Catalysis on Pristine 2D Materials via Dispersion and Electrostatic Interactions

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Supporting Information

(Total 131 Pages)

Top-down view of corannulene and sumanene bowl-to-bowl inversion on graphene (Figure S1), interaction energies between the catalyst and substrate in the RCs, TSSs, and PCs (Table S1); ALMO-EDA analysis (Table S2), optimized geometries for all structures (Table S3), and full references for references for quantum chemical software.

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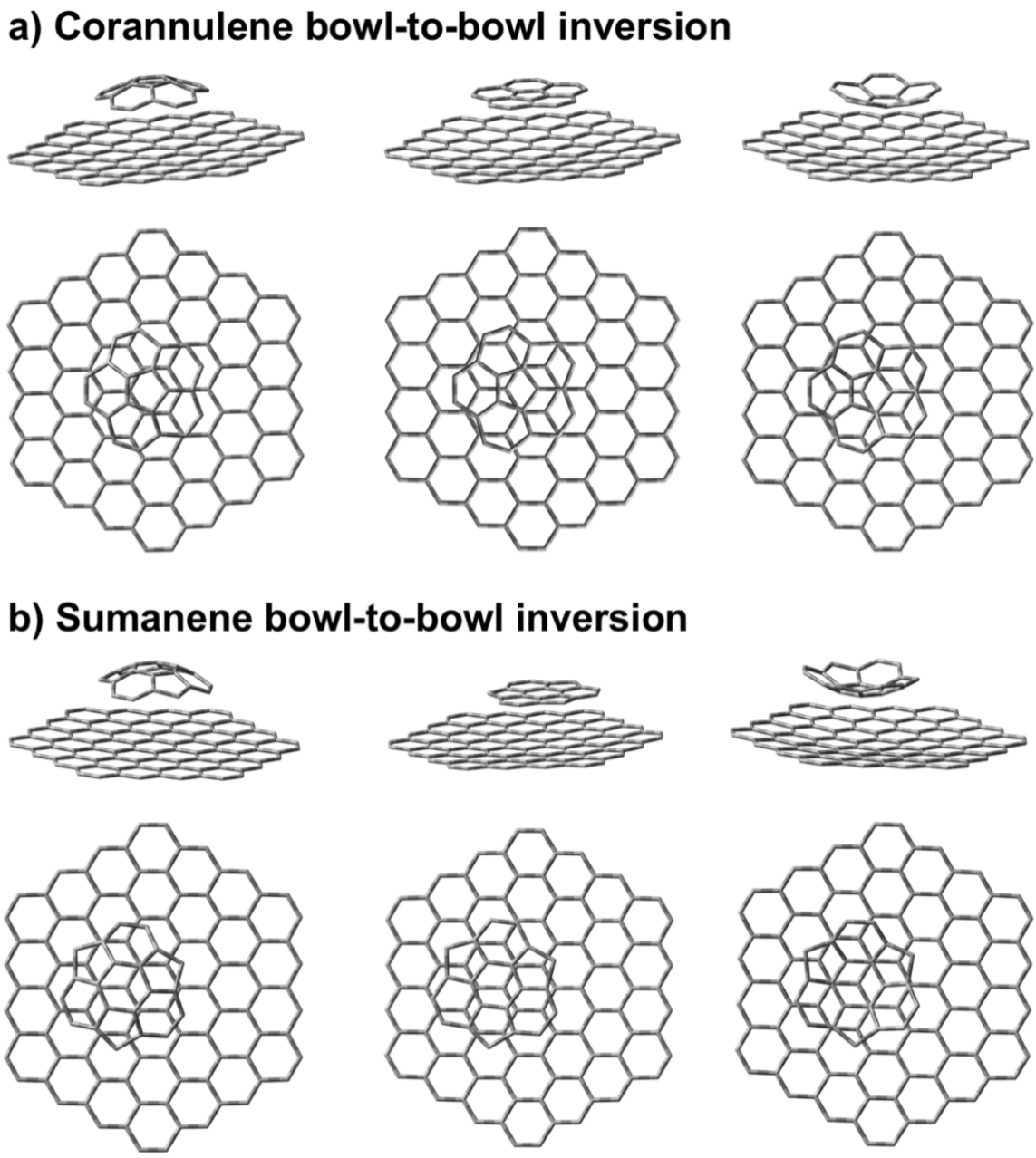


Figure S1. Side and top-down views of the optimized structures of the reactant complexes, transition state structures, and product complexes involved in the graphene-catalyzed bowl-to-bowl inversion in (a) corannulene and (b) sumanene. For clarity hydrogen atoms are omitted.

Table S1. Gibbs free interaction energies at 298 K between the catalyst and substrate in the RCs, TSSs, and PCs ($\Delta\Delta G_{298}$, revDSD-PBEP86-D3BJ/Def2-TZVPP, kJ mol^{-1}).

	Catalyst	RC[a,c]	TSS[b,c]	PC[a,c]
Corannulene bowl-to-bowl inversion	Graphene	–174.1	–195.2	–187.2
	h-BN	–68.1	–96.0	–83.9
	Graphane	–45.6	–59.0	–45.5
Sumanene bowl-to-bowl inversion	Graphene	–136.3	–182.1	–170.5
	h-BN	–65.1	–93.5	–79.1
	Graphane	–35.1	–47.9	–44.2
2,2'-dimethylbiphenyl rotation around central C–C bond	Graphene	–92.5	–142.7	–152.3
	h-BN	–12.7	–56.9	–31.5
	Graphane	8.2[d]	–25.5	–8.7

[a]Gibbs free energy at 298 K for the formation of the reactant complex: $\Delta\Delta G_{298} = G_{298}(\text{RC}) - \Delta G_{298}(\text{reactant}) - \Delta G_{298}(\text{catalyst})$, a similar definition applies for the product complex. [b]The Gibbs free energy at 298 K for the formation of the TSS complex is estimated as $\Delta\Delta G_{298} = \Delta G_{298}(\text{catalyzed TSS}) - \Delta G_{298}(\text{free TSS}) - \Delta G_{298}(\text{catalyst})$. [c]We note that the use of the Def2-TZVPP basis set may lead to overbinding of these complexes due to the slow basis-set convergence of the MP2-like correlation energy. Due to the large size of these systems we were unable to use a larger basis set in the DHDFT calculations. [d]It should be noted that on the enthalpic PES we obtain a binding energy of $\Delta H_{298} = -35.5$ kJ mol^{-1} at the revDSD-PBEP86-D3BJ/Def2-TZVPP level of theory.

Table S2. Electrostatic ($\Delta\Delta E_{ELEC}$), dispersion ($\Delta\Delta E_{DISP}$), polarisation ($\Delta\Delta E_{POL}$), charge transfer ($\Delta\Delta E_{CT}$), and Pauli repulsion ($\Delta\Delta E_{PAULI}$) contributions to the reaction barrier heights and reaction energies of the catalyzed reactions obtained from second generation ALMO-EDA at the ωB97M-V/Def2-SVP level of theory (in kJ mol^{-1}).

Reaction	Catalyst	Specie	$\Delta\Delta E_{DISP}$	$\Delta\Delta E_{ELEC}$	$\Delta\Delta E_{POL}$	$\Delta\Delta E_{CT}$	$\Delta\Delta E_{PAULI}$
Corannulene bowl-to-bowl inversion	**Graphene**	**TS**	-36.7	-30.7	-0.6	0.5	45.2
		PC	-8.4	-4.4	0.0	-0.1	11.0
	h-BN	**TS**	-36.5	-34.5	-1.0	-0.4	49.8
		PC	-13.8	-15.7	-0.7	-0.1	22.8
	Graphane	**TS**	-28.3	-19.7	-0.8	0.3	26.4
		PC	-3.1	-0.4	-0.2	0.4	-2.4
Sumanene bowl-to-bowl inversion	**Graphene**	**TS**	-49.2	-30.2	-0.9	1.1	45.8
		PC	-5.0	1.8	0.6	1.6	1.7
	h-BN	**TS**	-59.6	-55.6	-2.4	-4.7	81.5
		PC	-22.5	-24.1	-0.9	-1.7	36.1
	Graphane	**TS**	-41.0	-25.5	-1.3	0.4	34.5
		PC	-6.2	0.6	0.0	1.2	-4.4
Dimethylbiphenyl rotation around central C–C bond	**Graphene**	**TS**	-51.1	-40.0	-1.4	0.1	57.8
		PC	-3.9	-10.9	-0.6	0.6	13.7
	h-BN	**TS**	-46.7	-46.4	-1.9	-0.6	66.6
		PC	-2.1	-9.6	-0.6	-0.3	12.6
	Graphane	**TS**	-41.5	-33.0	-1.7	-1.2	48.6
		PC	-3.8	-7.6	-0.7	0.3	9.2

[a] The tabulated values are contributions to the catalyzed reaction barrier heights (i.e., $\Delta\Delta E_{COMPONENT} = \Delta E_{COMPONENT}(TS) - \Delta E_{COMPONENT}(RC)$. A negative $\Delta\Delta E_{COMPONENT}$ value indicates stabilization of the TS relative to the RC.

Table S3. PBE-D3BJ/6-31G(d) optimized geometries

C96H24

C	-2.470547	-2.854814	0.003079
C	-2.471326	-1.426821	-0.004695
C	-1.236293	-0.713774	0.005377
C	-0.000000	-1.427548	-0.005377
C	-0.000000	-2.853642	0.004695
C	-1.237068	-3.566963	-0.003079
C	-1.236293	0.713774	-0.005377
C	1.236293	-0.713774	0.005377
C	1.236293	0.713774	-0.005377
C	0.000000	1.427548	0.005377
C	2.471326	1.426821	0.004695
C	3.707615	0.712150	-0.003079
C	3.707615	-0.712150	0.003079
C	2.471326	-1.426821	-0.004695
C	2.470547	-2.854814	0.003079
C	1.237068	-3.566963	-0.003079
C	-3.707615	-0.712150	0.003079
C	-3.707615	0.712150	-0.003079
C	-2.471326	1.426821	0.004695
C	-2.470547	2.854814	-0.003079
C	-1.237068	3.566963	0.003079
C	0.000000	2.853642	-0.004695
C	2.470547	2.854814	-0.003079
C	1.237068	3.566963	0.003079
C	-3.710370	3.569834	0.002039
C	-4.946752	1.428358	0.002039
C	-4.946752	-1.428358	-0.002039
C	-3.710370	-3.569834	-0.002039
C	-1.236382	-4.998192	0.002039
C	1.236382	-4.998192	0.002039
C	3.710370	-3.569834	-0.002039
C	4.946752	-1.428358	-0.002039
C	4.946752	1.428358	0.002039
C	3.710370	3.569834	0.002039
C	1.236382	4.998192	-0.002039
C	-1.236382	4.998192	-0.002039
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C	2.473810	5.708630	0.000073
C	-3.706913	4.996697	-0.000073
C	-6.180723	-0.711933	0.000073
C	-2.473810	-5.708630	-0.000073
C	3.706913	-4.996697	0.000073
C	-3.706913	-4.996697	0.000073

C	2.473810	-5.708630	-0.000073
C	6.180723	-0.711933	0.000073
C	3.706913	4.996697	-0.000073
C	-6.180723	0.711933	-0.000073
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C	-4.944863	2.854918	0.000195
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C	4.944863	-2.854918	-0.000195
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C	7.426175	-1.440148	-0.000713
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C	4.960292	-5.711182	-0.000713
C	2.465883	-7.151330	0.000713
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C	-7.426175	-1.440148	-0.000713
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C	-1.244339	-7.832685	0.001899
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C	-7.405474	2.838713	0.001899
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C	8.654500	0.684815	0.000621
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C	-3.734183	7.837424	-0.000621
C	-4.920317	7.152609	0.000621
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C	-8.654500	-0.684815	-0.000621
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H	9.600195	1.237681	0.000647
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H	3.728234	8.932853	-0.000647
H	1.243997	8.928970	-0.001783
H	-1.243997	8.928970	-0.001783
H	-3.728234	8.932853	-0.000647
H	-5.871961	7.695172	0.000647
H	-7.110716	5.541818	0.001783
H	-8.354713	3.387152	0.001783
H	-9.600195	1.237681	0.000647
H	-9.600195	-1.237681	-0.000647
H	-8.354713	-3.387152	-0.001783
H	-7.110716	-5.541818	-0.001783
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H	1.243997	-8.928970	0.001783
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B48N48H24

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H	7.336806	5.678901	-0.000166
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C96H120

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C	-1.273608	-0.735318	-0.230093
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H	0.000000	-1.471757	1.343806
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C	-3.820658	-0.735921	-0.227411
C	2.547655	2.940827	0.227411
C	-2.547655	-2.940827	-0.227411
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C	5.092754	-1.468350	0.241139
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C	-1.274748	-5.144630	-0.241139
C	-3.818006	-3.676279	0.241139
C	-5.092754	-1.468350	0.241139
C	-5.092754	1.468350	-0.241139
C	-3.818006	3.676279	-0.241139
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C	-5.094211	2.941144	0.210884
C	-5.094211	-2.941144	-0.210884
C	0.000000	-5.882288	0.210884
H	-5.105095	-2.947428	-1.324885
H	-5.088823	-1.460873	1.354869
H	-3.809565	-3.676613	1.354869
H	-1.279258	-5.137486	-1.354869
H	-0.000000	-5.894856	1.324885
H	1.279258	-5.137486	-1.354869
H	3.809565	-3.676613	1.354869
H	5.105095	-2.947428	-1.324885
H	5.088823	-1.460873	1.354869

H	5.088823	1.460873	-1.354869
H	5.105095	2.947428	1.324885
H	3.809565	3.676613	-1.354869
H	1.279258	5.137486	1.354869
H	0.000000	5.894856	-1.324885
H	-1.279258	5.137486	1.354869
H	-3.809565	3.676613	-1.354869
H	-5.105095	2.947428	1.324885
H	-5.088823	1.460873	-1.354869
C	-6.368877	0.737723	0.221385
C	-6.368877	-0.737723	-0.221385
C	-3.823325	-5.146747	-0.221385
C	-2.545551	-5.884470	0.221385
C	2.545551	-5.884470	0.221385
C	3.823325	-5.146747	-0.221385
C	6.368877	-0.737723	-0.221385
C	6.368877	0.737723	0.221385
C	3.823325	5.146747	0.221385
C	2.545551	5.884470	-0.221385
C	-2.545551	5.884470	-0.221385
C	-3.823325	5.146747	0.221385
H	-2.536044	-5.896301	1.335351
H	-3.838325	-5.144430	-1.335351
H	-6.374369	-0.751872	-1.335351
H	-6.374369	0.751872	1.335351
H	-3.838325	5.144430	1.335351
H	-2.536044	5.896301	-1.335351
H	2.536044	5.896301	-1.335351
H	3.838325	5.144430	1.335351
H	6.374369	0.751872	1.335351
H	6.374369	-0.751872	-1.335351
H	3.838325	-5.144430	-1.335351
H	2.536044	-5.896301	1.335351
C	2.549983	7.353192	0.252719
C	0.000000	7.349436	0.264196
C	-2.549983	7.353192	0.252719
C	-5.093060	5.884946	-0.252719
C	-6.364799	3.674718	-0.264196
C	-7.643043	1.468246	-0.252719
C	-7.643043	-1.468246	0.252719
C	-6.364799	-3.674718	0.264196
C	-5.093060	-5.884946	0.252719
C	-2.549983	-7.353192	-0.252719
C	-0.000000	-7.349436	-0.264196
C	2.549983	-7.353192	-0.252719
C	5.093060	-5.884946	0.252719

C	6.364799	-3.674718	0.264196
C	7.643043	-1.468246	0.252719
C	7.643043	1.468246	-0.252719
C	6.364799	3.674718	-0.264196
C	5.093060	5.884946	-0.252719
C	-6.355062	5.137928	0.196876
C	-7.627107	2.934681	0.196876
C	-8.907725	0.734518	0.219610
C	-8.907725	-0.734518	-0.219610
C	-7.627107	-2.934681	-0.196876
C	-6.355062	-5.137928	-0.196876
C	-3.817751	-8.081575	0.219610
C	-1.272046	-8.072609	0.196876
C	1.272046	-8.072609	0.196876
C	5.089974	-7.347057	-0.219610
C	6.355062	-5.137928	-0.196876
C	8.907725	-0.734518	-0.219610
C	7.627107	2.934681	0.196876
C	6.355062	5.137928	0.196876
C	5.089974	7.347057	0.219610
C	1.272046	8.072609	-0.196876
C	-1.272046	8.072609	-0.196876
C	-3.817751	8.081575	-0.219610
H	7.683515	2.973088	1.305015
H	8.529470	3.455943	-0.178439
H	6.416528	5.167576	1.305015
H	7.257669	5.658766	-0.178439
C	3.817751	8.081575	-0.219610
H	5.161952	7.364922	1.326327
H	5.990248	7.865929	-0.160545
H	3.816971	9.120672	0.160545
H	3.797233	8.152842	-1.326327
H	1.271801	9.114709	0.178439
H	1.266988	8.140664	-1.305015
H	-1.271801	9.114709	0.178439
H	-1.266988	8.140664	-1.305015
C	-5.089974	7.347057	0.219610
H	-3.816971	9.120672	0.160545
H	-3.797233	8.152842	-1.326327
H	-5.990248	7.865929	-0.160545
H	-5.161952	7.364922	1.326327
H	-7.257669	5.658766	-0.178439
H	-6.416528	5.167576	1.305015
H	-8.529470	3.455943	-0.178439
H	-7.683515	2.973088	1.305015
H	-9.807219	1.254742	-0.160545

H	-8.959185	0.787921	1.326327
H	-9.807219	-1.254742	0.160545
H	-8.959185	-0.787921	-1.326327
H	-8.529470	-3.455943	0.178439
H	-7.683515	-2.973088	-1.305015
H	-7.257669	-5.658766	0.178439
H	-6.416528	-5.167576	-1.305015
C	-5.089974	-7.347057	-0.219610
H	-5.990248	-7.865929	0.160545
H	-5.161952	-7.364922	-1.326327
H	-3.797233	-8.152842	1.326327
H	-3.816971	-9.120672	-0.160545
H	-1.266988	-8.140664	1.305015
H	-1.271801	-9.114709	-0.178439
H	1.266988	-8.140664	1.305015
H	1.271801	-9.114709	-0.178439
C	3.817751	-8.081575	0.219610
C	7.627107	-2.934681	-0.196876
C	8.907725	0.734518	0.219610
H	3.797233	-8.152842	1.326327
H	3.816971	-9.120672	-0.160545
H	5.161952	-7.364922	-1.326327
H	5.990248	-7.865929	0.160545
H	6.416528	-5.167576	-1.305015
H	7.257669	-5.658766	0.178439
H	7.683515	-2.973088	-1.305015
H	8.529470	-3.455943	0.178439
H	9.807219	-1.254742	0.160545
H	8.959185	-0.787921	-1.326327
H	8.959185	0.787921	1.326327
H	9.807219	1.254742	-0.160545
H	6.351812	3.667220	-1.376348
H	5.074548	5.887336	-1.364942
H	2.561309	7.338355	1.364942
H	0.000000	7.334441	1.376348
H	-2.561309	7.338355	1.364942
H	-5.074548	5.887336	-1.364942
H	-6.351812	3.667220	-1.376348
H	-7.635856	1.451019	-1.364942
H	-7.635856	-1.451019	1.364942
H	-6.351812	-3.667220	1.376348
H	-5.074548	-5.887336	1.364942
H	-2.561309	-7.338355	-1.364942
H	-0.000000	-7.334441	-1.376348
H	2.561309	-7.338355	-1.364942
H	5.074548	-5.887336	1.364942

H	6.351812	-3.667220	1.376348
H	7.635856	-1.451019	1.364942
H	7.635856	1.451019	-1.364942

Free corannulene reactant

C	1.311816	2.994008	-0.263423
C	2.442097	2.172811	-0.263423
C	-1.311816	2.994008	-0.263423
C	0.000000	2.495838	0.098931
C	0.000000	1.210755	0.643137
C	2.373683	0.771256	0.098931
C	-2.442097	2.172811	-0.263423
C	3.252844	-0.322412	-0.263423
C	0.698552	-3.193270	-0.263423
C	-0.698552	-3.193270	-0.263423
C	1.467017	-2.019175	0.098931
C	0.711664	-0.979521	0.643137
C	-0.711664	-0.979521	0.643137
C	-1.467017	-2.019175	0.098931
C	-2.821116	-1.651137	-0.263423
C	-3.252844	-0.322412	-0.263423
C	-2.373683	0.771256	0.098931
C	-1.151497	0.374144	0.643137
C	2.821116	-1.651137	-0.263423
C	1.151497	0.374144	0.643137
H	-4.256011	-0.100709	-0.645665
H	-3.502381	-2.420145	-0.645665
H	-1.219400	-4.078828	-0.645665
H	1.219400	-4.078828	-0.645665
H	3.502381	-2.420145	-0.645665
H	4.256011	-0.100709	-0.645665
H	3.383990	2.583096	-0.645665
H	1.410960	4.016586	-0.645665
H	-1.410960	4.016586	-0.645665
H	-3.383990	2.583096	-0.645665

