1.390430000	-2.123428000	-2.096704000
C	-1.766895000	-2.581435000	-0.791119000
C	-1.112271000	-2.391200000	1.975140000
C	-0.317749000	-3.231392000	1.114243000
C	-0.632440000	-3.316465000	-0.252262000
C	0.423658000	-3.338246000	-1.237690000
C	-0.027642000	-2.575404000	-2.360729000
C	0.877415000	-1.744399000	-3.067171000
C	0.464792000	-0.439933000	-3.507259000
C	1.587509000	0.457885000	-3.351851000
C	1.374170000	1.794769000	-2.935659000
C	-0.630124000	3.261479000	0.816510000
C	3.709605000	1.751352000	-0.054651000
C	2.920662000	2.589595000	0.810820000
C	2.547832000	2.126522000	2.104860000
C	2.947825000	0.831089000	2.535843000
C	3.749554000	-0.010558000	1.674133000
C	4.060421000	-0.442431000	-0.737375000
C	3.597807000	0.312964000	-1.880049000
C	3.382090000	1.662937000	-1.459795000
C	2.270103000	2.412413000	-1.984396000
C	1.485918000	3.240674000	-1.117329000
C	1.797809000	3.333919000	0.266468000

C	1.193665000	2.594386000	2.377345000
C	0.281964000	1.755495000	3.083100000
C	0.688171000	0.453620000	3.512164000
C	2.012235000	-0.013427000	3.246452000
C	2.229121000	-1.372737000	2.824031000
C	3.300007000	-1.373581000	1.850307000
C	3.248016000	-2.261347000	0.739575000
C	3.622553000	-1.801186000	-0.555573000
C	2.702917000	-0.298193000	-2.827861000
C	2.266721000	-1.649333000	-2.639224000
C	2.714264000	-2.401235000	-1.518435000
C	1.799071000	-3.254897000	-0.811201000
C	2.112627000	-3.162887000	0.585490000
C	1.065643000	-3.156360000	1.553533000
C	1.121125000	-2.261543000	2.667159000
C	-0.222949000	-1.782163000	2.928018000
C	-0.435990000	-0.448126000	3.343414000
C	0.744406000	3.351001000	1.244599000
C	-1.099097000	1.663565000	2.637496000
C	4.139947000	0.450436000	0.391391000
C	-4.809313000	-0.652320000	-0.653972000
C	-6.473431000	0.076798000	0.940062000
C	-6.362783000	1.044996000	-0.049418000
C	-5.452475000	0.661987000	-1.025816000
H	-5.179570000	1.232151000	-1.905228000
H	-6.918561000	1.977550000	-0.062743000
H	-7.118982000	0.126805000	1.809189000
H	-4.898469000	-1.392088000	-1.459933000
C	-5.592520000	-1.100788000	0.617416000
H	-6.188544000	-2.000915000	0.409345000
H	-4.926760000	-1.366851000	1.446527000

Print[6,6]

E=-2480.306886

G=-2479.90317

C	-2.542281000	1.132398000	-1.417488000
C	-3.254388000	-0.024623000	-0.680125000
C	-2.910782000	0.037290000	0.792477000
C	-2.428040000	1.226031000	1.439654000
C	-2.026240000	2.360171000	0.678706000
C	-2.063079000	2.292516000	-0.752916000
C	-1.815642000	0.623547000	-2.516100000
C	-1.818908000	-0.829750000	-2.456352000
C	-2.550232000	-1.242941000	-1.320047000
C	-2.069389000	-2.340841000	-0.558227000
C	-2.430388000	-1.091849000	1.537554000
C	-1.675626000	0.836180000	2.602962000
C	-0.513589000	1.561517000	2.986427000
C	-0.086015000	2.693480000	2.210807000
C	-0.820192000	3.085726000	1.064593000
C	-0.133856000	3.495592000	-0.123054000
C	-0.878388000	2.979463000	-1.247370000
C	-0.200946000	2.495049000	-2.378704000
C	-0.673794000	1.301433000	-3.035002000
C	-0.677699000	-1.551093000	-2.914556000
C	0.477431000	-0.851910000	-3.411073000
C	0.479458000	0.560326000	-3.470911000
C	1.667170000	1.306518000	-3.099274000
C	1.251821000	2.499456000	-2.430487000
C	1.993946000	2.994521000	-1.318790000
C	1.308326000	3.494910000	-0.162456000
C	2.052803000	3.081220000	0.995523000
C	1.370200000	2.684664000	2.177822000
C	-1.677376000	-0.606662000	2.664719000

C	2.984138000	-0.610659000	2.569664000
C	1.825190000	-1.309443000	3.060338000
C	1.363214000	-2.492418000	2.398136000
C	2.044690000	-2.990577000	1.253881000
C	3.220009000	-2.300156000	0.749609000
C	4.132172000	0.021354000	0.631902000
C	3.688920000	1.213590000	1.309363000
C	2.985682000	0.818486000	2.508816000
C	1.828735000	1.560029000	2.938073000
C	0.666824000	0.854206000	3.429496000
C	0.664954000	-0.561089000	3.489895000
C	-0.093014000	-2.494067000	2.430795000
C	-0.827887000	-2.981284000	1.321616000
C	-0.142882000	-3.490670000	0.173100000
C	1.299280000	-3.498441000	0.134231000
C	1.986352000	-3.099018000	-1.059996000
C	3.180984000	-2.358148000	-0.672996000
C	3.595209000	-1.233829000	-1.440596000
C	4.075024000	-0.038605000	-0.783535000
C	3.226138000	2.347247000	0.551657000
C	3.187534000	2.285575000	-0.870414000
C	3.598080000	1.099170000	-1.540046000
C	2.833500000	0.604417000	-2.664313000
C	2.831294000	-0.833629000	-2.603267000
C	1.663160000	-1.566881000	-2.977272000
C	1.245026000	-2.698595000	-2.210636000
C	-0.207711000	-2.686194000	-2.159684000
C	-0.886656000	-3.069777000	-0.991187000
C	-0.517640000	-1.300099000	3.108130000
C	-2.032185000	-2.287812000	0.875062000
C	3.685924000	-1.108364000	1.407999000
C	-4.804323000	-0.012291000	-0.935390000

C	-6.447221000	-0.577157000	0.747302000
C	-6.362359000	0.806411000	0.665708000
C	-5.456602000	1.197667000	-0.312228000
H	-5.194024000	2.215961000	-0.572510000
H	-6.931210000	1.494519000	1.283532000
H	-4.925479000	-0.025454000	-2.026432000
H	-7.080321000	-1.136418000	1.426223000
C	-5.540578000	-1.216375000	-0.271097000
H	-6.109892000	-1.787824000	-1.017501000
H	-4.842761000	-1.930255000	0.184107000

TS[5,6]

E=-2480.283584

G=-2479.876129

C	3.268436000	-0.778315000	-0.209095000
C	3.116113000	0.787438000	-0.292749000
C	2.585983000	1.508128000	0.834474000
C	2.238505000	0.863979000	2.081293000
C	2.244163000	-0.553208000	2.164445000
C	2.615165000	-1.348241000	1.025491000
C	2.495185000	-1.244058000	-1.449229000
C	2.132052000	-0.127344000	-2.248551000
C	2.457596000	1.092645000	-1.563868000
C	1.598348000	2.226399000	-1.725973000
C	1.713741000	2.653462000	0.679162000
C	1.153522000	1.604366000	2.672465000
C	0.112042000	0.931304000	3.361931000
C	0.124736000	-0.497447000	3.454128000
C	1.180315000	-1.233838000	2.855132000
C	0.898513000	-2.460549000	2.139212000
C	1.773727000	-2.513478000	1.007740000
C	1.317241000	-3.066839000	-0.232385000

C	1.651376000	-2.386844000	-1.444335000
C	1.020628000	-0.185397000	-3.134511000
C	0.186305000	-1.360742000	-3.157105000
C	0.493206000	-2.449417000	-2.320224000
C	-0.562258000	-3.161472000	-1.641828000
C	-0.073750000	-3.510129000	-0.340999000
C	-0.935607000	-3.445852000	0.774519000
C	-0.457752000	-2.925503000	2.034748000
C	-1.522122000	-2.163926000	2.622167000
C	-1.245231000	-0.963551000	3.336509000
C	0.848881000	2.729722000	1.814191000
C	-3.553916000	1.237720000	1.440926000
C	-2.728301000	2.406830000	1.455474000
C	-2.389556000	3.061101000	0.233559000
C	-2.864930000	2.540825000	-1.000558000
C	-3.707668000	1.358252000	-1.013772000
C	-4.026742000	-0.736956000	0.294991000
C	-3.524789000	-1.093106000	1.592365000
C	-3.241280000	0.118325000	2.309590000
C	-2.095619000	0.185968000	3.183956000
C	-1.269968000	1.355839000	3.190104000
C	-1.568942000	2.459564000	2.333171000
C	-1.008923000	3.514696000	0.345127000
C	-0.148383000	3.454394000	-0.774536000
C	-0.624606000	2.935418000	-2.017845000
C	-1.979229000	2.469575000	-2.135048000
C	-2.264593000	1.251964000	-2.844551000
C	-3.334128000	0.566124000	-2.153701000
C	-3.322361000	-0.882859000	-2.066661000
C	-3.667462000	-1.523447000	-0.847434000
C	-2.676762000	-2.237658000	1.744950000
C	-2.319524000	-3.029557000	0.607101000

C	-2.804775000	-2.684600000	-0.683753000
C	-1.926138000	-2.746756000	-1.817837000
C	-2.235151000	-1.632185000	-2.673083000
C	-1.184424000	-0.937958000	-3.343668000
C	-1.196786000	0.498110000	-3.432424000
C	0.161602000	0.964142000	-3.296069000
C	0.447009000	2.157713000	-2.600669000
C	-0.521011000	3.158409000	1.655002000
C	1.247156000	3.036880000	-0.608516000
C	-4.055197000	0.723148000	0.204569000
C	4.832094000	-1.113696000	-0.284349000
C	5.210134000	1.141567000	-0.436327000
C	5.602013000	0.731519000	0.895243000
C	5.446687000	-0.615795000	1.000478000
H	5.572048000	-1.215052000	1.894070000
H	5.863101000	1.409739000	1.700009000
H	5.311572000	2.155200000	-0.809078000
H	4.984497000	-2.168869000	-0.517893000
C	5.369835000	-0.088624000	-1.302753000
H	6.428487000	-0.278598000	-1.523998000
H	4.813749000	-0.059500000	-2.241923000

Prod[5,6]

E=-2480.303788

G=-2479.892930

C	-3.277847000	0.811988000	-0.259336000
C	-3.277859000	-0.811968000	-0.259344000
C	-2.609382000	-1.436760000	0.933980000
C	-2.244777000	-0.708727000	2.122254000
C	-2.244772000	0.708713000	2.122262000
C	-2.609369000	1.436760000	0.933994000
C	-2.472448000	1.168147000	-1.508860000

C	-2.125888000	0.000021000	-2.241493000
C	-2.472447000	-1.168110000	-1.508868000
C	-1.627954000	-2.300779000	-1.587612000
C	-1.754550000	-2.587060000	0.847529000
C	-1.176717000	-1.419753000	2.772719000
C	-0.128999000	-0.715351000	3.423720000
C	-0.128996000	0.715312000	3.423728000
C	-1.176709000	1.419726000	2.772735000
C	-0.881878000	2.597639000	1.981428000
C	-1.754535000	2.587059000	0.847558000
C	-1.292781000	3.066644000	-0.422360000
C	-1.627946000	2.300811000	-1.587588000
C	-1.014337000	0.000023000	-3.138318000
C	-0.172831000	1.164524000	-3.238529000
C	-0.472495000	2.304702000	-2.467990000
C	0.585354000	3.049406000	-1.833864000
C	0.097886000	3.486516000	-0.557358000
C	0.962718000	3.489280000	0.560318000
C	0.479099000	3.043367000	1.850741000
C	1.534079000	2.322154000	2.488706000
C	1.246479000	1.162807000	3.283747000
C	-0.881892000	-2.597657000	1.981398000
C	3.519987000	-1.169756000	1.519578000
C	2.687241000	-2.329409000	1.605244000
C	2.342170000	-3.056410000	0.421762000
C	2.826514000	-2.621338000	-0.843332000
C	3.677233000	-1.448036000	-0.929859000
C	4.022458000	0.735539000	0.253506000
C	3.519993000	1.169722000	1.519592000
C	3.224856000	-0.000021000	2.316210000
C	2.079799000	-0.000023000	3.197749000
C	1.246473000	-1.162851000	3.283734000

C	1.534067000	-2.322189000	2.488678000
C	0.962701000	-3.489290000	0.560276000
C	0.097868000	-3.486508000	-0.557400000
C	0.585339000	-3.049386000	-1.833900000
C	1.945141000	-2.612719000	-1.980619000
C	2.247880000	-1.447492000	-2.766348000
C	3.323998000	-0.729829000	-2.113121000
C	3.324002000	0.729839000	-2.113111000
C	3.677241000	1.448030000	-0.929842000
C	2.687253000	2.329379000	1.605272000
C	2.342185000	3.056395000	0.421799000
C	2.826527000	2.621336000	-0.843301000
C	1.945154000	2.612734000	-1.980587000
C	2.247887000	1.447516000	-2.766330000
C	1.191863000	0.721184000	-3.401563000
C	1.191859000	-0.721147000	-3.401572000
C	-0.172837000	-1.164482000	-3.238542000
C	-0.472506000	-2.304667000	-2.468016000
C	0.479084000	-3.043390000	1.850704000
C	-1.292796000	-3.066631000	-0.422395000
C	4.022455000	-0.735561000	0.253497000
C	-4.834065000	1.128870000	-0.372075000
C	-4.834081000	-1.128850000	-0.372120000
C	-5.451544000	-0.669849000	0.939024000
C	-5.451440000	0.669822000	0.939094000
H	-5.721800000	1.328129000	1.756674000
H	-5.721981000	-1.328196000	1.756545000
H	-5.026310000	-2.159067000	-0.675230000
H	-5.026291000	2.159102000	-0.675135000
C	-5.300326000	0.000028000	-1.314073000
H	-6.384653000	0.000035000	-1.451691000
H	-4.806004000	0.000036000	-2.288616000

TS[6,6]

E=-2480.260792

G=-2479.856169

C	-2.601530000	0.859912000	-1.543991000
C	-3.258841000	-0.275480000	-0.748774000
C	-3.106214000	-0.107242000	0.781174000
C	-2.546314000	1.148753000	1.312252000
C	-2.172911000	2.226731000	0.479572000
C	-2.198257000	2.100318000	-0.945957000
C	-1.825452000	0.325597000	-2.587479000
C	-1.757203000	-1.118489000	-2.438844000
C	-2.474700000	-1.487144000	-1.279416000
C	-1.964327000	-2.514690000	-0.447455000
C	-2.482396000	-1.158471000	1.575480000
C	-1.800265000	0.876797000	2.507868000
C	-0.682863000	1.687731000	2.869011000
C	-0.293779000	2.784832000	2.020572000
C	-1.024601000	3.056879000	0.840325000
C	-0.347166000	3.428873000	-0.365594000
C	-1.046579000	2.813657000	-1.462356000
C	-0.319412000	2.304425000	-2.568653000
C	-0.715636000	1.030483000	-3.146468000
C	-0.573797000	-1.809243000	-2.843308000
C	0.547891000	-1.089419000	-3.391685000
C	0.470462000	0.327695000	-3.524223000
C	1.609422000	1.158250000	-3.180345000
C	1.119940000	2.374215000	-2.594850000
C	1.828635000	2.978231000	-1.508456000
C	1.092043000	3.507423000	-0.383204000
C	1.836262000	3.212272000	0.809102000
C	1.153218000	2.870687000	2.026681000

C	-1.721630000	-0.546439000	2.644859000
C	2.906049000	-0.312773000	2.654022000
C	1.779486000	-1.030413000	3.165665000
C	1.387113000	-2.284301000	2.563665000
C	2.133410000	-2.817094000	1.472159000
C	3.263789000	-2.092732000	0.947335000
C	4.034382000	0.254922000	0.693896000
C	3.545989000	1.459083000	1.279291000
C	2.839091000	1.109812000	2.501014000
C	1.650496000	1.811234000	2.859782000
C	0.514048000	1.086707000	3.398229000
C	0.579705000	-0.321291000	3.531579000
C	-0.045864000	-2.378346000	2.586754000
C	-0.743201000	-2.966745000	1.477989000
C	-0.000996000	-3.504385000	0.375054000
C	1.433957000	-3.429794000	0.360730000
C	2.123375000	-3.074933000	-0.842256000
C	3.259554000	-2.250070000	-0.486235000
C	3.625370000	-1.159862000	-1.324403000
C	4.012294000	0.097056000	-0.742415000
C	3.036558000	2.514213000	0.434396000
C	3.029907000	2.360722000	-1.003187000
C	3.517808000	1.163225000	-1.589036000
C	2.799136000	0.553755000	-2.681064000
C	2.873770000	-0.880905000	-2.527666000
C	1.755595000	-1.697112000	-2.878004000
C	1.388083000	-2.805293000	-2.043831000
C	-0.059304000	-2.863937000	-2.009285000
C	-0.739868000	-3.210851000	-0.825873000
C	-0.551355000	-1.142416000	3.162351000
C	-1.960452000	-2.376758000	0.974965000
C	3.656650000	-0.846092000	1.536882000

C	-4.827450000	-0.405768000	-1.055190000
C	-5.145340000	-0.146696000	1.190930000
C	-5.571379000	1.082666000	0.560037000
C	-5.443459000	0.942473000	-0.787442000
H	-5.589293000	1.709939000	-1.537917000
H	-5.826108000	1.994617000	1.088490000
H	-4.987693000	-0.821749000	-2.050900000
H	-5.218424000	-0.329781000	2.257475000
C	-5.336205000	-1.226511000	0.144492000
H	-6.398078000	-1.478761000	0.026559000
H	-4.768864000	-2.141890000	0.329283000

Prod[6,6]

E=-2480.282913

G=-2479.874139

C	2.587607000	-1.006643000	-1.443163000
C	3.253953000	0.204226000	-0.799495000
C	3.254001000	0.202293000	0.799675000
C	2.587887000	-1.010064000	1.440528000
C	2.211635000	-2.173125000	0.714898000
C	2.211378000	-2.171014000	-0.720404000
C	1.818439000	-0.597189000	-2.548247000
C	1.737918000	0.853846000	-2.543519000
C	2.458037000	1.343138000	-1.436854000
C	1.952560000	2.459904000	-0.714263000
C	2.457925000	1.339640000	1.439513000
C	1.818511000	-0.603330000	2.546414000
C	0.709564000	-1.370303000	3.020670000
C	0.325929000	-2.564000000	2.304262000
C	1.065172000	-2.956793000	1.154624000
C	0.377899000	-3.449710000	-0.004354000
C	1.064647000	-2.953813000	-1.161918000

C	0.325759000	-2.558391000	-2.310572000
C	0.709015000	-1.363229000	-3.023863000
C	0.551228000	1.493295000	-3.018684000
C	-0.560100000	0.717474000	-3.492328000
C	-0.481336000	-0.713814000	-3.495091000
C	-1.608927000	-1.497406000	-3.050040000
C	-1.110041000	-2.646175000	-2.333079000
C	-1.806092000	-3.123374000	-1.169358000
C	-1.063625000	-3.530129000	-0.004394000
C	-1.806197000	-3.126322000	1.162088000
C	-1.109330000	-2.651615000	2.326677000
C	1.738396000	0.847998000	2.545703000
C	-2.878985000	0.586434000	2.613780000
C	-1.767152000	1.363229000	3.049674000
C	-1.398688000	2.560366000	2.332146000
C	-2.144599000	2.957994000	1.168887000
C	-3.264552000	2.174225000	0.728821000
C	-3.996839000	-0.195761000	0.730355000
C	-3.505672000	-1.337172000	1.445696000
C	-2.799351000	-0.854376000	2.611966000
C	-1.608396000	-1.504450000	3.046824000
C	-0.480801000	-0.721988000	3.493232000
C	-0.559686000	0.709294000	3.494513000
C	0.037156000	2.632309000	2.309720000
C	0.727349000	3.108871000	1.162085000
C	-0.010567000	3.525436000	0.004012000
C	-1.451658000	3.444236000	0.004021000
C	-2.144768000	2.961042000	-1.162067000
C	-3.264806000	2.175923000	-0.723594000
C	-3.635007000	0.994399000	-1.445852000
C	-3.997219000	-0.194091000	-0.730183000
C	-3.005229000	-2.469798000	0.723306000

C	-3.005592000	-2.468056000	-0.728696000
C	-3.505716000	-1.333633000	-1.448139000
C	-2.800032000	-0.848181000	-2.613499000
C	-2.879574000	0.592749000	-2.611847000
C	-1.767637000	1.370643000	-3.046127000
C	-1.399010000	2.565838000	-2.325779000
C	0.036901000	2.638110000	-2.303850000
C	0.727177000	3.111675000	-1.154737000
C	0.551679000	1.486125000	3.022125000
C	1.952774000	2.458070000	0.719737000
C	-3.634801000	0.990727000	1.448539000
C	4.814282000	0.313872000	-1.123146000
C	4.814234000	0.311411000	1.123609000
C	5.445352000	-0.989776000	0.668581000
C	5.444881000	-0.988510000	-0.671000000
H	5.718168000	-1.802688000	-1.332369000
H	5.718937000	-1.805252000	1.328217000
H	4.992435000	0.616413000	-2.155414000
H	4.992320000	0.611635000	2.156559000
C	5.264476000	1.265072000	0.001303000
H	6.345474000	1.427512000	0.001503000
H	4.742251000	2.226597000	0.002435000

S=6

¹³C₆₀

E=-2286.034540

G=-2285.727302

C	2.752119000	-1.236341000	-0.133928000
C	2.612438000	-0.641947000	-1.438815000
C	2.515466000	0.786956000	-1.570049000
C	2.562233000	1.623408000	-0.397765000
C	2.686966000	1.033901000	0.892206000

C	2.779065000	-0.411431000	1.024645000
C	1.974130000	-2.465573000	-0.115636000
C	1.365478000	-2.627879000	-1.402800000
C	1.740559000	-1.488789000	-2.213828000
C	0.809104000	-0.924381000	-3.120517000
C	1.564773000	1.360303000	-2.482319000
C	1.644668000	2.728762000	-0.595938000
C	0.877042000	3.226980000	0.506572000
C	1.018983000	2.628971000	1.811329000
C	1.928070000	1.534359000	1.998311000
C	1.530127000	0.400507000	2.805109000
C	2.080487000	-0.797310000	2.216191000
C	1.323125000	-2.016289000	2.241315000
C	1.270412000	-2.849118000	1.063808000
C	0.044064000	-3.172513000	-1.512943000
C	-0.673292000	-3.562672000	-0.324625000
C	-0.060537000	-3.401766000	0.963758000
C	-0.830418000	-2.897634000	2.066849000
C	0.024374000	-2.040236000	2.856689000
C	-0.511364000	-0.854248000	3.452146000
C	0.253677000	0.375008000	3.420507000
C	-0.661061000	1.475904000	3.243174000
C	-0.277986000	2.599443000	2.432551000
C	1.029357000	2.563995000	-1.880915000
C	-3.155532000	2.464339000	0.115747000
C	-2.449404000	2.850405000	-1.068596000
C	-2.499333000	2.015516000	-2.243691000
C	-3.257578000	0.796360000	-2.222281000
C	-3.962898000	0.408165000	-1.030797000
C	-3.785802000	0.642457000	1.439473000
C	-2.921940000	1.493266000	2.218777000
C	-2.544750000	2.626988000	1.404356000

C	-1.224284000	3.175572000	1.510553000
C	-0.511044000	3.567838000	0.322954000
C	-1.124031000	3.405304000	-0.966392000
C	-1.200094000	2.043356000	-2.860552000
C	-0.661583000	0.855798000	-3.455249000
C	-1.425524000	-0.374364000	-3.424243000
C	-2.710165000	-0.400215000	-2.814793000
C	-3.104997000	-1.529843000	-2.005836000
C	-3.871845000	-1.027561000	-0.899126000
C	-3.733567000	-1.617247000	0.397400000
C	-3.693558000	-0.782078000	1.572954000
C	-1.983313000	0.924349000	3.127985000
C	-1.892860000	-0.513051000	3.267811000
C	-2.743511000	-1.358029000	2.487160000
C	-2.209644000	-2.557505000	1.883882000
C	-2.826573000	-2.719422000	0.594769000
C	-2.058394000	-3.222473000	-0.510780000
C	-2.198208000	-2.623123000	-1.815221000
C	-0.899004000	-2.596903000	-2.436096000
C	-0.514868000	-1.475035000	-3.245273000
C	-0.349201000	2.899745000	-2.068830000
C	0.717222000	0.518409000	-3.260473000
C	-3.916537000	1.234196000	0.133870000
C	5.862797000	-1.218004000	-0.075540000
C	5.911108000	1.070455000	-0.524625000
C	5.865311000	0.862944000	0.905332000
C	5.840580000	-0.478498000	1.173309000
H	5.791974000	-0.931643000	2.155727000
H	5.838796000	1.657836000	1.640722000
H	5.910192000	2.033626000	-1.018953000
H	5.833889000	-2.296340000	-0.166854000
C	5.960857000	-0.259475000	-1.236321000

H	6.887675000	-0.394689000	-1.827324000
H	5.138116000	-0.386820000	-1.963507000

TS_{bir}

E=-2480.181820

G=-2479.785864

C	-2.263938000	-1.894004000	0.978939000
C	-2.923452000	-0.699004000	0.449052000
C	-2.811600000	-0.426675000	-0.948434000
C	-2.146491000	-1.354040000	-1.834334000
C	-1.551190000	-2.547701000	-1.310859000
C	-1.606356000	-2.809952000	0.103115000
C	-1.678008000	-1.561238000	2.238353000
C	-1.920551000	-0.151940000	2.486796000
C	-2.680412000	0.379694000	1.393587000
C	-2.417316000	1.713285000	0.925044000
C	-2.547373000	0.919739000	-1.420658000
C	-1.460312000	-0.586818000	-2.830646000
C	-0.187472000	-1.003137000	-3.312665000
C	0.423070000	-2.203949000	-2.787645000
C	-0.251556000	-2.962332000	-1.785929000
C	0.486287000	-3.503629000	-0.672544000
C	-0.343328000	-3.398614000	0.496271000
C	0.236396000	-3.072712000	1.760558000
C	-0.439216000	-2.145340000	2.642611000
C	-0.936569000	0.632275000	3.138056000
C	0.311273000	0.041657000	3.554539000
C	0.558987000	-1.347730000	3.303262000
C	1.849332000	-1.770002000	2.817771000
C	1.649871000	-2.845513000	1.874297000
C	2.484984000	-2.938389000	0.706187000
C	1.901207000	-3.268955000	-0.569774000

C	2.577940000	-2.500362000	-1.581178000
C	1.841432000	-1.971378000	-2.692710000
C	-1.716285000	0.822491000	-2.578365000
C	2.848126000	1.570376000	-2.250724000
C	1.605246000	2.162563000	-2.648084000
C	0.940453000	3.092656000	-1.771591000
C	1.521318000	3.417962000	-0.500899000
C	2.773550000	2.822197000	-0.104908000
C	4.034121000	0.700058000	-0.447177000
C	3.840578000	-0.366978000	-1.396820000
C	3.095182000	0.165986000	-2.504695000
C	2.099701000	-0.629876000	-3.151449000
C	0.850562000	-0.035989000	-3.553712000
C	0.602431000	1.360813000	-3.300418000
C	-0.479006000	2.859094000	-1.871961000
C	-1.307758000	2.956271000	-0.710870000
C	-0.726765000	3.285792000	0.558905000
C	0.687430000	3.515190000	0.666047000
C	1.422552000	2.978419000	1.785291000
C	2.711712000	2.552345000	1.309952000
C	3.315232000	1.360283000	1.842515000
C	3.973382000	0.433318000	0.960754000
C	3.583780000	-1.698057000	-0.933388000
C	3.520454000	-1.967477000	0.484081000
C	3.720308000	-0.902151000	1.429714000
C	2.878744000	-0.807598000	2.595710000
C	2.625575000	0.591937000	2.848555000
C	1.346938000	1.010044000	3.319351000
C	0.738384000	2.213939000	2.789089000
C	-0.669261000	1.981749000	2.674777000
C	-1.405095000	2.510432000	1.570569000
C	-0.683367000	1.784469000	-2.812260000

C	-2.362297000	1.985114000	-0.485465000
C	3.430813000	1.899613000	-0.982127000
C	-5.404202000	-1.075441000	0.533990000
C	-6.176954000	1.089403000	0.090112000
C	-6.036896000	0.393742000	-1.133018000
C	-5.608207000	-0.898030000	-0.901655000
H	-5.425973000	-1.658487000	-1.649377000
H	-6.230894000	0.820938000	-2.110136000
H	-5.271168000	-2.032874000	1.021342000
H	-6.501649000	2.117127000	0.197009000
C	-5.865626000	0.173143000	1.247542000
H	-6.752392000	-0.013652000	1.881563000
H	-5.100865000	0.580694000	1.929010000

Print[5,6]

E=-2480.216105

G=-2479.814145

C	-3.228742000	-0.414831000	-0.493849000
C	-2.907845000	0.339518000	0.813229000
C	-2.459481000	1.692871000	0.835133000
C	-2.091572000	2.370637000	-0.377994000
C	-2.113336000	1.644671000	-1.611080000
C	-2.548808000	0.274715000	-1.654342000
C	-2.541936000	-1.769792000	-0.225924000
C	-2.181385000	-1.855571000	1.138406000
C	-2.407320000	-0.567541000	1.773274000
C	-1.545755000	-0.145358000	2.828627000
C	-1.559058000	2.142684000	1.875957000
C	-0.951674000	3.222686000	-0.084577000
C	0.097445000	3.381893000	-1.037122000
C	0.047262000	2.663649000	-2.283956000
C	-1.058052000	1.803885000	-2.563254000

C	-0.833646000	0.514979000	-3.199538000
C	-1.753887000	-0.420551000	-2.630062000
C	-1.366665000	-1.783462000	-2.425474000
C	-1.738347000	-2.435840000	-1.199684000
C	-1.104046000	-2.675761000	1.581162000
C	-0.302101000	-3.379786000	0.601245000
C	-0.617239000	-3.249625000	-0.781040000
C	0.441001000	-3.105231000	-1.748669000
C	-0.006582000	-2.183774000	-2.748952000
C	0.907135000	-1.248743000	-3.318580000
C	0.493479000	0.111675000	-3.542562000
C	1.608514000	0.978001000	-3.263529000
C	1.384554000	2.260949000	-2.631920000
C	-0.643824000	3.100122000	1.309356000
C	3.669432000	1.758602000	0.227897000
C	2.893833000	2.449898000	1.208489000
C	2.508061000	1.778493000	2.432940000
C	2.915046000	0.415446000	2.671232000
C	3.691381000	-0.280797000	1.690653000
C	4.032242000	-0.319792000	-0.795640000
C	3.585250000	0.599046000	-1.798823000
C	3.359960000	1.886986000	-1.164205000
C	2.262274000	2.712797000	-1.583534000
C	1.478187000	3.409486000	-0.602909000
C	1.786729000	3.272936000	0.788822000
C	1.176886000	2.194991000	2.763219000
C	0.247664000	1.255968000	3.335591000
C	0.656166000	-0.115190000	3.564576000
C	1.978000000	-0.529216000	3.239635000
C	2.200744000	-1.807138000	2.609250000
C	3.274734000	-1.649385000	1.652654000
C	3.228796000	-2.354521000	0.396048000

C	3.616535000	-1.685668000	-0.828794000
C	2.710407000	0.150105000	-2.845993000
C	2.288114000	-1.221561000	-2.884315000
C	2.732439000	-2.135425000	-1.875462000
C	1.812966000	-3.081017000	-1.306154000
C	2.121365000	-3.214166000	0.097942000
C	1.056160000	-3.375805000	1.053074000
C	1.099726000	-2.657100000	2.310854000
C	-0.238774000	-2.244439000	2.645919000
C	-0.460048000	-0.977553000	3.270199000
C	0.729362000	3.120035000	1.749067000
C	-1.108268000	1.234736000	2.874998000
C	4.079138000	0.391299000	0.463299000
C	-4.779090000	-0.548691000	-0.767599000
C	-6.452899000	-0.087838000	0.913410000
C	-6.339302000	1.026946000	0.092823000
C	-5.422421000	0.808058000	-0.926747000
H	-5.146430000	1.512027000	-1.701914000
H	-6.898200000	1.948109000	0.225845000
H	-7.103744000	-0.179633000	1.775108000
H	-4.863740000	-1.150226000	-1.681470000
C	-5.564427000	-1.195868000	0.413986000
H	-6.153752000	-2.055263000	0.063653000
H	-4.900870000	-1.585391000	1.194678000

Print[6,6]

E=-2480.216700

G=-2479.814898

C	-2.512052000	1.106601000	-1.446052000
C	-3.220408000	-0.036614000	-0.689686000
C	-2.895371000	0.052628000	0.783061000

C	-2.424835000	1.257897000	1.413144000
C	-2.025884000	2.389505000	0.632888000
C	-2.043547000	2.288299000	-0.800686000
C	-1.784476000	0.576102000	-2.534357000
C	-1.788264000	-0.874059000	-2.447494000
C	-2.521952000	-1.266992000	-1.304871000
C	-2.051786000	-2.360081000	-0.518651000
C	-2.428294000	-1.067093000	1.554785000
C	-1.684855000	0.890178000	2.579826000
C	-0.522401000	1.625645000	2.965737000
C	-0.094292000	2.752634000	2.178063000
C	-0.827560000	3.119824000	1.011479000
C	-0.132739000	3.497561000	-0.183113000
C	-0.869426000	2.970749000	-1.303052000
C	-0.174495000	2.460030000	-2.435558000
C	-0.644168000	1.244557000	-3.069109000
C	-0.649374000	-1.605584000	-2.895286000
C	0.497846000	-0.925773000	-3.433079000
C	0.500560000	0.501092000	-3.520500000
C	1.676718000	1.243067000	-3.143264000
C	1.256386000	2.464877000	-2.487411000
C	2.005048000	2.971459000	-1.366660000
C	1.308844000	3.490410000	-0.213107000
C	2.047548000	3.112843000	0.959521000
C	1.353457000	2.748638000	2.157837000
C	-1.687256000	-0.562411000	2.669072000
C	2.948092000	-0.573899000	2.594732000
C	1.796464000	-1.260835000	3.108697000
C	1.344514000	-2.467659000	2.476133000
C	2.036673000	-2.978291000	1.331294000
C	3.197646000	-2.291985000	0.820545000
C	4.070010000	0.033280000	0.651629000

C	3.645943000	1.248991000	1.311681000
C	2.950087000	0.876461000	2.506125000
C	1.800825000	1.624998000	2.931923000
C	0.645492000	0.935135000	3.445036000
C	0.643182000	-0.509738000	3.533679000
C	-0.103190000	-2.464254000	2.496151000
C	-0.837344000	-2.969661000	1.382784000
C	-0.144619000	-3.491030000	0.243083000
C	1.296949000	-3.493644000	0.212808000
C	1.994780000	-3.120970000	-0.995218000
C	3.163264000	-2.378268000	-0.625234000
C	3.589797000	-1.259974000	-1.428521000
C	4.035259000	-0.055153000	-0.797533000
C	3.205647000	2.365141000	0.536473000
C	3.171741000	2.275796000	-0.909050000
C	3.593801000	1.065733000	-1.570440000
C	2.836357000	0.553901000	-2.691878000
C	2.833567000	-0.885464000	-2.604030000
C	1.671280000	-1.620386000	-2.968342000
C	1.247106000	-2.752590000	-2.169586000
C	-0.183898000	-2.737318000	-2.119351000
C	-0.880771000	-3.102562000	-0.932883000
C	-0.527568000	-1.249426000	3.141672000
C	-2.033667000	-2.286777000	0.917454000
C	3.642017000	-1.091507000	1.454033000
C	-4.773614000	-0.027096000	-0.956187000
C	-6.430897000	-0.566502000	0.719863000
C	-6.343305000	0.815684000	0.619921000
C	-5.428051000	1.192683000	-0.354618000
H	-5.161539000	2.206749000	-0.626832000
H	-6.917271000	1.512956000	1.222452000
H	-4.885448000	-0.056151000	-2.047695000

H	-7.072114000	-1.115506000	1.399455000
C	-5.514367000	-1.221436000	-0.279431000
H	-6.076057000	-1.804825000	-1.022328000
H	-4.820614000	-1.927400000	0.193617000

TS[5,6]

E=-2480.189226

G=-2479.783956

C	3.252095000	-0.798483000	-0.174524000
C	3.117187000	0.767842000	-0.311510000
C	2.576660000	1.525595000	0.794254000
C	2.221875000	0.924923000	2.059369000
C	2.218923000	-0.489476000	2.189456000
C	2.590568000	-1.322480000	1.074916000
C	2.509489000	-1.306457000	-1.412725000
C	2.138707000	-0.209831000	-2.231930000
C	2.484351000	1.033297000	-1.603277000
C	1.609192000	2.174458000	-1.807902000
C	1.706912000	2.665690000	0.597192000
C	1.143440000	1.690281000	2.627934000
C	0.094108000	1.047087000	3.348393000
C	0.098124000	-0.382677000	3.481733000
C	1.154353000	-1.141761000	2.897608000
C	0.864888000	-2.387801000	2.214604000
C	1.739835000	-2.483677000	1.088324000
C	1.290481000	-3.078017000	-0.133625000
C	1.641525000	-2.458899000	-1.373104000
C	1.038253000	-0.292884000	-3.130718000
C	0.201436000	-1.473385000	-3.134638000
C	0.506963000	-2.553101000	-2.252447000
C	-0.565767000	-3.218582000	-1.543480000
C	-0.094074000	-3.535820000	-0.233739000

C	-0.969403000	-3.425608000	0.891082000
C	-0.494802000	-2.857030000	2.124877000
C	-1.560500000	-2.086336000	2.708041000
C	-1.267531000	-0.848398000	3.390698000
C	0.842862000	2.779290000	1.727606000
C	-3.542051000	1.296813000	1.414783000
C	-2.725142000	2.464021000	1.395097000
C	-2.365352000	3.071107000	0.127770000
C	-2.832756000	2.502149000	-1.108018000
C	-3.653404000	1.335808000	-1.097140000
C	-4.005402000	-0.710530000	0.308633000
C	-3.530921000	-1.031149000	1.627940000
C	-3.237191000	0.212003000	2.308608000
C	-2.106599000	0.300211000	3.190658000
C	-1.278708000	1.473017000	3.168978000
C	-1.582011000	2.550008000	2.267250000
C	-1.007897000	3.529500000	0.229335000
C	-0.129577000	3.441553000	-0.898318000
C	-0.595426000	2.870597000	-2.129846000
C	-1.936539000	2.403140000	-2.241865000
C	-2.221674000	1.164138000	-2.923390000
C	-3.285643000	0.503816000	-2.215753000
C	-3.283145000	-0.934679000	-2.076620000
C	-3.649733000	-1.540581000	-0.815421000
C	-2.699207000	-2.175439000	1.831680000
C	-2.336929000	-3.003514000	0.706670000
C	-2.808284000	-2.681506000	-0.606984000
C	-1.919041000	-2.791732000	-1.739853000
C	-2.215377000	-1.709334000	-2.643900000
C	-1.146498000	-1.054312000	-3.346395000
C	-1.150084000	0.396221000	-3.483507000
C	0.196081000	0.859431000	-3.361189000

C	0.487543000	2.091928000	-2.696975000
C	-0.527011000	3.209976000	1.550499000
C	1.247251000	3.013436000	-0.708533000
C	-4.015401000	0.723658000	0.174690000
C	4.817743000	-1.135045000	-0.211322000
C	5.157596000	1.116098000	-0.421813000
C	5.546234000	0.751236000	0.928384000
C	5.408078000	-0.593271000	1.069227000
H	5.536428000	-1.168042000	1.978440000
H	5.785816000	1.456922000	1.715826000
H	5.265590000	2.118665000	-0.822401000
H	4.978907000	-2.195863000	-0.409774000
C	5.365075000	-0.136004000	-1.249552000
H	6.431849000	-0.310970000	-1.439384000
H	4.828901000	-0.143881000	-2.200386000

Prod[5,6]

E=-2480.204745

G=-2479.797339

C	-3.272625000	0.811406000	-0.250145000
C	-3.272585000	-0.811412000	-0.250060000
C	-2.593404000	-1.431877000	0.937762000
C	-2.224869000	-0.708166000	2.128951000
C	-2.224861000	0.708398000	2.128863000
C	-2.593405000	1.431982000	0.937615000
C	-2.511419000	1.174644000	-1.521785000
C	-2.137543000	-0.000108000	-2.226947000
C	-2.511400000	-1.174779000	-1.521644000
C	-1.628762000	-2.322083000	-1.596353000
C	-1.730260000	-2.581015000	0.844338000
C	-1.155570000	-1.419927000	2.774481000
C	-0.104975000	-0.716918000	3.433829000

C	-0.104972000	0.717283000	3.433751000
C	-1.155568000	1.420228000	2.774336000
C	-0.861034000	2.592266000	1.977911000
C	-1.730251000	2.581128000	0.844078000
C	-1.277516000	3.058832000	-0.426293000
C	-1.628745000	2.321932000	-1.596595000
C	-1.034904000	-0.000163000	-3.134098000
C	-0.198792000	1.171639000	-3.259085000
C	-0.500238000	2.333065000	-2.485464000
C	0.577168000	3.058506000	-1.843923000
C	0.108073000	3.504004000	-0.569490000
C	0.983276000	3.491033000	0.561467000
C	0.505544000	3.045620000	1.844757000
C	1.564486000	2.327582000	2.498886000
C	1.265944000	1.165826000	3.297206000
C	-0.861046000	-2.592049000	1.978189000
C	3.529647000	-1.169614000	1.531633000
C	2.707163000	-2.329548000	1.623209000
C	2.346926000	-3.050186000	0.419540000
C	2.816240000	-2.602386000	-0.859457000
C	3.647938000	-1.447184000	-0.960323000
C	4.004985000	0.720473000	0.246420000
C	3.529646000	1.169759000	1.531516000
C	3.229664000	0.000120000	2.322658000
C	2.097975000	0.000161000	3.208832000
C	1.265951000	-1.165475000	3.297316000
C	1.564484000	-2.327330000	2.499133000
C	0.983255000	-3.490972000	0.561837000
C	0.108056000	-3.504066000	-0.569129000
C	0.577153000	-3.058710000	-1.843593000
C	1.924386000	-2.609214000	-1.999677000
C	2.216607000	-1.444523000	-2.797336000

C	3.281144000	-0.723607000	-2.157458000
C	3.281143000	0.723365000	-2.157534000
C	3.647932000	1.447072000	-0.960474000
C	2.707166000	2.329711000	1.622974000
C	2.346932000	3.050241000	0.419226000
C	2.816240000	2.602277000	-0.859732000
C	1.924393000	2.608999000	-1.999952000
C	2.216616000	1.444216000	-2.797495000
C	1.147423000	0.729875000	-3.433161000
C	1.147420000	-0.730239000	-3.433087000
C	-0.198803000	-1.171972000	-3.258942000
C	-0.500257000	-2.333318000	-2.485216000
C	0.505538000	-3.045415000	1.845064000
C	-1.277547000	-3.058883000	-0.425973000
C	4.004974000	-0.720459000	0.246491000
C	-4.837296000	1.128848000	-0.321527000
C	-4.837311000	-1.128895000	-0.321398000
C	-5.424840000	-0.669854000	1.002565000
C	-5.424899000	0.669954000	1.002468000
H	-5.676124000	1.328147000	1.826333000
H	-5.676031000	-1.327948000	1.826521000
H	-5.035665000	-2.158903000	-0.620927000
H	-5.035712000	2.158809000	-0.621182000
C	-5.320419000	-0.000080000	-1.254217000
H	-6.407156000	-0.000076000	-1.372882000
H	-4.841527000	-0.000133000	-2.236268000

TS[6,6]

E=-2480.162547

G=-2479.760492

C	-2.590313000	1.039438000	-1.425481000
C	-3.252954000	-0.182871000	-0.777961000

C	-3.158189000	-0.189043000	0.776901000
C	-2.610384000	1.002628000	1.455474000
C	-2.183055000	2.180827000	0.728613000
C	-2.193860000	2.205072000	-0.688618000
C	-1.807780000	0.629767000	-2.529896000
C	-1.733308000	-0.818985000	-2.540562000
C	-2.460964000	-1.321254000	-1.437857000
C	-1.953697000	-2.451672000	-0.727034000
C	-2.504295000	-1.335282000	1.439108000
C	-1.800522000	0.574294000	2.589479000
C	-0.689432000	1.345209000	3.029977000
C	-0.313029000	2.556965000	2.343014000
C	-1.054015000	2.959778000	1.181223000
C	-0.358110000	3.465906000	0.028792000
C	-1.046792000	2.989182000	-1.132582000
C	-0.311072000	2.595320000	-2.281321000
C	-0.704431000	1.397884000	-3.003525000
C	-0.557485000	-1.464709000	-3.026726000
C	0.567518000	-0.685893000	-3.483748000
C	0.494946000	0.742700000	-3.471277000
C	1.615333000	1.519421000	-3.024575000
C	1.120568000	2.676149000	-2.303546000
C	1.819551000	3.140274000	-1.144506000
C	1.077824000	3.537595000	0.028330000
C	1.821431000	3.120054000	1.191324000
C	1.126684000	2.633391000	2.347264000
C	-1.735503000	-0.842614000	2.585997000
C	2.903390000	-0.625365000	2.582084000
C	1.776840000	-1.407909000	3.028978000
C	1.390289000	-2.590601000	2.306176000
C	2.131229000	-2.986152000	1.144510000
C	3.258771000	-2.207254000	0.705063000