Free corannulene inversion TS

C	1.369531	3.086892	0.000000
C	2.512600	2.256404	-0.000000
C	-1.369531	3.086892	-0.000000
C	0.000000	2.570169	0.000000
C	0.000000	1.193160	0.000000
C	2.444376	0.794226	0.000000
C	-2.512600	2.256404	0.000000
C	3.359017	-0.348600	0.000000
C	0.706455	-3.302338	0.000000

C	-0.706455	-3.302338	-0.000000
C	1.510707	-2.079310	0.000000
C	0.701322	-0.965287	0.000000
C	-0.701322	-0.965287	0.000000
C	-1.510707	-2.079310	0.000000
C	-2.922403	-1.692358	0.000000
C	-3.359017	-0.348600	0.000000
C	-2.444376	0.794226	0.000000
C	-1.134763	0.368707	0.000000
C	2.922403	-1.692358	0.000000
C	1.134763	0.368707	0.000000
H	-3.698829	-2.465997	0.000000
H	-4.441892	-0.179084	-0.000000
H	-3.488303	2.755760	0.000000
H	-1.542939	4.169150	0.000000
H	1.542939	4.169150	0.000000
H	3.488303	2.755760	-0.000000
H	4.441892	-0.179084	0.000000
H	3.698829	-2.465997	0.000000
H	1.202301	-4.279830	0.000000
H	-1.202301	-4.279830	-0.000000

Free sumanene reactant

C	-3.230872	1.037015	0.456720
C	-2.513517	2.279510	0.456720
C	-1.214635	2.371564	-0.072279
C	-2.661152	-0.133877	-0.072279
C	-2.858748	-1.650499	0.195104
C	3.230872	1.037015	0.456720
C	2.661152	-0.133877	-0.072279
C	2.858748	-1.650499	0.195104
C	2.513517	2.279510	0.456720
C	1.214635	2.371564	-0.072279
C	0.718813	1.220881	-0.713336
C	1.416720	0.012070	-0.713336
C	0.697907	-1.232951	-0.713336
C	1.446517	-2.237687	-0.072279
C	0.717355	-3.316525	0.456720
C	-0.717355	-3.316525	0.456720
C	-1.446517	-2.237687	-0.072279
C	-0.697907	-1.232951	-0.713336
C	-1.416720	0.012070	-0.713336
C	-0.718813	1.220881	-0.713336
C	0.000000	3.300998	0.195104
H	2.955979	3.119326	1.004804
H	4.179405	1.000290	1.004804

H	0.000000	3.680024	1.232210
H	-2.955979	3.119326	1.004804
H	-4.179405	1.000290	1.004804
H	-3.629163	-2.095298	-0.465702
H	-1.223426	-4.119616	1.004804
H	1.223426	-4.119616	1.004804
H	3.186994	-1.840012	1.232210
H	-3.186994	-1.840012	1.232210
H	0.000000	4.190597	-0.465702
H	3.629163	-2.095298	-0.465702

Free sumanene inversion TS

C	2.685259	-2.392891	0.000000
C	3.414934	-1.129057	-0.000000
C	2.764276	0.137341	0.000000
C	1.263198	-2.462604	0.000000
C	0.000000	-3.438568	-0.000000
C	-0.729675	3.521948	0.000000
C	-1.501079	2.325263	0.000000
C	-2.977887	1.719284	-0.000000
C	0.729675	3.521948	0.000000
C	1.501079	2.325263	0.000000
C	0.686652	1.206308	0.000000
C	-0.686652	1.206308	-0.000000
C	-1.388020	-0.008496	0.000000
C	-2.764276	0.137341	-0.000000
C	-3.414934	-1.129057	0.000000
C	-2.685259	-2.392891	-0.000000
C	-1.263198	-2.462604	0.000000
C	-0.701368	-1.197812	0.000000
C	0.701368	-1.197812	0.000000
C	1.388020	-0.008496	-0.000000
C	2.977887	1.719284	-0.000000
H	1.204961	4.509619	0.000000
H	-1.204961	4.509619	-0.000000
H	4.507926	-1.211282	-0.000000
H	3.302964	-3.298337	0.000000
H	-3.302964	-3.298337	0.000000
H	-4.507926	-1.211282	0.000000
H	-3.551097	2.050227	0.884871
H	-3.551097	2.050227	-0.884871
H	3.551097	2.050227	-0.884871
H	3.551097	2.050227	0.884871
H	0.000000	-4.100454	-0.884871
H	-0.000000	-4.100454	0.884871

Free 2,2prime-dimethylbiphenyl reactant

C	-0.000153	0.747904	-0.308536
C	0.842880	1.447044	-1.190937
C	0.866991	2.848137	-1.209202
C	0.038849	3.563782	-0.335797
C	-0.806450	2.873771	0.543583
C	-0.842880	1.468862	0.574678
C	0.000153	-0.747904	-0.308536
C	0.842880	-1.468862	0.574678
C	0.806450	-2.873771	0.543583
C	-0.038849	-3.563782	-0.335797
C	-0.866991	-2.848137	-1.209202
C	-0.842880	-1.447044	-1.190937
H	1.485271	0.875038	-1.869539
H	1.529275	3.375793	-1.903336
H	0.047308	4.658789	-0.338551
H	-1.458338	3.435073	1.223229
H	1.458338	-3.435073	1.223229
H	-0.047308	-4.658789	-0.338551
H	-1.529275	-3.375793	-1.903336
H	-1.485271	-0.875038	-1.869539
C	1.768942	-0.741538	1.521886
H	2.478568	-0.095799	0.974891
H	1.212685	-0.075694	2.206144
H	2.349678	-1.451457	2.133112
C	-1.768942	0.741538	1.521886
H	-2.478568	0.095799	0.974891
H	-1.212685	0.075694	2.206144
H	-2.349678	1.451457	2.133112

Free 2,2prime-dimethylbiphenyl rotation TS

C	0.753223	-0.070618	0.000008
C	1.328146	-1.368744	0.000012
C	2.699215	-1.633058	0.000017
C	3.603986	-0.573612	0.000019
C	3.085284	0.721565	0.000024
C	1.705880	1.017610	0.000023
C	-0.753223	0.070618	-0.000008
C	-1.705880	-1.017610	-0.000023
C	-3.085284	-0.721565	-0.000024
C	-3.603986	0.573612	-0.000019
C	-2.699215	1.633058	-0.000017
C	-1.328146	1.368744	-0.000012
H	0.685276	-2.236644	0.000015
H	3.044458	-2.672252	0.000019
H	4.685699	-0.740930	0.000021

H	3.783427	1.565972	0.000033
H	-3.783427	-1.565972	-0.000033
H	-4.685699	0.740930	-0.000021
H	-3.044458	2.672252	-0.000019
H	-0.685276	2.236644	-0.000015
C	-1.424698	-2.511594	-0.000064
H	-0.866553	-2.845585	-0.892798
H	-0.866627	-2.845644	0.892695
H	-2.379225	-3.062519	-0.000122
C	1.424698	2.511594	0.000064
H	0.866627	2.845644	-0.892695
H	0.866553	2.845585	0.892798
H	2.379225	3.062519	0.000122

Graphene-catalyzed corannulene reactant

C	1.732146	-2.456647	2.612628
C	2.564787	-1.332587	2.621809
C	-0.780639	-3.250722	2.593711
C	0.321767	-2.374596	2.941155
C	-0.072044	-1.141053	3.458718
C	2.071556	-0.010464	2.956772
C	-2.107334	-2.806689	2.578579
C	2.587823	1.301668	2.616487
C	-0.722293	3.278945	2.583654
C	-2.056646	2.858690	2.569976
C	0.363996	2.384335	2.934116
C	-0.051537	1.159751	3.455712
C	-1.407758	0.732406	3.441571
C	-2.440805	1.501085	2.906495
C	-3.624581	0.739721	2.554972
C	-3.637252	-0.659279	2.556741
C	-2.467177	-1.441023	2.910087
C	-1.420494	-0.689680	3.443326
C	1.775321	2.440239	2.604168
C	0.774027	0.001871	3.466740
H	-4.510616	1.264778	2.181211
H	-4.532725	-1.168871	2.184146
H	-2.877839	-3.492240	2.208587
H	-0.570066	-4.264708	2.236039
H	2.145944	-3.404299	2.249322
H	3.594737	-1.448665	2.266899
H	3.619428	1.398033	2.260511
H	2.205152	3.379287	2.237294
H	-0.493519	4.287494	2.221592
H	-2.814448	3.556016	2.195577
C	-2.815040	2.399715	-0.774762

C	-1.388011	2.434104	-0.783369
C	-0.646790	1.216691	-0.782033
C	-1.331612	-0.035627	-0.802231
C	-2.756478	-0.068652	-0.802795
C	-3.498062	1.150786	-0.793834
C	0.780064	1.249640	-0.767124
C	-0.589542	-1.254887	-0.781576
C	0.837288	-1.221699	-0.766160
C	1.521667	0.030523	-0.745958
C	1.578013	-2.439086	-0.724966
C	0.891733	-3.690793	-0.707961
C	-0.531681	-3.723536	-0.732424
C	-1.273617	-2.505301	-0.782773
C	-2.700652	-2.537169	-0.775098
C	-3.440770	-1.321245	-0.793465
C	-0.703191	3.685464	-0.736592
C	0.720269	3.718694	-0.713727
C	1.463746	2.500081	-0.728797
C	2.890422	2.532764	-0.689378
C	3.630643	1.316414	-0.674611
C	2.946884	0.063595	-0.711888
C	3.004510	-2.405609	-0.681994
C	3.687713	-1.156151	-0.669580
C	3.575250	3.787272	-0.614793
C	1.405867	4.972846	-0.634410
C	-1.447872	4.906654	-0.685388
C	-3.559253	3.621564	-0.725922
C	-4.928631	1.117109	-0.757040
C	-4.871405	-1.353887	-0.756793
C	-3.387513	-3.792241	-0.726874
C	-1.219055	-4.978085	-0.681810
C	1.634533	-4.911815	-0.625273
C	3.746501	-3.626830	-0.602547
C	5.117097	-1.122415	-0.597267
C	5.060090	1.349030	-0.603270
C	0.946890	-6.161468	-0.581963
C	5.855070	-2.342261	-0.534800
C	5.000650	3.817615	-0.551774
C	-0.762001	6.156154	-0.614076
C	-5.668415	2.336665	-0.713502
C	-4.813861	-3.822385	-0.697996
C	-4.985440	3.585651	-0.696422
C	-5.553923	-2.606376	-0.714376
C	-0.476084	-6.194383	-0.608409
C	5.171651	-3.590959	-0.536924
C	0.661056	6.189337	-0.590745

C	5.741030	2.601878	-0.546238
C	-5.611891	-0.134801	-0.742786
C	-2.873915	4.871952	-0.680282
C	2.831525	5.004534	-0.591329
C	5.799727	0.129791	-0.565950
C	3.059984	-4.877241	-0.578416
C	-2.645130	-5.009488	-0.679304
C	1.701916	-7.388295	-0.501255
C	-1.175588	-7.455129	-0.552470
C	-3.336484	-6.271714	-0.617979
C	-5.499471	-5.090685	-0.641222
C	-6.995992	-2.631908	-0.672975
C	-7.051219	-0.168160	-0.695560
C	3.806913	-6.106117	-0.495752
C	5.913121	-4.826247	-0.460645
C	7.295320	-2.300904	-0.459913
C	7.237521	0.163153	-0.487587
C	7.181663	2.627355	-0.472224
C	5.684209	5.086092	-0.480110
C	3.520828	6.266879	-0.512552
C	1.358564	7.449993	-0.513415
C	-1.519110	7.383147	-0.557424
C	-3.622968	6.100811	-0.618124
C	-5.728977	4.820834	-0.638978
C	-7.110128	2.295442	-0.671685
C	-2.573753	-7.466834	-0.562115
C	-4.755298	-6.273979	-0.606870
C	3.098729	-7.335196	-0.463239
C	5.223460	-6.042601	-0.444210
C	-7.705314	-1.426943	-0.667916
C	-7.762913	1.058943	-0.667333
C	-5.040354	6.037321	-0.605047
C	-2.916331	7.330022	-0.564151
C	2.756426	7.461825	-0.479526
C	4.938923	6.269226	-0.464766
C	7.890668	1.422273	-0.449381
C	7.947980	-1.064331	-0.442698
C	-7.652909	-3.914616	-0.628734
C	-6.941019	-5.084272	-0.613939
C	-0.393748	-8.664462	-0.481388
C	0.975043	-8.632686	-0.456993
C	7.351709	-4.753252	-0.397157
C	8.009246	-3.552034	-0.397754
C	7.837102	3.910369	-0.416067
C	7.124747	5.079914	-0.418941
C	0.574814	8.659330	-0.468317

C	-0.794041	8.627501	-0.489090
C	-7.168657	4.747697	-0.611023
C	-7.825665	3.546353	-0.626360
H	-0.925731	-9.621239	-0.442902
H	1.549121	-9.563840	-0.399555
H	3.667844	-8.270079	-0.401340
H	5.791208	-6.978438	-0.384202
H	7.914127	-5.691783	-0.344626
H	9.102925	-3.520016	-0.345240
H	9.042305	-1.038135	-0.383492
H	8.985051	1.446823	-0.390532
H	8.931151	3.929108	-0.364858
H	7.643276	6.043604	-0.370526
H	5.462831	7.230485	-0.407913
H	3.281730	8.422183	-0.420380
H	1.105195	9.616185	-0.413219
H	-1.369740	9.558604	-0.450027
H	-3.487260	8.264713	-0.518164
H	-5.609606	6.972999	-0.558447
H	-7.732312	5.686142	-0.571995
H	-8.920272	3.513962	-0.599963
H	-8.858283	1.032529	-0.632957
H	-8.800735	-1.451272	-0.633623
H	-8.747852	-3.932911	-0.602740
H	-7.460653	-6.047818	-0.575627
H	-5.280664	-7.235012	-0.560817
H	-3.100846	-8.426948	-0.516543

Graphene-catalyzed corannulene inversion TS

C	-1.532398	2.510225	2.638752
C	-2.361826	1.365748	2.655134
C	1.070763	3.361172	2.594447
C	-0.070829	2.444530	2.594879
C	0.355526	1.135679	2.544786
C	-1.843569	-0.002640	2.628466
C	2.415353	2.926432	2.569434
C	-2.358271	-1.372337	2.656670
C	1.079404	-3.358914	2.597183
C	2.422878	-2.920758	2.571888
C	-0.064550	-2.445245	2.597101
C	0.358452	-1.135322	2.545934
C	1.692667	-0.699937	2.519814
C	2.807413	-1.508179	2.541880
C	4.029401	-0.701939	2.534238
C	4.027577	0.711706	2.533769
C	2.803537	1.514816	2.540724

C	1.690870	0.703700	2.519256
C	-1.525876	-2.514682	2.641299
C	-0.467598	-0.000890	2.560719
H	5.007167	-1.196199	2.519708
H	5.004065	1.208497	2.518754
H	3.187867	3.703319	2.563456
H	0.899520	4.443368	2.605653
H	-2.032964	3.485107	2.649074
H	-3.443696	1.537669	2.679037
H	-3.439665	-1.547139	2.681224
H	-2.023843	-3.490876	2.652940
H	0.910894	-4.441527	2.609384
H	3.197370	-3.695678	2.566294
C	2.689320	-2.472501	-0.789264
C	1.261698	-2.472308	-0.798263
C	0.549202	-1.237151	-0.822118
C	1.264703	-0.001922	-0.854747
C	2.690903	-0.003754	-0.843190
C	3.403017	-1.240952	-0.822304
C	-0.878604	-1.235595	-0.792125
C	0.552325	1.235083	-0.822203
C	-0.875483	1.237181	-0.792295
C	-1.590353	0.001697	-0.766770
C	-1.584705	2.471888	-0.715325
C	-0.867291	3.706024	-0.684542
C	0.556344	3.703631	-0.717616
C	1.267930	2.468460	-0.798468
C	2.695554	2.464997	-0.789449
C	3.406135	1.231680	-0.822452
C	0.546964	-3.705697	-0.717618
C	-0.876674	-3.704440	-0.684241
C	-1.590953	-2.468503	-0.714965
C	-3.017071	-2.466181	-0.641807
C	-3.727089	-1.232211	-0.622433
C	-3.014254	0.003493	-0.689580
C	-3.010837	2.473175	-0.642548
C	-3.723985	1.241016	-0.622966
C	-3.730236	-3.702549	-0.535976
C	-1.591033	-4.940210	-0.572262
C	1.262318	-4.943667	-0.646179
C	3.403271	-3.711119	-0.715449
C	4.833697	-1.241813	-0.773799
C	4.836834	1.228831	-0.773859
C	3.412637	3.701804	-0.715409
C	1.274827	4.939799	-0.646190
C	-1.578538	4.943568	-0.572535

C	-3.720905	3.711339	-0.536986
C	-5.151935	1.242015	-0.518239
C	-5.155032	-1.229643	-0.517607
C	-0.859979	6.174972	-0.514569
C	-5.858851	2.478973	-0.438419
C	-5.154423	-3.697978	-0.445605
C	0.547342	-6.174839	-0.548220
C	5.542963	-2.478273	-0.710363
C	4.839082	3.696646	-0.680202
C	4.829722	-3.709619	-0.680316
C	5.549205	2.463513	-0.710379
C	0.562965	6.172747	-0.548060
C	-5.145123	3.710350	-0.446949
C	-0.875595	-6.173436	-0.514535
C	-5.865031	-2.464806	-0.437263
C	5.547078	-0.007372	-0.759663
C	2.688245	-4.943160	-0.646437
C	-3.016030	-4.936991	-0.508734
C	-5.864188	0.007080	-0.471377
C	-3.003558	4.943964	-0.509478
C	2.700743	4.935636	-0.646267
C	-1.583286	7.419023	-0.408472
C	1.293410	7.414764	-0.472114
C	3.423032	6.179136	-0.560328
C	5.555649	4.946384	-0.598420
C	6.991062	2.453928	-0.655478
C	6.985889	-0.009211	-0.693448
C	-3.718640	6.189720	-0.401480
C	-5.854901	4.962726	-0.349201
C	-7.298099	2.472882	-0.336180
C	-7.300543	0.008875	-0.363390
C	-7.304251	-2.455117	-0.334883
C	-5.867333	-4.948555	-0.347578
C	-3.734229	-6.180942	-0.400616
C	-1.602024	-7.415671	-0.408413
C	1.274660	-7.418699	-0.472420
C	3.407400	-6.188478	-0.560610
C	5.543146	-4.961159	-0.598559
C	6.984829	-2.472355	-0.655323
C	2.691146	7.391868	-0.482997
C	4.841105	6.146848	-0.545881
C	-2.980363	7.400418	-0.359608
C	-5.135370	6.161338	-0.331972
C	7.670870	1.232377	-0.653094
C	7.667725	-1.252516	-0.652943
C	4.825545	-6.159809	-0.546134

C	2.672444	-7.399356	-0.483352
C	-2.999029	-7.393518	-0.359149
C	-5.150851	-6.148982	-0.330598
C	-7.983444	-1.233409	-0.306267
C	-7.980350	1.252886	-0.307010
C	7.679471	3.719015	-0.590961
C	6.996353	4.905290	-0.564286
C	0.542955	8.642221	-0.378643
C	-0.825942	8.644341	-0.348883
C	-7.293601	4.925173	-0.262956
C	-7.980364	3.740564	-0.257836
C	-7.989674	-3.721060	-0.255965
C	-7.305901	-4.907390	-0.260959
C	-0.847770	-8.642910	-0.349056
C	0.521119	-8.644264	-0.378975
C	6.983937	-4.923713	-0.564244
C	7.670047	-3.739158	-0.590724
H	1.099330	9.584456	-0.327183
H	-1.376723	9.588296	-0.274121
H	-3.525561	8.348079	-0.278860
H	-5.678602	7.110399	-0.254481
H	-7.831525	5.877138	-0.196597
H	-9.073495	3.734718	-0.186875
H	-9.073664	1.253135	-0.226464
H	-9.076751	-1.230908	-0.225663
H	-9.082771	-3.712471	-0.184774
H	-7.846176	-5.857998	-0.194240
H	-5.696446	-7.096674	-0.252949
H	-3.546595	-8.339806	-0.278330
H	-1.400917	-9.585478	-0.274270
H	1.075132	-9.587899	-0.327620
H	3.221264	-8.346339	-0.421200
H	5.371721	-7.108166	-0.481739
H	7.523748	-5.875358	-0.509575
H	8.764985	-3.732458	-0.557601
H	8.763028	-1.252318	-0.606458
H	8.766173	1.229447	-0.606688
H	8.774394	3.709583	-0.558011
H	7.538563	5.855576	-0.509671
H	5.389692	7.093813	-0.481491
H	3.242357	8.337454	-0.420787

Graphene-catalyzed corannulene product

C	1.394090	-2.467545	2.874835
C	2.217722	-1.331210	2.885293
C	-1.143901	-3.296778	2.841227

C	-0.028955	-2.398914	2.583045
C	-0.432728	-1.145132	2.143779
C	1.711012	0.003087	2.606417
C	-2.479010	-2.865024	2.824810
C	2.214566	1.338525	2.885546
C	-1.151663	3.296215	2.841657
C	-2.485756	2.861334	2.825129
C	-0.034601	2.401002	2.583406
C	-0.435409	1.146344	2.143925
C	-1.781752	0.707054	2.128331
C	-2.853948	1.481236	2.549380
C	-4.052186	0.698111	2.806650
C	-4.050536	-0.705494	2.806574
C	-2.850457	-1.485765	2.549220
C	-1.780093	-0.709000	2.128263
C	1.388266	2.472922	2.875270
C	0.398112	0.001578	2.154331
H	-4.984106	1.208920	3.073903
H	-4.981251	-1.218527	3.073770
H	-3.255404	-3.590264	3.093051
H	-0.945396	-4.337339	3.121654
H	1.841269	-3.426686	3.159424
H	3.265599	-1.460749	3.178456
H	3.262128	1.470483	3.178753
H	1.833184	3.433062	3.160039
H	-0.955617	4.337206	3.122220
H	-3.263856	3.584720	3.093435
C	-2.673978	2.465761	-0.864223
C	-1.245934	2.469440	-0.890668
C	-0.529593	1.236298	-0.957382
C	-1.242703	-0.001379	-1.004725
C	-2.670015	-0.002712	-0.962342
C	-3.385137	1.232756	-0.908987
C	0.898893	1.237856	-0.905705
C	-0.527259	-1.237707	-0.957355
C	0.901224	-1.236576	-0.905684
C	1.613540	0.001312	-0.873666
C	1.610280	-2.468012	-0.775819
C	0.895001	-3.703094	-0.724248
C	-0.528374	-3.703968	-0.768899
C	-1.241290	-2.472177	-0.890508
C	-2.669337	-2.471174	-0.864055
C	-3.382818	-1.239515	-0.908937
C	-0.535328	3.702574	-0.769151
C	0.888044	3.704369	-0.724445
C	1.605635	2.470627	-0.775905

C	3.030405	2.471312	-0.671896
C	3.743391	1.239265	-0.654655
C	3.034645	0.002652	-0.748549
C	3.035048	-2.466014	-0.671795
C	3.745714	-1.232629	-0.654603
C	3.739204	3.708201	-0.540213
C	1.597958	4.940030	-0.582046
C	-1.253746	4.937233	-0.669214
C	-3.390718	3.700939	-0.755518
C	-4.814912	1.230171	-0.828231
C	-4.812593	-1.239603	-0.828182
C	-3.383765	-3.707689	-0.755284
C	-1.244477	-4.939966	-0.668869
C	1.607230	-4.937410	-0.581738
C	3.746162	-3.701563	-0.540013
C	5.171788	-1.230624	-0.523916
C	5.169468	1.239945	-0.523978
C	0.891054	-6.169248	-0.508338
C	5.880306	-2.465266	-0.426213
C	5.162174	3.706896	-0.433222
C	-0.542801	6.168588	-0.547516
C	-5.526818	2.463807	-0.743694
C	-4.809728	-3.705507	-0.707745
C	-4.816673	3.696082	-0.707940
C	-5.522189	-2.474571	-0.743601
C	-0.531223	-6.169974	-0.547074
C	5.169127	-3.697580	-0.433014
C	0.879475	6.170529	-0.508757
C	5.875667	2.475921	-0.426353
C	-5.525541	-0.005385	-0.805222
C	-2.679264	4.933467	-0.668425
C	3.021984	4.940109	-0.506112
C	5.881010	0.005329	-0.470143
C	3.031254	-4.934813	-0.505827
C	-2.669999	-4.938872	-0.668072
C	1.615484	-7.410595	-0.379418
C	-1.259113	-7.412224	-0.452517
C	-3.389652	-6.182194	-0.560060
C	-5.523790	-4.955221	-0.604736
C	-6.963410	-2.468122	-0.672470
C	-6.963352	-0.006731	-0.719612
C	3.747536	-6.177812	-0.375137
C	5.880437	-4.947450	-0.315680
C	7.318174	-2.456214	-0.305714
C	7.315757	0.006681	-0.341474
C	7.313549	2.469578	-0.305861

C	5.871139	4.958108	-0.315981
C	3.735934	6.184461	-0.375527
C	1.601577	7.413246	-0.379940
C	-1.273017	7.409478	-0.453060
C	-3.401245	6.175442	-0.560477
C	-5.533076	4.944460	-0.604994
C	-6.968024	2.454656	-0.672541
C	-2.656431	-7.392321	-0.464922
C	-4.807207	-6.153335	-0.541209
C	3.011843	-7.389180	-0.322640
C	5.163179	-6.146888	-0.293140
C	-7.645774	-1.248701	-0.669382
C	-7.648100	1.233959	-0.669409
C	-4.818744	6.143922	-0.541581
C	-2.670296	7.386952	-0.465451
C	2.997973	7.394452	-0.323141
C	5.151633	6.156200	-0.293527
C	7.995404	1.249806	-0.273633
C	7.997737	-1.235162	-0.273558
C	-7.649562	-3.733225	-0.591581
C	-6.964077	-4.917686	-0.559986
C	-0.507707	-8.637176	-0.338782
C	0.860865	-8.636567	-0.304820
C	7.317963	-4.907295	-0.214828
C	8.002430	-3.721562	-0.211215
C	7.995430	3.736215	-0.211445
C	7.308738	4.920660	-0.215135
C	0.844661	8.637808	-0.305463
C	-0.523910	8.635848	-0.339435
C	-6.973289	4.904222	-0.560199
C	-7.656548	3.718473	-0.591701
H	-1.063294	-9.579144	-0.274900
H	1.413558	-9.578031	-0.214180
H	3.558279	-8.334552	-0.224915
H	5.706925	-7.094255	-0.199835
H	7.856324	-5.858023	-0.135276
H	9.094711	-3.712590	-0.128284
H	9.089910	-1.232679	-0.178639
H	9.087580	1.249381	-0.178718
H	9.087726	3.729300	-0.128521
H	7.845311	5.872404	-0.135654
H	5.693598	7.104595	-0.200299
H	3.542633	8.340857	-0.225498
H	1.395587	9.580315	-0.214912
H	-1.081263	9.576778	-0.275649
H	-3.221909	8.331248	-0.388496

H	-5.366689	7.090092	-0.461493
H	-7.514207	5.854385	-0.491975
H	-8.751147	3.707889	-0.549049
H	-8.742826	1.230649	-0.610510
H	-8.740505	-1.247444	-0.610492
H	-8.744180	-3.724698	-0.548956
H	-7.503208	-5.868862	-0.491714
H	-5.353374	-7.100527	-0.461062
H	-3.206270	-8.337645	-0.387891

Graphene-catalyzed sumanene reactant

C	5.277184	-3.703576	-0.447215
C	5.278176	-1.233330	-0.466452
C	5.276659	1.239262	-0.462886
C	5.272649	3.709597	-0.443245
C	3.133875	4.946108	-0.566401
C	0.992579	6.180583	-0.661444
C	-1.142486	4.944789	-0.792773
C	-3.281142	3.706974	-0.881412
C	-5.418028	2.469294	-0.958284
C	-5.415994	-0.003945	-0.988966
C	-5.414259	-2.476366	-0.973007
C	-3.276680	-3.711472	-0.885008
C	-1.136965	-4.947051	-0.782968
C	0.999664	-6.179763	-0.654857
C	3.139832	-4.942771	-0.566703
C	3.139826	-2.468918	-0.611803
C	3.137376	0.001575	-0.614621
C	3.136679	2.472434	-0.602636
C	0.996605	3.707640	-0.721910
C	-1.138166	2.469847	-0.826499
C	-3.275206	1.233889	-0.910201
C	-3.273984	-1.238877	-0.916552
C	-1.135347	-2.471101	-0.823448
C	1.001586	-3.706551	-0.720262
C	-0.422445	-6.180657	-0.719982
C	-2.563058	-4.945753	-0.832297
C	-4.702953	-3.709378	-0.929261
C	-4.703586	-1.239422	-0.970216
C	-4.705746	1.232521	-0.958567
C	-4.707738	3.703098	-0.917977
C	-2.568659	4.942102	-0.836104
C	-0.429610	6.179363	-0.728767
C	1.709798	4.946877	-0.653438
C	3.849014	3.712333	-0.538559
C	5.984247	2.476924	-0.405093

C	5.987348	0.003418	-0.415017
C	5.987413	-2.470154	-0.409132
C	3.853539	-3.707838	-0.543963
C	1.715588	-4.945279	-0.650818
C	3.850156	-1.234874	-0.564235
C	3.848442	1.238925	-0.558194
C	1.710819	2.471887	-0.687141
C	-0.426286	1.235729	-0.788140
C	-0.425845	3.706210	-0.788367
C	-2.564758	2.467793	-0.873771
C	-2.562305	-0.002423	-0.880050
C	-2.562217	-2.471227	-0.876160
C	-0.421239	-3.707141	-0.779072
C	-0.423798	-1.236242	-0.788782
C	1.714648	-2.469814	-0.696457
C	1.713201	0.000518	-0.691444
C	-1.137766	-0.000962	-0.824027
C	1.002111	-1.235880	-0.737557
C	7.426572	-2.461437	-0.307801
C	-5.424011	4.955648	-0.910047
C	7.423975	0.004220	-0.313906
C	-3.290471	6.188451	-0.827520
C	7.423514	2.469931	-0.305137
C	-1.159388	7.423993	-0.723946
C	-1.150792	-7.426029	-0.716090
C	-5.417630	-4.962761	-0.920930
C	-3.283249	-6.193131	-0.826001
C	-6.856839	-2.469744	-1.002108
C	1.725923	-7.424433	-0.584689
C	-6.856080	-0.004450	-1.015669
C	3.857874	-6.189178	-0.495628
C	-6.860547	2.460837	-0.989370
C	5.989984	-4.956256	-0.381322
C	1.717270	7.426161	-0.591738
C	5.984058	4.963157	-0.379688
C	3.850491	6.193481	-0.497441
C	-6.858652	-4.923645	-0.959122
C	-4.701334	-6.162999	-0.871357
C	-2.548254	-7.405827	-0.769643
C	8.111460	-3.729179	-0.250835
C	8.105780	-1.239550	-0.265020
C	8.104194	1.248805	-0.263587
C	-0.407300	8.652731	-0.660304
C	-2.556895	7.402201	-0.774709
C	-4.708834	6.156641	-0.866148
C	0.970869	-8.652978	-0.589143

C	3.122353	-7.402815	-0.510082
C	5.273978	-6.157390	-0.407803
C	7.428237	-4.915565	-0.285079
C	7.422392	4.924132	-0.283694
C	5.266591	6.163406	-0.408326
C	3.113622	7.406279	-0.515267
C	-7.548118	3.728337	-0.982249
C	-7.540330	1.239077	-1.017304
C	-7.538759	-1.248856	-1.023644
C	-7.543019	-3.738049	-0.996925
C	0.960743	8.653772	-0.597973
C	-0.397197	-8.653781	-0.651585
C	-6.865020	4.914704	-0.944716
C	8.106946	3.738510	-0.248781
H	-8.638390	-3.732453	-1.021026
H	-8.635193	-1.248946	-1.041471
H	-8.636762	1.237557	-1.036263
H	-8.643496	3.721538	-1.006083
H	-7.408806	5.865870	-0.938329
H	-5.257939	7.105815	-0.857961
H	-3.106923	8.350850	-0.767909
H	-0.961585	9.597837	-0.659574
H	1.511222	9.599765	-0.547572
H	3.659594	8.355835	-0.462255
H	5.811935	7.113446	-0.357436
H	7.962766	5.876154	-0.237401
H	9.200050	3.733204	-0.174001
H	9.198078	1.249037	-0.186110
H	9.199619	-1.238533	-0.187006
H	9.204513	-3.722590	-0.175461
H	7.969599	-5.866961	-0.237585
H	5.820432	-7.106696	-0.355266
H	3.669494	-8.351646	-0.456116
H	1.522576	-9.598234	-0.538234
H	-0.950235	-9.599627	-0.650710
H	-3.097134	-8.355168	-0.764036
H	-5.249528	-7.112700	-0.863594
H	-7.401337	-5.875429	-0.953277
C	-4.573457	-0.606288	2.396775
C	-4.025090	-1.934339	2.417899
C	-2.760664	-2.195391	2.975578
C	-3.865464	0.486659	2.928756
C	-3.849935	2.020413	2.671033
C	1.858392	-1.465311	2.669573
C	1.419311	-0.219430	3.152457
C	1.827495	1.261226	2.909404

C	0.983355	-2.604549	2.634810
C	-0.348906	-2.518111	3.078287
C	-0.717470	-1.303386	3.684036
C	0.132726	-0.198475	3.720156
C	-0.413709	1.128545	3.696331
C	0.492287	2.032492	3.112896
C	-0.067616	3.212056	2.589206
C	-1.490761	3.400848	2.527176
C	-2.380803	2.416039	2.991923
C	-1.794824	1.313135	3.638622
C	-2.669828	0.175973	3.601345
C	-2.138930	-1.113404	3.624276
C	-1.667523	-3.280761	2.763803
H	1.349448	-3.503826	2.127517
H	2.834861	-1.566637	2.182971
H	-4.565366	-2.709822	1.863463
H	-5.499362	-0.454438	1.831474
H	-1.858082	4.278030	1.982892
H	0.560276	3.959718	2.092516
H	2.615346	1.597661	3.612229
H	2.232926	1.409863	1.894510
H	-1.676788	-3.672117	1.732782
H	-1.812850	-4.154146	3.430147
H	-4.118577	2.261646	1.628948
H	-4.575793	2.558209	3.312810
C	0.999795	1.236366	-0.732808

Graphene-catalyzed sumanene inversion TS

C	-5.231143	3.752113	-0.381738
C	-5.258102	1.282853	-0.433658
C	-5.282857	-1.189274	-0.450499
C	-5.302854	-3.659212	-0.416244
C	-3.174857	-4.916179	-0.514130
C	-1.044220	-6.170097	-0.562908
C	1.102197	-4.956069	-0.706982
C	3.251909	-3.740413	-0.811676
C	5.401897	-2.524081	-0.869433
C	5.424274	-0.051409	-0.887304
C	5.446742	2.419885	-0.847069
C	3.320957	3.676095	-0.815781
C	1.192632	4.933301	-0.735320
C	-0.930719	6.186045	-0.585300
C	-3.081971	4.969907	-0.498067
C	-3.107853	2.497006	-0.575618
C	-3.131800	0.027564	-0.613615
C	-3.155634	-2.443701	-0.598476

C	-1.026212	-3.699410	-0.682873
C	1.119831	-2.483159	-0.805290
C	3.270110	-1.268480	-0.876649
C	3.293523	1.204349	-0.874122
C	1.165913	2.458359	-0.812005
C	-0.958020	3.713954	-0.683854
C	0.491105	6.173427	-0.653909
C	2.619474	4.917441	-0.765085
C	4.747469	3.659245	-0.816143
C	4.723986	1.190629	-0.877338
C	4.701414	-1.280483	-0.887462
C	4.678957	-3.750761	-0.830292
C	2.527898	-4.967270	-0.742586
C	0.378259	-6.182479	-0.618932
C	-1.750349	-4.930363	-0.589454
C	-3.879270	-3.675930	-0.512891
C	-6.002536	-2.419727	-0.385462
C	-5.980415	0.053441	-0.390350
C	-5.954268	2.526037	-0.356006
C	-3.808042	3.742119	-0.486250
C	-1.658532	4.958688	-0.591938
C	-3.830662	1.270505	-0.540834
C	-3.855245	-1.202725	-0.556773
C	-1.729485	-2.457200	-0.680287
C	0.418893	-1.241961	-0.796546
C	0.396545	-3.711709	-0.736663
C	2.547266	-2.494869	-0.835851
C	2.568458	-0.025001	-0.866044
C	2.593378	2.443820	-0.838766
C	0.464131	3.700690	-0.750789
C	0.441271	1.230322	-0.797857
C	-1.683483	2.484490	-0.670412
C	-1.708313	0.014290	-0.700238
C	1.142819	-0.012248	-0.837383
C	-0.984594	1.244086	-0.740434
C	-7.392948	2.531470	-0.247007
C	5.383657	-5.009493	-0.791527
C	-7.416390	0.066694	-0.279374
C	3.238268	-6.219643	-0.701310
C	-7.441189	-2.398481	-0.277947
C	1.096400	-7.433286	-0.580908
C	1.232197	7.411125	-0.628356
C	5.474687	4.904833	-0.775854
C	3.352291	6.157089	-0.727537
C	6.889171	2.398755	-0.830677
C	-1.643618	7.437259	-0.495193

C	6.864204	-0.065190	-0.870107
C	-3.786779	6.222726	-0.407676
C	6.844826	-2.529807	-0.863615
C	-5.930649	5.011196	-0.296283
C	-1.780206	-7.407713	-0.471488
C	-6.025768	-4.905231	-0.335613
C	-3.902897	-6.155662	-0.423111
C	6.915639	4.851648	-0.768830
C	4.770425	6.112399	-0.737623
C	2.629637	7.376914	-0.668237
C	-8.064318	3.805355	-0.170700
C	-8.085015	1.316673	-0.214579
C	-8.109328	-1.170813	-0.231735
C	0.333482	-8.653865	-0.494546
C	2.494142	-7.425359	-0.624104
C	4.656891	-6.202519	-0.731549
C	-0.876432	8.658205	-0.486950
C	-3.039543	7.429103	-0.412394
C	-5.202477	6.204982	-0.311651
C	-7.368712	4.984730	-0.193256
C	-7.463666	-4.852144	-0.240729
C	-5.319062	-6.111971	-0.342761
C	-3.176870	-7.374775	-0.408211
C	7.520275	-3.803527	-0.839169
C	7.536673	-1.314693	-0.865736
C	7.559462	1.171569	-0.843335
C	7.588445	3.659195	-0.793431
C	-1.034892	-8.641791	-0.443092
C	0.491470	8.645814	-0.549907
C	6.825312	-4.983007	-0.805639
C	-8.136940	-3.659935	-0.214253
H	8.684006	3.641782	-0.783678
H	8.655982	1.160461	-0.828714
H	8.633255	-1.323675	-0.854611
H	8.615979	-3.806892	-0.842122
H	7.359417	-5.939420	-0.781711
H	5.196757	-7.156541	-0.699165
H	3.035705	-8.378453	-0.592638
H	0.879726	-9.603358	-0.468445
H	-1.594375	-9.581513	-0.376110
H	-3.731507	-8.318297	-0.339030
H	-5.872881	-7.056268	-0.277585
H	-8.012734	-5.798769	-0.185921
H	-9.229844	-3.643448	-0.137698
H	-9.202711	-1.160017	-0.147743
H	-9.178362	1.326233	-0.130065

H	-9.157057	3.809089	-0.090185
H	-7.899524	5.941290	-0.131454
H	-5.738597	7.159330	-0.244930
H	-3.576818	8.382679	-0.343960
H	-1.418690	9.608238	-0.423891
H	1.054489	9.585712	-0.536575
H	3.188565	8.320088	-0.642182
H	5.328165	7.056094	-0.705709
H	7.467265	5.797915	-0.739141
C	4.728874	0.700550	2.536677
C	4.159418	2.044573	2.558052
C	2.756893	2.287260	2.602178
C	3.929601	-0.477991	2.560508
C	3.948779	-2.074388	2.579974
C	-2.048129	1.533287	2.754035
C	-1.556921	0.196645	2.736682
C	-1.960642	-1.347100	2.768668
C	-1.169587	2.698934	2.725117
C	0.250221	2.595628	2.679153
C	0.652686	1.270955	2.650042
C	-0.173729	0.173872	2.675782
C	0.374226	-1.117782	2.657099
C	-0.570381	-2.129326	2.702248
C	0.050167	-3.411191	2.683146
C	1.498446	-3.589663	2.638930
C	2.409759	-2.495737	2.609363
C	1.737038	-1.285448	2.614514
C	2.581058	-0.164835	2.588366
C	2.044721	1.099792	2.607025
C	1.623615	3.409610	2.658478
H	-1.672626	3.672831	2.731075
H	-3.122444	1.748263	2.780919
H	4.882254	2.867711	2.526726
H	5.822754	0.649142	2.489295
H	1.848943	-4.627855	2.619352
H	-0.541875	-4.333650	2.691226
H	-2.515332	-1.596049	3.691535
H	-2.621691	-1.613749	1.926196
H	1.682636	4.093077	1.794050
H	1.728460	4.038200	3.561409
H	4.468880	-2.488999	1.699260
H	4.484529	-2.456342	3.467956
C	-1.007630	-1.228731	-0.744403