C	4.019574000	0.173957000	0.709129000
C	3.516925000	1.319052000	1.444699000
C	2.830661000	0.827976000	2.593567000
C	1.632472000	1.484655000	3.052916000
C	0.516913000	0.692113000	3.483010000
C	0.587403000	-0.738171000	3.471207000
C	-0.050616000	-2.661446000	2.304561000
C	-0.746259000	-3.116528000	1.133457000
C	-0.002420000	-3.531554000	-0.025433000
C	1.434122000	-3.459242000	-0.025818000
C	2.131326000	-2.970280000	-1.191090000
C	3.254965000	-2.192404000	-0.743264000
C	3.637787000	-1.002695000	-1.457425000
C	4.009901000	0.182463000	-0.731660000
C	3.020724000	2.464936000	0.739077000
C	3.015844000	2.473068000	-0.708337000
C	3.516185000	1.337554000	-1.441352000
C	2.811435000	0.863523000	-2.594719000
C	2.885213000	-0.584747000	-2.604772000
C	1.763070000	-1.352619000	-3.046475000
C	1.389498000	-2.562379000	-2.345541000
C	-0.044867000	-2.625805000	-2.323879000
C	-0.734818000	-3.108294000	-1.181649000
C	-0.547773000	-1.501405000	3.007368000
C	-1.948986000	-2.453589000	0.692829000
C	3.635095000	-1.027794000	1.428169000
C	-4.801173000	-0.292369000	-1.131807000
C	-5.068664000	-0.331779000	1.121555000
C	-5.553984000	0.967465000	0.660176000
C	-5.440792000	1.007388000	-0.688858000
H	-5.628484000	1.853033000	-1.339562000
H	-5.826845000	1.792871000	1.308195000

H	-4.950188000	-0.574505000	-2.175384000
H	-5.182952000	-0.654434000	2.151839000
C	-5.305161000	-1.268944000	-0.052940000
H	-6.369059000	-1.502633000	-0.181231000
H	-4.735175000	-2.200473000	-0.002611000

Prod[6,6]

E=-2480.172341

G=-2479.768814

C	2.592914000	-0.972123000	-1.455401000
C	3.262390000	0.211405000	-0.771629000
C	3.300090000	0.159356000	0.823233000
C	2.676279000	-1.091433000	1.449448000
C	2.178863000	-2.204574000	0.639029000
C	2.193043000	-2.166762000	-0.769920000
C	1.806482000	-0.519918000	-2.545020000
C	1.739970000	0.926942000	-2.494440000
C	2.457790000	1.368551000	-1.366036000
C	1.960827000	2.474726000	-0.610288000
C	2.520309000	1.283591000	1.516291000
C	1.809905000	-0.681521000	2.570668000
C	0.685849000	-1.470673000	2.967106000
C	0.310905000	-2.656881000	2.242535000
C	1.050109000	-3.005490000	1.056927000
C	0.354159000	-3.456962000	-0.115482000
C	1.044959000	-2.932969000	-1.255101000
C	0.317663000	-2.492526000	-2.388563000
C	0.714119000	-1.269794000	-3.059384000
C	0.561702000	1.597863000	-2.958733000
C	-0.563775000	0.836156000	-3.446709000
C	-0.490748000	-0.593114000	-3.500118000
C	-1.606473000	-1.390467000	-3.089302000

C	-1.118764000	-2.572165000	-2.419657000
C	-1.821460000	-3.084864000	-1.282698000
C	-1.082973000	-3.529234000	-0.124110000
C	-1.829383000	-3.160479000	1.055231000
C	-1.136169000	-2.726352000	2.233992000
C	1.729575000	0.722408000	2.595762000
C	-2.904208000	0.512196000	2.601948000
C	-1.785520000	1.273736000	3.083245000
C	-1.391736000	2.492747000	2.410225000
C	-2.127601000	2.938698000	1.266216000
C	-3.252288000	2.177833000	0.788118000
C	-4.024790000	-0.214484000	0.696646000
C	-3.527352000	-1.379193000	1.377864000
C	-2.835200000	-0.933965000	2.554790000
C	-1.639655000	-1.612209000	2.982234000
C	-0.518286000	-0.837079000	3.445970000
C	-0.590906000	0.584968000	3.490122000
C	0.044048000	2.559492000	2.413176000
C	0.749925000	3.067268000	1.270156000
C	0.008007000	3.532079000	0.123978000
C	-1.425303000	3.462116000	0.119003000
C	-2.122090000	3.026603000	-1.066737000
C	-3.246052000	2.231986000	-0.652529000
C	-3.627454000	1.062768000	-1.426354000
C	-4.009474000	-0.167121000	-0.745549000
C	-3.027654000	-2.489308000	0.629647000
C	-3.021680000	-2.439639000	-0.822811000
C	-3.520300000	-1.281376000	-1.501293000
C	-2.808187000	-0.752364000	-2.631030000
C	-2.879625000	0.698521000	-2.582357000
C	-1.758606000	1.484278000	-2.991642000
C	-1.382468000	2.667696000	-2.233020000

C	0.051468000	2.725658000	-2.204733000
C	0.740730000	3.160227000	-1.044502000
C	0.537394000	1.367726000	3.060045000
C	1.944701000	2.407342000	0.805344000
C	-3.638674000	0.960475000	1.464274000
C	4.817469000	0.341374000	-1.135718000
C	4.868183000	0.275197000	1.111069000
C	5.492895000	-1.011213000	0.604130000
C	5.461307000	-0.971854000	-0.734415000
H	5.720195000	-1.765626000	-1.426026000
H	5.788875000	-1.843332000	1.232615000
H	4.970796000	0.674244000	-2.163087000
H	5.071495000	0.548066000	2.147034000
C	5.285918000	1.263914000	0.006632000
H	6.364711000	1.440971000	-0.016167000
H	4.753364000	2.218911000	0.046980000

C60 + indene asymm

S=0

Indene (C₉H₈)

E=-347.7947401

C	-2.171016000	-0.713586000	0.000000000
C	-0.955547000	-1.410500000	0.000000000
C	-2.190116000	0.684294000	0.000000000
C	0.229664000	-0.689429000	0.000000000
C	-0.998953000	1.415469000	0.000000000
C	0.211702000	0.722685000	0.000000000
H	-3.107195000	-1.264763000	0.000000000
H	-0.947382000	-2.497790000	0.000000000
H	-3.142092000	1.208075000	0.000000000
H	-1.018521000	2.502129000	0.000000000

C	1.667876000	-1.155624000	0.000000000
H	1.904436000	-1.772688000	0.878926000
C	2.440205000	0.143958000	0.000000000
H	3.523294000	0.191115000	0.000000000
C	1.599304000	1.196582000	0.000000000
H	1.884315000	2.243516000	0.000000000
H	1.904436000	-1.772688000	-0.878926000

Pre-complex

E=-2634.302526

C	-2.586223000	-0.023801000	0.117338000
C	-2.242149000	-0.483432000	1.453277000
C	-1.663894000	0.396287000	2.366655000
C	-1.400250000	1.775949000	1.980018000
C	-1.729548000	2.213290000	0.697339000
C	-2.338746000	1.295473000	-0.252601000
C	-2.315641000	-1.106247000	-0.813863000
C	-1.804256000	-2.236891000	-0.054505000
C	-1.758676000	-1.850966000	1.348589000
C	-0.707552000	-2.282225000	2.157183000
C	-0.565287000	-0.052745000	3.207876000
C	-0.138003000	2.176747000	2.582016000
C	0.739884000	3.003479000	1.879633000
C	0.393846000	3.462729000	0.543503000
C	-0.814750000	3.075213000	-0.035176000
C	-0.859946000	2.690093000	-1.438178000
C	-1.803355000	1.590042000	-1.571901000
C	-1.543659000	0.553398000	-2.468950000
C	-1.806984000	-0.825450000	-2.082096000
C	-0.796750000	-3.037845000	-0.591330000
C	-0.259451000	-2.742105000	-1.910706000
C	-0.753721000	-1.659655000	-2.640367000

C	0.161493000	-0.796705000	-3.371510000
C	-0.326445000	0.570240000	-3.265194000
C	0.578269000	1.625085000	-3.137148000
C	0.305347000	2.707505000	-2.204282000
C	1.566779000	3.110760000	-1.600284000
C	1.609986000	3.479679000	-0.255823000
C	0.377698000	1.047236000	3.341296000
C	4.232274000	1.102168000	0.810905000
C	3.716675000	0.819676000	2.075848000
C	3.452035000	-0.557954000	2.462068000
C	3.714609000	-1.596059000	1.568219000
C	4.251760000	-1.301023000	0.248632000
C	4.158369000	0.478575000	-1.458280000
C	3.671012000	1.845091000	-1.351401000
C	3.716397000	2.230315000	0.050783000
C	2.707663000	3.030552000	0.587173000
C	2.169779000	2.735889000	1.906736000
C	2.664066000	1.653819000	2.635464000
C	2.236156000	-0.575302000	3.260562000
C	1.332202000	-1.630083000	3.132350000
C	1.605987000	-2.713271000	2.199896000
C	2.771810000	-2.696096000	1.434138000
C	2.726601000	-3.080875000	0.032146000
C	3.641072000	-2.218888000	-0.700833000
C	3.309229000	-1.779196000	-1.982095000
C	3.573435000	-0.401435000	-2.368602000
C	2.618557000	2.275485000	-2.159337000
C	2.007883000	1.357378000	-3.108588000
C	2.475533000	0.047230000	-3.211204000
C	1.532632000	-1.052456000	-3.345128000
C	2.047801000	-2.181495000	-2.585703000
C	1.170754000	-3.007539000	-1.882683000

C	1.517602000	-3.467635000	-0.546350000
C	0.302042000	-3.486540000	0.252479000
C	0.345286000	-3.117528000	1.596945000
C	1.748744000	0.791274000	3.366894000
C	-0.097691000	-1.363752000	3.105986000
C	4.505508000	0.019424000	-0.121934000
C	-5.625578000	-0.211480000	-0.677019000
C	-5.601275000	-2.421530000	0.153272000
C	-5.536118000	-1.582632000	1.206118000
C	-5.547640000	-0.195472000	0.734080000
H	-5.468781000	-1.868707000	2.250234000
H	-5.602328000	-3.504498000	0.199305000
C	-5.680385000	-1.647945000	-1.143033000
H	-6.603397000	-1.871891000	-1.697100000
H	-4.847025000	-1.891630000	-1.815891000
C	-5.598502000	0.972642000	-1.398171000
H	-5.641994000	0.966312000	-2.484292000
C	-5.454952000	1.012319000	1.426465000
H	-5.383938000	1.027836000	2.510503000
C	-5.421685000	2.201175000	0.694833000
H	-5.332044000	3.150594000	1.214896000
C	-5.488953000	2.183581000	-0.702997000
H	-5.452766000	3.118700000	-1.254305000

TS[5,6]

E=-2634.239511

C	-2.816526000	-0.112436000	-0.403071000
C	-2.577895000	-1.631100000	-0.082197000
C	-1.866389000	-1.866746000	1.206227000
C	-1.730831000	-0.877772000	2.182214000
C	-2.062407000	0.487898000	1.906908000
C	-2.501345000	0.857043000	0.620223000

C	-2.173100000	0.165396000	-1.709172000
C	-1.581851000	-1.038739000	-2.236025000
C	-1.685406000	-2.082160000	-1.248521000
C	-0.628938000	-2.964270000	-1.099187000
C	-0.760572000	-2.797482000	1.345229000
C	-0.541941000	-1.178504000	3.003360000
C	0.265170000	-0.156407000	3.475420000
C	-0.064127000	1.243759000	3.178797000
C	-1.188829000	1.550016000	2.422444000
C	-1.113427000	2.593025000	1.416810000
C	-1.917888000	2.156411000	0.292185000
C	-1.506249000	2.434245000	-1.002340000
C	-1.637042000	1.401246000	-2.034356000
C	-0.474330000	-0.958305000	-3.096838000
C	0.091577000	0.334118000	-3.432071000
C	-0.476746000	1.491070000	-2.897972000
C	0.374220000	2.566288000	-2.410027000
C	-0.260965000	3.147002000	-1.237335000
C	0.519701000	3.564746000	-0.156990000
C	0.083675000	3.281846000	1.200725000
C	1.256844000	2.957525000	1.990135000
C	1.180777000	1.954029000	2.960914000
C	0.052833000	-2.387564000	2.479938000
C	3.990750000	-0.120540000	1.747926000
C	3.451957000	-1.367091000	2.061247000
C	3.316878000	-2.384094000	1.025811000
C	3.732513000	-2.110790000	-0.276262000
C	4.298651000	-0.808146000	-0.603146000
C	4.102789000	1.550179000	0.093635000
C	3.467050000	2.126050000	1.269921000
C	3.394906000	1.091313000	2.291201000
C	2.275013000	1.006275000	3.117390000

C	1.709538000	-0.293884000	3.441804000
C	2.289128000	-1.458642000	2.930627000
C	2.075192000	-3.104015000	1.263954000
C	1.283864000	-3.505367000	0.181986000
C	1.714568000	-3.210070000	-1.175336000
C	2.913735000	-2.533785000	-1.401356000
C	2.985797000	-1.501210000	-2.426022000
C	3.841018000	-0.436164000	-1.930232000
C	3.530280000	0.898268000	-2.214005000
C	3.667447000	1.910873000	-1.182397000
C	2.423348000	3.038045000	1.123534000
C	1.967444000	3.414883000	-0.207614000
C	2.573982000	2.861964000	-1.333658000
C	1.761253000	2.429936000	-2.461103000
C	2.354927000	1.217615000	-3.007112000
C	1.536794000	0.193474000	-3.485728000
C	1.860198000	-1.195913000	-3.190593000
C	0.611020000	-1.902158000	-2.955273000
C	0.536203000	-2.877568000	-1.959508000
C	1.441456000	-2.529550000	2.438106000
C	-0.160552000	-3.371481000	0.234552000
C	4.426317000	0.165404000	0.388173000
C	-4.838785000	-0.228336000	-0.719866000
C	-4.091987000	-2.316921000	-0.122370000
C	-4.859150000	-1.747569000	1.007870000
C	-5.250395000	-0.474872000	0.667561000
H	-4.898449000	-2.174194000	2.003408000
H	-3.988269000	-3.400909000	-0.165860000
C	-4.714636000	-1.603081000	-1.339308000
H	-5.711004000	-2.011345000	-1.544675000
H	-4.117540000	-1.649387000	-2.251389000
C	-5.225102000	1.003032000	-1.348618000

H	-5.021458000	1.155705000	-2.404115000
C	-5.814639000	0.592892000	1.431509000
H	-6.049453000	0.444689000	2.481484000
C	-6.034964000	1.794929000	0.820124000
H	-6.445707000	2.623627000	1.389616000
C	-5.762463000	1.994530000	-0.580371000
H	-6.004151000	2.956261000	-1.023355000

Prod[5,6]

E= -2634.24925519

C	-2.951534000	-0.104133000	-0.462464000
C	-2.604940000	-1.663689000	-0.136969000
C	-1.892641000	-1.881333000	1.164120000
C	-1.763752000	-0.901975000	2.137043000
C	-2.080758000	0.476341000	1.852009000
C	-2.524727000	0.863283000	0.596428000
C	-2.180650000	0.180875000	-1.749377000
C	-1.564930000	-1.012084000	-2.257752000
C	-1.674777000	-2.065753000	-1.286747000
C	-0.623338000	-2.952929000	-1.139186000
C	-0.782662000	-2.819526000	1.311921000
C	-0.581015000	-1.204456000	2.971154000
C	0.221491000	-0.187219000	3.457695000
C	-0.102566000	1.219787000	3.166926000
C	-1.212261000	1.536977000	2.402796000
C	-1.131669000	2.591164000	1.416224000
C	-1.930048000	2.161925000	0.281741000
C	-1.506547000	2.450257000	-1.003699000
C	-1.623688000	1.411238000	-2.043557000
C	-0.446089000	-0.930448000	-3.110747000
C	0.121645000	0.358857000	-3.431609000
C	-0.453062000	1.508752000	-2.887379000

C	0.392443000	2.581956000	-2.386094000
C	-0.255167000	3.157462000	-1.218847000
C	0.517533000	3.573409000	-0.130513000
C	0.068360000	3.280629000	1.219182000
C	1.232494000	2.944942000	2.017250000
C	1.145188000	1.932476000	2.978115000
C	0.019907000	-2.411973000	2.452452000
C	3.965553000	-0.135506000	1.780690000
C	3.424490000	-1.384806000	2.078827000
C	3.302212000	-2.394215000	1.034465000
C	3.728622000	-2.109230000	-0.260775000
C	4.299071000	-0.804488000	-0.572507000
C	4.096695000	1.548476000	0.141204000
C	3.448064000	2.115619000	1.315050000
C	3.364207000	1.072431000	2.326882000
C	2.234595000	0.980878000	3.138860000
C	1.664178000	-0.322487000	3.444602000
C	2.251606000	-1.484433000	2.933708000
C	2.056063000	-3.114925000	1.253498000
C	1.277324000	-3.507329000	0.160410000
C	1.721244000	-3.200963000	-1.189146000
C	2.922433000	-2.524273000	-1.398624000
C	3.005778000	-1.483829000	-2.414746000
C	3.853954000	-0.422775000	-1.900222000
C	3.546078000	0.915105000	-2.176905000
C	3.673007000	1.918949000	-1.136033000
C	2.408436000	3.031560000	1.164768000
C	1.965412000	3.419184000	-0.168386000
C	2.582839000	2.873690000	-1.291602000
C	1.779587000	2.448441000	-2.428369000
C	2.379303000	1.240183000	-2.978721000
C	1.567538000	0.220221000	-3.475514000

C	1.887733000	-1.171592000	-3.187928000
C	0.635639000	-1.877235000	-2.969889000
C	0.549903000	-2.859990000	-1.982279000
C	1.410384000	-2.551887000	2.426096000
C	-0.168746000	-3.368740000	0.199758000
C	4.415379000	0.161540000	0.428001000
C	-4.558023000	-0.167219000	-0.683525000
C	-4.058998000	-2.324771000	-0.202581000
C	-4.838095000	-1.775919000	0.967168000
C	-5.136432000	-0.485123000	0.690112000
H	-4.998287000	-2.292951000	1.906191000
H	-4.002210000	-3.410590000	-0.290512000
C	-4.690820000	-1.539385000	-1.373816000
H	-5.739322000	-1.805764000	-1.527361000
H	-4.146527000	-1.624390000	-2.318019000
C	-5.082351000	1.074095000	-1.306860000
H	-4.845660000	1.270659000	-2.348709000
C	-5.793803000	0.546124000	1.443717000
H	-6.077716000	0.358725000	2.475748000
C	-6.077799000	1.728241000	0.839219000
H	-6.582925000	2.514382000	1.393162000
C	-5.762424000	1.969526000	-0.562680000
H	-6.099833000	2.902230000	-1.006764000

TS[6,6]

E=-2634.265706

C	-2.471084000	0.913820000	0.591025000
C	-2.732908000	-0.132911000	-0.400828000
C	-2.551426000	-1.583458000	-0.028009000
C	-1.861774000	-1.781110000	1.315317000
C	-1.726702000	-0.768200000	2.243351000
C	-2.055263000	0.625494000	1.884508000

C	-1.964868000	2.094253000	-0.080896000
C	-1.788730000	1.761623000	-1.482319000
C	-2.181874000	0.377740000	-1.656920000
C	-1.505870000	-0.424994000	-2.564260000
C	-1.593043000	-2.318847000	-0.964789000
C	-0.842876000	-2.788377000	1.209549000
C	0.260613000	-2.792053000	2.070080000
C	0.397216000	-1.738955000	3.050095000
C	-0.578460000	-0.738746000	3.126420000
C	-0.184982000	0.648522000	3.309141000
C	-1.096775000	1.486228000	2.540738000
C	-0.608594000	2.633335000	1.897798000
C	-1.055935000	2.942878000	0.556323000
C	-0.716011000	2.288652000	-2.204213000
C	0.238786000	3.164628000	-1.538536000
C	0.073172000	3.481946000	-0.190531000
C	1.223541000	3.500185000	0.698830000
C	0.800754000	2.971869000	1.988870000
C	1.670304000	2.168947000	2.729463000
C	1.164954000	0.983824000	3.405743000
C	2.181093000	-0.055837000	3.315108000
C	1.804922000	-1.388466000	3.142267000
C	-0.674837000	-3.120260000	-0.195733000
C	3.794455000	-2.048361000	0.095956000
C	2.876159000	-2.885746000	-0.539571000
C	2.419430000	-2.575476000	-1.886095000
C	2.898373000	-1.438839000	-2.539037000
C	3.855451000	-0.568573000	-1.878833000
C	4.431219000	0.197013000	0.396845000
C	4.014988000	-0.328411000	1.687488000
C	3.622765000	-1.716131000	1.502726000
C	2.541018000	-2.235716000	2.214991000

C	1.584741000	-3.106725000	1.550312000
C	1.747367000	-3.423097000	0.203462000
C	1.010177000	-2.922767000	-1.972665000
C	0.134498000	-2.114970000	-2.703227000
C	0.635363000	-0.933151000	-3.385994000
C	1.987830000	-0.602111000	-3.308657000
C	2.388725000	0.785340000	-3.129555000
C	3.538126000	0.806433000	-2.241784000
C	3.675118000	1.825391000	-1.298286000
C	4.126808000	1.513367000	0.048775000
C	3.308447000	0.483706000	2.576579000
C	2.991473000	1.858324000	2.212706000
C	3.396145000	2.362794000	0.976402000
C	2.492365000	3.199574000	0.203436000
C	2.665403000	2.867923000	-1.203359000
C	1.561366000	2.850235000	-2.055779000
C	1.417588000	1.785162000	-3.039193000
C	0.009338000	1.444290000	-3.131517000
C	-0.378700000	0.107876000	-3.296360000
C	0.594602000	-3.441043000	-0.688413000
C	-1.185640000	-1.812277000	-2.184729000
C	4.293247000	-0.865753000	-0.587179000
C	-4.956521000	-0.271310000	-0.726664000
C	-4.083061000	-2.302288000	-0.055226000
C	-4.849215000	-1.724036000	1.056807000
C	-5.286080000	-0.469040000	0.677099000
H	-4.855216000	-2.114090000	2.067911000
H	-3.942071000	-3.382440000	-0.066106000
C	-4.699269000	-1.641834000	-1.302263000
H	-5.651688000	-2.129474000	-1.548608000
H	-4.057874000	-1.658224000	-2.186132000
C	-5.327180000	0.938958000	-1.371809000

H	-5.140743000	1.067235000	-2.433761000
C	-5.853590000	0.608724000	1.424458000
H	-6.058677000	0.485891000	2.483798000
C	-6.109401000	1.790743000	0.785227000
H	-6.521728000	2.628369000	1.340151000
C	-5.853260000	1.956093000	-0.617071000
H	-6.096044000	2.906598000	-1.082826000

Prod[6,6]

E= -2634.28011530

C	-2.510436000	0.897393000	0.601623000
C	-2.930834000	-0.113436000	-0.456719000
C	-2.589346000	-1.634793000	-0.109434000
C	-1.882995000	-1.840205000	1.226236000
C	-1.758937000	-0.860028000	2.186001000
C	-2.081542000	0.549775000	1.864130000
C	-1.980115000	2.078440000	-0.024877000
C	-1.792323000	1.794678000	-1.437377000
C	-2.204434000	0.437278000	-1.680463000
C	-1.499788000	-0.333917000	-2.577413000
C	-1.588458000	-2.292242000	-1.061164000
C	-0.856047000	-2.838052000	1.096861000
C	0.240603000	-2.868289000	1.964878000
C	0.364026000	-1.849145000	2.981182000
C	-0.616793000	-0.855473000	3.077323000
C	-0.226599000	0.525123000	3.311845000
C	-1.129406000	1.386169000	2.564520000
C	-0.642201000	2.558231000	1.974345000
C	-1.079833000	2.914321000	0.644779000
C	-0.716840000	2.359496000	-2.129983000
C	0.229896000	3.215289000	-1.428009000
C	0.053135000	3.484209000	-0.071998000

C	1.196189000	3.476354000	0.826666000
C	0.765034000	2.901593000	2.093125000
C	1.628689000	2.071824000	2.809687000
C	1.120452000	0.861478000	3.439395000
C	2.140618000	-0.170972000	3.322653000
C	1.769270000	-1.497622000	3.098644000
C	-0.673724000	-3.118729000	-0.316898000
C	3.786773000	-2.043810000	0.047877000
C	2.877452000	-2.861663000	-0.624671000
C	2.428394000	-2.503834000	-1.962500000
C	2.908739000	-1.342886000	-2.570561000
C	3.856878000	-0.494068000	-1.872013000
C	4.411590000	0.192204000	0.433128000
C	3.987694000	-0.380329000	1.701064000
C	3.602136000	-1.761855000	1.464388000
C	2.516698000	-2.309754000	2.149111000
C	1.569440000	-3.160508000	1.446140000
C	1.745172000	-3.429448000	0.090084000
C	1.021803000	-2.852726000	-2.071381000
C	0.145447000	-2.018951000	-2.773500000
C	0.648870000	-0.811147000	-3.407008000
C	2.000517000	-0.481526000	-3.314663000
C	2.396608000	0.900389000	-3.083081000
C	3.539642000	0.892748000	-2.188437000
C	3.666999000	1.878702000	-1.208653000
C	4.109097000	1.519856000	0.129866000
C	3.271668000	0.397562000	2.612474000
C	2.954974000	1.784248000	2.295302000
C	3.368955000	2.334536000	1.081149000
C	2.470832000	3.197327000	0.331305000
C	2.655458000	2.915793000	-1.084999000
C	1.557498000	2.925619000	-1.946465000

C	1.424776000	1.896034000	-2.967736000
C	0.017240000	1.552225000	-3.076917000
C	-0.365544000	0.222878000	-3.285270000
C	0.600568000	-3.418104000	-0.810357000
C	-1.179510000	-1.744092000	-2.256626000
C	4.286185000	-0.835772000	-0.588468000
C	-4.539896000	-0.173928000	-0.677708000
C	-4.032521000	-2.317448000	-0.175046000
C	-4.827195000	-1.769830000	0.982927000
C	-5.128197000	-0.483422000	0.694450000
H	-4.994829000	-2.285187000	1.921662000
H	-3.960830000	-3.403094000	-0.251308000
C	-4.648821000	-1.549813000	-1.364567000
H	-5.689170000	-1.829380000	-1.549214000
H	-4.071043000	-1.630518000	-2.290777000
C	-5.083532000	1.053698000	-1.314268000
H	-4.849948000	1.242289000	-2.358365000
C	-5.804132000	0.546897000	1.435892000
H	-6.088584000	0.364470000	2.468653000
C	-6.107023000	1.715730000	0.817660000
H	-6.628189000	2.500022000	1.359057000
C	-5.787836000	1.943164000	-0.586292000
H	-6.144330000	2.860706000	-1.046832000

S=1

Pre-complex

E=-2634.241763

C	-2.552927000	0.256130000	0.367228000
C	-2.243134000	1.501996000	-0.249563000
C	-1.804425000	1.540482000	-1.599477000
C	-1.686523000	0.294722000	-2.359665000
C	-1.990904000	-0.919573000	-1.756418000

C	-2.427996000	-0.953442000	-0.359729000
C	-2.112562000	0.310724000	1.763531000
C	-1.528094000	1.618526000	2.000764000
C	-1.595223000	2.354757000	0.747912000
C	-0.550129000	3.190646000	0.374847000
C	-0.732874000	2.399587000	-1.981814000
C	-0.525769000	0.402866000	-3.226964000
C	0.287065000	-0.712940000	-3.451675000
C	-0.034956000	-1.982930000	-2.823088000
C	-1.158110000	-2.084323000	-1.994928000
C	-1.075645000	-2.819515000	-0.742389000
C	-1.879482000	-2.112563000	0.256518000
C	-1.441010000	-2.062754000	1.605579000
C	-1.570983000	-0.817752000	2.365448000
C	-0.405829000	1.743793000	2.827103000
C	0.163874000	0.563490000	3.454086000
C	-0.410200000	-0.691862000	3.230152000
C	0.436706000	-1.847768000	2.988074000
C	-0.217229000	-2.690232000	1.985520000
C	0.568004000	-3.367210000	1.020547000
C	0.115792000	-3.429393000	-0.370805000
C	1.282838000	-3.333240000	-1.231371000
C	1.211054000	-2.620736000	-2.433416000
C	0.074302000	1.704312000	-2.985845000
C	4.012096000	-0.312282000	-1.757697000
C	3.465511000	0.816245000	-2.359256000
C	3.334578000	2.059631000	-1.601857000
C	3.773421000	2.110782000	-0.257474000
C	4.334040000	0.948995000	0.361036000
C	4.138930000	-1.507687000	0.254108000
C	3.491266000	-2.357078000	-0.742401000
C	3.423450000	-1.619152000	-1.992843000

C	2.303867000	-1.745385000	-2.820717000
C	1.733210000	-0.565766000	-3.449779000
C	2.305608000	0.689131000	-3.224911000
C	2.108131000	2.687716000	-1.983329000
C	1.323813000	3.364291000	-1.019222000
C	1.777879000	3.425268000	0.370954000
C	2.970860000	2.814336000	0.740574000
C	3.054065000	2.078019000	1.991531000
C	3.889943000	0.914604000	1.754149000
C	3.581603000	-0.300178000	2.356569000
C	3.700485000	-1.544486000	1.599106000
C	2.444112000	-3.193175000	-0.370920000
C	1.989340000	-3.223818000	1.019878000
C	2.624419000	-2.404693000	1.982823000
C	1.819483000	-1.708686000	2.985356000
C	2.420952000	-0.407091000	3.224105000
C	1.610414000	0.708477000	3.451310000
C	1.933140000	1.978444000	2.821827000
C	0.687024000	2.617778000	2.436025000
C	0.613373000	3.330154000	1.233661000
C	1.456770000	1.844689000	-2.985152000
C	-0.097023000	3.220203000	-1.017546000
C	4.456057000	-0.257215000	-0.365568000
C	-5.517095000	0.354496000	0.636444000
C	-5.412543000	2.386057000	-0.557146000
C	-5.466413000	1.378742000	-1.455044000
C	-5.531157000	0.098367000	-0.755083000
H	-5.445791000	1.482910000	-2.534412000
H	-5.349036000	3.443044000	-0.787970000
C	-5.462474000	1.848335000	0.853485000
H	-6.341334000	2.220778000	1.399283000
H	-4.584595000	2.151164000	1.440181000

C	-5.525813000	-0.692687000	1.547807000
H	-5.500400000	-0.500798000	2.617110000
C	-5.554092000	-1.213194000	-1.233721000
H	-5.552209000	-1.415339000	-2.301077000
C	-5.555852000	-2.261354000	-0.311562000
H	-5.559919000	-3.288283000	-0.665306000
C	-5.539918000	-2.006118000	1.064905000
H	-5.533264000	-2.836560000	1.764656000

TS_{bir}[5,6]

E=-2634.231881

C	2.530632000	-0.161093000	0.551457000
C	2.370235000	-1.471662000	-0.087127000
C	1.903508000	-1.466243000	-1.478446000
C	1.795984000	-0.235414000	-2.217165000
C	2.052578000	0.993233000	-1.596495000
C	2.428074000	1.025733000	-0.168998000
C	2.018094000	-0.225570000	1.906258000
C	1.437393000	-1.543537000	2.102364000
C	1.595754000	-2.285587000	0.866719000
C	0.580553000	-3.135540000	0.440974000
C	0.854371000	-2.342706000	-1.905955000
C	0.673447000	-0.354608000	-3.143268000
C	-0.143639000	0.747133000	-3.395830000
C	0.126309000	2.020304000	-2.747257000
C	1.213067000	2.131438000	-1.860791000
C	1.056885000	2.867630000	-0.610844000
C	1.823040000	2.186518000	0.425293000
C	1.330432000	2.133162000	1.743542000
C	1.434557000	0.900277000	2.494887000
C	0.279788000	-1.692156000	2.875367000
C	-0.339041000	-0.516916000	3.475078000

C	0.223770000	0.746028000	3.290701000
C	-0.629362000	1.891836000	3.021022000
C	0.057960000	2.745562000	2.060633000
C	-0.676166000	3.400185000	1.064267000
C	-0.162189000	3.462354000	-0.299046000
C	-1.286738000	3.344403000	-1.216244000
C	-1.140764000	2.633150000	-2.415398000
C	0.086507000	-1.666790000	-2.949449000
C	-3.946630000	0.280792000	-1.900615000
C	-3.355124000	-0.839073000	-2.482299000
C	-3.240042000	-2.078772000	-1.726350000
C	-3.732505000	-2.141686000	-0.414934000
C	-4.348110000	-0.977641000	0.185594000
C	-4.188242000	1.483468000	0.108270000
C	-3.508546000	2.337798000	-0.847110000
C	-3.359552000	1.597341000	-2.092622000
C	-2.204330000	1.742897000	-2.859122000
C	-1.587379000	0.574484000	-3.468519000
C	-2.150382000	-0.687923000	-3.283738000
C	-1.973264000	-2.690242000	-2.054999000
C	-1.228694000	-3.345637000	-1.056976000
C	-1.741200000	-3.407338000	0.307184000
C	-2.965105000	-2.822131000	0.618803000
C	-3.122748000	-2.083142000	1.865253000
C	-3.971379000	-0.940976000	1.595907000
C	-3.720658000	0.284255000	2.218667000
C	-3.827082000	1.519507000	1.463929000
C	-2.488359000	3.191549000	-0.422506000
C	-2.110418000	3.227654000	0.987503000
C	-2.771931000	2.408702000	1.908545000
C	-2.011791000	1.727058000	2.945127000
C	-2.599827000	0.410534000	3.137771000

C	-1.781146000	-0.688402000	3.398244000
C	-2.045272000	-1.965433000	2.749584000
C	-0.771926000	-2.582132000	2.432931000
C	-0.618812000	-3.288864000	1.227193000
C	-1.294647000	-1.834441000	-3.016130000
C	0.195925000	-3.171700000	-0.984132000
C	-4.456491000	0.212911000	-0.537413000
C	5.537290000	-0.430178000	0.658599000
C	4.444856000	-2.316920000	-0.229787000
C	4.918128000	-1.532092000	-1.286640000
C	5.495486000	-0.332206000	-0.761098000
H	4.756284000	-1.736981000	-2.337843000
H	4.104725000	-3.339585000	-0.340886000
C	5.024365000	-1.790667000	1.069208000
H	5.852818000	-2.443980000	1.384697000
H	4.313743000	-1.762724000	1.901106000
C	5.982386000	0.634089000	1.424405000
H	6.004273000	0.571190000	2.508809000
C	5.912174000	0.845964000	-1.404542000
H	5.869701000	0.928438000	-2.486526000
C	6.350421000	1.910207000	-0.623902000
H	6.661857000	2.835268000	-1.099819000
C	6.384520000	1.809168000	0.775551000
H	6.722604000	2.656926000	1.363955000

Print[5,6]

E=-2634.257204

C	-2.541585000	0.161127000	-0.266430000
C	-2.571964000	-1.348780000	0.044403000
C	-1.835597000	-1.625448000	1.343120000
C	-1.577769000	-0.606650000	2.316970000
C	-1.812164000	0.744710000	2.033572000

C	-2.288608000	1.124302000	0.691157000
C	-2.101508000	0.378342000	-1.615182000
C	-1.620044000	-0.885435000	-2.155796000
C	-1.758226000	-1.896395000	-1.145189000
C	-0.773585000	-2.856666000	-1.009815000
C	-0.812477000	-2.620096000	1.456664000
C	-0.398732000	-0.990150000	3.090157000
C	0.505459000	-0.022511000	3.519578000
C	0.271599000	1.378395000	3.205998000
C	-0.864890000	1.743960000	2.469842000
C	-0.751007000	2.747411000	1.420133000
C	-1.629737000	2.361709000	0.327982000
C	-1.245480000	2.596258000	-0.995813000
C	-1.487829000	1.579770000	-1.993403000
C	-0.544281000	-0.899284000	-3.053312000
C	0.105747000	0.349032000	-3.424278000
C	-0.354808000	1.559242000	-2.906801000
C	0.592829000	2.570107000	-2.465090000
C	0.041603000	3.210104000	-1.279510000
C	0.886373000	3.575630000	-0.230382000
C	0.479279000	3.343329000	1.148933000
C	1.657956000	2.956361000	1.909180000
C	1.552647000	1.990877000	2.914517000
C	0.078931000	-2.247271000	2.553561000
C	4.148925000	-0.310079000	1.634609000
C	3.525006000	-1.504187000	1.992612000
C	3.270733000	-2.524293000	0.983988000
C	3.660257000	-2.305731000	-0.340421000
C	4.311701000	-1.061992000	-0.710740000
C	4.320724000	1.317302000	-0.057509000
C	3.774681000	1.957956000	1.126996000
C	3.667595000	0.953081000	2.174308000

C	2.583638000	0.970336000	3.050521000
C	1.935039000	-0.276205000	3.426797000
C	2.395828000	-1.487344000	2.909337000
C	1.989846000	-3.136463000	1.275557000
C	1.130998000	-3.500368000	0.228089000
C	1.537765000	-3.266457000	-1.150795000
C	2.774975000	-2.688377000	-1.429692000
C	2.888210000	-1.683690000	-2.478503000
C	3.835407000	-0.678051000	-2.033073000
C	3.619195000	0.668500000	-2.333631000
C	3.866132000	1.686714000	-1.325895000
C	2.789392000	2.937739000	0.999202000
C	2.312612000	3.322067000	-0.323032000
C	2.842352000	2.709934000	-1.461101000
C	1.964030000	2.326302000	-2.554180000
C	2.444368000	1.062758000	-3.093891000
C	1.534182000	0.095895000	-3.522571000
C	1.761557000	-1.307758000	-3.210998000
C	0.472898000	-1.917502000	-2.924813000
C	0.362340000	-2.872625000	-1.909676000
C	1.445776000	-2.495086000	2.462561000
C	-0.289400000	-3.257497000	0.323951000
C	4.551967000	-0.083276000	0.254367000
C	-5.748122000	-0.413901000	-0.674179000
C	-4.044260000	-1.933730000	0.109389000
C	-4.803140000	-1.303233000	1.246952000
C	-5.708602000	-0.346238000	0.752282000
H	-4.567809000	-1.470671000	2.290888000
H	-3.927824000	-3.017690000	0.221834000
C	-4.884669000	-1.560726000	-1.144317000
H	-5.512471000	-2.415136000	-1.429765000
H	-4.274270000	-1.315017000	-2.017556000

C	-6.526802000	0.465896000	-1.401731000
H	-6.550975000	0.418681000	-2.487543000
C	-6.496657000	0.614037000	1.428498000
H	-6.475628000	0.673782000	2.512921000
C	-7.276788000	1.488749000	0.682735000
H	-7.878154000	2.238204000	1.189784000
C	-7.293185000	1.425988000	-0.719827000
H	-7.904695000	2.125314000	-1.282205000

TS[5,6]

E=-2634.224067

C	-2.830671000	-0.159271000	-0.461067000
C	-2.591401000	-1.632881000	0.038596000
C	-1.901127000	-1.703012000	1.381348000
C	-1.767013000	-0.563274000	2.256494000
C	-2.064934000	0.722397000	1.801865000
C	-2.506815000	0.934023000	0.430237000
C	-2.157250000	-0.047546000	-1.785489000
C	-1.549410000	-1.302133000	-2.146838000
C	-1.666941000	-2.209546000	-1.043113000
C	-0.631070000	-3.081476000	-0.766431000
C	-0.826706000	-2.595394000	1.653226000
C	-0.617047000	-0.773806000	3.122416000
C	0.197718000	0.300228000	3.491780000
C	-0.114156000	1.636904000	3.018597000
C	-1.228926000	1.839164000	2.194210000
C	-1.133785000	2.727687000	1.051196000
C	-1.929726000	2.151566000	-0.031165000
C	-1.499794000	2.293649000	-1.364155000
C	-1.609649000	1.141153000	-2.251645000
C	-0.432882000	-1.340472000	-3.001698000
C	0.142919000	-0.099905000	-3.477090000

C	-0.431491000	1.116434000	-3.102794000
C	0.412275000	2.237524000	-2.729245000
C	-0.250109000	2.957420000	-1.646911000
C	0.519117000	3.503140000	-0.607414000
C	0.059440000	3.385816000	0.770574000
C	1.220625000	3.171968000	1.622035000
C	1.133536000	2.313729000	2.721964000
C	-0.022049000	-2.038410000	2.740603000
C	3.942372000	0.091208000	1.807638000
C	3.385702000	-1.102347000	2.264178000
C	3.258746000	-2.239590000	1.360459000
C	3.705740000	-2.131660000	0.038084000
C	4.285034000	-0.889287000	-0.433562000
C	4.088347000	1.539414000	-0.039627000
C	3.436780000	2.258256000	1.043369000
C	3.348034000	1.364145000	2.188813000
C	2.223642000	1.391947000	3.011527000
C	1.641655000	0.145374000	3.488582000
C	2.213216000	-1.075548000	3.123220000
C	2.012744000	-2.911458000	1.656089000
C	1.238946000	-3.451130000	0.615543000
C	1.704910000	-3.333132000	-0.761340000
C	2.911113000	-2.694233000	-1.043317000
C	3.009342000	-1.799985000	-2.189459000
C	3.854231000	-0.682430000	-1.809991000
C	3.556602000	0.604417000	-2.263372000
C	3.673843000	1.739922000	-1.360317000
C	2.393772000	3.141300000	0.766875000
C	1.956447000	3.346135000	-0.609689000
C	2.592195000	2.660920000	-1.652128000
C	1.800183000	2.095791000	-2.732502000
C	2.400729000	0.824981000	-3.114812000

C	1.589593000	-0.249065000	-3.482688000
C	1.900552000	-1.590134000	-3.010466000
C	0.644403000	-2.261270000	-2.717044000
C	0.548649000	-3.109036000	-1.611112000
C	1.360935000	-2.191144000	2.741590000
C	-0.194636000	-3.311402000	0.618832000
C	4.399772000	0.203025000	0.430859000
C	-4.764886000	-0.289113000	-0.696572000
C	-4.038099000	-2.321386000	0.058635000
C	-4.797259000	-1.648321000	1.170696000
C	-5.161385000	-0.406040000	0.726366000
H	-4.848261000	-2.008485000	2.191303000
H	-3.953030000	-3.407779000	0.110791000
C	-4.710286000	-1.725176000	-1.195116000
H	-5.720694000	-2.125664000	-1.333223000
H	-4.141836000	-1.863692000	-2.117286000
C	-5.185410000	0.878398000	-1.425451000
H	-5.031088000	0.924660000	-2.499355000
C	-5.668517000	0.745672000	1.404165000
H	-5.870525000	0.702938000	2.470379000
C	-5.870180000	1.895288000	0.691428000
H	-6.228905000	2.787176000	1.197102000
C	-5.660174000	1.953867000	-0.732620000
H	-5.906134000	2.873746000	-1.254810000

Prod[5,6]

E=-2634.275165

Pro-int[6,6]

E=-2634.258049

C	-2.220828000	1.118925000	0.908628000
C	-2.539482000	0.157557000	-0.103788000

C	-2.563126000	-1.337016000	0.164252000
C	-1.762028000	-1.655085000	1.442798000
C	-1.469855000	-0.708310000	2.405605000
C	-1.718863000	0.723705000	2.154599000
C	-1.688449000	2.316668000	0.262601000
C	-1.657101000	2.060579000	-1.162330000
C	-2.169983000	0.708072000	-1.372374000
C	-1.618133000	-0.093368000	-2.380404000
C	-1.713304000	-2.076172000	-0.887782000
C	-0.831257000	-2.718587000	1.191291000
C	0.338456000	-2.849171000	1.952088000
C	0.634145000	-1.870262000	2.973608000
C	-0.252952000	-0.810803000	3.185487000
C	0.256138000	0.531633000	3.411380000
C	-0.650340000	1.474873000	2.770381000
C	-0.132643000	2.620773000	2.149288000
C	-0.667300000	3.046079000	0.865246000
C	-0.605791000	2.540974000	-1.937754000
C	0.464575000	3.303518000	-1.313091000
C	0.434550000	3.550708000	0.059807000
C	1.651544000	3.432660000	0.847499000
C	1.297302000	2.856633000	2.138477000
C	2.164233000	1.951793000	2.757819000
C	1.630068000	0.766211000	3.410252000
C	2.555108000	-0.334774000	3.176250000
C	2.067193000	-1.624920000	2.963596000
C	-0.800638000	-2.977235000	-0.241566000
C	3.745323000	-2.236179000	-0.274422000
C	2.719805000	-2.968020000	-0.874028000
C	2.179795000	-2.546844000	-2.158280000
C	2.686299000	-1.408193000	-2.786306000
C	3.753898000	-0.647516000	-2.163071000

C	4.570238000	-0.063453000	0.092081000
C	4.223233000	-0.635257000	1.382647000
C	3.714247000	-1.978429000	1.157639000
C	2.658492000	-2.462889000	1.930687000
C	1.587112000	-3.220371000	1.303501000
C	1.616948000	-3.467512000	-0.068524000
C	0.746818000	-2.791804000	-2.143477000
C	-0.122388000	-1.879726000	-2.749445000
C	0.406172000	-0.696201000	-3.407371000
C	1.780598000	-0.465122000	-3.428571000
C	2.295471000	0.877421000	-3.208195000
C	3.511754000	0.765850000	-2.422657000
C	3.799734000	1.713919000	-1.440182000
C	4.335386000	1.291230000	-0.157036000
C	3.653505000	0.169074000	2.371938000
C	3.410950000	1.581797000	2.111824000
C	3.748761000	2.130483000	0.874302000
C	2.848518000	3.074736000	0.228846000
C	2.879918000	2.817163000	-1.203384000
C	1.712830000	2.927170000	-1.957659000
C	1.409961000	1.934569000	-2.980694000
C	-0.019935000	1.698740000	-2.969493000
C	-0.519459000	0.404405000	-3.174903000
C	0.399653000	-3.355547000	-0.858424000
C	-1.369511000	-1.520851000	-2.105368000
C	4.273914000	-1.052090000	-0.931602000
C	-5.776745000	-0.460347000	-0.647701000
C	-4.040386000	-1.888984000	0.251123000
C	-4.805576000	-1.175619000	1.333692000
C	-5.745209000	-0.292316000	0.770243000
H	-4.559930000	-1.250021000	2.386379000
H	-3.950686000	-2.966507000	0.434647000