Graphene-catalyzed sumanene product

C	5.171189	-3.811855	-0.404864

C	5.230241	-1.344873	-0.481192
C	5.284515	1.125396	-0.485147
C	5.333030	3.593181	-0.414491
C	3.222608	4.875527	-0.529844
C	1.109094	6.154885	-0.578649
C	-1.049344	4.969234	-0.761326
C	-3.212229	3.780795	-0.874661
C	-5.375700	2.590988	-0.881191
C	-5.428599	0.120992	-0.938625
C	-5.482614	-2.348361	-0.895594
C	-3.373469	-3.629957	-0.891541
C	-1.263285	-4.911242	-0.774667
C	0.841729	-6.188719	-0.582772
C	3.008020	-5.001346	-0.523982
C	3.068231	-2.531674	-0.659814
C	3.124162	-0.063921	-0.724938
C	3.175747	2.405197	-0.665265
C	1.063598	3.687411	-0.764714
C	-1.094311	2.500649	-0.965684
C	-3.260103	1.311916	-1.018234
C	-3.314381	-1.161327	-1.025696
C	-1.201708	-2.441821	-0.972121
C	0.903564	-3.721039	-0.766449
C	-0.579344	-6.157988	-0.650522
C	-2.688866	-4.877832	-0.801596
C	-4.799316	-3.595527	-0.863477
C	-4.744093	-1.129463	-0.962648
C	-4.690471	1.340881	-0.955478
C	-4.638549	3.807780	-0.843622
C	-2.474404	4.997539	-0.783700
C	-0.312127	6.184902	-0.639603
C	1.800119	4.907627	-0.626830
C	3.911811	3.627181	-0.539043
C	6.017539	2.345815	-0.388458
C	5.966575	-0.125199	-0.419777
C	5.909518	-2.595605	-0.380873
C	3.750215	-3.783920	-0.532076
C	1.585953	-4.972218	-0.626784
C	3.806109	-1.314630	-0.626101
C	3.860063	1.156459	-0.628915
C	1.752615	2.436804	-0.790348
C	-0.406200	1.250895	-1.008698
C	-0.358238	3.717888	-0.837658
C	-2.522276	2.529474	-0.968180
C	-2.573157	0.059734	-1.061945
C	-2.629884	-2.409341	-0.979062

C	-0.518092	-3.690113	-0.845641
C	-0.459385	-1.223388	-1.011703
C	1.646210	-2.501554	-0.789724
C	1.704951	-0.033056	-0.870681
C	-1.145776	0.029122	-1.064747
C	0.966404	-1.254366	-0.922282
C	7.345656	-2.619064	-0.243420
C	-5.328119	5.072416	-0.754801
C	7.399553	-0.156196	-0.276578
C	-3.169505	6.256020	-0.694539
C	7.453474	2.306982	-0.251891
C	-1.015152	7.442781	-0.567919
C	-1.336503	-7.384511	-0.583734
C	-5.542698	-4.829492	-0.780775
C	-3.437643	-6.105681	-0.717794
C	-6.923712	-2.309139	-0.838923
C	1.536351	-7.446993	-0.454127
C	-6.866991	0.152081	-0.869113
C	3.694652	-6.261078	-0.395620
C	-6.817571	2.613737	-0.823498
C	5.852963	-5.078173	-0.288557
C	1.857958	7.381861	-0.452680
C	6.069174	4.828935	-0.300959
C	3.963576	6.104352	-0.403506
C	-6.982224	-4.759094	-0.750932
C	-4.854458	-6.044359	-0.719776
C	-2.732748	-7.332781	-0.621689
C	8.000025	-3.900086	-0.145791
C	8.052140	-1.413454	-0.200508
C	8.106407	1.071707	-0.205151
C	-0.239591	8.652880	-0.455387
C	-2.412453	7.451570	-0.599455
C	-4.587666	6.256054	-0.691822
C	0.753323	-8.656658	-0.407841
C	2.931653	-7.456576	-0.370400
C	5.109175	-6.261786	-0.288947
C	7.289524	-5.070291	-0.166280
C	7.504235	4.758636	-0.180852
C	5.377158	6.043581	-0.300900
C	3.252807	7.331523	-0.375184
C	-7.478393	3.893079	-0.753290
C	-7.524079	1.407944	-0.824234
C	-7.577876	-1.074336	-0.832481
C	-7.639696	-3.558755	-0.777069
C	1.128107	8.624119	-0.401873
C	-0.614072	-8.626829	-0.468328

C	-6.769334	5.063661	-0.722102
C	8.163060	3.558589	-0.158449
H	-8.734439	-3.525437	-0.744540
H	-8.673171	-1.048413	-0.784324
H	-8.619464	1.429118	-0.775586
H	-8.573495	3.907177	-0.719226
H	-7.290200	6.025837	-0.662748
H	-5.115522	7.214906	-0.623637
H	-2.943573	8.409055	-0.537633
H	-0.775899	9.607244	-0.408539
H	1.698910	9.555150	-0.312562
H	3.817762	8.266599	-0.279605
H	5.940207	6.980286	-0.210106
H	8.062361	5.698301	-0.102541
H	9.254051	3.527533	-0.061607
H	9.197564	1.046891	-0.098181
H	9.143312	-1.436023	-0.093253
H	9.091233	-3.916352	-0.047754
H	7.805997	-6.033256	-0.085177
H	5.630857	-7.221964	-0.196254
H	3.455474	-8.415128	-0.273051
H	1.283110	-9.611429	-0.316470
H	-1.191028	-9.557345	-0.425073
H	-3.304862	-8.266586	-0.563585
H	-5.423443	-6.979682	-0.655813
H	-7.544216	-5.698181	-0.697211
C	-4.472553	-0.913405	3.114541
C	-3.804381	-2.187910	3.128665
C	-2.475667	-2.327368	2.682250
C	-3.829086	0.251466	2.652615
C	-3.973379	1.786774	2.887627
C	2.054217	-1.180690	3.239519
C	1.522749	0.033253	2.761362
C	1.782013	1.551852	3.005544
C	1.284755	-2.396676	3.222897
C	-0.033251	-2.428393	2.726156
C	-0.480880	-1.237259	2.134825
C	0.262928	-0.060960	2.151066
C	-0.401749	1.206789	2.138238
C	0.388299	2.199155	2.738139
C	-0.312458	3.332266	3.196122
C	-1.750012	3.390869	3.167393
C	-2.521114	2.316824	2.681111
C	-1.792105	1.263187	2.109573
C	-2.557614	0.053410	2.092821
C	-1.911016	-1.179195	2.106396

C	-1.297499	-3.316241	2.941183
H	1.719442	-3.271143	3.720588
H	3.024696	-1.208661	3.748085
H	-4.326260	-3.022158	3.611337
H	-5.459496	-0.860191	3.588415
H	-2.226070	4.252858	3.648664
H	0.212475	4.153389	3.697682
H	2.133108	1.746614	4.034023
H	2.558862	1.950680	2.323427
H	-1.321290	-4.174607	2.240701
H	-1.333176	-3.737636	3.961039
H	-4.682755	2.246965	2.171267
H	-4.352047	2.012815	3.899786
C	1.019591	1.219270	-0.920986

Graphene-catalyzed 2,2prime-dimethylbiphenyl reactant

C	1.692792	-3.223474	-0.799711
C	0.357227	-2.720242	-0.752711
C	0.126225	-1.312930	-0.736568
C	1.230817	-0.408913	-0.732726
C	2.564741	-0.912314	-0.741832
C	2.794671	-2.320728	-0.781845
C	-1.207696	-0.809419	-0.673274
C	0.999968	0.999381	-0.704222
C	-0.335397	1.504082	-0.692204
C	-1.439236	0.599093	-0.673220
C	-0.565400	2.911196	-0.650289
C	0.539917	3.813827	-0.601089
C	1.871989	3.309309	-0.592680
C	2.103317	1.901126	-0.643081
C	3.437977	1.394694	-0.617599
C	3.668273	-0.009084	-0.672631
C	-0.746516	-3.624532	-0.694069
C	-2.076103	-3.121499	-0.607902
C	-2.308667	-1.713027	-0.612134
C	-3.641160	-1.208776	-0.520481
C	-3.873300	0.196201	-0.522781
C	-2.771276	1.102084	-0.590798
C	-1.900653	3.414671	-0.591638
C	-3.002406	2.511457	-0.566609
C	-4.744633	-2.116118	-0.434952
C	-3.180323	-4.028271	-0.526587
C	-0.513727	-5.036810	-0.687849
C	1.923973	-4.635789	-0.786857
C	4.133537	-2.826778	-0.753074
C	5.005841	-0.516147	-0.637604

C	4.543510	2.299224	-0.531139
C	2.979040	4.213377	-0.516207
C	0.308472	5.225158	-0.540133
C	-2.131284	4.826284	-0.535689
C	-4.339232	3.015626	-0.475192
C	-5.208924	0.701638	-0.424259
C	1.414499	6.124713	-0.481471
C	-4.566775	4.423790	-0.441485
C	-6.075593	-1.609962	-0.341833
C	-1.616868	-5.938571	-0.612196
C	4.361590	-4.235623	-0.764230
C	5.875994	1.790817	-0.491595
C	3.259969	-5.137481	-0.784530
C	6.106526	0.386993	-0.544733
C	2.745681	5.620077	-0.466014
C	-3.466078	5.326385	-0.470695
C	-2.946161	-5.435699	-0.529147
C	-6.307362	-0.205263	-0.339858
C	5.235498	-1.923246	-0.681747
C	0.820166	-5.538666	-0.743739
C	-4.511126	-3.523305	-0.434541
C	-5.439124	2.109547	-0.411990
C	-1.026214	5.727999	-0.518062
C	4.311531	3.705750	-0.482302
C	1.174154	7.546260	-0.425491
C	3.866365	6.525675	-0.391280
C	5.424915	4.615527	-0.398751
C	6.986197	2.707884	-0.401487
C	7.452343	-0.131529	-0.502930
C	6.581778	-2.433685	-0.639083
C	-1.258494	7.148095	-0.457544
C	-3.691270	6.750556	-0.420130
C	-5.917199	4.925022	-0.359251
C	-6.783807	2.617258	-0.320002
C	-7.651551	0.310796	-0.247434
C	-7.183139	-2.530385	-0.252804
C	-5.621835	-4.436011	-0.347417
C	-4.063875	-6.344043	-0.444016
C	-1.375284	-7.360911	-0.609417
C	1.053961	-6.959757	-0.730739
C	3.486264	-6.562470	-0.777610
C	5.713612	-4.738957	-0.733657
C	5.166005	6.010265	-0.358611
C	6.740027	4.083840	-0.358284
C	-0.140945	8.022001	-0.421730
C	-2.596206	7.620458	-0.421021

C	7.658816	-1.513760	-0.552641
C	6.781618	-3.838170	-0.676082
C	2.391652	-7.432469	-0.760078
C	-0.061246	-7.835357	-0.672162
C	-5.361915	-5.831091	-0.355661
C	-6.935563	-3.906784	-0.257649
C	-7.858661	1.693876	-0.242537
C	-6.983761	4.022129	-0.303448
C	8.541095	0.809291	-0.408499
C	8.319365	2.159803	-0.360632
C	3.594928	7.941257	-0.347407
C	2.314580	8.426747	-0.365304
C	-5.052709	7.221782	-0.357629
C	-6.111327	6.353572	-0.327824
C	-8.737770	-0.633656	-0.160332
C	-8.514955	-1.984843	-0.162729
C	-3.791460	-7.760090	-0.451896
C	-2.512735	-8.243763	-0.530952
C	4.848622	-7.034943	-0.772430
C	5.908067	-6.167641	-0.750509
H	4.446491	8.628850	-0.296041
H	2.131817	9.506458	-0.328100
H	-0.318264	9.103282	-0.376728
H	-2.772581	8.701966	-0.377828
H	-5.223664	8.303620	-0.326745
H	-7.137410	6.734062	-0.273664
H	-8.008107	4.408157	-0.237667
H	-8.882377	2.080902	-0.173006
H	-9.758551	-0.241541	-0.091025
H	-9.355751	-2.684153	-0.094862
H	-7.780772	-4.602280	-0.190054
H	-6.208003	-6.525661	-0.289638
H	-4.640779	-8.449586	-0.389965
H	-2.328977	-9.323949	-0.532743
H	0.117609	-8.917299	-0.665375
H	2.568877	-8.514669	-0.752331
H	5.019728	-8.117184	-0.777108
H	6.935171	-6.548976	-0.737311
H	7.807079	-4.225761	-0.647510
H	8.683516	-1.902999	-0.519631
H	9.562859	0.414936	-0.376053
H	9.162069	2.856543	-0.289982
H	7.587345	4.776878	-0.291891
H	6.014344	6.702602	-0.298145
C	-0.111608	-0.715348	3.450813
C	-0.581633	-1.976511	3.881869

C	-1.927437	-2.344959	3.787597
C	-2.853838	-1.440650	3.255526
C	-2.418700	-0.167119	2.875033
C	-1.071100	0.229154	2.976557
C	1.355233	-0.426492	3.446989
C	2.309696	-1.355522	2.933431
C	3.654567	-0.952976	2.822413
C	4.092625	0.309829	3.234348
C	3.172950	1.195165	3.808489
C	1.828982	0.821852	3.909903
H	0.132046	-2.684158	4.310693
H	-2.244974	-3.338497	4.120693
H	-3.906559	-1.718822	3.139361
H	-3.142381	0.550707	2.472279
H	4.372926	-1.655943	2.384768
H	5.142561	0.594770	3.109652
H	3.493916	2.178634	4.167230
H	1.119574	1.515232	4.368421
C	1.964158	-2.760880	2.493959
H	1.911624	-3.453872	3.353880
H	0.992789	-2.817589	1.978251
H	2.741427	-3.153212	1.820255
C	-0.731377	1.645810	2.570065
H	-0.692408	2.320696	3.445210
H	0.242958	1.722321	2.063237
H	-1.507255	2.045789	1.898878

Graphene-catalyzed 2,2prime-dimethylbiphenyl rotation TS

C	-3.072531	2.030766	-0.630858
C	-1.659384	2.234734	-0.647723
C	-0.777620	1.114128	-0.649093
C	-1.309307	-0.210580	-0.658663
C	-2.720477	-0.413338	-0.647783
C	-3.602139	0.708974	-0.639987
C	0.635405	1.317348	-0.628174
C	-0.426878	-1.332062	-0.630727
C	0.986268	-1.129238	-0.614253
C	1.517327	0.195730	-0.603637
C	1.866285	-2.250249	-0.562317
C	1.334867	-3.575913	-0.548119
C	-0.075209	-3.778563	-0.567237
C	-0.957981	-2.655906	-0.611519
C	-2.371510	-2.857723	-0.597714
C	-3.251007	-1.738365	-0.621922
C	-1.127939	3.560432	-0.603091
C	0.281991	3.762854	-0.576645

C	1.164953	2.640663	-0.584363
C	2.577201	2.842969	-0.529362
C	3.456738	1.723501	-0.509417
C	2.927267	0.398339	-0.550668
C	3.278427	-2.046310	-0.504211
C	3.807640	-0.724192	-0.495007
C	3.107275	4.171136	-0.464475
C	0.813069	5.090852	-0.512081
C	-2.013063	4.684980	-0.562510
C	-3.956041	3.155974	-0.582180
C	-5.017812	0.505433	-0.595514
C	-4.666854	-1.941068	-0.581746
C	-2.902837	-4.185925	-0.546978
C	-0.608308	-5.106314	-0.522224
C	2.217972	-4.700116	-0.476424
C	4.160677	-3.171449	-0.431904
C	5.221780	-0.520747	-0.409283
C	4.870803	1.926432	-0.422784
C	1.683994	-6.023097	-0.445200
C	6.099723	-1.643932	-0.345493
C	4.518287	4.370913	-0.391027
C	-1.480432	6.007722	-0.508926
C	-5.896718	1.628364	-0.549527
C	-4.315360	-4.385243	-0.513936
C	-5.367596	2.950129	-0.543096
C	-5.194624	-3.265622	-0.528767
C	0.275076	-6.225546	-0.466829
C	5.570820	-2.965563	-0.358391
C	-0.071516	6.210160	-0.487047
C	5.397564	3.251567	-0.368940
C	-5.546546	-0.818751	-0.570312
C	-3.424555	4.479575	-0.550920
C	2.224358	5.291582	-0.461996
C	5.750028	0.803975	-0.375228
C	3.628661	-4.495108	-0.424192
C	-2.020560	-5.306427	-0.512681
C	2.580386	-7.151681	-0.378332
C	-0.269099	-7.560998	-0.421060
C	-2.556361	-6.642327	-0.458689
C	-4.844756	-5.726360	-0.458571
C	-6.623105	-3.462790	-0.479514
C	-6.971189	-1.023037	-0.510905
C	4.517016	-5.626603	-0.352309
C	6.454593	-4.104003	-0.289466
C	7.524304	-1.431189	-0.260696
C	7.172966	1.008516	-0.285867

C	6.824286	3.448669	-0.282981
C	5.046044	5.712350	-0.329410
C	2.758383	6.627689	-0.396641
C	0.470906	7.545784	-0.425287
C	-2.378389	7.136205	-0.465386
C	-4.314497	5.610917	-0.497598
C	-6.252740	4.088356	-0.489293
C	-7.322925	1.416219	-0.495933
C	-1.656181	-7.738689	-0.420924
C	-3.964886	-6.813051	-0.436768
C	3.960864	-6.932032	-0.337322
C	5.915576	-5.394357	-0.290950
C	-7.470729	-2.350685	-0.472593
C	-7.823821	0.110769	-0.480415
C	-5.714042	5.378689	-0.472330
C	-3.759324	6.916370	-0.463225
C	1.857326	7.723871	-0.385574
C	4.165740	6.798897	-0.336814
C	7.671341	2.336562	-0.246582
C	8.024456	-0.125548	-0.235102
C	-7.122573	-4.814599	-0.430108
C	-6.276738	-5.891479	-0.421783
C	0.651943	-8.669224	-0.368072
C	2.007291	-8.474544	-0.347798
C	7.873761	-3.859730	-0.214695
C	8.382503	-2.588429	-0.200553
C	7.322337	4.800968	-0.232181
C	6.476533	5.877706	-0.254545
C	-0.451349	8.653911	-0.397881
C	-1.806666	8.459071	-0.416356
C	-7.673301	3.844426	-0.448453
C	-8.182284	2.573201	-0.450560
H	0.238282	-9.683432	-0.339122
H	2.688664	-9.331452	-0.302925
H	4.637959	-7.793091	-0.284685
H	6.591482	-6.256275	-0.237181
H	8.544660	-4.724635	-0.165698
H	9.464435	-2.426181	-0.139904
H	9.107849	0.030923	-0.168600
H	8.754914	2.491576	-0.179659
H	8.406139	4.950049	-0.171160
H	6.876931	6.896739	-0.211794
H	4.571697	7.816484	-0.288274
H	2.264612	8.740929	-0.336973
H	-0.038751	9.668117	-0.356451
H	-2.489213	9.315787	-0.389218

H	-4.437826	7.777089	-0.425309
H	-6.391067	6.240387	-0.430548
H	-8.344870	4.709373	-0.410768
H	-9.265289	2.410739	-0.414441
H	-8.908383	-0.045648	-0.436434
H	-8.555635	-2.505171	-0.430275
H	-8.207670	-4.963145	-0.396968
H	-6.678214	-6.910212	-0.382178
H	-4.372310	-7.830321	-0.394236
H	-2.064971	-8.755564	-0.382150
C	0.130035	0.123070	2.868921
C	0.693246	1.426243	2.888000
C	2.061673	1.703058	2.848536
C	2.974621	0.651626	2.796346
C	2.468279	-0.648653	2.798049
C	1.091942	-0.957105	2.833984
C	-1.374860	-0.031085	2.856939
C	-2.335847	1.049361	2.808774
C	-3.710636	0.739323	2.734786
C	-4.216970	-0.560727	2.719882
C	-3.305035	-1.611533	2.798709
C	-1.938097	-1.334677	2.869032
H	0.042526	2.287678	2.929235
H	2.398101	2.745035	2.845729
H	4.053437	0.829269	2.742104
H	3.173259	-1.485920	2.753436
H	-4.414937	1.576481	2.673967
H	-5.293837	-0.738592	2.640236
H	-3.641093	-2.653827	2.791352
H	-1.288815	-2.195614	2.932362
C	-2.070068	2.545613	2.838728
H	-1.577450	2.871660	3.772461
H	-1.457793	2.897840	1.992181
H	-3.027621	3.087840	2.776407
C	0.822721	-2.452289	2.827135
H	0.324751	-2.801080	3.749890
H	0.212022	-2.778910	1.969459
H	1.778481	-2.996336	2.754958

Graphene-catalyzed 2,2prime-dimethylbiphenyl product

C	0.236188	-3.613198	-0.740461
C	-0.747666	-2.577140	-0.732763
C	-0.342322	-1.209756	-0.731465
C	1.046017	-0.877739	-0.709392
C	2.028080	-1.911355	-0.731346
C	1.621844	-3.280415	-0.741093

C	-1.325435	-0.175554	-0.697890
C	1.451230	0.489363	-0.649295
C	0.468058	1.523679	-0.609585
C	-0.919734	1.192159	-0.655247
C	0.873024	2.889458	-0.538356
C	2.261113	3.220498	-0.484705
C	3.241474	2.187936	-0.515987
C	2.836891	0.820514	-0.590200
C	3.819543	-0.214993	-0.611871
C	3.415525	-1.578819	-0.676017
C	-2.136149	-2.909837	-0.709128
C	-3.115769	-1.876792	-0.693065
C	-2.711343	-0.508039	-0.703634
C	-3.693329	0.527216	-0.667154
C	-3.289378	1.892064	-0.630116
C	-1.901183	2.225414	-0.608800
C	-0.110441	3.924015	-0.495391
C	-1.495116	3.592798	-0.537479
C	-5.084207	0.192351	-0.636263
C	-4.506560	-2.211183	-0.652970
C	-2.541268	-4.282344	-0.675063
C	-0.170629	-4.985549	-0.709548
C	2.606607	-4.319254	-0.719448
C	4.400118	-2.617588	-0.664366
C	5.209951	0.117796	-0.545588
C	4.632444	2.519937	-0.456630
C	2.666595	4.591052	-0.407569
C	0.296292	5.294250	-0.418390
C	-2.480433	4.629684	-0.483871
C	-4.273647	2.929323	-0.563993
C	4.054177	4.919478	-0.355980
C	-2.072334	5.994958	-0.408622
C	-6.064190	1.228180	-0.579690
C	-3.928594	-4.612786	-0.631620
C	2.198014	-5.686538	-0.706116
C	6.189843	-0.919265	-0.548989
C	0.813697	-6.018559	-0.700093
C	5.786056	-2.283259	-0.603824
C	5.034104	3.886979	-0.380281
C	-0.688110	6.326288	-0.376658
C	-4.908323	-3.579947	-0.620036
C	-5.660359	2.593110	-0.549120
C	3.993406	-3.984936	-0.687943
C	-1.558065	-5.316312	-0.678428
C	-5.487153	-1.175927	-0.625691
C	-3.867059	4.295410	-0.501030

C	1.683420	5.624018	-0.374258
C	5.612931	1.484253	-0.474056
C	4.455999	6.302933	-0.277139
C	6.438067	4.214612	-0.324076
C	7.012457	1.818746	-0.412965
C	7.589997	-0.576751	-0.486158
C	6.772863	-3.335774	-0.590513
C	4.983954	-5.030487	-0.663518
C	2.092028	7.002822	-0.294801
C	-0.271248	7.705319	-0.297963
C	-3.071070	7.034980	-0.358314
C	-4.858296	5.338683	-0.440945
C	-6.647538	3.643458	-0.486826
C	-7.464670	0.883180	-0.539101
C	-6.886659	-1.512823	-0.574533
C	-6.312091	-3.909854	-0.570339
C	-4.330175	-5.998106	-0.595381
C	-1.966687	-6.697079	-0.643112
C	0.396389	-7.399366	-0.671143
C	3.196264	-6.727963	-0.684811
C	7.385570	3.186091	-0.341425
C	7.966852	0.768530	-0.422862
C	3.478423	7.302752	-0.250269
C	1.093133	8.010382	-0.261107
C	6.355994	-4.670337	-0.623367
C	4.551185	-6.381882	-0.670088
C	-0.967991	-7.705191	-0.644785
C	-3.352808	-6.998325	-0.603140
C	-7.259815	-2.881738	-0.551421
C	-7.841444	-0.463581	-0.539852
C	-6.230671	4.977606	-0.440357
C	-4.425979	6.688831	-0.375997
C	8.164549	-2.962208	-0.535232
C	8.553115	-1.649940	-0.486173
C	6.808956	5.606086	-0.248573
C	5.866351	6.599312	-0.226893
C	-1.292298	8.722779	-0.257112
C	-2.623860	8.403952	-0.285041
C	-8.039586	3.267812	-0.465575
C	-8.428170	1.954895	-0.489011
C	-6.682842	-5.302988	-0.537499
C	-5.740221	-6.296292	-0.549247
C	1.417000	-8.417950	-0.662665
C	2.748645	-8.098632	-0.670072
H	7.875314	5.854710	-0.207892
H	6.171383	7.650078	-0.168350

H	3.789148	8.352721	-0.189586
H	1.404791	9.060072	-0.200388
H	-0.975493	9.770115	-0.199618
H	-3.382522	9.193761	-0.250279
H	-5.181238	7.482854	-0.333965
H	-6.985094	5.772168	-0.393906
H	-8.789187	4.065887	-0.423843
H	-9.491669	1.692266	-0.465030
H	-8.906882	-0.720837	-0.503584
H	-8.325522	-3.137357	-0.511568
H	-7.749089	-5.552686	-0.500636
H	-6.044872	-7.348448	-0.522488
H	-3.663367	-8.049706	-0.575558
H	-1.279780	-8.756279	-0.619896
H	1.099752	-9.466574	-0.645841
H	3.507121	-8.889276	-0.658698
H	5.305910	-7.177274	-0.651389
H	7.109929	-5.466550	-0.608024
H	8.913903	-3.761579	-0.529745
H	9.616478	-1.389341	-0.442117
H	9.032379	1.023697	-0.375813
H	8.451437	3.440300	-0.296986
C	-1.073753	-0.788474	3.012150
C	-2.017931	-1.851588	2.985604
C	-3.375977	-1.542347	2.773707
C	-3.817417	-0.228295	2.588755
C	-2.884610	0.817354	2.591043
C	-1.531872	0.530083	2.792753
C	0.381417	-1.011718	3.262100
C	1.082965	-1.960287	2.489671
C	2.454577	-2.177496	2.651121
C	3.159841	-1.436804	3.607173
C	2.474215	-0.508504	4.398985
C	1.093212	-0.278544	4.252133
H	-4.102928	-2.363008	2.758503
H	-4.880527	-0.023735	2.427157
H	-3.206278	1.850017	2.422708
H	2.967640	-2.917097	2.028054
H	4.235560	-1.588701	3.744507
H	3.019011	0.053869	5.166751
C	0.421078	0.711052	5.180487
H	0.409721	1.734451	4.761970
H	-0.626999	0.438863	5.383030
H	0.961475	0.762995	6.140940
C	-1.632237	-3.299733	3.195669
H	-1.372090	-3.795802	2.241561

H	-0.760228	-3.404586	3.860585
H	-2.475236	-3.864038	3.628822
H	0.535864	-2.525520	1.731968
H	-0.798003	1.341830	2.766381

h-BN-catalyzed corannulene reactant

C	-2.557500	-1.352413	2.559556
C	-1.720406	-2.473303	2.554048
C	-2.592593	1.281474	2.559529
C	-2.071875	-0.028757	2.899891
C	-0.777271	-0.011526	3.417231
C	-0.312118	-2.385186	2.890478
C	-1.785679	2.424299	2.554256
C	0.795083	-3.255607	2.545114
C	3.640664	-0.651843	2.525102
C	3.621995	0.746923	2.525526
C	2.472080	-1.439010	2.873040
C	1.420228	-0.693449	3.403949
C	1.401221	0.728784	3.404251
C	2.432825	1.502380	2.873845
C	2.044364	2.858654	2.537452
C	0.707989	3.273605	2.546131
C	-0.375627	2.373815	2.891077
C	0.043068	1.150232	3.412736
C	2.119888	-2.805041	2.536211
C	0.073805	-1.150973	3.412329
H	2.801207	3.558684	2.166125
H	0.477355	4.281995	2.184652
H	-2.219254	3.362879	2.190762
H	-3.624367	1.374064	2.201920
H	-3.586496	-1.472530	2.202168
H	-2.128858	-3.423091	2.190552
H	0.591201	-4.269816	2.183773
H	2.894949	-3.484466	2.164197
H	4.542045	-1.157834	2.161370
H	4.509473	1.277151	2.162101
N	-0.730183	-6.291685	-0.562459
N	1.423534	-5.006552	-0.676827
N	3.581841	-3.723209	-0.727906
N	5.740543	-2.442414	-0.696096
N	5.709422	0.074508	-0.727738
N	5.674835	2.591326	-0.690889
N	3.483539	3.815567	-0.723755
N	1.292527	5.042375	-0.675613
N	-0.894008	6.271093	-0.564781
N	-3.059516	4.986149	-0.564171

N	-5.223395	3.698550	-0.534064
N	-5.187565	1.188792	-0.588670
N	-5.154829	-1.323064	-0.588022
N	-5.125146	-3.832852	-0.531044
N	-2.928441	-5.063605	-0.560985
N	-0.770733	-3.780396	-0.707610
N	1.388619	-2.495776	-0.825311
N	3.550325	-1.211294	-0.822948
N	3.517567	1.303742	-0.821603
N	1.323160	2.531523	-0.824631
N	-0.869004	3.759496	-0.708438
N	-3.031140	2.476037	-0.701193
N	-2.997876	-0.038849	-0.731929
N	-2.965613	-2.553740	-0.700622
B	-5.865928	-2.587965	-0.527158
B	-5.894019	-0.076551	-0.552840
B	-5.931447	2.434766	-0.529156
B	-3.771170	3.721161	-0.605629
B	-1.608679	5.005673	-0.616717
B	0.554383	6.290103	-0.596392
B	2.741517	5.059555	-0.674037
B	4.934373	3.836682	-0.681594
B	4.967145	1.321829	-0.753536
B	4.999925	-1.191701	-0.755709
B	5.032770	-3.706621	-0.687712
B	2.872475	-4.986080	-0.677577
B	0.718168	-6.273021	-0.596236
B	-1.477618	-5.045346	-0.614605
B	-3.672860	-3.817640	-0.603372
B	0.679945	-3.757284	-0.739872
B	2.837824	-2.474019	-0.796986
B	2.806839	0.036766	-0.826636
B	0.613686	1.264746	-0.815857
B	2.772425	2.547479	-0.794951
B	0.581808	3.774147	-0.739558
B	-1.578418	2.491718	-0.735331
B	-3.735759	1.208684	-0.680904
B	-3.703009	-1.305150	-0.680529
B	-1.544848	-0.019924	-0.771418
B	-1.512982	-2.531565	-0.734878
B	0.646425	-1.247906	-0.816128
N	-0.837444	1.246412	-0.792027
N	-0.804684	-1.267393	-0.792069
N	1.356312	0.017899	-0.830197
N	1.471542	-7.523511	-0.540439
N	1.274938	7.559745	-0.539547

N	3.618878	-6.238847	-0.612992
N	3.455039	6.331249	-0.607646
N	5.773459	-4.964526	-0.626490
N	5.642020	5.113339	-0.617668
N	-7.324728	-2.599192	-0.452080
N	-7.390064	2.407975	-0.454489
N	-7.351088	-0.095535	-0.474073
B	-5.968660	4.946949	-0.453188
B	-5.837544	-5.100185	-0.448446
B	-3.802859	6.237656	-0.478449
B	-3.638840	-6.333993	-0.473638
B	-1.633664	7.522765	-0.479515
B	-1.436910	-7.562157	-0.475924
B	7.129884	2.613749	-0.634157
B	7.195724	-2.426987	-0.640519
B	7.165464	0.093447	-0.662282
B	-8.135288	3.653298	-0.391168
B	-8.092402	1.146948	-0.431955
B	-8.059728	-1.356897	-0.430711
B	0.767471	-8.791582	-0.461449
B	2.914763	-7.501856	-0.553113
B	5.065869	-6.222302	-0.596150
B	7.093646	5.136733	-0.573417
B	4.901929	6.352278	-0.587716
B	2.718253	7.575552	-0.549155
N	-7.281987	-5.073358	-0.387231
N	-5.078015	-6.319878	-0.427717
N	-2.873181	-7.553013	-0.436133
N	-0.658312	-8.779813	-0.432134
N	7.895507	-3.691422	-0.592984
N	7.873301	-1.160169	-0.630849
N	7.840298	1.365029	-0.627144
N	-0.887042	8.760271	-0.435091
N	-3.069254	7.476255	-0.441373
N	-5.241212	6.186067	-0.433507
N	-7.411937	4.882490	-0.392485
N	7.796431	3.895874	-0.582998
B	-8.037173	-3.863466	-0.387100
B	0.538001	8.809092	-0.462030
B	7.225271	-4.950177	-0.584558
H	-7.949761	5.746929	-0.341655
H	-5.763150	7.060135	-0.374388
H	-3.586721	8.352896	-0.381032
H	-1.388960	9.645660	-0.377990
H	1.117912	9.863986	-0.419227
H	3.310065	8.622360	-0.502944

H	5.486725	7.402939	-0.539691
H	7.691261	6.181515	-0.526474
H	8.814622	3.929278	-0.547489
H	8.858969	1.380438	-0.582872
H	8.892044	-1.149087	-0.586912
H	8.914270	-3.698385	-0.558851
H	7.849973	-5.979115	-0.540346
H	5.677867	-7.257450	-0.550220
H	3.533646	-8.532950	-0.508267
H	1.374688	-9.831029	-0.419446
H	-1.136982	-9.677926	-0.374146
H	-3.367591	-8.442802	-0.374909
H	-5.576959	-7.207208	-0.367610
H	-7.797038	-5.951487	-0.335214
H	-9.240133	-3.889722	-0.330999
H	-9.261648	-1.368565	-0.372078
H	-9.294225	1.127302	-0.373465
H	-9.338540	3.648205	-0.335429

h-BN-catalyzed corannulene inversion TS

C	2.249960	1.374506	2.575743
C	1.416337	2.516297	2.567528
C	2.257066	-1.364427	2.575557
C	1.736638	0.003703	2.570880
C	0.359507	0.000129	2.547381
C	-0.045817	2.444786	2.554741
C	1.429370	-2.510518	2.567380
C	-1.190209	3.357100	2.548590
C	-4.138602	0.695093	2.493778
C	-4.134934	-0.718216	2.493952
C	-2.917117	1.503517	2.517411
C	-1.801356	0.696546	2.523592
C	-1.797713	-0.707495	2.523634
C	-2.909260	-1.520264	2.517691
C	-2.518897	-2.931421	2.530584
C	-1.172757	-3.364847	2.548947
C	-0.033130	-2.446594	2.554814
C	-0.462206	-1.137613	2.539086
C	-2.534077	2.916679	2.530078
C	-0.468096	1.133598	2.539062
H	-3.289826	-3.709737	2.520430
H	-1.000506	-4.446810	2.549791
H	1.931944	-3.484298	2.558018
H	3.339509	-1.534929	2.573517
H	3.331506	1.550597	2.573879
H	1.913867	3.492662	2.558242

H	-1.023594	4.439945	2.549276
H	-3.309028	3.690989	2.519679
H	-5.116542	1.188434	2.460583
H	-5.110290	-1.216654	2.460846
N	0.884100	6.280976	-0.475645
N	-1.281455	5.019976	-0.628290
N	-3.452387	3.760698	-0.726954
N	-5.624567	2.503227	-0.730170
N	-5.621628	-0.012626	-0.797500
N	-5.612979	-2.528362	-0.726492
N	-3.435100	-3.775934	-0.724015
N	-1.258383	-5.025299	-0.627069
N	0.913045	-6.276474	-0.477293
N	3.092477	-5.016456	-0.473179
N	5.269908	-3.752824	-0.425044
N	5.262894	-1.243526	-0.494794
N	5.257064	1.268025	-0.493318
N	5.252422	3.777243	-0.420554
N	3.069239	5.030890	-0.469485
N	0.900083	3.771624	-0.657580
N	-1.271214	2.510495	-0.810420
N	-3.446688	1.249485	-0.860741
N	-3.440924	-1.264818	-0.859780
N	-1.259700	-2.515830	-0.809728
N	0.917419	-3.767018	-0.658390
N	3.093599	-2.507090	-0.626830
N	3.088374	0.007313	-0.673893
N	3.082017	2.521683	-0.625281
B	5.980058	2.524684	-0.417226
B	5.982167	0.013898	-0.451853
B	5.991737	-2.496916	-0.420600
B	3.817895	-3.759428	-0.512603
B	1.641941	-5.019390	-0.539953
B	-0.535237	-6.278528	-0.517864
B	-2.707044	-5.024821	-0.635775
B	-4.885330	-3.780121	-0.688577
B	-4.890949	-1.266579	-0.799631
B	-4.896733	1.244671	-0.801204
B	-4.902663	3.758330	-0.693086
B	-2.730095	5.012938	-0.638772
B	-0.564121	6.276481	-0.518260
B	1.618777	5.027243	-0.537906
B	3.800463	3.777237	-0.509354
B	-0.550670	3.763689	-0.700780
B	-2.721435	2.504206	-0.802466
B	-2.716140	-0.006004	-0.870548

B	-0.535701	-1.257057	-0.824738
B	-2.709925	-2.516172	-0.800963
B	-0.533390	-3.765705	-0.700382
B	1.641254	-2.507335	-0.690498
B	3.811995	-1.247913	-0.604776
B	3.806197	1.265804	-0.603785
B	1.636067	0.003984	-0.751805
B	1.629713	2.515280	-0.689707
B	-0.541450	1.255054	-0.824951
N	0.916095	-1.255062	-0.785373
N	0.910332	1.259722	-0.785267
N	-1.264336	-0.002671	-0.870083
N	-1.304919	7.534071	-0.441307
N	-1.270242	-7.539442	-0.439698
N	-3.463904	6.272669	-0.548093
N	-3.435043	-6.287790	-0.543228
N	-5.631131	5.023062	-0.606995
N	-5.607964	-5.048041	-0.600118
N	7.438599	2.520709	-0.327287
N	7.450293	-2.486283	-0.331431
N	7.438979	0.017224	-0.357079
B	6.000342	-5.008664	-0.331293
B	5.976978	5.036323	-0.324602
B	3.820587	-6.274722	-0.368667
B	3.791475	6.292386	-0.363061
B	1.637360	-7.534825	-0.369666
B	1.602552	7.542552	-0.366423
B	-7.067690	-2.535043	-0.678489
B	-7.079325	2.503307	-0.683122
B	-7.075997	-0.015919	-0.730807
B	8.180868	-3.739300	-0.256137
B	8.166123	-1.233019	-0.305898
B	8.160264	1.270756	-0.303631
B	-0.589195	8.793496	-0.339121
B	-2.748058	7.526695	-0.458777
B	-4.910599	6.271670	-0.541835
B	-7.059699	-5.056191	-0.568825
B	-4.881714	-6.293321	-0.534799
B	-2.713426	-7.538555	-0.454658
N	7.420720	4.994621	-0.250242
N	5.230183	6.263764	-0.303390
N	3.038447	7.519160	-0.318957
N	0.836281	8.767637	-0.307034
N	-7.766868	3.774195	-0.617862
N	-7.771692	1.244703	-0.693842
N	-7.765853	-1.279666	-0.691168

N	0.876721	-8.763379	-0.309445
N	3.073211	-7.504950	-0.324473
N	5.259228	-6.239560	-0.310798
N	7.443946	-4.960370	-0.258193
N	-7.749369	-3.808944	-0.610461
B	8.163299	3.776983	-0.249559
B	-0.548682	-8.795644	-0.338945
B	-7.082924	5.024634	-0.577353
H	7.971399	-5.830667	-0.199536
H	5.770577	-7.119097	-0.241424
H	3.580205	-8.386603	-0.250204
H	1.368435	-9.653339	-0.237044
H	-1.141149	-9.842918	-0.279246
H	-3.317535	-8.577448	-0.387972
H	-5.478252	-7.336454	-0.465897
H	-7.668581	-6.093781	-0.504681
H	-8.768134	-3.830408	-0.583984
H	-8.784694	-1.283768	-0.649124
H	-8.790555	1.244184	-0.652115
H	-8.785745	3.791060	-0.592369
H	-7.696604	6.059526	-0.515397
H	-5.511942	7.312162	-0.474772
H	-3.356941	8.562884	-0.393469
H	-1.186475	9.838082	-0.280342
H	1.323851	9.659791	-0.233624
H	3.541320	8.403074	-0.243537
H	5.737402	7.145581	-0.232656
H	7.944077	5.867276	-0.189957
H	9.366036	3.790672	-0.182141
H	9.361769	1.269698	-0.233334
H	9.367628	-1.226463	-0.235912
H	9.383701	-3.747507	-0.189545

h-BN-catalyzed corannulene product

C	2.435061	-3.011517	2.799028
C	1.075871	-3.360938	2.793657
C	4.132474	-0.957283	2.808499
C	2.894062	-1.661125	2.516857
C	1.883905	-0.823721	2.060596
C	0.025760	-2.398266	2.505525
C	4.220338	0.443084	2.807275
C	-1.400461	-2.379657	2.785089
C	-1.985626	1.464075	2.781208
C	-1.091628	2.545444	2.782559
C	-1.561064	0.102541	2.500222
C	-0.247544	0.019932	2.054810