C	-4.850277000	-1.586682000	-1.043287000
H	-5.426994000	-2.473391000	-1.336136000
H	-4.210441000	-1.335392000	-1.894687000
C	-6.591101000	0.332642000	-1.433663000
H	-6.609276000	0.210662000	-2.513786000
C	-6.573253000	0.679746000	1.378123000
H	-6.557258000	0.815353000	2.455800000
C	-7.389201000	1.465864000	0.574139000
H	-8.023560000	2.221883000	1.028538000
C	-7.400858000	1.303482000	-0.820090000
H	-8.041897000	1.933405000	-1.429640000

TS[6,6]

E=-2634.214836

C	-2.494247000	0.962215000	0.405901000
C	-2.789948000	-0.198282000	-0.436968000
C	-2.576403000	-1.612311000	0.123901000
C	-1.889789000	-1.621307000	1.496149000
C	-1.770350000	-0.469463000	2.294332000
C	-2.074473000	0.825715000	1.757770000
C	-1.994408000	2.027873000	-0.391981000
C	-1.803130000	1.524964000	-1.745153000
C	-2.202479000	0.139646000	-1.757225000
C	-1.501692000	-0.775071000	-2.525790000
C	-1.595647000	-2.444693000	-0.702152000
C	-0.882638000	-2.611691000	1.531823000
C	0.229423000	-2.500209000	2.404915000
C	0.353822000	-1.318840000	3.243641000
C	-0.618737000	-0.324530000	3.185589000
C	-0.230629000	1.073581000	3.207198000
C	-1.124108000	1.784004000	2.311963000
C	-0.637096000	2.826329000	1.525096000

C	-1.082426000	2.969016000	0.137876000
C	-0.723060000	1.962545000	-2.514904000
C	0.227001000	2.916723000	-1.956269000
C	0.036229000	3.400980000	-0.644003000
C	1.185488000	3.546942000	0.249214000
C	0.759925000	3.200933000	1.594720000
C	1.628449000	2.508258000	2.450881000
C	1.123697000	1.427067000	3.274800000
C	2.137690000	0.388272000	3.326681000
C	1.761260000	-0.958272000	3.315568000
C	-0.687935000	-3.123511000	0.178062000
C	3.774399000	-2.002861000	0.389810000
C	2.858845000	-2.928077000	-0.142445000
C	2.416869000	-2.793034000	-1.527070000
C	2.898470000	-1.750413000	-2.315651000
C	3.846831000	-0.793269000	-1.761834000
C	4.401229000	0.258010000	0.408014000
C	3.980932000	-0.092544000	1.756265000
C	3.583490000	-1.491044000	1.741878000
C	2.497519000	-1.912741000	2.505518000
C	1.538542000	-2.860696000	1.944239000
C	1.730067000	-3.358979000	0.639474000
C	1.012270000	-3.162827000	-1.591954000
C	0.140698000	-2.464264000	-2.437301000
C	0.645390000	-1.379136000	-3.259216000
C	1.998466000	-1.031936000	-3.204023000
C	2.389733000	0.367626000	-3.190076000
C	3.537191000	0.508105000	-2.299661000
C	3.653806000	1.651279000	-1.493166000
C	4.094987000	1.516008000	-0.110612000
C	3.270489000	0.826931000	2.529665000
C	2.953712000	2.141378000	1.987502000

C	3.361312000	2.476167000	0.694538000
C	2.456073000	3.192069000	-0.193674000
C	2.648907000	2.684692000	-1.547045000
C	1.544983000	2.554695000	-2.409035000
C	1.420493000	1.367297000	-3.246246000
C	0.013294000	1.007838000	-3.315122000
C	-0.368168000	-0.340467000	-3.316524000
C	0.586676000	-3.502243000	-0.255094000
C	-1.185973000	-2.107033000	-1.977507000
C	4.274799000	-0.925951000	-0.426969000
C	-4.801480000	-0.319715000	-0.667863000
C	-4.043558000	-2.305703000	0.178771000
C	-4.793547000	-1.591189000	1.254940000
C	-5.163684000	-0.366913000	0.759813000
H	-4.829138000	-1.901383000	2.292505000
H	-3.945783000	-3.386387000	0.281952000
C	-4.699140000	-1.768353000	-1.107202000
H	-5.696454000	-2.199620000	-1.252934000
H	-4.102688000	-1.926194000	-2.009015000
C	-5.198145000	0.820956000	-1.437661000
H	-5.056666000	0.821007000	-2.513885000
C	-5.642727000	0.817959000	1.399437000
H	-5.825986000	0.821406000	2.469627000
C	-5.838091000	1.941282000	0.642710000
H	-6.173401000	2.859713000	1.115268000
C	-5.642145000	1.935889000	-0.781785000
H	-5.875483000	2.837404000	-1.340356000

Prod[6,6]

E=-2634.265379

C₆₀ + isoindene

S=0

Indene symm (C₉H₈)

E=-347.7586564

G=-347.649589

C	-2.162417000	0.725394000	0.000000000
C	-1.006866000	1.441145000	0.000000000
C	-2.162289000	-0.725586000	0.000000000
C	0.253734000	0.742007000	0.000000000
C	-1.006625000	-1.441300000	0.000000000
C	0.254022000	-0.742096000	0.000000000
H	-3.119927000	1.239038000	0.000000000
H	-1.019519000	2.527809000	0.000000000
H	-3.119747000	-1.239359000	0.000000000
H	-1.019210000	-2.527980000	0.000000000
C	1.540355000	1.186491000	0.000000000
C	2.461253000	0.000437000	0.000000000
H	3.129564000	0.000033000	-0.876160000
C	1.540821000	-1.186481000	0.000000000
H	1.874496000	-2.217257000	0.000000000
H	1.872846000	2.217626000	0.000000000
H	3.129564000	0.000033000	0.876160000

Pre-complex

E=-2634.249165

G=-2633.806112

C	-5.623022000	-0.290015000	0.730351000
C	-5.560607000	-0.282912000	-0.750208000
C	-5.610950000	0.976472000	-1.446458000
C	-5.710249000	2.127525000	-0.728397000
C	-5.771299000	2.120759000	0.719525000

C	-5.731548000	0.962949000	1.432104000
C	-5.522767000	-1.574953000	1.173052000
C	-5.420883000	-1.563410000	-1.195737000
H	-5.555282000	0.993927000	-2.531310000
H	-5.738146000	3.085718000	-1.239521000
H	-5.843900000	3.074184000	1.235185000
H	-5.769123000	0.969941000	2.517889000
C	-2.416410000	-0.867975000	0.649523000
C	-2.314953000	-1.120520000	-0.780286000
C	-2.265609000	0.165883000	-1.460082000
C	-1.542205000	-2.184532000	-1.246535000
C	-1.454624000	0.334656000	-2.579476000
C	-2.345200000	1.211527000	-0.452437000
C	-0.690225000	-2.007468000	-2.414181000
C	-0.840453000	-3.041518000	-0.304347000
C	-2.436001000	0.573277000	0.851157000
C	-1.744884000	-1.690631000	1.552816000
C	-0.647420000	-0.775486000	-3.066661000
C	-0.681647000	1.557612000	-2.739379000
C	-1.606744000	2.384405000	-0.604634000
C	0.537516000	-2.754808000	-2.192322000
C	0.445233000	-3.393720000	-0.888291000
C	-0.940300000	-2.800164000	1.067285000
C	-1.786261000	1.132836000	1.949637000
C	-1.062712000	-1.106379000	2.698504000
C	0.623810000	-0.238445000	-3.524395000
C	0.603013000	1.202713000	-3.322226000
C	-0.755624000	2.560279000	-1.772083000
C	-0.925319000	2.967778000	0.540858000
C	1.757506000	-2.240955000	-2.633533000
C	1.576781000	-3.491302000	-0.078535000
C	0.240941000	-2.901264000	1.911330000

C	-1.083707000	0.274453000	2.893518000
C	-1.013100000	2.354921000	1.791492000
C	0.164452000	-1.854818000	2.920018000
C	1.801653000	-0.956018000	-3.313846000
C	1.760978000	1.866499000	-2.916608000
C	0.452051000	3.251349000	-1.347921000
C	0.347455000	3.502794000	0.081629000
C	2.937463000	-2.342829000	-1.788432000
C	1.472565000	-3.239984000	1.350886000
C	2.848857000	-2.954886000	-0.538029000
C	0.123821000	0.966474000	3.316339000
C	0.167713000	2.252127000	2.635571000
C	1.322354000	-1.191329000	3.326676000
C	3.009019000	-0.263286000	-2.890073000
C	2.988525000	1.117652000	-2.695059000
C	1.683953000	2.912591000	-1.908447000
C	1.479210000	3.405009000	0.891234000
C	3.711070000	-1.120792000	-1.947061000
C	2.680061000	-2.547605000	1.774794000
C	3.530152000	-2.371136000	0.607264000
C	1.301452000	0.249052000	3.528436000
C	1.387455000	2.766105000	2.195027000
C	2.606998000	-1.545452000	2.742349000
C	3.670599000	1.701471000	-1.550180000
C	2.864179000	2.810502000	-1.063701000
C	2.763826000	3.051517000	0.306699000
C	4.364053000	-0.561309000	-0.848739000
C	4.272161000	-1.199979000	0.455350000
C	2.573054000	0.785904000	3.069034000
C	2.615507000	2.018091000	2.416856000
C	3.379905000	-0.323027000	2.582859000
C	4.343330000	0.879282000	-0.646189000

C	3.465991000	2.194107000	1.249332000
C	4.194993000	-0.154184000	1.463882000
C	4.239022000	1.130956000	0.782934000
C	-5.395753000	-2.487075000	-0.012611000
H	-5.524413000	-1.910167000	2.203043000
H	-5.338801000	-1.888553000	-2.225563000
H	-6.212967000	-3.224860000	-0.051515000
H	-4.466592000	-3.076345000	0.024448000

TS[5,6]

E=-2634.247916

G=-2633.782191

C	5.274531000	-0.358578000	-0.721463000
C	5.274469000	-0.358581000	0.721462000
C	5.734217000	0.779118000	1.427100000
C	6.203783000	1.858814000	0.711714000
C	6.203826000	1.858817000	-0.711664000
C	5.734319000	0.779121000	-1.427079000
C	4.632258000	-1.536992000	-1.167296000
C	4.632135000	-1.537002000	1.167259000
H	5.716904000	0.793139000	2.513006000
H	6.575327000	2.734201000	1.236433000
H	6.575402000	2.734207000	-1.236357000
H	5.717073000	0.793135000	-2.512987000
C	2.558599000	-0.938017000	-0.755403000
C	2.558552000	-0.938326000	0.755531000
C	2.383910000	0.474977000	1.173043000
C	1.708137000	-1.883295000	1.420210000
C	1.647276000	0.827937000	2.292819000
C	2.359957000	1.321109000	0.000511000
C	0.927058000	-1.509463000	2.596379000
C	0.986546000	-2.876799000	0.709418000

C	2.384083000	0.475452000	-1.172366000
C	1.708311000	-1.882699000	-1.420590000
C	0.900988000	-0.192810000	3.034862000
C	0.854620000	2.042696000	2.295419000
C	1.607644000	2.504996000	0.000697000
C	-0.288900000	-2.302688000	2.607685000
C	-0.261707000	-3.148793000	1.429199000
C	0.986643000	-2.876521000	-0.710323000
C	1.647607000	0.828875000	-2.292104000
C	0.927427000	-1.508395000	-2.596736000
C	-0.346208000	0.400706000	3.483472000
C	-0.374957000	1.782659000	3.029424000
C	0.839734000	2.874628000	1.174689000
C	0.839907000	2.875109000	-1.173258000
C	-1.490574000	-1.738397000	3.043107000
C	-1.437178000	-3.400166000	0.731368000
C	-0.261499000	-3.148213000	-1.430400000
C	0.901432000	-0.191561000	-3.034682000
C	0.854957000	2.043639000	-2.294327000
C	-0.288522000	-2.301621000	-2.608548000
C	-1.520245000	-0.356399000	3.490661000
C	-1.573303000	2.353247000	2.601814000
C	-0.410907000	3.467455000	0.728838000
C	-0.410801000	3.467754000	-0.727350000
C	-2.718139000	-2.000446000	2.311806000
C	-1.437074000	-3.399871000	-0.732849000
C	-2.689685000	-2.815280000	1.177665000
C	-0.345697000	0.402137000	-3.483237000
C	-0.374509000	1.783905000	-3.028626000
C	-1.490129000	-1.737153000	-3.043917000
C	-2.768665000	0.238553000	3.036745000
C	-2.795567000	1.563237000	2.604651000

C	-1.592401000	3.210728000	1.425377000
C	-1.592190000	3.211315000	-1.424174000
C	-3.511157000	-0.780539000	2.307910000
C	-2.689512000	-2.814795000	-1.179091000
C	-3.461691000	-2.451374000	-0.000696000
C	-1.519730000	-0.354969000	-3.490902000
C	-1.572918000	2.354318000	-2.600959000
C	-2.717806000	-1.999502000	-2.312909000
C	-3.566419000	1.930226000	1.424968000
C	-2.823724000	2.946840000	0.699360000
C	-2.823622000	2.947127000	-0.698446000
C	-4.247579000	-0.430252000	1.177133000
C	-4.226193000	-1.284525000	-0.000512000
C	-2.768214000	0.239799000	-3.036925000
C	-2.795179000	1.564306000	-2.604297000
C	-3.510821000	-0.779595000	-2.308627000
C	-4.277654000	0.953854000	0.726514000
C	-3.566209000	1.930810000	-1.424581000
C	-4.247404000	-0.429770000	-1.177810000
C	-4.277542000	0.954149000	-0.726630000
C	4.611612000	-2.494519000	-0.000029000
H	4.593137000	-1.858247000	-2.201725000
H	4.593082000	-1.858296000	2.201680000
H	5.559183000	-3.060203000	0.000010000
H	3.796041000	-3.220965000	-0.000084000

Prod[5,6]

E=-2634.294613

G=-2633.822328

C	2.738389000	-0.980575000	-0.821330000
C	2.738397000	-0.980699000	0.821268000
C	1.713684000	-1.894826000	1.434312000

C	0.992391000	-2.838028000	0.722213000
C	0.992394000	-2.837899000	-0.722599000
C	1.713679000	-1.894573000	-1.434505000
C	2.394840000	0.466059000	-1.176028000
C	2.341974000	1.287479000	0.000123000
C	2.394805000	0.465873000	1.176182000
C	1.650742000	0.821057000	2.284946000
C	0.925621000	-1.512452000	2.608868000
C	-0.268995000	-3.125259000	1.435871000
C	-1.437377000	-3.372834000	0.736465000
C	-1.437353000	-3.372711000	-0.737013000
C	-0.268958000	-3.125024000	-1.436344000
C	-0.296755000	-2.295705000	-2.619308000
C	0.925703000	-1.512067000	-2.609051000
C	0.900897000	-0.198346000	-3.042581000
C	1.650820000	0.821439000	-2.284765000
C	1.602792000	2.488839000	0.000203000
C	0.844926000	2.868029000	-1.169592000
C	0.857048000	2.029642000	-2.286031000
C	-0.371057000	1.779346000	-3.026253000
C	-0.346049000	0.400962000	-3.486648000
C	-1.525352000	-0.349320000	-3.499580000
C	-1.499849000	-1.730588000	-3.054074000
C	-2.723689000	-1.987497000	-2.318461000
C	-2.692025000	-2.800149000	-1.180554000
C	-0.296828000	-2.296124000	2.618986000
C	-4.246810000	-0.416378000	1.178143000
C	-3.515662000	-0.767357000	2.311768000
C	-2.771109000	0.250331000	3.042102000
C	-2.792325000	1.573233000	2.607088000
C	-3.560210000	1.942341000	1.425117000
C	-4.273900000	0.967604000	-0.725835000

C	-4.246768000	-0.416186000	-1.178278000
C	-4.226242000	-1.270791000	-0.000133000
C	-3.462424000	-2.437051000	-0.000224000
C	-2.692054000	-2.800334000	1.180060000
C	-2.723754000	-1.987860000	2.318106000
C	-1.525453000	-0.349863000	3.499528000
C	-0.346160000	0.400432000	3.486707000
C	-0.371143000	1.778888000	3.026532000
C	-1.566308000	2.357728000	2.602588000
C	-1.583366000	3.216504000	1.425939000
C	-2.814069000	2.954848000	0.700417000
C	-2.814052000	2.954951000	-0.700008000
C	-3.560187000	1.942555000	-1.424887000
C	-3.515596000	-0.766993000	-2.311946000
C	-2.771048000	0.250802000	-3.042141000
C	-2.792272000	1.573637000	-2.606912000
C	-1.566228000	2.358117000	-2.602243000
C	-1.583325000	3.216724000	-1.425463000
C	-0.401950000	3.470463000	-0.728153000
C	-0.401970000	3.470338000	0.728701000
C	0.844885000	2.867840000	1.170068000
C	0.856970000	2.029286000	2.286357000
C	-1.499942000	-1.731068000	3.053788000
C	0.900818000	-0.198811000	3.042597000
C	-4.273901000	0.967488000	0.725897000
C	5.134528000	-0.294615000	0.703300000
C	4.467778000	-2.445126000	-0.000122000
C	4.230118000	-1.424365000	-1.137089000
C	5.134526000	-0.294541000	-0.703310000
H	4.347303000	-1.773499000	-2.163697000
H	5.487557000	-2.840511000	-0.000149000
C	4.230139000	-1.424500000	1.136966000

H	4.347313000	-1.773752000	2.163532000
C	5.802809000	0.690554000	1.415621000
H	5.787262000	0.705749000	2.502014000
C	5.802840000	0.690671000	-1.415530000
H	5.787410000	0.705902000	-2.501925000
C	6.504636000	1.669127000	-0.698455000
H	7.052148000	2.438641000	-1.235151000
C	6.504531000	1.669134000	0.698645000
H	7.051783000	2.438785000	1.235411000
H	3.752215000	-3.272164000	-0.000178000

TS[6,6]

E=-2634.264395

G=-2633.798611

C	5.320997000	-0.362890000	-0.726826000
C	5.321020000	-0.362888000	0.726811000
C	5.727951000	0.805013000	1.431222000
C	6.132088000	1.903226000	0.715465000
C	6.132066000	1.903229000	-0.715486000
C	5.727907000	0.805021000	-1.431239000
C	4.780180000	-1.567183000	-1.173259000
C	4.780203000	-1.567168000	1.173264000
H	5.714528000	0.817829000	2.517150000
H	6.452586000	2.800555000	1.236780000
H	6.452548000	2.800562000	-1.236805000
H	5.714465000	0.817847000	-2.517166000
C	2.491018000	-0.935911000	-0.715016000
C	2.491090000	-0.935649000	0.715009000
C	1.474822000	0.102587000	-2.591525000
C	2.200551000	1.538576000	-0.734459000
C	0.582683000	1.080961000	-3.035540000
C	1.082765000	-1.297215000	-2.591935000

C	1.262298000	2.551930000	-1.179509000
C	2.200628000	1.538851000	0.733542000
C	1.667590000	-1.925407000	-1.421779000
C	2.296804000	0.335893000	-1.421776000
C	0.471494000	2.333083000	-2.312116000
C	-0.747045000	0.695790000	-3.486439000
C	-0.188588000	-1.667569000	-3.033543000
C	0.681985000	3.178623000	-0.000689000
C	1.262426000	2.552379000	1.178308000
C	2.296973000	0.336431000	1.421313000
C	0.953629000	-2.899786000	-0.732121000
C	1.667734000	-1.924865000	1.422239000
C	-0.928532000	2.725557000	-2.308530000
C	-1.682236000	1.714641000	-3.036019000
C	-1.123943000	-0.646814000	-3.485571000
C	-0.936302000	-2.678807000	-2.309980000
C	-0.659683000	3.559765000	-0.000689000
C	0.471747000	2.333964000	2.311084000
C	1.475110000	0.103574000	2.591237000
C	0.953703000	-2.899507000	0.733033000
C	-0.375618000	-3.276898000	-1.177645000
C	1.083048000	-1.296228000	2.592224000
C	-1.482847000	3.327384000	-1.178294000
C	-2.956511000	1.347836000	-2.602632000
C	-2.452720000	-1.029667000	-3.035183000
C	-2.335744000	-2.284907000	-2.306901000
C	-1.482719000	3.327836000	1.177094000
C	0.583012000	1.082117000	3.034969000
C	-0.928280000	2.726444000	2.307500000
C	-0.375493000	-3.276447000	1.178846000
C	-1.196905000	-3.510046000	0.000690000
C	-0.188258000	-1.666411000	3.034113000

C	-2.811427000	2.946394000	-0.728463000
C	-3.533751000	1.977056000	-1.425356000
C	-3.350298000	-0.053212000	-2.602639000
C	-3.122934000	-2.510227000	-1.176999000
C	-2.811352000	2.946677000	0.727555000
C	-0.746666000	0.697119000	3.486162000
C	-1.681904000	1.715800000	3.035451000
C	-0.936052000	-2.677920000	2.311014000
C	-2.540924000	-3.136070000	0.000691000
C	-1.123565000	-0.645484000	3.485850000
C	-4.284477000	0.965468000	-0.697502000
C	-4.170361000	-0.289459000	-1.424753000
C	-4.059176000	-1.492835000	-0.727614000
C	-3.533598000	1.977601000	1.424895000
C	-2.956226000	1.348829000	2.602346000
C	-2.335493000	-2.284024000	2.307935000
C	-3.122806000	-2.509775000	1.178203000
C	-2.452392000	-1.028510000	3.035755000
C	-4.284398000	0.965735000	0.697507000
C	-4.059095000	-1.492555000	0.728532000
C	-3.350011000	-0.052217000	2.602930000
C	-4.170201000	-0.288914000	1.425223000
C	4.700223000	-2.503214000	0.000011000
H	4.711127000	-1.883845000	-2.206788000
H	4.711152000	-1.883817000	2.206797000
H	5.616771000	-3.121230000	0.000012000
H	3.855541000	-3.196164000	0.000027000

Prod[6,6]

E=-2634.326798

G=-2633.853285

C	-2.319876000	0.339270000	-1.439667000
---	--------------	-------------	--------------

C	-2.718104000	-0.990570000	-0.806230000
C	-2.718104000	-0.990619000	0.806208000
C	-2.319853000	0.339161000	1.439738000
C	-2.207060000	1.520512000	0.741305000
C	-2.207077000	1.520575000	-0.741143000
C	-1.479255000	0.110028000	-2.583372000
C	-1.084742000	-1.288498000	-2.582323000
C	-1.682361000	-1.923432000	-1.436801000
C	-0.965949000	-2.871626000	-0.741450000
C	-1.682342000	-1.923538000	1.436686000
C	-1.479216000	0.109835000	2.583416000
C	-0.588582000	1.087946000	3.038294000
C	-0.480869000	2.333737000	2.315461000
C	-1.270534000	2.535631000	1.177874000
C	-0.692506000	3.161688000	0.000133000
C	-1.270556000	2.535725000	-1.177648000
C	-0.480903000	2.333915000	-2.315258000
C	-0.588627000	1.088179000	-3.038188000
C	0.185810000	-1.656914000	-3.036597000
C	1.119493000	-0.635904000	-3.491224000
C	0.740983000	0.705312000	-3.491255000
C	1.673800000	1.725774000	-3.040503000
C	0.916512000	2.733327000	-2.311730000
C	1.468269000	3.332704000	-1.178365000
C	0.643870000	3.558870000	0.000140000
C	1.468285000	3.332613000	1.178616000
C	0.916547000	2.733151000	2.311943000
C	-1.084714000	-1.288694000	2.582251000
C	3.344145000	-0.040768000	2.605383000
C	2.448271000	-1.018325000	3.040614000
C	2.330040000	-2.273183000	2.311559000
C	3.114096000	-2.496140000	1.178453000