C	0.654928	1.112116	2.053797
C	0.325613	2.385508	2.502482
C	1.487832	3.209763	2.789695
C	2.792786	2.693385	2.795286
C	3.079612	1.295911	2.514419
C	1.972667	0.590753	2.059223
C	-2.152356	-1.195054	2.782521
C	0.511416	-1.176418	2.055488
H	1.348806	4.256223	3.083339
H	3.607714	3.362376	3.093634
H	5.170718	0.897975	3.108147
H	5.018590	-1.527014	3.109958
H	3.160159	-3.776867	3.097617
H	0.807266	-4.381629	3.088022
H	-1.905524	-3.307466	3.076378
H	-3.207333	-1.256073	3.072470
H	-3.024738	1.656811	3.070791
H	-1.476866	3.529461	3.072515
N	-1.267072	-6.211386	-0.456623
N	0.965348	-5.075986	-0.623555
N	3.203220	-3.943560	-0.737919
N	5.442686	-2.813096	-0.750411
N	5.583308	-0.304815	-0.866509
N	5.719471	2.205691	-0.811644
N	3.616726	3.573470	-0.792738
N	1.516899	4.942038	-0.648609
N	-0.575588	6.311786	-0.434688
N	-2.822555	5.180261	-0.427868
N	-5.067658	4.044531	-0.366610
N	-5.207390	1.542121	-0.487348
N	-5.346730	-0.963894	-0.511360
N	-5.485320	-3.468189	-0.436416
N	-3.377651	-4.842624	-0.484976
N	-1.141679	-3.709441	-0.702893
N	1.096608	-2.577867	-0.908285
N	3.340567	-1.441319	-0.956904
N	3.478250	1.068581	-0.976089
N	1.372090	2.443378	-0.921066
N	-0.727146	3.812128	-0.690728
N	-2.969894	2.678896	-0.632756
N	-3.111334	0.170967	-0.730382
N	-3.247416	-2.338276	-0.661772
B	-6.140051	-2.176627	-0.430225
B	-5.997984	0.328682	-0.451021
B	-5.861180	2.833271	-0.377813
B	-3.619009	3.968258	-0.477693

B	-1.375811	5.100308	-0.519125
B	0.869427	6.231262	-0.495029
B	2.962886	4.859488	-0.670613
B	5.064825	3.495660	-0.759764
B	4.925956	0.988263	-0.889203
B	4.787923	-1.518151	-0.861786
B	4.650539	-4.022837	-0.683210
B	2.411840	-5.149998	-0.616382
B	0.179177	-6.287264	-0.483423
B	-1.929433	-4.920050	-0.549889
B	-4.035861	-3.550221	-0.530145
B	0.306970	-3.784493	-0.748660
B	2.545618	-2.652097	-0.874767
B	2.681561	-0.146783	-1.009156
B	0.575677	1.227571	-0.974786
B	2.820875	2.359756	-0.903849
B	0.720322	3.729211	-0.757148
B	-1.522883	2.597854	-0.748657
B	-3.760505	1.463959	-0.622590
B	-3.899407	-1.043892	-0.640208
B	-1.664996	0.091720	-0.864030
B	-1.799258	-2.415416	-0.763801
B	0.437965	-1.282617	-0.971934
N	-0.875105	1.309357	-0.913331
N	-1.013337	-1.204944	-0.917527
N	1.230346	-0.067368	-1.057529
N	0.847309	-7.581989	-0.364054
N	1.675889	7.446471	-0.395602
N	3.072657	-6.445554	-0.477686
N	3.762517	6.077083	-0.559549
N	5.306126	-5.323232	-0.548878
N	5.859836	4.719074	-0.660378
N	-7.595825	-2.090054	-0.331696
N	-7.317032	2.906233	-0.269466
N	-7.451821	0.408348	-0.340055
B	-5.722912	5.337851	-0.236658
B	-6.280296	-4.683439	-0.336178
B	-3.474785	6.475176	-0.281751
B	-4.169660	-6.059847	-0.364359
B	-1.223782	7.606625	-0.285218
B	-2.054865	-7.428831	-0.329068
B	7.171816	2.129696	-0.758674
B	6.894209	-2.895180	-0.685136
B	7.034997	-0.383775	-0.787216
B	-7.972691	4.197144	-0.158673
B	-8.104631	1.696985	-0.259787

B	-8.244199	-0.801334	-0.293538
B	0.062781	-8.797466	-0.242888
B	2.288299	-7.654779	-0.362014
B	4.516293	-6.526279	-0.453521
B	7.309490	4.645519	-0.637650
B	5.206687	6.001669	-0.567937
B	3.115924	7.364081	-0.432296
N	-7.719453	-4.560457	-0.260767
N	-5.604680	-5.950945	-0.310193
N	-3.487511	-7.326159	-0.299169
N	-1.359256	-8.693130	-0.233547
N	7.508932	-4.200002	-0.575484
N	7.658186	-1.680155	-0.723812
N	7.797437	0.837405	-0.765559
N	-0.393783	8.788149	-0.204968
N	-2.657917	7.659188	-0.220482
N	-4.911832	6.522905	-0.201177
N	-7.165883	5.372812	-0.144378
N	7.926681	3.361784	-0.690862
B	-8.391183	-3.302599	-0.255117
B	1.030389	8.739039	-0.253931
B	6.754654	-5.407283	-0.503536
H	-7.640234	6.271207	-0.061345
H	-5.369706	7.428978	-0.105305
H	-3.112072	8.566389	-0.117885
H	-0.833068	9.702420	-0.104368
H	1.683396	9.748632	-0.176879
H	3.779404	8.365134	-0.350664
H	5.861854	7.008401	-0.488576
H	7.976390	5.646702	-0.569185
H	8.944984	3.323743	-0.666973
H	8.814506	0.782870	-0.717606
H	8.674976	-1.736346	-0.672001
H	8.524967	-4.272576	-0.538547
H	7.307306	-6.473219	-0.402705
H	5.057010	-7.596454	-0.346702
H	2.838017	-8.720718	-0.259174
H	0.601031	-9.871418	-0.150346
H	-1.896840	-9.554838	-0.147207
H	-4.039344	-8.179208	-0.212021
H	-6.160436	-6.802361	-0.232453
H	-8.291033	-5.402272	-0.200232
H	-9.592594	-3.247516	-0.183648
H	-9.443234	-0.731537	-0.214769
H	-9.303823	1.758963	-0.176999
H	-9.172234	4.273584	-0.076368

h-BN-catalyzed sumanene reactant

N	0.919621	6.293148	-0.653332
N	-1.233518	5.006399	-0.779121
N	-3.391209	3.722209	-0.864717
N	-5.549968	2.442039	-0.929641
N	-5.519373	-0.075786	-0.978929
N	-5.484858	-2.593402	-0.946847
N	-3.294198	-3.818088	-0.875885
N	-1.105180	-5.046221	-0.773261
N	1.079312	-6.277699	-0.640366
N	3.243157	-4.992344	-0.545851
N	5.403770	-3.703264	-0.426436
N	5.369614	-1.192350	-0.457051
N	5.338684	1.320090	-0.467357
N	5.309442	3.831287	-0.453207
N	3.116775	5.064632	-0.573993
N	0.960668	3.780179	-0.736061
N	-1.197550	2.493301	-0.854987
N	-3.358636	1.208975	-0.914496
N	-3.325166	-1.304512	-0.943439
N	-1.133806	-2.533275	-0.836066
N	1.056750	-3.763722	-0.723895
N	3.213657	-2.478328	-0.602359
N	3.181846	0.036230	-0.619012
N	3.149653	2.550372	-0.608013
B	6.049029	2.585698	-0.413719
B	6.076225	0.073011	-0.413962
B	6.111679	-2.439368	-0.393426
B	3.953916	-3.726811	-0.527073
B	1.794997	-5.012342	-0.640656
B	-0.367786	-6.295957	-0.705776
B	-2.554501	-5.062965	-0.822430
B	-4.745357	-3.838834	-0.908948
B	-4.775724	-1.323247	-0.959710
B	-4.809995	1.189415	-0.947885
B	-4.842308	3.706633	-0.891779
B	-2.682343	4.985557	-0.817122
B	-0.528227	6.273922	-0.712828
B	1.667889	5.046892	-0.658853
B	3.859183	3.818165	-0.547032
B	-0.490026	3.756744	-0.792017
B	-2.646744	2.472611	-0.878392
B	-2.616347	-0.039489	-0.896518
B	-0.424135	-1.265918	-0.812050
B	-2.584479	-2.548351	-0.885272

B	-0.392158	-3.778649	-0.785188
B	1.764029	-2.494780	-0.700078
B	3.920585	-1.211990	-0.563697
B	3.889538	1.302000	-0.568140
B	1.731306	0.016184	-0.711306
B	1.699522	2.531606	-0.704459
B	-0.457936	1.245813	-0.811385
N	1.025734	-1.248802	-0.768246
N	0.992977	1.265299	-0.748563
N	-1.282271	7.524934	-0.699307
N	-1.089802	-7.565610	-0.698434
N	-3.429134	6.239191	-0.796255
N	-3.268453	-6.335471	-0.809059
N	-5.583613	4.965101	-0.872456
N	-5.454142	-5.116140	-0.891593
N	7.506338	2.596455	-0.316944
N	7.568603	-2.412770	-0.293333
N	7.531674	0.091669	-0.314095
B	6.148102	-4.953000	-0.353972
B	6.022374	5.099927	-0.393286
B	3.985345	-6.245171	-0.469148
B	3.826892	6.336253	-0.504866
B	1.817643	-7.530795	-0.563614
B	1.625858	7.565090	-0.583569
B	-6.940661	-2.615518	-0.960420
B	-7.006306	2.427138	-0.948513
B	-6.976276	-0.093987	-0.983431
B	8.312253	-3.658999	-0.227094
B	8.270917	-1.151748	-0.256280
B	8.239807	1.353530	-0.269144
B	-0.578562	8.794275	-0.635020
B	-2.725049	7.503058	-0.742166
B	-4.876175	6.222915	-0.826561
B	-6.906473	-5.139219	-0.914850
B	-4.715298	-6.355769	-0.845820
B	-2.532455	-7.580685	-0.751251
N	7.465335	5.072016	-0.303771
N	5.264681	6.320845	-0.423019
N	3.061498	7.556173	-0.518789
N	0.846638	8.783145	-0.581318
N	-7.705982	3.692349	-0.931488
N	-7.683985	1.160456	-0.978627
N	-7.651136	-1.366277	-0.979398
N	1.070031	-8.768602	-0.566934
N	3.251841	-7.484554	-0.485954
N	5.421653	-6.192860	-0.379069

N	7.589489	-4.888298	-0.258647
N	-7.608278	-3.898037	-0.947882
B	8.218726	3.861427	-0.263981
B	-0.353973	-8.816483	-0.630874
B	-7.035952	4.950963	-0.894590
H	8.126956	-5.753029	-0.208884
H	5.943284	-7.067490	-0.325624
H	3.768113	-8.362273	-0.431087
H	1.570246	-9.655375	-0.516609
H	-0.934234	-9.872031	-0.627189
H	-3.124861	-8.628126	-0.744293
H	-5.301434	-7.406679	-0.834975
H	-7.505582	-6.184083	-0.903981
H	-8.627013	-3.931984	-0.959733
H	-8.670761	-1.382555	-0.980972
H	-8.703693	1.150073	-0.983165
H	-8.725227	3.700525	-0.945584
H	-7.661667	5.980095	-0.880511
H	-5.488786	7.258556	-0.811129
H	-3.344235	8.534831	-0.730136
H	-1.185785	9.834505	-0.626284
H	1.324124	9.682533	-0.534258
H	3.555127	8.447109	-0.468745
H	5.764136	7.208693	-0.375996
H	7.981215	5.950282	-0.263418
H	9.420511	3.887969	-0.186902
H	9.440555	1.365344	-0.190129
H	9.471475	-1.132871	-0.175774
H	9.514076	-3.654738	-0.146255
C	1.168703	-2.457489	2.589363
C	1.970710	-1.264616	2.620619
C	1.452578	-0.045012	3.093489
C	-0.168608	-2.452906	3.028048
C	-1.438341	-3.301680	2.732363
C	-1.684735	3.388339	2.490584
C	-2.509292	2.344706	2.949106
C	-3.954337	1.858675	2.643366
C	-0.251416	3.289848	2.545506
C	0.384940	2.143212	3.056549
C	-0.460619	1.183520	3.640063
C	-1.850426	1.280378	3.588778
C	-2.651452	0.090841	3.556096
C	-3.868443	0.325660	2.892167
C	-4.512232	-0.812859	2.373109
C	-3.881213	-2.104613	2.394168
C	-2.595871	-2.283641	2.937256

C	-2.040314	-1.161915	3.577218
C	-0.610305	-1.261604	3.630119
C	0.168108	-0.105537	3.661460
C	1.767869	1.459408	2.857808
H	0.325098	4.082876	2.057136
H	-2.108023	4.249823	1.962757
H	2.956836	-1.311097	2.146092
H	1.595352	-3.335958	2.093128
H	-4.383321	-2.916540	1.856926
H	-5.453649	-0.723250	1.820321
H	-4.701734	2.343523	3.301284
H	-4.252239	2.089631	1.607590
H	2.172240	1.638592	1.848124
H	2.524389	1.840625	3.571170
H	-1.431082	-3.710921	1.708974
H	-1.524249	-4.168261	3.416619
N	-1.166444	-0.019850	-0.838377

h-BN-catalyzed sumanene inversion TS

N	1.015109	6.281666	-0.532808
N	-1.155476	5.028112	-0.682578
N	-3.330707	3.776125	-0.799752
N	-5.507518	2.527317	-0.866989
N	-5.513301	0.008863	-0.874113
N	-5.515753	-2.508982	-0.814916
N	-3.342197	-3.765859	-0.792788
N	-1.170121	-5.025649	-0.721320
N	0.996204	-6.287300	-0.578457
N	3.177404	-5.032613	-0.470453
N	5.356308	-3.774899	-0.348668
N	5.359700	-1.264376	-0.400327
N	5.366678	1.247770	-0.435042
N	5.373371	3.758959	-0.413843
N	3.196325	5.022930	-0.497976
N	1.021869	3.770259	-0.662119
N	-1.154359	2.515411	-0.786818
N	-3.333718	1.262530	-0.855581
N	-3.337375	-1.251450	-0.853695
N	-1.162791	-2.512202	-0.782697
N	1.009708	-3.773518	-0.664245
N	3.185629	-2.519221	-0.543155
N	3.191375	-0.004682	-0.583913
N	3.195609	2.509647	-0.574525
B	6.095029	2.502679	-0.382379
B	6.084983	-0.009950	-0.370612
B	6.082528	-2.521385	-0.325071

B	3.905702	-3.776583	-0.455618
B	1.729194	-5.030761	-0.573865
B	-0.450566	-6.285101	-0.651228
B	-2.620826	-5.019994	-0.752514
B	-4.793337	-3.763199	-0.784380
B	-4.787941	-1.249387	-0.842320
B	-4.784565	1.262377	-0.874925
B	-4.780203	3.781534	-0.829957
B	-2.603360	5.026848	-0.723779
B	-0.433423	6.282400	-0.590349
B	1.745501	5.024745	-0.567347
B	3.922001	3.766588	-0.499580
B	-0.429981	3.767767	-0.705462
B	-2.603822	2.515546	-0.812219
B	-2.609294	0.002985	-0.833866
B	-0.434435	-1.254761	-0.763190
B	-2.614252	-2.505919	-0.807412
B	-0.438498	-3.766503	-0.731967
B	1.735209	-2.514614	-0.635293
B	3.909361	-1.263450	-0.510628
B	3.916749	1.249477	-0.537836
B	1.739583	-0.004042	-0.668402
B	1.742750	2.511519	-0.659345
B	-0.432351	1.257331	-0.764081
N	1.015393	-1.258875	-0.714777
N	1.019958	1.255798	-0.712772
N	-1.169596	7.544585	-0.550176
N	-1.190779	-7.544852	-0.641966
N	-3.333403	6.291449	-0.683511
N	-3.352439	-6.283032	-0.723603
N	-5.504860	5.050413	-0.803239
N	-5.520862	-5.030955	-0.740310
N	7.553002	2.492721	-0.289323
N	7.540263	-2.516105	-0.223326
N	7.541187	-0.011966	-0.270631
B	6.081616	-5.034683	-0.268145
B	6.103841	5.016843	-0.345796
B	3.900744	-6.295213	-0.389079
B	3.923858	6.283277	-0.415485
B	1.716173	-7.550263	-0.498684
B	1.738777	7.541861	-0.446420
B	-6.969754	-2.508914	-0.790733
B	-6.963757	2.532925	-0.872456
B	-6.968695	0.011577	-0.853881
B	8.264855	-3.772613	-0.145658
B	8.261469	-1.265635	-0.199704

B	8.268027	1.239298	-0.236996
B	-0.448540	8.802078	-0.462155
B	-2.612328	7.543459	-0.599400
B	-4.779575	6.296770	-0.730878
B	-6.973136	-5.032238	-0.722146
B	-4.800011	-6.281114	-0.718579
B	-2.634118	-7.538524	-0.679426
N	7.547247	4.968498	-0.268622
N	5.362670	6.248106	-0.353060
N	3.175057	7.513395	-0.396080
N	0.976688	8.770643	-0.413883
N	-7.645278	3.808696	-0.867390
N	-7.659707	1.276182	-0.869863
N	-7.663115	-1.249703	-0.808069
N	0.951630	-8.778053	-0.508971
N	3.150317	-7.524687	-0.410001
N	5.337456	-6.264085	-0.290261
N	7.523878	-4.991173	-0.168428
N	-7.657205	-3.781129	-0.744078
B	8.283510	3.747171	-0.237873
B	-0.472792	-8.805772	-0.575780
B	-6.956774	5.057326	-0.830913
H	8.048130	-5.863599	-0.112617
H	5.846102	-7.146173	-0.234535
H	3.653976	-8.409605	-0.353852
H	1.439497	-9.671695	-0.459245
H	-1.067720	-9.853333	-0.574012
H	-3.241380	-8.577604	-0.666549
H	-5.401120	-7.323555	-0.690869
H	-7.587485	-6.068054	-0.686517
H	-8.676293	-3.799429	-0.730357
H	-8.682734	-1.250589	-0.792827
H	-8.679429	1.280156	-0.862883
H	-8.664302	3.831376	-0.880036
H	-7.567843	6.095505	-0.817890
H	-5.377749	7.340937	-0.704993
H	-3.217058	8.583704	-0.567753
H	-1.041095	9.850551	-0.429740
H	1.466984	9.662269	-0.353299
H	3.681076	8.396774	-0.337021
H	5.874305	7.128573	-0.298968
H	8.075515	5.839292	-0.226991
H	9.486109	3.756536	-0.167642
H	9.469175	1.233898	-0.161189
H	9.462310	-1.264055	-0.118807
H	9.466638	-3.785874	-0.062722

C	1.327609	-2.510943	2.640940
C	2.113934	-1.281200	2.667499
C	1.521453	0.014551	2.670063
C	-0.097132	-2.516345	2.617997
C	-1.403106	-3.433284	2.596745
C	-1.813353	3.554195	2.542292
C	-2.639525	2.393478	2.536010
C	-4.141180	1.856049	2.505122
C	-0.355676	3.487773	2.587820
C	0.360404	2.256623	2.632168
C	-0.504987	1.176315	2.617110
C	-1.876763	1.238946	2.573317
C	-2.632505	0.057127	2.549072
C	-3.999608	0.266527	2.491415
C	-4.705973	-0.970187	2.447078
C	-4.034910	-2.266414	2.471604
C	-2.618199	-2.401350	2.538641
C	-2.000903	-1.162797	2.570525
C	-0.600067	-1.226644	2.614833
C	0.140098	-0.069400	2.638620
C	1.806186	1.584030	2.697596
H	0.164414	4.452409	2.575961
H	-2.241940	4.561947	2.502310
H	3.201812	-1.413069	2.674479
H	1.903710	-3.443203	2.629198
H	-4.691414	-3.142435	2.422711
H	-5.799288	-1.002722	2.379235
H	-4.700826	2.194605	3.395699
H	-4.695283	2.229563	1.627659
H	2.448247	1.902240	1.859167
H	2.334666	1.874124	3.623590
H	-1.408564	-4.126674	1.739056
H	-1.459431	-4.059961	3.505061
N	-1.158354	0.001869	-0.798387

h-BN-catalyzed sumanene product

N	1.132923	6.257371	-0.542297
N	-1.057305	5.046993	-0.739956
N	-3.254331	3.837568	-0.861567
N	-5.453133	2.629397	-0.845108
N	-5.506563	0.115780	-0.929455
N	-5.558728	-2.398993	-0.881307
N	-3.410982	-3.696080	-0.886245
N	-1.266619	-4.994123	-0.745006
N	0.870390	-6.295172	-0.540824
N	3.075446	-5.085548	-0.477484