C	4.048847000	-1.480653000	0.728711000
C	4.272326000	0.977555000	0.697533000
C	3.521653000	1.988551000	1.426309000
C	2.948395000	1.360233000	2.605115000
C	1.673843000	1.725540000	3.040629000
C	0.741035000	0.705038000	3.491310000
C	1.119545000	-0.636177000	3.491171000
C	0.930122000	-2.662987000	2.314572000
C	0.363151000	-3.248582000	1.177571000
C	1.182623000	-3.480548000	-0.000137000
C	2.529409000	-3.119380000	-0.000134000
C	3.114077000	-2.496049000	-1.178680000
C	4.048835000	-1.480596000	-0.728873000
C	4.160903000	-0.276567000	-1.426049000
C	4.272315000	0.977607000	-0.697507000
C	2.795758000	2.955494000	0.728857000
C	2.795749000	2.955552000	-0.728656000
C	3.521633000	1.988660000	-1.426192000
C	2.948359000	1.360435000	-2.605039000
C	3.344105000	-0.040566000	-2.605421000
C	2.448227000	-1.018088000	-3.040719000
C	2.330008000	-2.273003000	-2.311759000
C	0.930089000	-2.662809000	-2.314785000
C	0.363138000	-3.248488000	-1.177818000
C	0.185852000	-1.657145000	3.036471000
C	-0.965944000	-2.871692000	0.741252000
C	4.160926000	-0.276677000	1.425980000
C	-5.104667000	-0.297856000	-0.702840000
C	-4.456101000	-2.454202000	-0.000026000
C	-4.204731000	-1.434763000	1.132580000
C	-5.104772000	-0.297953000	0.702831000
H	-4.313796000	-1.779264000	2.161883000

H	-5.480741000	-2.836002000	-0.000032000
C	-4.204717000	-1.434723000	-1.132610000
H	-4.313782000	-1.779179000	-2.161928000
C	-5.776953000	0.683750000	-1.415779000
H	-5.763543000	0.697821000	-2.502206000
C	-5.777080000	0.683623000	1.415789000
H	-5.763556000	0.697750000	2.502214000
C	-6.481623000	1.660025000	0.698497000
H	-7.031145000	2.428030000	1.235281000
C	-6.481728000	1.659967000	-0.698467000
H	-7.031665000	2.427686000	-1.235234000
H	-3.750772000	-3.290435000	-0.000017000

S=1

Pre-complex

E=-2634.227761

G=-2633.765911

C	-1.734716000	-0.919767000	-2.135087000
C	-2.373613000	-0.923791000	-0.830487000
C	-2.570843000	0.278285000	-0.151679000
C	-2.157640000	1.534892000	-0.750701000
C	-1.547316000	1.539680000	-2.004906000
C	-1.329929000	0.286485000	-2.711974000
C	-0.873498000	-2.090546000	-2.216085000
C	-0.983160000	-2.818906000	-0.960213000
C	-1.910703000	-2.098067000	-0.103351000
C	-1.677592000	-2.020123000	1.270501000
C	-2.332856000	0.358556000	1.277706000
C	-1.655299000	2.394744000	0.309983000
C	-0.556038000	3.220832000	0.075598000
C	0.085956000	3.222390000	-1.230822000

C	-0.399213000	2.400385000	-2.248607000
C	0.528600000	1.678162000	-3.105217000
C	-0.046304000	0.371593000	-3.389981000
C	0.779236000	-0.750990000	-3.468401000
C	0.356816000	-2.007327000	-2.868022000
C	0.141820000	-3.434968000	-0.409267000
C	1.424445000	-3.347169000	-1.090348000
C	1.529498000	-2.648777000	-2.293358000
C	2.676496000	-1.788264000	-2.538058000
C	2.212620000	-0.615349000	-3.264104000
C	2.764089000	0.637001000	-2.991091000
C	1.904012000	1.807685000	-2.909771000
C	2.410234000	2.664763000	-1.848351000
C	1.519977000	3.355669000	-1.026095000
C	-1.764205000	1.666332000	1.565766000
C	2.779048000	2.094181000	2.212358000
C	1.548650000	2.011741000	2.864278000
C	1.125059000	0.754933000	3.464231000
C	1.950747000	-0.367400000	3.387285000
C	3.232998000	-0.281116000	2.706025000
C	4.280420000	0.927223000	0.825797000
C	3.817349000	2.100156000	0.099747000
C	2.889192000	2.821457000	0.956944000
C	1.764840000	3.436718000	0.406037000
C	0.481914000	3.352198000	1.087003000
C	0.376837000	2.654236000	2.290717000
C	-0.308308000	0.620133000	3.263060000
C	-0.859795000	-0.632757000	2.988145000
C	0.001257000	-1.803322000	2.906325000
C	1.376714000	-1.672941000	3.101620000
C	2.304807000	-2.394514000	2.243909000
C	3.452272000	-1.533990000	1.999641000

C	4.067108000	-1.530245000	0.747613000
C	4.489924000	-0.274020000	0.148139000
C	3.582587000	2.022962000	-1.273148000
C	3.801203000	0.770009000	-1.979670000
C	4.245687000	-0.354425000	-1.283661000
C	3.671893000	-1.660534000	-1.569291000
C	3.561576000	-2.387459000	-0.313592000
C	2.462197000	-3.213001000	-0.079189000
C	1.819986000	-3.216217000	1.226659000
C	0.385966000	-3.352546000	1.021979000
C	-0.504772000	-2.660871000	1.844651000
C	-0.770722000	1.793730000	2.535727000
C	-1.899327000	-0.767241000	1.979116000
C	3.639225000	0.923690000	2.131402000
C	-5.545109000	-1.575771000	-1.164408000
C	-5.430702000	-1.576112000	1.179443000
H	-5.562806000	-1.887606000	-2.202110000
H	-5.338189000	-1.887902000	2.213020000
C	-5.439772000	-2.522696000	0.004879000
H	-6.273556000	-3.246931000	0.044052000
H	-4.524086000	-3.139528000	-0.038310000
C	-5.602170000	-0.231078000	-0.711058000
C	-5.522720000	-0.232938000	0.734258000
C	-5.655321000	0.974813000	-1.405322000
H	-5.699193000	0.986582000	-2.490508000
C	-5.492113000	0.975635000	1.430358000
C	-5.623891000	2.187430000	-0.679958000
H	-5.414128000	0.986405000	2.513398000
H	-5.655079000	3.129964000	-1.218190000
C	-5.545493000	2.187962000	0.707259000
H	-5.513671000	3.130487000	1.245349000

TS_{bir}[5,6]

E=-2634.226205

G=-2633.763378

C	-2.526624000	-0.256340000	0.528094000
C	-2.419097000	-0.981901000	-0.743037000
C	-1.708023000	-2.205652000	-0.754981000
C	-1.188004000	-2.767371000	0.475965000
C	-1.354532000	-2.092793000	1.689362000
C	-2.039945000	-0.803441000	1.709235000
C	-2.380807000	1.160231000	0.267953000
C	-2.116408000	1.330581000	-1.152807000
C	-2.104662000	0.017167000	-1.767988000
C	-1.202377000	-0.265763000	-2.789645000
C	-0.759657000	-2.492979000	-1.813971000
C	0.079890000	-3.419619000	0.177972000
C	1.127966000	-3.362684000	1.096416000
C	0.955890000	-2.654571000	2.356025000
C	-0.261912000	-2.029824000	2.640766000
C	-0.274321000	-0.708873000	3.255687000
C	-1.376414000	0.046342000	2.681852000
C	-1.233785000	1.414783000	2.433191000
C	-1.749900000	1.985056000	1.203103000
C	-1.227610000	2.317305000	-1.586815000
C	-0.560452000	3.169658000	-0.611339000
C	-0.814472000	3.005896000	0.750319000
C	0.279560000	3.066260000	1.706924000
C	0.020922000	2.080605000	2.746332000
C	1.078063000	1.355871000	3.297757000
C	0.927430000	-0.068780000	3.558415000
C	2.193776000	-0.718242000	3.259543000
C	2.205830000	-1.983648000	2.668228000
C	0.345092000	-3.249558000	-1.240832000

C	4.313844000	-1.129057000	-0.246154000
C	3.674327000	-1.946077000	-1.178356000
C	3.155838000	-1.375345000	-2.412273000
C	3.300253000	-0.009484000	-2.663230000
C	3.966336000	0.841684000	-1.690520000
C	4.291487000	1.004177000	0.750553000
C	4.034487000	0.019998000	1.789687000
C	4.047757000	-1.298621000	1.174124000
C	3.153649000	-2.278531000	1.604297000
C	2.487673000	-3.132097000	0.632114000
C	2.742017000	-2.968878000	-0.729441000
C	1.905148000	-2.044924000	-2.726683000
C	0.844221000	-1.321304000	-3.277532000
C	0.994853000	0.103995000	-3.537160000
C	2.196967000	0.744637000	-3.237407000
C	2.183972000	2.063931000	-2.621582000
C	3.278156000	2.124156000	-1.666601000
C	3.114014000	2.804546000	-0.459284000
C	3.631712000	2.233818000	0.774289000
C	3.126067000	0.303036000	2.810010000
C	2.437070000	1.585448000	2.835118000
C	2.685343000	2.530132000	1.838446000
C	1.583793000	3.285675000	1.262467000
C	1.849037000	3.455613000	-0.157829000
C	0.798850000	3.399230000	-1.074880000
C	0.970006000	2.689015000	-2.334257000
C	-0.283568000	2.021702000	-2.648362000
C	-0.270955000	0.754242000	-3.238394000
C	1.648065000	-3.028906000	-1.686801000
C	-0.512441000	-1.552702000	-2.817218000
C	4.463318000	0.294627000	-0.507699000
C	-5.317547000	-0.224953000	-0.749162000

C	-4.995909000	-2.536189000	-0.174065000
C	-5.546691000	-1.753069000	0.988804000
C	-5.748954000	-0.401895000	0.616336000
H	-5.769575000	-2.178327000	1.959916000
H	-5.711664000	-3.295886000	-0.539022000
C	-4.759360000	-1.460542000	-1.209523000
H	-4.514313000	-1.674166000	-2.242325000
C	-5.409229000	1.021111000	-1.361135000
H	-5.072503000	1.160576000	-2.383818000
C	-6.256497000	0.690708000	1.329730000
H	-6.580163000	0.574008000	2.359865000
C	-6.344778000	1.939120000	0.692900000
H	-6.738073000	2.789834000	1.241694000
C	-5.934995000	2.104653000	-0.629607000
H	-6.009391000	3.080563000	-1.099270000
H	-4.080828000	-3.098983000	0.070295000

Print[5,6]

E=-2634.258969

G=-2633.794332

C	-2.476829000	-0.546401000	0.736558000
C	-2.695140000	-0.833660000	-0.764176000
C	-1.743511000	-1.922524000	-1.227474000
C	-1.096643000	-2.822079000	-0.318974000
C	-1.151965000	-2.620295000	1.066097000
C	-1.848995000	-1.432288000	1.591088000
C	-2.326317000	0.864946000	0.951601000
C	-2.198729000	1.519143000	-0.341878000
C	-2.270010000	0.518770000	-1.368824000
C	-1.465223000	0.631023000	-2.485097000
C	-0.906407000	-1.780207000	-2.381645000
C	0.142420000	-3.294678000	-0.931482000

C	1.272906000	-3.515761000	-0.149419000
C	1.218877000	-3.285518000	1.285959000
C	0.025739000	-2.839659000	1.872449000
C	0.068410000	-1.807706000	2.899546000
C	-1.088176000	-0.944787000	2.723125000
C	-0.980191000	0.428452000	2.961864000
C	-1.614948000	1.356999000	2.054468000
C	-1.375306000	2.642790000	-0.483988000
C	-0.622008000	3.137411000	0.658771000
C	-0.738492000	2.508847000	1.898192000
C	0.444215000	2.284943000	2.713937000
C	0.295415000	0.994378000	3.370476000
C	1.406179000	0.165874000	3.535504000
C	1.289058000	-1.266902000	3.299895000
C	2.524587000	-1.725829000	2.683736000
C	2.486117000	-2.713580000	1.695401000
C	0.261941000	-2.643524000	-2.219114000
C	4.288756000	-0.831014000	-0.926611000
C	3.566999000	-1.306729000	-2.020373000
C	2.919479000	-0.370100000	-2.929131000
C	3.030099000	1.005072000	-2.705808000
C	3.783887000	1.498495000	-1.567059000
C	4.349412000	0.830227000	0.739771000
C	4.205040000	-0.458204000	1.396335000
C	4.167214000	-1.486702000	0.367144000
C	3.329841000	-2.591314000	0.513871000
C	2.578887000	-3.089753000	-0.628171000
C	2.694501000	-2.460773000	-1.868363000
C	1.651883000	-0.942557000	-3.337902000
C	0.528809000	-0.119029000	-3.498934000
C	0.646411000	1.313570000	-3.261363000
C	1.868757000	1.864194000	-2.879360000

C	1.911335000	2.895028000	-1.851041000
C	3.092736000	2.667074000	-1.039214000
C	3.048999000	2.889865000	0.338560000
C	3.689114000	1.952300000	1.246682000
C	3.399839000	-0.577264000	2.529731000
C	2.709183000	0.591888000	3.058225000
C	2.852923000	1.830797000	2.429551000
C	1.696827000	2.694743000	2.254620000
C	1.818061000	3.349927000	0.960658000
C	0.681887000	3.568785000	0.180693000
C	0.729528000	3.338893000	-1.255981000
C	-0.545244000	2.769433000	-1.660866000
C	-0.584098000	1.771831000	-2.639163000
C	1.509524000	-2.232774000	-2.681323000
C	-0.769759000	-0.547244000	-3.032932000
C	4.401599000	0.601498000	-0.694617000
C	-5.148524000	-0.111241000	-0.660557000
C	-4.663166000	-2.446515000	-0.291167000
C	-5.527097000	-1.874157000	0.797399000
C	-5.842342000	-0.531848000	0.514455000
H	-5.910241000	-2.447988000	1.633215000
H	-5.245249000	-3.121329000	-0.938509000
C	-4.196425000	-1.202027000	-1.103135000
H	-4.230142000	-1.376383000	-2.183084000
C	-5.350907000	1.150750000	-1.188993000
H	-4.830332000	1.465049000	-2.088831000
C	-6.707161000	0.373608000	1.172814000
H	-7.232234000	0.070899000	2.074285000
C	-6.887249000	1.643380000	0.638054000
H	-7.555368000	2.343532000	1.132042000
C	-6.229257000	2.033484000	-0.538543000
H	-6.393273000	3.026823000	-0.944974000

H -3.826826000 -3.043235000 0.088550000

TS_{bir}[6,6]

E=-2634.224571

G=-2633.762188

C -2.087047000 -0.092767000 -1.809400000

C -2.452230000 -0.961017000 -0.684203000

C -2.515684000 -0.379784000 0.606095000

C -2.347450000 1.043467000 0.788807000

C -2.065105000 1.868665000 -0.303126000

C -1.927101000 1.278165000 -1.632912000

C -1.189102000 -0.821437000 -2.684287000

C -0.939594000 -2.125131000 -2.088484000

C -1.686543000 -2.201369000 -0.845659000

C -1.133518000 -2.848992000 0.257143000

C -1.941693000 -1.053436000 1.749819000

C -1.667123000 1.260370000 2.059596000

C -0.721723000 2.278347000 2.179545000

C -0.419456000 3.130636000 1.039788000

C -1.077321000 2.921996000 -0.177046000

C -0.331061000 2.993119000 -1.426236000

C -0.857867000 1.977772000 -2.325119000

C 0.004217000 1.279380000 -3.174029000

C -0.165518000 -0.151208000 -3.357817000

C 0.326139000 -2.706265000 -2.186133000

C 1.395382000 -2.003991000 -2.880658000

C 1.155018000 -0.754895000 -3.453295000

C 2.142493000 0.306113000 -3.327587000

C 1.430523000 1.563398000 -3.153694000

C 1.935679000 2.535477000 -2.289571000

C 1.036388000 3.266427000 -1.408730000

C 1.720409000 3.480584000 -0.142588000

C	1.005934000	3.409781000	1.054992000
C	-1.416145000	-0.040518000	2.656669000
C	3.103202000	0.854734000	2.710873000
C	2.078498000	0.183436000	3.377321000
C	1.905511000	-1.250055000	3.191050000
C	2.767682000	-1.951399000	2.346521000
C	3.835876000	-1.250611000	1.652605000
C	4.305300000	0.973191000	0.690368000
C	3.596164000	2.230649000	0.865139000
C	2.851979000	2.157424000	2.113622000
C	1.586218000	2.735044000	2.207416000
C	0.517341000	2.035315000	2.903170000
C	0.758359000	0.786200000	3.476095000
C	0.480207000	-1.533042000	3.175653000
C	-0.029051000	-2.505477000	2.309719000
C	0.870346000	-3.236071000	1.428259000
C	2.238468000	-2.965566000	1.447156000
C	2.983091000	-2.893702000	0.198701000
C	3.970168000	-1.833887000	0.325613000
C	4.263170000	-1.017917000	-0.767851000
C	4.434926000	0.414270000	-0.582284000
C	3.039649000	2.877145000	-0.238987000
C	3.173134000	2.293868000	-1.566041000
C	3.856786000	1.089060000	-1.733633000
C	3.329960000	0.074067000	-2.633069000
C	3.580299000	-1.228761000	-2.035203000
C	2.633795000	-2.246093000	-2.156974000
C	2.328806000	-3.097602000	-1.016786000
C	0.902714000	-3.382049000	-1.036464000
C	0.187577000	-3.448517000	0.161300000
C	-0.229184000	-0.275188000	3.350321000
C	-1.265352000	-2.265510000	1.589747000

C	4.001351000	0.123025000	1.830487000
C	-4.756325000	-1.494479000	-1.184433000
C	-5.604163000	-1.725032000	1.001622000
H	-4.507087000	-1.734526000	-2.210751000
H	-5.863340000	-2.127604000	1.973454000
C	-5.039732000	-2.544122000	-0.131929000
H	-5.756622000	-3.301380000	-0.499219000
H	-4.141298000	-3.113605000	0.153515000
C	-5.284371000	-0.231151000	-0.751196000
C	-5.733026000	-0.372118000	0.611664000
C	-5.320644000	1.005991000	-1.381824000
H	-4.973358000	1.116107000	-2.404226000
C	-6.185612000	0.756459000	1.311110000
C	-5.786217000	2.126003000	-0.663450000
H	-6.518385000	0.668374000	2.341245000
H	-5.809623000	3.098314000	-1.145757000
C	-6.204491000	1.999170000	0.661370000
H	-6.550152000	2.876803000	1.199795000

Print[6,6]

E=-2634.259110

G=-2633.794527

C	-2.167935000	0.318372000	-1.657923000
C	-2.688735000	-0.857216000	-0.805243000
C	-2.490969000	-0.549647000	0.668791000
C	-2.296544000	0.779689000	1.162557000
C	-2.072054000	1.853582000	0.292421000
C	-1.984080000	1.591881000	-1.155273000
C	-1.292592000	-0.165315000	-2.687667000
C	-1.011591000	-1.571181000	-2.433894000
C	-1.712600000	-1.968881000	-1.245590000
C	-1.101141000	-2.832119000	-0.356125000

C	-1.846150000	-1.458235000	1.567809000
C	-1.558086000	0.704964000	2.421987000
C	-0.614921000	1.677346000	2.743475000
C	-0.367952000	2.780315000	1.826983000
C	-1.082696000	2.852852000	0.622624000
C	-0.390288000	3.228587000	-0.603056000
C	-0.951033000	2.450980000	-1.695515000
C	-0.127223000	1.998468000	-2.730109000
C	-0.301914000	0.657931000	-3.240321000
C	0.249924000	-2.098814000	-2.740929000
C	1.283321000	-1.235361000	-3.293253000
C	1.013638000	0.110828000	-3.536711000
C	2.003851000	1.123235000	-3.205513000
C	1.296539000	2.291817000	-2.703580000
C	1.835380000	3.033313000	-1.651464000
C	0.973155000	3.516639000	-0.580865000
C	1.713264000	3.432286000	0.668705000
C	1.052720000	3.066836000	1.845370000
C	-1.277307000	-0.692898000	2.675508000
C	3.230732000	0.217866000	2.745668000
C	2.240280000	-0.606966000	3.276340000
C	2.058585000	-1.955383000	2.754993000
C	2.884830000	-2.422185000	1.728905000
C	3.917446000	-1.561710000	1.179109000
C	4.336947000	0.833330000	0.761109000
C	3.634152000	2.001962000	1.263821000
C	2.948922000	1.622712000	2.490712000
C	1.688771000	2.145034000	2.777382000
C	0.655933000	1.285507000	3.334177000
C	0.926211000	-0.061523000	3.578422000
C	0.638254000	-2.243022000	2.735721000
C	0.086188000	-2.980741000	1.678870000

C	0.948714000	-3.462166000	0.608295000
C	2.316269000	-3.193901000	0.634526000
C	3.006642000	-2.816656000	-0.591485000
C	3.993937000	-1.806885000	-0.255108000
C	4.237687000	-0.747934000	-1.132001000
C	4.412636000	0.599005000	-0.614206000
C	3.026583000	2.887600000	0.372988000
C	3.102690000	2.642797000	-1.061418000
C	3.783579000	1.522920000	-1.543885000
C	3.221977000	0.747530000	-2.637941000
C	3.503209000	-0.657637000	-2.383368000
C	2.554815000	-1.628869000	-2.707231000
C	2.302489000	-2.733686000	-1.793509000
C	0.877305000	-3.020482000	-1.821284000
C	0.213176000	-3.370760000	-0.642114000
C	-0.063484000	-1.073135000	3.241072000
C	-1.179039000	-2.596935000	1.097811000
C	4.088979000	-0.268980000	1.675346000
C	-4.191245000	-1.214986000	-1.131025000
C	-5.545603000	-1.875603000	0.762044000
H	-4.242413000	-1.390107000	-2.210457000
H	-5.950004000	-2.449601000	1.587696000
C	-4.671526000	-2.453191000	-0.315504000
H	-5.243444000	-3.133855000	-0.965337000
H	-3.838944000	-3.046615000	0.078626000
C	-5.114695000	-0.104013000	-0.673298000
C	-5.819337000	-0.521891000	0.497388000
C	-5.281284000	1.170922000	-1.181531000
H	-4.757773000	1.483974000	-2.079112000
C	-6.653594000	0.399978000	1.173261000
C	-6.126305000	2.071509000	-0.510669000
H	-7.185267000	0.098803000	2.071397000