N	5.276821	-3.871848	-0.353271
N	5.330142	-1.364286	-0.436459
N	5.383711	1.145448	-0.448323
N	5.436449	3.653783	-0.383063
N	3.286742	4.957934	-0.496243
N	1.094574	3.749317	-0.751133
N	-1.100727	2.542649	-0.990846
N	-3.305219	1.328812	-1.039715
N	-3.358332	-1.186956	-1.055426
N	-1.205356	-2.489291	-0.989862
N	0.937236	-3.787252	-0.747670
N	3.135922	-2.576513	-0.627978
N	3.191705	-0.064410	-0.700932
N	3.240226	2.447538	-0.628609
B	6.134017	2.384599	-0.356520
B	6.077793	-0.124999	-0.380067
B	6.026941	-2.633363	-0.331828
B	3.828535	-3.845134	-0.486743
B	1.628840	-5.054944	-0.589075
B	-0.575391	-6.264378	-0.613464
B	-2.715813	-4.960967	-0.779271
B	-4.861388	-3.666134	-0.841690
B	-4.807085	-1.156140	-0.957712
B	-4.754524	1.355520	-0.945870
B	-4.703037	3.868509	-0.808978
B	-2.505047	5.072565	-0.752478
B	-0.314369	6.285145	-0.601198
B	1.838368	4.987697	-0.597281
B	3.987813	3.688387	-0.505273
B	-0.355154	3.776761	-0.829719
B	-2.551872	2.567746	-0.970754
B	-2.604076	0.055145	-1.073369
B	-0.450473	-1.246155	-1.017438
B	-2.657787	-2.454787	-0.984246
B	-0.510098	-3.753487	-0.835635
B	1.690291	-2.544932	-0.772969
B	3.883784	-1.335411	-0.591073
B	3.937457	1.174825	-0.598464
B	1.746449	-0.035302	-0.863056
B	1.793206	2.477584	-0.778685
B	-0.400252	1.269171	-1.015951
N	1.000515	-1.278204	-0.936688
N	1.051624	1.238930	-0.930779
N	-1.026462	7.559026	-0.518523
N	-1.340625	-7.507542	-0.546223
N	-3.210875	6.347064	-0.646838

N	-3.472538	-6.206567	-0.688839
N	-5.404040	5.147070	-0.703656
N	-5.613936	-4.916455	-0.748058
N	7.589329	2.347399	-0.229817
N	7.482400	-2.656596	-0.199201
N	7.531170	-0.154763	-0.244355
B	5.975482	-5.143425	-0.235573
B	6.188907	4.895940	-0.278663
B	3.771071	-6.359252	-0.346396
B	4.035787	6.202447	-0.375110
B	1.562196	-7.569520	-0.409638
B	1.877407	7.501686	-0.415463
B	-7.011094	-2.371483	-0.804955
B	-6.907183	2.662141	-0.774713
B	-6.959799	0.145088	-0.837302
B	8.181315	-3.925319	-0.095603
B	8.226848	-1.420930	-0.162214
B	8.280393	1.081148	-0.179420
B	-0.284744	8.801374	-0.401500
B	-2.468778	7.583960	-0.542380
B	-4.656177	6.378978	-0.633228
B	-7.064820	-4.890881	-0.702167
B	-4.919003	-6.178196	-0.683983
B	-2.782754	-7.473243	-0.586024
N	7.629094	4.820996	-0.170190
N	5.471713	6.140550	-0.282794
N	3.311713	7.446303	-0.348383
N	1.139478	8.743982	-0.358877
N	-7.566111	3.946816	-0.690917
N	-7.626904	1.420291	-0.781914
N	-7.679636	-1.100442	-0.799815
N	0.772966	-8.780653	-0.365723
N	2.996130	-7.572790	-0.325880
N	5.207136	-6.357294	-0.239755
N	7.416822	-5.128833	-0.116066
N	-7.724327	-3.627775	-0.732341
B	8.341987	3.586222	-0.142507
B	-0.651497	-8.780016	-0.426901
B	-6.854288	5.181450	-0.653925
H	7.921314	-6.011200	-0.039052
H	5.695573	-7.248169	-0.152696
H	3.480747	-8.465252	-0.233916
H	1.242876	-9.681062	-0.279433
H	-1.269762	-9.812891	-0.377774
H	-3.411930	-8.497603	-0.526201
H	-5.539645	-7.207351	-0.616477

H	-7.697283	-5.914228	-0.634395
H	-8.742775	-3.623164	-0.691644
H	-8.697271	-1.080063	-0.739227
H	-8.644751	1.441325	-0.724661
H	-8.583900	3.984726	-0.650473
H	-7.443798	6.229405	-0.577316
H	-5.234299	7.431801	-0.554199
H	-3.055213	8.632647	-0.469491
H	-0.859399	9.858545	-0.339661
H	1.646724	9.624073	-0.274536
H	3.833209	8.318196	-0.260911
H	5.997569	7.010585	-0.203109
H	8.171107	5.681699	-0.103609
H	9.542721	3.571664	-0.045312
H	9.479307	1.052444	-0.077193
H	9.425721	-1.441843	-0.057377
H	9.381095	-3.960713	0.008381
C	-3.832454	-2.249868	3.006402
C	-4.534584	-0.992650	2.987324
C	-3.916994	0.191289	2.535789
C	-2.494540	-2.354341	2.574688
C	-1.289283	-3.310523	2.834555
C	-0.478925	3.375338	3.044013
C	0.251470	2.251740	2.607068
C	1.665306	1.644215	2.864975
C	-1.918855	3.395296	3.017292
C	-2.663776	2.292305	2.552593
C	-1.905372	1.252103	1.997102
C	-0.515130	1.232534	2.024030
C	0.182164	-0.015420	2.043066
C	1.444291	0.116160	2.639280
C	2.012694	-1.085122	3.109601
C	1.274996	-2.322111	3.100876
C	-0.048677	-2.388881	2.620497
C	-0.529875	-1.209958	2.033187
C	-1.959357	-1.190264	2.005035
C	-2.637649	0.023969	1.986445
C	-4.102143	1.724428	2.759160
H	-2.415453	4.254694	3.481490
H	0.023773	4.221134	3.526277
H	-5.528622	-0.968656	3.447785
H	-4.339035	-3.098414	3.479683
H	1.740570	-3.185040	3.590015
H	2.990345	-1.089620	3.604426
H	2.415738	2.052951	2.160123
H	2.029585	1.863132	3.883212

H	-4.490799	1.948341	3.767456
H	-4.819570	2.158908	2.035702
H	-1.314237	-3.734541	3.853086
H	-1.288659	-4.166898	2.132107
N	-1.150104	0.026017	-1.090821

h-BN-catalyzed 2,2prime-dimethylbiphenyl reactant

N	2.989269	-5.286554	-1.020546
N	3.935436	-2.960546	-1.030541
N	4.889314	-0.646912	-0.807532
N	5.841802	1.659951	-0.524536
N	4.304586	3.654347	-0.438258
N	2.765226	5.648800	-0.405784
N	0.278948	5.316814	-0.536236
N	-2.211311	4.979117	-0.529136
N	-4.698018	4.640931	-0.419636
N	-5.646208	2.308801	-0.307290
N	-6.583808	-0.024091	-0.137426
N	-5.038941	-2.004583	-0.188797
N	-3.498238	-3.988590	-0.277352
N	-1.966668	-5.974266	-0.419894
N	0.507977	-5.633912	-0.751222
N	1.447327	-3.305518	-0.885280
N	2.399265	-0.979380	-0.852016
N	3.354289	1.340719	-0.694906
N	1.816869	3.328244	-0.600442
N	-0.674411	2.992697	-0.634669
N	-3.161883	2.651141	-0.494410
N	-4.103673	0.323201	-0.366847
N	-2.563077	-1.662516	-0.457307
N	-1.027881	-3.649081	-0.601591
B	-3.299640	-5.426489	-0.262573
B	-4.834062	-3.439377	-0.150932
B	-6.380508	-1.458550	-0.087309
B	-5.446129	0.871198	-0.271116
B	-4.504827	3.199922	-0.408862
B	-3.554046	5.529379	-0.473190
B	-1.063579	5.864758	-0.521214
B	1.426292	6.202530	-0.448970
B	2.965646	4.210581	-0.484863
B	4.500162	2.218918	-0.547992
B	6.036662	0.231353	-0.668613
B	5.081354	-2.075957	-0.950516
B	4.132982	-4.396707	-1.084069
B	1.645839	-4.743249	-0.895059
B	-0.828198	-5.086206	-0.593099

B	2.591432	-2.414450	-0.934183
B	3.546064	-0.092686	-0.787779
B	2.012939	1.890308	-0.682812
B	-0.477512	1.553482	-0.665862
B	0.474925	3.878735	-0.601417
B	-2.016720	3.539474	-0.558097
B	-2.962755	1.212776	-0.486308
B	-3.900392	-1.113664	-0.336953
B	-2.360043	-3.099306	-0.441975
B	-1.422785	-0.773802	-0.585108
B	0.111459	-2.758269	-0.727893
B	1.058266	-0.431471	-0.769603
N	-1.622515	0.664882	-0.590480
N	-0.085868	-1.320801	-0.708229
N	0.863410	1.006399	-0.739280
N	5.485961	-4.941347	-1.170532
N	-3.743410	6.978042	-0.462301
N	6.432108	-2.628275	-0.991667
N	-1.259157	7.310344	-0.481166
N	7.385332	-0.331577	-0.679238
N	1.222924	7.648091	-0.393076
N	-4.446627	-6.315612	-0.092142
N	-7.520537	-2.359944	0.063590
N	-5.976723	-4.333517	0.009394
B	-7.930729	0.522198	-0.049814
B	-1.769481	-7.416784	-0.416984
B	-6.993899	2.858639	-0.227170
B	0.707434	-7.077953	-0.759203
B	-6.043816	5.193088	-0.353678
B	3.189719	-6.728893	-1.048448
B	3.913711	6.535428	-0.281337
B	6.991637	2.537115	-0.366237
B	5.454667	4.536962	-0.292716
B	-8.864428	-1.815646	0.154665
B	-7.313952	-3.788434	0.117023
B	-5.775828	-5.766943	0.044468
B	5.683441	-6.378633	-1.239100
B	6.626868	-4.056105	-1.128515
B	7.576974	-1.752153	-0.855211
B	2.369356	8.534348	-0.287822
B	-0.113899	8.194810	-0.424890
B	-2.599202	7.859627	-0.468261
N	-2.926696	-8.265835	-0.237737
N	-0.439262	-7.933983	-0.592143
N	2.043810	-7.589047	-0.929167
N	4.539398	-7.229984	-1.185695

N	8.310518	1.942793	-0.353267
N	6.770456	3.952526	-0.235718
N	5.228807	5.958361	-0.214238
N	-6.194584	6.631708	-0.371576
N	-7.159092	4.289587	-0.268538
N	-8.104405	1.948447	-0.106584
N	-9.035658	-0.400546	0.092189
N	3.674706	7.961148	-0.228843
B	-4.249136	-7.754690	-0.077060
B	-5.086837	7.529751	-0.419274
B	8.533580	0.542805	-0.515969
H	-9.986064	-0.037403	0.156557
H	-9.048438	2.329598	-0.046156
H	-8.100724	4.677666	-0.215135
H	-7.129021	7.037620	-0.334791
H	-5.262656	8.721583	-0.419782
H	-2.758181	9.052570	-0.453612
H	-0.277538	9.386815	-0.394488
H	2.221444	9.729216	-0.246106
H	4.466191	8.598754	-0.149353
H	6.032261	6.579727	-0.121936
H	7.578051	4.567243	-0.135452
H	9.128667	2.540938	-0.243189
H	9.652543	0.096016	-0.516640
H	8.689516	-2.210964	-0.881541
H	7.741038	-4.507190	-1.191081
H	6.790766	-6.844369	-1.330225
H	4.698552	-8.236273	-1.222377
H	2.186597	-8.598839	-0.938559
H	-0.302975	-8.944707	-0.593358
H	-2.808262	-9.278345	-0.228301
H	-5.182725	-8.502494	0.066400
H	-6.718838	-6.501745	0.184040
H	-8.254310	-4.528153	0.248315
H	-9.815998	-2.543918	0.279376
C	1.203785	-1.261252	3.295898
C	-0.098297	-1.069574	3.810717
C	-1.089911	-2.051888	3.719084
C	-0.793852	-3.274513	3.104752
C	0.505237	-3.505278	2.639452
C	1.522401	-2.535893	2.737905
C	2.179531	-0.128794	3.292139
C	1.813948	1.182250	2.862208
C	2.819435	2.162459	2.749244
C	4.155158	1.904287	3.074550
C	4.504102	0.639270	3.562613

C	3.523176	-0.351906	3.669797
H	-0.334265	-0.122755	4.302972
H	-2.089690	-1.856408	4.120221
H	-1.562906	-4.045889	2.991258
H	0.746131	-4.466406	2.170120
H	2.537217	3.155585	2.381838
H	4.911490	2.686339	2.949994
H	5.536204	0.418036	3.853327
H	3.801408	-1.331303	4.066596
C	0.400476	1.591802	2.514141
H	-0.167997	0.786792	2.023024
H	-0.170886	1.885022	3.414481
H	0.410872	2.468022	1.847762
C	2.897756	-2.914553	2.237384
H	3.411047	-2.080421	1.733331
H	3.555689	-3.241905	3.063571
H	2.829495	-3.760123	1.535775

h-BN-catalyzed 2,2prime-dimethylbiphenyl rotation TS

N	0.992868	-6.084180	-0.619616
N	2.667493	-4.215535	-0.723635
N	4.348784	-2.349085	-0.738796
N	6.033071	-0.486897	-0.695037
N	5.258280	1.908971	-0.628598
N	4.480363	4.300843	-0.503498
N	2.024089	4.821975	-0.477548
N	-0.432415	5.345089	-0.396749
N	-2.885697	5.870337	-0.277914
N	-4.572474	3.999742	-0.245887
N	-6.254219	2.125618	-0.179534
N	-5.476745	-0.261204	-0.263547
N	-4.700882	-2.650182	-0.324004
N	-3.927896	-5.039122	-0.353771
N	-1.468422	-5.563154	-0.500368
N	0.207845	-3.694563	-0.651663
N	1.888998	-1.825017	-0.706642
N	3.573762	0.042754	-0.708199
N	2.798689	2.433367	-0.613079
N	0.339432	2.955337	-0.536937
N	-2.116832	3.477986	-0.399485
N	-3.797940	1.608913	-0.350553
N	-3.024813	-0.781431	-0.465748
N	-2.249049	-3.173210	-0.519108
B	-5.003118	-4.069923	-0.289392
B	-5.774926	-1.679680	-0.246079
B	-6.554597	0.707821	-0.176977

B	-4.875403	2.580010	-0.259194
B	-3.193937	4.449749	-0.308738
B	-1.507914	6.317685	-0.317010
B	0.947199	5.790154	-0.410357
B	3.405060	5.270695	-0.458851
B	4.181194	2.878790	-0.585489
B	4.954178	0.488938	-0.673642
B	5.729238	-1.902235	-0.717215
B	4.046132	-3.764438	-0.740124
B	2.369358	-5.635953	-0.685766
B	-0.090743	-5.114076	-0.594781
B	-2.547739	-4.592359	-0.461266
B	1.585164	-3.242141	-0.703926
B	3.269517	-1.373962	-0.714321
B	2.496643	1.011627	-0.653162
B	0.036239	1.533039	-0.576966
B	1.722357	3.401576	-0.549808
B	-0.737384	3.924967	-0.448305
B	-2.418662	2.057104	-0.430890
B	-4.097613	0.188458	-0.362871
B	-3.322033	-2.201183	-0.440504
B	-1.643820	-0.334023	-0.537782
B	-0.869796	-2.721172	-0.596202
B	0.809767	-0.854349	-0.655031
N	-1.344048	1.087884	-0.531400
N	-0.569585	-1.302835	-0.626686
N	1.114146	0.565885	-0.640894
N	3.460007	-6.608215	-0.701538
N	-1.194974	7.744161	-0.272294
N	5.130151	-4.742800	-0.741340
N	1.252435	7.216141	-0.349337
N	6.810619	-2.886899	-0.709887
N	3.703002	6.699603	-0.388620
N	-6.390991	-4.515022	-0.183819
N	-7.938655	0.248406	-0.085497
N	-7.159304	-2.131420	-0.144514
B	-7.336179	3.096664	-0.096542
B	-4.230955	-6.462352	-0.305582
B	-5.653438	4.974334	-0.162579
B	-1.768732	-6.988547	-0.449386
B	-3.963450	6.846406	-0.198002
B	0.695806	-7.508847	-0.571688
B	5.864492	4.751960	-0.470725
B	7.416654	-0.043249	-0.640717
B	6.642602	2.355706	-0.571807
B	-9.018858	1.216416	-0.006697

B	-8.234296	-1.164836	-0.069384
B	-7.460213	-3.547046	-0.115989
B	3.164104	-8.029681	-0.666017
B	4.831790	-6.158614	-0.732821
B	6.507457	-4.297827	-0.730136
B	5.083605	7.150654	-0.363575
B	2.629116	7.663528	-0.341467
B	0.179518	8.186085	-0.288150
N	-5.616090	-6.866432	-0.204594
N	-3.145267	-7.402800	-0.357506
N	-0.676826	-7.927113	-0.491188
N	1.800099	-8.442286	-0.604196
N	8.461547	-1.044026	-0.642273
N	7.690311	1.366798	-0.575858
N	6.912533	3.769630	-0.502552
N	-3.616630	8.250307	-0.169449
N	-5.320646	6.375856	-0.148384
N	-7.010759	4.496745	-0.095545
N	-8.694202	2.605436	-0.016627
N	6.122096	6.173800	-0.402150
B	-6.694703	-5.934922	-0.144155
B	-2.269724	8.718907	-0.201358
B	8.193495	-2.444316	-0.678111
H	-9.464590	3.270643	0.040424
H	-7.769043	5.176150	-0.036481
H	-6.074763	7.059973	-0.090336
H	-4.357994	8.948094	-0.117193
H	-2.029081	9.898894	-0.168593
H	0.434886	9.361537	-0.247089
H	2.877470	8.840144	-0.291517
H	5.346531	8.325084	-0.309034
H	7.085213	6.507394	-0.382558
H	7.881890	4.084995	-0.471728
H	8.660983	1.677200	-0.537197
H	9.437256	-0.749968	-0.614827
H	9.095801	-3.242801	-0.676963
H	7.399211	-5.106352	-0.731092
H	5.728426	-6.961527	-0.743976
H	4.051791	-8.843964	-0.684936
H	1.610244	-9.443502	-0.576633
H	-0.884086	-8.925079	-0.457035
H	-3.357902	-8.399629	-0.323159
H	-5.847031	-7.858864	-0.173103
H	-7.833589	-6.318651	-0.060008
H	-8.602758	-3.916282	-0.032998
H	-9.375009	-1.540773	0.008520