H	-6.259784000	3.076005000	-0.900610000
C	-6.792435000	1.684229000	0.662205000
H	-7.434588000	2.397889000	1.171062000

TS[5,6]

E=-2634.248222

G=-2633.781759

C	-2.537504000	-0.928185000	0.764168000
C	-2.698578000	-0.975411000	-0.790754000
C	-1.689911000	-1.905735000	-1.432489000
C	-0.937390000	-2.886512000	-0.687952000
C	-0.944502000	-2.884570000	0.707785000
C	-1.704153000	-1.858702000	1.432087000
C	-2.379583000	0.472199000	1.161419000
C	-2.346483000	1.312008000	-0.016113000
C	-2.384339000	0.477147000	-1.181426000
C	-1.646390000	0.819532000	-2.296393000
C	-0.919336000	-1.533194000	-2.571499000
C	0.298510000	-3.167087000	-1.402877000
C	1.479888000	-3.418463000	-0.701904000
C	1.472140000	-3.408158000	0.749926000
C	0.277636000	-3.145278000	1.435563000
C	0.288275000	-2.276391000	2.600474000
C	-0.937834000	-1.488420000	2.587584000
C	-0.919165000	-0.160190000	3.041767000
C	-1.655927000	0.843708000	2.294412000
C	-1.616506000	2.512794000	-0.015867000
C	-0.854712000	2.887373000	1.159818000
C	-0.871813000	2.068352000	2.289903000
C	0.355202000	1.815038000	3.025144000
C	0.324800000	0.431676000	3.484082000
C	1.503866000	-0.323228000	3.490653000

C	1.480595000	-1.709571000	3.043336000
C	2.718935000	-1.976132000	2.326374000
C	2.711816000	-2.806852000	1.202707000
C	0.315171000	-2.317667000	-2.576174000
C	4.254085000	-0.417449000	-1.158804000
C	3.520321000	-0.779391000	-2.287500000
C	2.769093000	0.230293000	-3.022770000
C	2.793259000	1.563274000	-2.597256000
C	3.558200000	1.937098000	-1.423569000
C	4.267846000	0.976617000	0.736271000
C	4.244521000	-0.402857000	1.194330000
C	4.238403000	-1.267105000	0.022966000
C	3.491379000	-2.443986000	0.026894000
C	2.726781000	-2.823094000	-1.152121000
C	2.741820000	-2.007465000	-2.285087000
C	1.530833000	-0.368598000	-3.471313000
C	0.345363000	0.382782000	-3.473080000
C	0.373180000	1.771156000	-3.026912000
C	1.568974000	2.348921000	-2.603467000
C	1.582173000	3.216747000	-1.433463000
C	2.809772000	2.959242000	-0.702738000
C	2.807405000	2.968745000	0.693308000
C	3.549298000	1.955610000	1.428926000
C	3.499554000	-0.751617000	2.320913000
C	2.746744000	0.267975000	3.041140000
C	2.776707000	1.596461000	2.603612000
C	1.554919000	2.383717000	2.596407000
C	1.574739000	3.235218000	1.415109000
C	0.394671000	3.485048000	0.714004000
C	0.398147000	3.476643000	-0.741522000
C	-0.849207000	2.876511000	-1.186950000
C	-0.857456000	2.037094000	-2.303401000

C	1.508462000	-1.751004000	-3.013074000
C	-0.896682000	-0.205077000	-3.037410000
C	4.273470000	0.968595000	-0.715636000
C	-5.114428000	-0.286094000	-0.714888000
C	-4.516783000	-2.497763000	-0.092038000
C	-4.672900000	-1.612702000	1.123058000
C	-5.318999000	-0.405411000	0.685026000
H	-4.684225000	-1.978067000	2.143636000
H	-5.461885000	-3.003892000	-0.336119000
C	-4.194122000	-1.405043000	-1.136971000
H	-4.267679000	-1.701132000	-2.185049000
C	-5.606785000	0.802968000	-1.415823000
H	-5.433449000	0.903712000	-2.483562000
C	-5.992447000	0.604522000	1.387500000
H	-6.131888000	0.534302000	2.462364000
C	-6.498036000	1.688599000	0.672111000
H	-7.041050000	2.470148000	1.195705000
C	-6.318595000	1.785907000	-0.714664000
H	-6.722001000	2.641058000	-1.248682000
H	-3.736137000	-3.257131000	0.002465000

Prod[5,6]

E=-2634.275165

G=-2633.805611

C	2.718550000	-0.984584000	-0.810352000
C	2.718589000	-0.984536000	0.810298000
C	1.689514000	-1.891438000	1.435710000
C	0.926594000	-2.877390000	0.697936000
C	0.926588000	-2.877575000	-0.697717000
C	1.689460000	-1.891600000	-1.435575000
C	2.393829000	0.465828000	-1.171168000
C	2.348120000	1.291178000	-0.000101000

C	2.393884000	0.466008000	1.171044000
C	1.663291000	0.826724000	2.288223000
C	0.926929000	-1.517432000	2.572993000
C	-0.302910000	-3.154901000	1.418650000
C	-1.491999000	-3.408625000	0.726209000
C	-1.492033000	-3.408765000	-0.725782000
C	-0.302966000	-3.154966000	-1.418236000
C	-0.312096000	-2.296809000	-2.584734000
C	0.926850000	-1.517751000	-2.572787000
C	0.912988000	-0.186714000	-3.040259000
C	1.663227000	0.826517000	-2.288283000
C	1.628406000	2.504123000	-0.000202000
C	0.871406000	2.881599000	-1.171359000
C	0.880056000	2.046870000	-2.290819000
C	-0.348695000	1.792697000	-3.021543000
C	-0.324430000	0.405991000	-3.474900000
C	-1.514599000	-0.341025000	-3.479393000
C	-1.500225000	-1.726292000	-3.027037000
C	-2.738180000	-1.982187000	-2.305969000
C	-2.732122000	-2.806254000	-1.177533000
C	-0.312033000	-2.296576000	2.585067000
C	-4.246220000	-0.391565000	1.176293000
C	-3.509012000	-0.750850000	2.303594000
C	-2.749089000	0.260239000	3.030658000
C	-2.770296000	1.592475000	2.598623000
C	-3.535930000	1.962146000	1.426029000
C	-4.258883000	0.991162000	-0.724804000
C	-4.246258000	-0.391714000	-1.176221000
C	-4.241451000	-1.249442000	0.000094000
C	-3.502343000	-2.430988000	0.000164000
C	-2.732096000	-2.806092000	1.177882000
C	-2.738118000	-1.981886000	2.306224000

C	-1.514548000	-0.340583000	3.479487000
C	-0.324405000	0.406413000	3.474822000
C	-0.348664000	1.793047000	3.021356000
C	-1.542992000	2.373505000	2.598255000
C	-1.556668000	3.236186000	1.424044000
C	-2.786801000	2.977542000	0.698099000
C	-2.786807000	2.977446000	-0.698431000
C	-3.535930000	1.961980000	-1.426238000
C	-3.509068000	-0.751145000	-2.303465000
C	-2.749103000	0.259848000	-3.030598000
C	-2.770288000	1.592132000	-2.598727000
C	-1.543016000	2.373199000	-2.598513000
C	-1.556688000	3.235991000	-1.424397000
C	-0.374018000	3.488213000	-0.728073000
C	-0.373995000	3.488308000	0.727691000
C	0.871446000	2.881737000	1.171037000
C	0.880085000	2.047110000	2.290542000
C	-1.500169000	-1.725945000	3.027225000
C	0.913100000	-0.186367000	3.040367000
C	-4.258874000	0.991256000	0.724712000
C	5.122471000	-0.325268000	0.702950000
C	4.434797000	-2.469847000	0.000005000
C	4.204572000	-1.445786000	-1.137577000
C	5.122421000	-0.325222000	-0.703008000
H	4.314443000	-1.794882000	-2.165013000
H	5.450089000	-2.876299000	-0.000085000
C	4.204695000	-1.445776000	1.137573000
H	4.314429000	-1.794829000	2.165033000
C	5.805022000	0.649337000	1.415685000
H	5.791055000	0.663771000	2.502073000
C	5.804886000	0.649454000	-1.415716000
H	5.790818000	0.664014000	-2.502102000

C	6.518999000	1.619325000	-0.698429000
H	7.075909000	2.381830000	-1.235393000
C	6.519112000	1.619234000	0.698415000
H	7.076207000	2.381601000	1.235383000
H	3.711840000	-3.290769000	0.000049000

TS[6,6]

E=-2634.23249

G=-2633.76802

C	-2.288583000	0.302623000	-1.484996000
C	-2.681621000	-1.002287000	-0.787288000
C	-2.527653000	-0.911215000	0.738352000
C	-2.335439000	0.395797000	1.380945000
C	-2.219669000	1.565785000	0.643622000
C	-2.193699000	1.513849000	-0.831104000
C	-1.435139000	0.022530000	-2.599132000
C	-1.048889000	-1.383346000	-2.543427000
C	-1.657266000	-1.977990000	-1.405812000
C	-0.938736000	-2.912424000	-0.648667000
C	-1.707830000	-1.840787000	1.458224000
C	-1.526557000	0.212859000	2.567762000
C	-0.639864000	1.204649000	2.987455000
C	-0.517284000	2.426192000	2.214814000
C	-1.292710000	2.600809000	1.063112000
C	-0.696323000	3.183691000	-0.127534000
C	-1.252650000	2.515768000	-1.289273000
C	-0.442843000	2.259719000	-2.403692000
C	-0.539022000	0.986511000	-3.076820000
C	0.241325000	-1.767409000	-2.977115000
C	1.171480000	-0.765462000	-3.434306000
C	0.798373000	0.587076000	-3.493778000
C	1.723136000	1.615381000	-3.075363000

C	0.956900000	2.651748000	-2.390758000
C	1.490876000	3.290587000	-1.273120000
C	0.647641000	3.567404000	-0.119087000
C	1.450875000	3.375760000	1.074838000
C	0.882455000	2.817758000	2.220205000
C	-1.131710000	-1.184433000	2.605892000
C	3.297150000	0.048912000	2.640353000
C	2.395665000	-0.913854000	3.087096000
C	2.297802000	-2.194935000	2.405942000
C	3.117579000	-2.467301000	1.297129000
C	4.052614000	-1.459742000	0.832973000
C	4.262605000	0.996528000	0.721215000
C	3.498470000	2.031804000	1.403271000
C	2.908131000	1.450399000	2.591775000
C	1.622823000	1.835377000	3.000346000
C	0.683815000	0.840913000	3.468187000
C	1.055246000	-0.514428000	3.505981000
C	0.905983000	-2.576013000	2.385967000
C	0.364197000	-3.217296000	1.271256000
C	1.210248000	-3.505657000	0.125531000
C	2.560570000	-3.134491000	0.137876000
C	3.155617000	-2.546611000	-1.051393000
C	4.078714000	-1.508003000	-0.623599000
C	4.196324000	-0.329272000	-1.359433000
C	4.290493000	0.952179000	-0.674891000
C	2.791710000	2.980011000	0.656156000
C	2.815186000	2.930841000	-0.788957000
C	3.552945000	1.932671000	-1.448878000
C	2.996546000	1.267297000	-2.606961000
C	3.390122000	-0.134484000	-2.553597000
C	2.502695000	-1.128492000	-2.963164000
C	2.383719000	-2.358940000	-2.199488000

C	0.980820000	-2.748316000	-2.206469000
C	0.408911000	-3.303409000	-1.064273000
C	0.134983000	-1.536177000	3.083212000
C	-0.962046000	-2.870170000	0.788300000
C	4.145488000	-0.230076000	1.487667000
C	-5.096618000	-0.299608000	-0.719767000
C	-4.513469000	-2.502209000	-0.062427000
C	-4.674553000	-1.600137000	1.135429000
C	-5.312537000	-0.400668000	0.681667000
H	-4.660203000	-1.940655000	2.164356000
H	-5.464573000	-2.997674000	-0.305949000
C	-4.181323000	-1.428349000	-1.122806000
H	-4.253658000	-1.739294000	-2.166688000
C	-5.581874000	0.782526000	-1.434973000
H	-5.400573000	0.873738000	-2.501986000
C	-5.994611000	0.616185000	1.369222000
H	-6.142690000	0.556262000	2.443410000
C	-6.494873000	1.689683000	0.637911000
H	-7.044618000	2.476295000	1.146395000
C	-6.300353000	1.771817000	-0.749216000
H	-6.697949000	2.621833000	-1.295519000
H	-3.742664000	-3.268380000	0.047281000

Prod[6,6]

E=-2634.265379

G=-2633.798116

C	-2.319014000	-0.497643000	1.399205000
C	-2.736785000	0.884960000	0.911559000
C	-2.755083000	1.053853000	-0.693512000
C	-2.352009000	-0.198653000	-1.466927000
C	-2.220170000	-1.444400000	-0.889243000
C	-2.200092000	-1.592878000	0.579481000

C	-1.461691000	-0.375522000	2.552379000
C	-1.084247000	0.997468000	2.692363000
C	-1.698575000	1.750336000	1.624509000
C	-0.997245000	2.766560000	1.024196000
C	-1.729781000	2.052738000	-1.233597000
C	-1.523231000	0.156323000	-2.584352000
C	-0.619049000	-0.769030000	-3.138299000
C	-0.487577000	-2.065969000	-2.536749000
C	-1.266770000	-2.397196000	-1.425404000
C	-0.676713000	-3.134948000	-0.321592000
C	-1.234585000	-2.640551000	0.896872000
C	-0.432151000	-2.542421000	2.055907000
C	-0.547168000	-1.403565000	2.898297000
C	0.205853000	1.333083000	3.175758000
C	1.157005000	0.272780000	3.518222000
C	0.790646000	-1.058398000	3.383477000
C	1.731496000	-2.024105000	2.840779000
C	0.978240000	-2.940225000	2.008850000
C	1.522529000	-3.419841000	0.819868000
C	0.694091000	-3.525589000	-0.372992000
C	1.493190000	-3.173548000	-1.504791000
C	0.928164000	-2.449256000	-2.576925000
C	-1.140732000	1.544765000	-2.441867000
C	3.334996000	0.317557000	-2.594598000
C	2.413952000	1.345550000	-2.919721000
C	2.289754000	2.491412000	-2.073729000
C	3.087342000	2.612325000	-0.914909000
C	4.049574000	1.562630000	-0.583679000
C	4.303740000	-0.876385000	-0.807437000
C	3.546709000	-1.805523000	-1.631075000
C	2.957477000	-1.054212000	-2.734819000
C	1.660754000	-1.390188000	-3.198436000

C	0.711661000	-0.330880000	-3.536790000
C	1.078284000	1.000380000	-3.401750000
C	0.876195000	2.880366000	-2.033112000
C	0.317685000	3.346449000	-0.840295000
C	1.141450000	3.459821000	0.350368000
C	2.521742000	3.103351000	0.302349000
C	3.118272000	2.369018000	1.409573000
C	4.070065000	1.416363000	0.861690000
C	4.201140000	0.149082000	1.435974000
C	4.318924000	-1.021999000	0.580139000
C	2.836205000	-2.841154000	-1.032946000
C	2.852509000	-2.998812000	0.411700000
C	3.578861000	-2.107785000	1.205816000
C	3.011380000	-1.607553000	2.445901000
C	3.395022000	-0.216163000	2.587835000
C	2.484310000	0.709591000	3.118014000
C	2.344802000	2.018252000	2.513304000
C	0.927305000	2.390997000	2.558145000
C	0.347663000	3.099598000	1.482309000
C	0.134941000	1.968841000	-2.858853000
C	-1.013018000	2.927044000	-0.443840000
C	4.165893000	0.443586000	-1.401623000
C	-5.120811000	0.192338000	0.762582000
C	-4.489771000	2.414292000	0.283361000
C	-4.246528000	1.521053000	-0.952736000
C	-5.137238000	0.340594000	-0.635139000
H	-4.369288000	1.971642000	-1.938512000
H	-5.516086000	2.788143000	0.334948000
C	-4.221254000	1.282936000	1.299588000
H	-4.320105000	1.516663000	2.360634000
C	-5.781102000	-0.862003000	1.375979000
H	-5.755147000	-0.989845000	2.454760000

C	-5.814602000	-0.563449000	-1.439773000
H	-5.814123000	-0.462955000	-2.521677000
C	-6.506920000	-1.613375000	-0.821197000
H	-7.060503000	-2.322986000	-1.429405000
C	-6.490189000	-1.760854000	0.567734000
H	-7.031234000	-2.583429000	1.026656000
H	-3.787826000	3.249448000	0.364338000

S=0 OS

$^{10}\text{S}_{60}$

E=-2286.490269

G=-2286.156410

C	0.604226000	2.679813000	2.225513000
C	1.850038000	2.650138000	1.458005000
C	1.851802000	3.021914000	0.119408000
C	0.607306000	3.442766000	-0.525449000
C	-0.595192000	3.477763000	0.223938000
C	-0.596847000	3.096748000	1.599042000
C	0.601782000	1.563156000	3.113620000
C	1.846416000	0.819092000	2.914911000
C	2.624589000	1.502134000	1.895920000
C	3.367213000	0.763533000	0.969255000
C	2.628114000	2.263177000	-0.846089000
C	0.607464000	2.943933000	-1.862169000
C	-0.595211000	2.478200000	-2.449962000
C	-1.841213000	2.520155000	-1.683187000
C	-1.841535000	3.007197000	-0.381803000
C	-2.619601000	2.336991000	0.645745000
C	-1.843774000	2.381092000	1.873088000
C	-1.846285000	1.293699000	2.737903000
C	-0.601786000	0.862153000	3.375942000
C	1.844052000	-0.568933000	2.975394000

C	0.596861000	-1.288633000	3.237881000
C	-0.604325000	-0.563364000	3.437889000
C	-1.850266000	-1.044353000	2.839290000
C	-2.624611000	0.109822000	2.416826000
C	-3.367499000	0.059701000	1.233109000
C	-3.364928000	1.197037000	0.328556000
C	-3.364982000	0.688234000	-1.032685000
C	-2.619469000	1.340744000	-2.019706000
C	1.851978000	2.202991000	-2.072545000
C	-0.601782000	-1.563156000	-3.113620000
C	0.601786000	-0.862153000	-3.375942000
C	1.846285000	-1.293699000	-2.737903000
C	1.843774000	-2.381092000	-1.873088000
C	0.596847000	-3.096748000	-1.599042000
C	-1.850038000	-2.650138000	-1.458005000
C	-2.624589000	-1.502134000	-1.895920000
C	-1.846416000	-0.819092000	-2.914911000
C	-1.844052000	0.568933000	-2.975394000
C	-0.596861000	1.288633000	-3.237881000
C	0.604325000	0.563364000	-3.437889000
C	2.624611000	-0.109822000	-2.416826000
C	3.367499000	-0.059701000	-1.233109000
C	3.364928000	-1.197037000	-0.328556000
C	2.619601000	-2.336991000	-0.645745000
C	1.841535000	-3.007197000	0.381803000
C	0.595192000	-3.477763000	-0.223938000
C	-0.607306000	-3.442766000	0.525449000
C	-1.851802000	-3.021914000	-0.119408000
C	-3.367213000	-0.763533000	-0.969255000
C	-3.368969000	-1.152045000	0.430914000
C	-2.628114000	-2.263177000	0.846089000
C	-1.851978000	-2.202991000	2.072545000

C	-0.607464000	-2.943933000	1.862169000
C	0.595211000	-2.478200000	2.449962000
C	1.841213000	-2.520155000	1.683187000
C	2.619469000	-1.340744000	2.019706000
C	3.364982000	-0.688234000	1.032685000
C	1.850266000	1.044353000	-2.839290000
C	3.368969000	1.152045000	-0.430914000
C	-0.604226000	-2.679813000	-2.225513000

Pre-complex

E=-2634.267742

G=-2633.804985

C	-1.786486000	-0.929805000	2.066199000
C	-2.452082000	-0.586617000	0.821237000
C	-2.299450000	-1.398939000	-0.298825000
C	-1.473421000	-2.592507000	-0.223099000
C	-0.832034000	-2.923385000	0.971930000
C	-0.992911000	-2.075358000	2.142283000
C	-1.342921000	0.306782000	2.694212000
C	-1.737477000	1.413680000	1.835295000
C	-2.427190000	0.862989000	0.680171000
C	-2.244784000	1.433417000	-0.579539000
C	-2.114208000	-0.803610000	-1.614967000
C	-0.769413000	-2.731987000	-1.489482000
C	0.545997000	-3.195327000	-1.509735000
C	1.215153000	-3.537963000	-0.263634000
C	0.540738000	-3.404554000	0.950326000
C	1.228851000	-2.852244000	2.107513000
C	0.281195000	-2.029907000	2.844018000
C	0.706367000	-0.845226000	3.445647000
C	-0.123244000	0.348304000	3.369221000
C	-0.897990000	2.518381000	1.689487000

C	0.375415000	2.559442000	2.391015000
C	0.754710000	1.498462000	3.214329000
C	2.126487000	1.015819000	3.192615000
C	2.097059000	-0.432011000	3.336124000
C	3.005908000	-1.221115000	2.630728000
C	2.562299000	-2.456640000	2.003394000
C	3.265279000	-2.595964000	0.737419000
C	2.605890000	-3.125374000	-0.372078000
C	-1.165512000	-1.625501000	-2.348757000
C	3.243845000	-0.319056000	-2.691995000
C	2.023482000	-0.360467000	-3.366388000
C	1.193808000	0.832307000	-3.442721000
C	1.618650000	2.016825000	-2.840782000
C	2.891803000	2.060242000	-2.137864000
C	4.356468000	0.574058000	-0.819444000
C	4.325901000	-0.873652000	-0.676392000
C	3.638468000	-1.425318000	-1.833723000
C	2.796064000	-2.527158000	-1.684863000
C	1.523643000	-2.570854000	-2.388109000
C	1.144809000	-1.510076000	-3.211181000
C	-0.197561000	0.418879000	-3.335310000
C	-1.105614000	1.207655000	-2.627436000
C	-0.661884000	2.443611000	-1.999851000
C	0.671319000	2.840005000	-2.104443000
C	1.358393000	3.392499000	-0.947382000
C	2.730504000	2.909778000	-0.967549000
C	3.372412000	2.581386000	0.226465000
C	4.202054000	1.388628000	0.302127000
C	4.143248000	-1.446419000	0.582040000
C	3.982921000	-0.596651000	1.752182000
C	4.011592000	0.791204000	1.615299000
C	3.064181000	1.614486000	2.350688000

C	2.668678000	2.720559000	1.492369000
C	1.352963000	3.183705000	1.512468000
C	0.683447000	3.526585000	0.266609000
C	-0.707769000	3.115793000	0.375764000
C	-1.365780000	2.583047000	-0.733899000
C	-0.227707000	-1.028058000	-3.192736000
C	-2.082684000	0.583810000	-1.749712000
C	3.687616000	0.916923000	-2.065258000
C	-5.429289000	1.578983000	1.171529000
C	-5.339010000	1.562942000	-1.196687000
H	-5.437840000	1.915939000	2.200859000
H	-5.265470000	1.886140000	-2.227698000
C	-5.328019000	2.490556000	-0.016128000
H	-6.174836000	3.195237000	-0.052247000
H	-4.423416000	3.115114000	0.012357000
C	-5.536366000	0.291786000	0.730389000
C	-5.475457000	0.281937000	-0.748604000
C	-5.655447000	-0.957162000	1.433940000
H	-5.691968000	-0.962647000	2.519715000
C	-5.534068000	-0.977100000	-1.443310000
C	-5.712665000	-2.116297000	0.721885000
H	-5.478484000	-0.996338000	-2.527925000
H	-5.797344000	-3.067460000	1.239861000
C	-5.652186000	-2.126675000	-0.723578000
H	-5.692565000	-3.084897000	-1.233679000

TS_{bir}[5,6]

E=-2634.246856

G=-2633.783166

C	-1.687455000	-1.972363000	-1.308226000
C	-2.567516000	-0.853872000	-0.836252000
C	-2.267328000	0.428180000	-1.436890000

C	-1.395726000	0.553855000	-2.581526000
C	-0.710988000	-0.549910000	-3.088318000
C	-0.851921000	-1.839271000	-2.408714000
C	-1.243244000	-2.743875000	-0.169047000
C	-1.698482000	-2.074659000	1.039147000
C	-2.452139000	-0.898404000	0.656615000
C	-2.304792000	0.269954000	1.405160000
C	-2.144233000	1.613772000	-0.649989000
C	-0.740319000	1.853805000	-2.521459000
C	0.584975000	1.987275000	-2.934842000
C	1.309163000	0.831694000	-3.438594000
C	0.670955000	-0.411421000	-3.504234000
C	1.386227000	-1.613988000	-3.102541000
C	0.445279000	-2.492798000	-2.426869000
C	0.862388000	-3.260803000	-1.338127000
C	-0.001576000	-3.389309000	-0.181761000
C	-0.902598000	-2.082417000	2.185539000
C	0.394136000	-2.740819000	2.165608000
C	0.835081000	-3.384050000	1.009581000
C	2.219239000	-3.246417000	0.584602000
C	2.236201000	-3.170191000	-0.868794000
C	3.136828000	-2.320438000	-1.511372000
C	2.704300000	-1.528015000	-2.653911000
C	3.366373000	-0.234619000	-2.582346000
C	2.679176000	0.919136000	-2.961390000
C	-1.201175000	2.514180000	-1.316206000
C	3.141873000	2.808262000	0.182728000
C	1.897432000	3.437249000	0.200125000
C	1.027841000	3.302199000	1.360668000
C	1.445613000	2.548381000	2.459918000
C	2.742687000	1.890570000	2.438434000
C	4.298936000	0.860901000	0.822942000

C	4.318581000	0.937372000	-0.628859000
C	3.603522000	2.141577000	-1.025900000
C	2.803842000	2.134023000	-2.167843000
C	1.507006000	2.793781000	-2.151274000
C	1.062949000	3.430311000	-0.991021000
C	-0.342653000	3.213159000	0.890786000
C	-1.248955000	2.362656000	1.529383000
C	-0.811435000	1.574233000	2.672965000
C	0.504938000	1.665599000	3.128689000
C	1.221358000	0.461905000	3.524782000
C	2.605285000	0.600688000	3.099266000
C	3.302191000	-0.507899000	2.618118000
C	4.168448000	-0.375736000	1.456335000
C	4.200774000	-0.225439000	-1.390249000
C	4.061946000	-1.515029000	-0.731296000
C	4.045481000	-1.587767000	0.663126000
C	3.105787000	-2.471689000	1.334089000
C	2.645418000	-1.803764000	2.542305000
C	1.318341000	-1.936861000	2.950968000
C	0.591845000	-0.780698000	3.453897000
C	-0.780527000	-0.872296000	2.979295000
C	-1.464447000	0.279719000	2.594193000
C	-0.321233000	3.287383000	-0.565344000
C	-2.182624000	1.559208000	0.755978000
C	3.573259000	2.017321000	1.325305000
C	-4.473819000	-1.342536000	-1.247817000
C	-5.204192000	-1.768145000	0.962998000
H	-4.379729000	-1.541978000	-2.310812000
H	-5.299744000	-2.229407000	1.938217000
C	-4.736976000	-2.477321000	-0.269150000
H	-5.572244000	-3.070614000	-0.681062000
H	-3.909757000	-3.174201000	-0.114084000

C	-5.219412000	-0.228774000	-0.756706000
C	-5.575139000	-0.474084000	0.625149000
C	-5.482687000	1.023750000	-1.342651000
H	-5.203434000	1.215522000	-2.374056000
C	-6.168254000	0.569505000	1.393471000
C	-6.090856000	2.002594000	-0.580382000
H	-6.417061000	0.404138000	2.437628000
H	-6.305501000	2.972792000	-1.018592000
C	-6.424218000	1.775568000	0.786032000
H	-6.885065000	2.579204000	1.352976000

Proint[5,6]

E=-2634.259637

G=-2633.794132

C	-1.715866000	-1.964560000	-1.252549000
C	-2.685289000	-0.835357000	-0.848238000
C	-2.240052000	0.465270000	-1.475061000
C	-1.359755000	0.525465000	-2.605331000
C	-0.695586000	-0.614286000	-3.071190000
C	-0.872097000	-1.883921000	-2.344728000
C	-1.288163000	-2.688369000	-0.087046000
C	-1.739057000	-1.969967000	1.096088000
C	-2.457671000	-0.798935000	0.676671000
C	-2.297076000	0.380595000	1.382869000
C	-2.078837000	1.667108000	-0.720220000
C	-0.666391000	1.811185000	-2.586147000
C	0.661883000	1.898708000	-2.995072000
C	1.359590000	0.707609000	-3.453029000
C	0.687884000	-0.522509000	-3.479041000
C	1.372814000	-1.726755000	-3.030081000
C	0.408999000	-2.562427000	-2.332938000
C	0.804375000	-3.306662000	-1.217929000

C	-0.066103000	-3.373517000	-0.066159000
C	-0.951069000	-1.964405000	2.253681000
C	0.329474000	-2.655651000	2.262876000
C	0.761702000	-3.345809000	1.130846000
C	2.151099000	-3.257166000	0.710884000
C	2.177223000	-3.231546000	-0.744314000
C	3.099856000	-2.423070000	-1.409594000
C	2.690491000	-1.658350000	-2.579946000
C	3.383169000	-0.379396000	-2.548591000
C	2.726226000	0.778304000	-2.973269000
C	-1.114861000	2.523828000	-1.408508000
C	3.219348000	2.761541000	0.107914000
C	1.993124000	3.424321000	0.095459000
C	1.111193000	3.347485000	1.253180000
C	1.501896000	2.615920000	2.378243000
C	2.780997000	1.927734000	2.389278000
C	4.322526000	0.808571000	0.821042000
C	4.352809000	0.835387000	-0.631794000
C	3.670845000	2.042769000	-1.074464000
C	2.878197000	2.016773000	-2.220827000
C	1.599928000	2.711030000	-2.235397000
C	1.166656000	3.399654000	-1.101287000
C	-0.255374000	3.275913000	0.775441000
C	-1.187824000	2.461363000	1.433419000
C	-0.776592000	1.697319000	2.603344000
C	0.535646000	1.775765000	3.068197000
C	1.221673000	0.570546000	3.513485000
C	2.608327000	0.663678000	3.092621000
C	3.285213000	-0.476821000	2.655601000
C	4.159346000	-0.403306000	1.495881000
C	4.210300000	-0.349332000	-1.354640000
C	4.036932000	-1.613389000	-0.652203000

C	4.013552000	-1.638795000	0.744140000
C	3.051213000	-2.477747000	1.439169000
C	2.600016000	-1.758671000	2.621309000
C	1.267618000	-1.848147000	3.026338000
C	0.563713000	-0.659237000	3.483990000
C	-0.807825000	-0.738291000	3.006699000
C	-1.461694000	0.416021000	2.567906000
C	-0.222638000	3.304187000	-0.679464000
C	-2.127728000	1.660075000	0.681704000
C	3.622925000	1.997490000	1.279011000
C	-4.203686000	-1.165166000	-1.222649000
C	-5.397657000	-1.891250000	0.731715000
H	-4.234016000	-1.269187000	-2.310589000
H	-5.688649000	-2.484458000	1.590638000
C	-4.697289000	-2.436503000	-0.478511000
H	-5.413248000	-2.969658000	-1.124897000
H	-3.902011000	-3.150874000	-0.247419000
C	-5.116625000	-0.087914000	-0.693293000
C	-5.720518000	-0.537029000	0.520993000
C	-5.339252000	1.196712000	-1.160722000
H	-4.881305000	1.537604000	-2.084137000
C	-6.512150000	0.356036000	1.279605000
C	-6.153673000	2.061783000	-0.415770000
H	-6.961981000	0.031476000	2.213508000
H	-6.337016000	3.070120000	-0.774372000
C	-6.721069000	1.641677000	0.798959000
H	-7.337629000	2.333592000	1.365910000

TS[5,6]

E=-2634.257183

G=-2633.789825

C	-2.512530000	-0.873727000	0.727523000
---	--------------	--------------	-------------

C	-2.694963000	-0.945286000	-0.815867000
C	-1.702435000	-1.894890000	-1.436415000
C	-0.983940000	-2.853121000	-0.684615000
C	-1.010792000	-2.858091000	0.731229000
C	-1.738169000	-1.818102000	1.419016000
C	-2.381163000	0.518151000	1.121215000
C	-2.328980000	1.346431000	-0.068499000
C	-2.363935000	0.496940000	-1.227042000
C	-1.599883000	0.815860000	-2.330600000
C	-0.897905000	-1.535328000	-2.583356000
C	0.271795000	-3.159799000	-1.381055000
C	1.431839000	-3.415459000	-0.660947000
C	1.408189000	-3.395556000	0.799631000
C	0.214967000	-3.117186000	1.469925000
C	0.233070000	-2.244537000	2.633838000
C	-0.974388000	-1.439852000	2.598706000
C	-0.943523000	-0.113650000	3.020820000
C	-1.664185000	0.894341000	2.258473000
C	-1.574889000	2.530187000	-0.070154000
C	-0.821613000	2.910952000	1.111719000
C	-0.862862000	2.104879000	2.249909000
C	0.354123000	1.847537000	3.005826000
C	0.304440000	0.473312000	3.480696000
C	1.468541000	-0.296879000	3.508867000
C	1.431776000	-1.687530000	3.080420000
C	2.670754000	-1.974934000	2.376479000
C	2.653772000	-2.810584000	1.256072000
C	0.319150000	-2.336974000	-2.569135000
C	4.268448000	-0.476147000	-1.113225000
C	3.546752000	-0.838600000	-2.249476000
C	2.820689000	0.173588000	-3.005134000
C	2.855076000	1.506551000	-2.593758000

C	3.609807000	1.883928000	-1.409254000
C	4.280123000	0.938045000	0.768660000
C	4.231711000	-0.436819000	1.241126000
C	4.222516000	-1.311186000	0.077903000
C	3.451397000	-2.472962000	0.084984000
C	2.697095000	-2.850811000	-1.099869000
C	2.745301000	-2.052879000	-2.244743000
C	1.577897000	-0.418171000	-3.469786000
C	0.404125000	0.346195000	-3.486886000
C	0.441662000	1.735368000	-3.051201000
C	1.638716000	2.304720000	-2.619200000
C	1.648658000	3.182777000	-1.456958000
C	2.865841000	2.920698000	-0.709963000
C	2.847107000	2.944641000	0.687760000
C	3.569526000	1.934317000	1.441297000
C	3.472182000	-0.762906000	2.364659000
C	2.729144000	0.275630000	3.066317000
C	2.776947000	1.594194000	2.613670000
C	1.564571000	2.396820000	2.582969000
C	1.608821000	3.233217000	1.392013000
C	0.439756000	3.487500000	0.674129000
C	0.459873000	3.463660000	-0.781546000
C	-0.788787000	2.873958000	-1.234677000
C	-0.793851000	2.019636000	-2.340042000
C	1.529840000	-1.790672000	-2.997657000
C	-0.854150000	-0.226439000	-3.058848000
C	4.303424000	0.914501000	-0.684083000
C	-5.129622000	-0.250460000	-0.724546000
C	-4.559509000	-2.482074000	-0.150062000
C	-4.869617000	-1.668093000	1.074638000
C	-5.416395000	-0.426562000	0.661028000
H	-4.895784000	-2.060631000	2.084116000

H	-5.459672000	-3.019351000	-0.487230000
C	-4.218850000	-1.359860000	-1.155813000
H	-4.281158000	-1.632317000	-2.210708000
C	-5.543113000	0.893239000	-1.393423000
H	-5.305658000	1.039178000	-2.443323000
C	-6.091464000	0.583673000	1.375945000
H	-6.287754000	0.470976000	2.438166000
C	-6.515525000	1.712999000	0.688456000
H	-7.056002000	2.492766000	1.217280000
C	-6.257091000	1.865750000	-0.685670000
H	-6.603060000	2.758432000	-1.198058000
H	-3.762668000	-3.217459000	-0.014723000

CROSSINGS

Proint[5,6]

$E(S_0) = -2634.2503821$

$E(T_1) = -2634.2503697$

C	-2.402424000	-0.681203000	0.942803000
C	-2.742636000	-0.807121000	-0.573577000
C	-1.807139000	-1.839201000	-1.229796000
C	-1.067575000	-2.819076000	-0.466622000
C	-1.001818000	-2.742088000	0.922668000
C	-1.682012000	-1.639416000	1.635136000
C	-2.219838000	0.702724000	1.296840000
C	-2.192238000	1.496688000	0.080545000
C	-2.354252000	0.619648000	-1.043708000
C	-1.639234000	0.861994000	-2.201331000
C	-1.062425000	-1.548952000	-2.410440000
C	0.120587000	-3.195564000	-1.220711000
C	1.315634000	-3.479969000	-0.561679000
C	1.376300000	-3.402085000	0.887475000

C	0.233693000	-3.032171000	1.607356000
C	0.347090000	-2.123473000	2.736281000
C	-0.827985000	-1.268624000	2.748319000
C	-0.707156000	0.069817000	3.128472000
C	-1.419382000	1.081292000	2.382654000
C	-1.393510000	2.640545000	-0.001965000
C	-0.552975000	3.019122000	1.122481000
C	-0.566786000	2.258555000	2.290093000
C	0.678958000	1.964950000	2.978688000
C	0.592649000	0.607870000	3.497847000
C	1.718826000	-0.215953000	3.482974000
C	1.592150000	-1.615148000	3.100372000
C	2.777416000	-1.986035000	2.341096000
C	2.670478000	-2.862037000	1.258432000
C	0.128946000	-2.400754000	-2.432489000
C	4.235180000	-0.674943000	-1.276235000
C	3.429089000	-1.039428000	-2.353568000
C	2.702819000	-0.018887000	-3.097003000
C	2.822877000	1.326352000	-2.734113000
C	3.666972000	1.703907000	-1.613716000
C	4.421651000	0.795232000	0.552377000
C	4.339718000	-0.559617000	1.072886000
C	4.226045000	-1.470097000	-0.057166000
C	3.413716000	-2.599121000	0.033561000
C	2.574201000	-2.982011000	-1.092364000
C	2.581399000	-2.217817000	-2.259614000
C	1.409391000	-0.560930000	-3.457967000
C	0.273544000	0.257694000	-3.437372000
C	0.401552000	1.658155000	-3.060125000
C	1.649084000	2.182956000	-2.720834000
C	1.769368000	3.096052000	-1.593626000
C	3.014977000	2.798288000	-0.907238000

C	3.080766000	2.867838000	0.485081000
C	3.796861000	1.844000000	1.230270000
C	3.630365000	-0.813302000	2.247080000
C	2.977106000	0.279347000	2.953912000
C	3.060046000	1.581677000	2.455627000
C	1.888501000	2.442021000	2.470014000
C	1.901120000	3.237125000	1.250965000
C	0.704514000	3.522334000	0.592835000
C	0.637426000	3.450679000	-0.859509000
C	-0.662679000	2.908180000	-1.221910000
C	-0.776046000	2.027603000	-2.298210000
C	1.330616000	-1.921561000	-2.941221000
C	-0.981831000	-0.238179000	-2.917481000
C	4.357132000	0.725070000	-0.898021000
C	-5.165729000	-0.018977000	-0.494413000
C	-4.715272000	-2.419707000	-0.171245000
C	-5.956445000	-1.947588000	0.530262000
C	-6.137798000	-0.553822000	0.396610000
H	-6.682271000	-2.621276000	0.971811000
H	-4.925844000	-3.260443000	-0.840267000
C	-4.185800000	-1.147585000	-0.911999000
H	-4.254039000	-1.313787000	-2.001848000
C	-5.277067000	1.271035000	-0.968266000
H	-4.615160000	1.641421000	-1.743950000
C	-7.150399000	0.290725000	0.904599000
H	-7.919249000	-0.109223000	1.560031000
C	-7.174729000	1.628096000	0.515292000
H	-7.939727000	2.288242000	0.915204000
C	-6.261198000	2.122138000	-0.421552000
H	-6.309942000	3.159731000	-0.736525000
H	-3.940045000	-2.768274000	0.526649000

Proint[6,6] $E(S_0)=-2634.2571867$ $E(T_1)=-2634.2571472$

C	-2.110512000	0.095890000	-1.776926000
C	-2.690799000	-0.918337000	-0.763669000
C	-2.522791000	-0.374164000	0.651846000
C	-2.301843000	1.012444000	0.926632000
C	-2.031864000	1.926910000	-0.098519000
C	-1.908537000	1.429411000	-1.481574000
C	-1.219937000	-0.565033000	-2.686973000
C	-0.980008000	-1.916654000	-2.201632000
C	-1.724493000	-2.105136000	-0.987820000
C	-1.153346000	-2.820003000	0.048538000
C	-1.918601000	-1.137116000	1.705080000
C	-1.599184000	1.130151000	2.202183000
C	-0.643674000	2.124577000	2.390263000
C	-0.347994000	3.059206000	1.315208000
C	-1.028648000	2.947485000	0.094298000
C	-0.295485000	3.105230000	-1.154919000
C	-0.844106000	2.170146000	-2.123003000
C	-0.004281000	1.540853000	-3.046719000
C	-0.195994000	0.139001000	-3.337278000
C	0.278969000	-2.507669000	-2.379534000
C	1.346109000	-1.765408000	-3.033735000
C	1.114259000	-0.472536000	-3.501021000
C	2.118566000	0.562437000	-3.309610000
C	1.424477000	1.809713000	-3.025658000
C	1.951639000	2.701980000	-2.090934000
C	1.072499000	3.369026000	-1.139458000
C	1.776663000	3.475765000	0.128975000
C	1.077523000	3.319063000	1.329263000
C	-1.358604000	-0.212322000	2.688538000

C	3.166375000	0.616573000	2.745786000
C	2.143492000	-0.092775000	3.374548000
C	1.945611000	-1.504448000	3.073114000
C	2.787288000	-2.147335000	2.160652000
C	3.853687000	-1.407204000	1.509659000
C	4.336795000	0.880064000	0.721083000
C	3.648661000	2.128056000	1.006468000
C	2.923428000	1.966213000	2.257782000
C	1.667982000	2.550661000	2.417666000
C	0.601459000	1.812143000	3.075676000
C	0.833999000	0.518543000	3.543969000
C	0.519496000	-1.764894000	3.056390000
C	-0.020764000	-2.652601000	2.115322000
C	0.857951000	-3.318423000	1.164425000
C	2.230035000	-3.075942000	1.188601000
C	2.961532000	-2.916104000	-0.060916000
C	3.962272000	-1.883652000	0.136874000
C	4.253288000	-0.986354000	-0.892933000
C	4.443554000	0.423825000	-0.594779000
C	3.084573000	2.867028000	-0.034504000
C	3.192695000	2.390034000	-1.407069000
C	3.860990000	1.194537000	-1.680603000
C	3.311747000	0.262244000	-2.651299000
C	3.554101000	-1.087457000	-2.163699000
C	2.592286000	-2.080685000	-2.353580000
C	2.291036000	-3.016582000	-1.280987000
C	0.860787000	-3.278151000	-1.304521000
C	0.157057000	-3.419110000	-0.105386000
C	-0.169280000	-0.516625000	3.345274000
C	-1.260578000	-2.344694000	1.441836000
C	4.040290000	-0.053877000	1.794419000
C	-4.189249000	-1.257855000	-1.054862000

C	-5.767614000	-1.881636000	0.691412000
H	-4.274583000	-1.462704000	-2.128243000
H	-6.328914000	-2.458697000	1.417131000
C	-4.714948000	-2.466007000	-0.211143000
H	-5.124221000	-3.250653000	-0.863067000
H	-3.906286000	-2.946354000	0.354125000
C	-5.080902000	-0.098732000	-0.626895000
C	-5.922408000	-0.506980000	0.452247000
C	-5.153159000	1.186286000	-1.131833000
H	-4.556693000	1.480898000	-1.987820000
C	-6.774146000	0.446215000	1.066093000
C	-6.002809000	2.120192000	-0.516508000
H	-7.413339000	0.152998000	1.894315000
H	-6.048158000	3.135832000	-0.896578000
C	-6.791516000	1.747708000	0.583751000
H	-7.438406000	2.486032000	1.049921000

Experimental section

Indene and [60]fullerene dissolved in toluene, after degasification with argon, were irradiated with different lamps. Reactions were monitored by hplc. (Buckyprep, Toluene:Acetonitrile:Hexane 6:1:3, 1mL/min). The retention time of the [6,6] monoadduct¹ is 7.87 min.

Table S14. Reagents concentrations, type of irradiation and conditions in the cycloaddition of indene and C₆₀.

Entry	Equiv. Indene	Indene Concentration (M)	C ₆₀ Concentration (M)	Toluene Volume (mL)	hv (nm)	Photosensitizer	A
1	10	2.79E-03	2.78E-04	20	420	-	7%
2	41	1.41E-03	3.47E-05	20	420	-	8%
3	50	2.74E-02	5.56E-04	50	Hg lamp 300W/KMnO ₄	-	7%
4	100	6.86E-04	6.94E-06	20	420	-	5%
5	100	2.74E-02	2.78E-04	50	Hg lamp 300W/KMnO ₄	-	39%
6	186	2.58E-02	1.39E-04	10	UVA	-	16%
7	204	1.41E-03	6.94E-06	20	420	-	15%
8	436	6.05E-02	1.39E-04	10	UVA	-	16%
9	647	5.99E-02	9.26E-05	10	UVA	-	25%
10	1280	5.93E-02	4.63E-05	10	UVA	-	19%
11	2547	5.90E-02	2.31E-05	10	UVA	-	12%
12	5	4.63E-04	2.31E-04	40	Hg lamp 300W/KMnO ₄	[Ru(bpy) ₃](ClO ₄) ₂	1%
13	5	4.63E-04	2.31E-04	40	Hg lamp 300W/KMnO ₄	Methylene blue	<1%
14	5	4.63E-04	2.31E-04	40	Hg lamp 300W/CoSO ₄	Rose bengal	3%

¹ Puplovskis, A.; Kacens, J.; Neilands, O. *Tetrahedron Lett.* **1997**, *38*, 285-288.