H	-10.165572	0.854355	0.066288
C	0.887223	-0.964787	2.765951
C	-0.193931	-0.045851	2.825627
C	-1.544061	-0.402381	2.792913
C	-1.898186	-1.747492	2.704825
C	-0.868855	-2.689106	2.669425
C	0.502934	-2.358395	2.704191
C	2.304530	-0.437078	2.741528
C	2.686965	0.957626	2.697025
C	4.055329	1.288870	2.599840
C	5.083903	0.346769	2.556909
C	4.733589	-0.999733	2.638706
C	3.386535	-1.356806	2.732630
H	0.009836	1.012487	2.900330
H	-2.306961	0.382573	2.825636
H	-2.944912	-2.064569	2.659139
H	-1.131242	-3.750602	2.600948
H	4.315420	2.351659	2.544889
H	6.126437	0.664860	2.456701
H	5.496337	-1.785174	2.618560
H	3.185869	-2.416093	2.802136
C	1.787091	2.180257	2.751609
H	1.062749	2.226434	1.921989
H	1.223568	2.252052	3.699416
H	2.403215	3.091113	2.677522
C	1.404319	-3.580952	2.677325
H	2.099263	-3.595157	1.821579
H	2.002546	-3.687878	3.600488
H	0.786195	-4.489295	2.590991

h-BN-catalyzed 2,2prime-dimethylbiphenyl product

N	-0.558584	-6.211189	-0.418140
N	1.531403	-4.837334	-0.647217
N	3.625709	-3.464744	-0.861347
N	5.727723	-2.094059	-0.950807
N	5.592997	0.418138	-0.847311
N	5.456440	2.923986	-0.629230
N	3.216344	4.052413	-0.504297
N	0.976185	5.187407	-0.408377
N	-1.261671	6.325572	-0.329347
N	-3.374059	4.953830	-0.389152
N	-5.482867	3.575709	-0.400518
N	-5.342143	1.068742	-0.459733
N	-5.199431	-1.439398	-0.427210
N	-5.056381	-3.943774	-0.308798
N	-2.807723	-5.078492	-0.352925

N	-0.712324	-3.705185	-0.569154
N	1.384427	-2.330776	-0.771764
N	3.485673	-0.954355	-0.913317
N	3.351465	1.549938	-0.717163
N	1.109545	2.682292	-0.583839
N	-1.131960	3.818399	-0.485029
N	-3.238234	2.445032	-0.507558
N	-3.101743	-0.064157	-0.598023
N	-2.957593	-2.573943	-0.519899
B	-5.852230	-2.733014	-0.333497
B	-5.992605	-0.225918	-0.415392
B	-6.137251	2.282606	-0.408609
B	-4.031774	3.660604	-0.433670
B	-1.924483	5.033659	-0.401993
B	0.185837	6.402596	-0.326781
B	2.424349	5.262402	-0.408887
B	4.665966	4.132909	-0.515269
B	4.801315	1.629547	-0.730476
B	4.935354	-0.873219	-0.913104
B	5.074449	-3.387236	-0.925212
B	2.974788	-4.756180	-0.757150
B	0.884101	-6.131895	-0.525396
B	-1.361189	-4.998544	-0.446314
B	-3.606514	-3.866579	-0.395544
B	0.731834	-3.622577	-0.666520
B	2.831050	-2.246635	-0.864438
B	2.693874	0.258109	-0.792629
B	0.451953	1.389185	-0.661092
B	2.559689	2.758820	-0.598965
B	0.317475	3.894770	-0.493851
B	-1.788021	2.524290	-0.552384
B	-3.892309	1.149204	-0.529581
B	-3.750182	-1.359512	-0.522549
B	-1.651002	0.015743	-0.641935
B	-1.508954	-2.489970	-0.588462
B	0.587713	-1.114857	-0.735601
N	-0.997378	1.312700	-0.647415
N	-0.858408	-1.197787	-0.682935
N	1.245280	0.177958	-0.747052
N	1.692398	-7.348889	-0.512041
N	0.854409	7.698967	-0.241622
N	3.774459	-5.976997	-0.753702
N	3.085151	6.560740	-0.315635
N	5.867432	-4.614151	-0.942018
N	5.321196	5.435491	-0.414227
N	-7.309570	-2.807037	-0.256383

N	-7.594783	2.193702	-0.357819
N	-7.448259	-0.307326	-0.344925
B	-6.280746	4.792498	-0.342845
B	-5.710474	-5.239464	-0.193723
B	-4.169716	6.173421	-0.320504
B	-3.459340	-6.376644	-0.232212
B	-2.053579	7.545316	-0.256097
B	-1.206389	-7.509248	-0.293153
B	6.909473	3.006691	-0.642550
B	7.181942	-2.017240	-0.980960
B	7.047544	0.497638	-0.853517
B	-8.392091	3.407412	-0.317794
B	-8.242289	0.903238	-0.329300
B	-8.099467	-1.598217	-0.272080
B	1.047403	-8.644148	-0.382790
B	3.128967	-7.267121	-0.631815
B	5.216067	-5.900186	-0.860543
B	6.771282	5.518207	-0.423576
B	4.530792	6.639635	-0.314646
B	2.296810	7.771903	-0.232749
N	-7.154735	-5.274806	-0.122408
N	-4.897087	-6.424046	-0.154826
N	-2.639573	-7.560897	-0.197101
N	-0.374018	-8.692081	-0.273285
N	7.933124	-3.252331	-1.032294
N	7.806658	-0.723850	-0.947068
N	7.670724	1.792723	-0.758881
N	-1.357535	8.810890	-0.179616
N	-3.487411	7.440810	-0.261475
N	-5.606066	6.061420	-0.311469
N	-7.721456	4.666544	-0.315191
N	7.524172	4.311786	-0.535849
B	-7.963537	-4.100101	-0.154021
B	0.065226	8.916169	-0.167633
B	7.316601	-4.538328	-1.009567
H	-8.296876	5.507397	-0.281594
H	-6.165569	6.912847	-0.265384
H	-4.041165	8.295726	-0.210759
H	-1.895057	9.675532	-0.127420
H	0.600336	9.993318	-0.097902
H	2.844942	8.840857	-0.157684
H	5.072999	7.711143	-0.232810
H	7.327678	6.583515	-0.339024
H	8.540675	4.388624	-0.543019
H	8.688864	1.850968	-0.764838
H	8.825071	-0.670809	-0.957114

H	8.951352	-3.217556	-1.068041
H	7.984541	-5.540441	-1.039135
H	5.871622	-6.909418	-0.873248
H	3.791906	-8.271618	-0.628100
H	1.699045	-9.657298	-0.368280
H	-0.809874	-9.609441	-0.185275
H	-3.092767	-8.470689	-0.113575
H	-5.355880	-7.331275	-0.074066
H	-7.630371	-6.173300	-0.046629
H	-9.164147	-4.179511	-0.093859
H	-9.300111	-1.662530	-0.217769
H	-9.443012	0.832682	-0.285498
H	-9.595109	3.352493	-0.284313
C	0.492105	-0.710613	2.902146
C	-0.404515	0.348090	2.635226
C	-1.778694	0.135880	2.492867
C	-2.288381	-1.164839	2.596537
C	-1.411017	-2.228489	2.833100
C	-0.024700	-2.033712	2.992385
C	1.941536	-0.393262	3.066858
C	2.393433	0.648124	3.925690
C	3.771707	0.930944	3.975810
C	4.705462	0.213216	3.219775
C	4.265379	-0.834177	2.401649
C	2.899234	-1.123568	2.332529
H	-0.001342	1.358870	2.518743
H	-2.443617	0.980634	2.285661
H	-3.361186	-1.352289	2.483507
H	-1.807235	-3.248227	2.906637
H	4.116103	1.732594	4.639826
H	5.770173	0.461410	3.280380
H	4.978208	-1.420878	1.813297
H	2.551667	-1.923853	1.675371
C	1.463564	1.442728	4.818407
H	1.101716	2.364927	4.327102
H	0.572862	0.863007	5.107464
H	1.990298	1.754973	5.736040
C	0.841784	-3.242524	3.271788
H	1.216179	-3.701849	2.337120
H	1.722938	-2.990277	3.882799
H	0.260739	-4.018809	3.797409

Graphane-catalyzed corannulene reactant

C	0.294945	1.464098	-0.495865
C	1.524063	0.638218	-0.918757
C	1.391551	-0.827588	-0.466672

C	0.085739	-1.463018	-0.977702
C	-1.140219	-0.631740	-0.555630
C	-1.012219	0.833889	-1.010478
H	1.572103	0.648056	-2.031635
H	0.253181	1.452437	0.615381
H	0.122855	-1.468564	-2.091003
H	-1.175884	-0.632092	0.557409
H	-0.974945	0.839639	-2.123791
H	1.343893	-0.826224	0.643613
C	-2.450239	-1.267289	-1.057468
C	2.622483	-1.659384	-0.873269
C	2.826375	1.267968	-0.390305
C	0.425088	2.934295	-0.936356
C	-0.043151	-2.922111	-0.503541
C	-2.237549	1.659893	-0.578823
C	-3.549437	1.030834	-1.083481
C	-3.672621	-0.434794	-0.630187
C	3.925177	-1.025388	-0.349799
C	4.061359	0.442163	-0.794947
C	1.729690	3.562588	-0.411490
C	-1.354100	-3.565762	-0.991475
C	-0.802720	3.757442	-0.504717
C	1.182694	-3.762127	-0.906544
C	2.962648	2.738996	-0.825094
C	-2.112084	3.130851	-1.017580
H	4.122506	0.452065	-1.906747
H	3.868260	-1.026850	0.762219
H	1.224162	-3.788989	-2.019080
H	-1.323955	-3.594946	-2.104562
H	-3.694021	-0.433949	0.480719
H	-3.525647	1.042745	-2.197017
H	-2.270046	1.646484	0.532423
H	0.467097	2.951104	-2.049359
H	2.767464	1.254530	0.720858
H	2.674987	-1.665119	-1.985779
H	-0.081101	-2.900287	0.606985
H	-2.416525	-1.276720	-2.170830
C	2.489700	-3.120984	-0.406499
H	2.442532	-3.107430	0.705530
C	-2.576798	-2.725700	-0.579479
H	-2.602763	-2.702568	0.532108
H	-2.080903	3.150366	-2.130822
H	-0.840152	3.733513	0.607146
H	3.021911	2.756462	-1.937014
H	1.678034	3.543013	0.699192
C	-2.272613	3.006728	3.192802

C	-3.416510	2.201371	3.165350
C	0.358790	2.968150	3.266037
C	-0.973922	2.487288	3.575936
C	-1.007929	1.199209	4.109361
C	-3.376860	0.794605	3.516833
C	1.478190	2.129574	3.302449
C	-4.267265	-0.291048	3.152099
C	-1.746747	-3.205090	3.231428
C	-0.348360	-3.226257	3.273505
C	-2.508930	-2.013296	3.551297
C	-1.750696	-0.978707	4.097205
C	-0.329206	-0.999650	4.138496
C	0.429121	-2.057234	3.639270
C	1.804431	-1.710377	3.335503
C	2.255577	-0.385980	3.340788
C	1.377697	0.725555	3.652535
C	0.129872	0.346752	4.145924
C	-3.853714	-1.627609	3.168304
C	-2.170318	0.380125	4.079646
H	2.494982	-2.491469	2.997638
H	3.278796	-0.186948	3.002276
H	2.439197	2.532064	2.962428
H	0.489321	3.992571	2.899540
H	-2.353584	4.033596	2.820093
H	-4.345125	2.632505	2.775626
H	-5.265562	-0.060001	2.762905
H	-4.544194	-2.389446	2.789001
H	-2.268016	-4.092120	2.852177
H	0.167525	-4.129466	2.926017
C	1.863155	5.035308	-0.839417
C	-0.675876	5.230980	-0.932457
C	4.260246	3.366658	-0.282261
C	5.359188	1.070783	-0.253573
C	5.159211	-1.854676	-0.748567
C	3.719467	-3.958399	-0.802315
C	1.053557	-5.215122	-0.411322
C	-1.481955	-5.017600	-0.492237
C	-3.890144	-3.369548	-1.059730
C	-4.989010	-1.069744	-1.114832
C	-4.770248	1.855137	-0.633492
C	-3.335006	3.954235	-0.571342
C	5.496471	2.542291	-0.684972
C	0.632110	5.856506	-0.414246
C	-4.650784	3.327557	-1.066302
C	-5.111380	-2.530336	-0.642796
C	-0.258313	-5.862279	-0.890486

C	5.023341	-3.318472	-0.290818
H	-0.225611	-5.900018	-2.003228
H	-1.511444	-4.981519	0.620688
H	1.019496	-5.182185	0.702445
H	3.768308	-3.976190	-1.914570
H	4.975746	-3.313985	0.822801
H	5.215666	-1.854718	-1.860682
H	5.295753	1.055307	0.859086
H	5.560629	2.559516	-1.796847
H	4.196946	3.349257	0.830612
H	1.912807	5.058053	-1.951665
H	0.589716	5.839528	0.699919
H	-0.639448	5.253980	-2.045232
H	-3.356533	3.932179	0.541106
H	-4.636670	3.350395	-2.179878
H	-4.782821	1.838406	0.479487
H	-4.973215	-1.075577	-2.228380
H	-5.135419	-2.513825	0.470846
H	-3.864514	-3.395715	-2.172815
C	-4.017988	-4.823398	-0.565064
C	-2.795217	-5.667930	-0.966201
C	2.278699	-6.060958	-0.807126
C	3.588813	-5.416049	-0.319766
C	6.460957	-1.223114	-0.218525
C	6.597114	0.246670	-0.655718
C	4.399496	4.839784	-0.711158
C	3.164457	5.663634	-0.304390
C	-1.901473	6.054560	-0.492781
C	-3.214726	5.429407	-0.997229
C	-6.091445	1.228004	-1.115520
C	-6.209410	-0.240428	-0.670109
H	3.553681	-5.393583	0.793962
H	2.314621	-6.094246	-1.919898
H	-2.765780	-5.705967	-2.079070
H	-4.050040	-4.792180	0.549183
H	-6.219854	-0.248102	0.444576
H	-6.083267	1.241320	-2.229248
H	-3.192654	5.456008	-2.110547
H	-1.930964	6.036181	0.621733
H	3.106337	5.649290	0.808488
H	4.462375	4.857768	-1.823134
H	6.659263	0.261177	-1.767787
H	6.406140	-1.235107	0.894410
C	-4.437440	6.252125	-0.540998
C	-5.870041	4.149970	-0.604324
C	-7.310263	2.053448	-0.653701

C	-7.532414	-0.873504	-1.146105
C	-6.429613	-3.171784	-1.117291
C	-5.333637	-5.471796	-1.042037
C	-2.923556	-7.119685	-0.460268
C	-0.386332	-7.312950	-0.384874
C	2.150038	-7.514982	-0.307730
C	4.817101	-6.258195	-0.722132
C	6.255481	-4.152999	-0.693038
C	7.697077	-2.051498	-0.625428
C	7.897867	0.875680	-0.115254
C	6.794924	3.170195	-0.140987
C	5.699241	5.468363	-0.167853
C	3.300522	7.138143	-0.736827
C	0.761744	7.331382	-0.843340
C	-1.777204	7.531031	-0.922117
C	-7.633827	-2.330042	-0.679591
C	-6.538450	-4.620388	-0.626921
C	-5.451619	-6.918074	-0.539241
C	-4.234619	-7.758237	-0.940906
C	-1.697462	-7.945736	-0.864828
C	0.837518	-8.142188	-0.790707
C	4.679007	-7.707038	-0.231717
C	6.109778	-5.604329	-0.220417
C	7.545619	-3.508180	-0.172542
C	9.122886	0.047573	-0.529197
C	8.016019	2.339936	-0.553115
C	5.827714	6.934327	-0.606410
C	2.065252	7.942004	-0.315343
C	-0.467088	8.137316	-0.406652
C	-3.001468	8.342648	-0.473964
C	-5.738689	5.613891	-1.039383
C	-7.175894	3.514969	-1.094854
C	-8.622107	1.420053	-1.138334
H	2.021896	7.982305	0.793289
H	2.158953	8.990275	-0.660332
H	-0.498678	8.175077	0.702500
H	-0.373461	9.186106	-0.750061
C	-4.308778	7.719301	-0.974930
H	-3.015384	8.385202	0.634348
H	-2.907515	9.387576	-0.825260
H	-5.180074	8.296119	-0.611131
H	-4.340540	7.768635	-2.082409
H	-6.609155	6.195976	-0.678472
H	-5.766810	5.665870	-2.147773
H	-8.042409	4.101910	-0.732295
H	-7.208258	3.563454	-2.203276

C	-8.740113	-0.040965	-0.691366
H	-9.482666	2.010685	-0.771196
H	-8.656274	1.471155	-2.245648
H	-9.673707	-0.493325	-1.075984
H	-8.805172	-0.082530	0.415275
H	-8.571050	-2.785264	-1.055234
H	-7.701846	-2.348757	0.428622
H	-7.474460	-5.078641	-1.001902
H	-6.614720	-4.620441	0.480915
H	-6.384103	-7.373775	-0.922588
H	-5.540960	-6.905346	0.566320
H	-4.320663	-8.785814	-0.539821
H	-4.201307	-7.854735	-2.045266
H	-1.787214	-8.976380	-0.469317
H	-1.671711	-8.037600	-1.970747
H	0.743439	-9.173458	-0.397862
H	0.863696	-8.231315	-1.896843
C	3.373809	-8.347791	-0.716035
H	3.275743	-9.377066	-0.322182
H	3.393643	-8.435810	-1.821434
H	4.701579	-7.712020	0.877201
H	5.551800	-8.300085	-0.564421
H	6.116102	-5.624150	0.889566
H	6.986193	-6.197992	-0.546233
H	7.543297	-3.542221	0.937092
H	8.422897	-4.100051	-0.499289
C	8.988998	-1.415168	-0.091872
C	6.918039	4.634386	-0.578421
C	4.599622	7.755182	-0.198202
H	8.981869	-1.468424	1.015970
H	9.863410	-2.004238	-0.427334
H	9.229889	0.094663	-1.632111
H	10.040759	0.498263	-0.106574
H	8.125096	2.380342	-1.657044
H	8.937700	2.788070	-0.133079
H	7.028699	4.674425	-1.682204
H	7.840903	5.078937	-0.157181
H	6.749456	7.373930	-0.180571
H	5.944374	6.968882	-1.708794
H	4.540287	7.803162	0.908333
H	4.693294	8.799498	-0.551448
H	0.803040	7.346443	-1.954504
H	-1.747643	7.546349	-2.033812
H	-4.450129	6.227661	0.571422
H	-5.877782	4.126043	0.508488
H	-7.314935	2.032701	0.459039

H	-7.515569	-0.869706	-2.258138
H	-6.407245	-3.186904	-2.228942
H	-5.299894	-5.499915	-2.153384
H	-2.954674	-7.076719	0.651152
H	-0.415749	-7.270734	0.726450
H	2.121224	-7.477259	0.803781
H	4.850757	-6.277288	-1.833661
H	6.299469	-4.157767	-1.804188
H	7.746571	-2.040985	-1.736521
H	7.834136	0.855713	0.995178
H	6.728579	3.151004	0.969184
H	5.631613	5.451387	0.942418
H	3.354205	7.149611	-1.847707

Graphane-catalyzed corannulene inversion TS

C	-0.495903	-1.432884	-0.485890
C	-1.608264	-0.454561	-0.905339
C	-1.280419	0.981995	-0.458510
C	0.093183	1.440757	-0.981539
C	1.200074	0.456523	-0.561914
C	0.882417	-0.983508	-1.004773
H	-1.665275	-0.460457	-2.017767
H	-0.448769	-1.419535	0.624248
H	0.049239	1.451627	-2.094434
H	1.232603	0.457056	0.549087
H	0.848800	-0.998300	-2.118003
H	-1.222265	0.975427	0.650882
C	2.585649	0.912484	-1.054918
C	-2.395654	1.968289	-0.851163
C	-2.977558	-0.907044	-0.364366
C	-0.818520	-2.877042	-0.912064
C	0.415889	2.869651	-0.506954
C	1.985929	-1.957692	-0.553220
C	3.375008	-1.510570	-1.044117
C	3.682705	-0.068495	-0.602702
C	-3.764142	1.509359	-0.313712
C	-4.096064	0.073948	-0.759722
C	-2.192510	-3.324166	-0.379218
C	1.797634	3.336522	-0.999861
C	0.290137	-3.849174	-0.467904
C	-0.693224	3.863670	-0.896081
C	-3.308111	-2.348259	-0.794149
C	1.673480	-3.404855	-0.976628
H	-4.165852	0.074635	-1.871166
H	-3.694629	1.502856	0.797451
H	-0.743375	3.898555	-2.008104

H	1.770650	3.368642	-2.112853
H	3.689787	-0.059293	0.508109
H	3.365039	-1.531185	-2.157767
H	2.007261	-1.936212	0.557546
H	-0.863225	-2.900084	-2.024805
H	-2.908983	-0.900663	0.746065
H	-2.458335	1.984226	-1.963125
H	0.458498	2.842059	0.602892
H	2.567513	0.916297	-2.168577
C	-2.067125	3.397622	-0.381350
H	-2.011005	3.371659	0.730189
C	2.897840	2.344569	-0.582494
H	2.913739	2.324292	0.528371
H	1.649854	-3.434460	-2.089851
H	0.324401	-3.820952	0.643667
H	-3.373472	-2.361688	-1.905826
H	-2.134604	-3.304079	0.731379
C	1.929221	-3.272312	3.229798
C	3.188997	-2.630596	3.205247
C	-0.775165	-2.843633	3.294631
C	0.658082	-2.547032	3.261678
C	0.873490	-1.186720	3.255836
C	3.350545	-1.175485	3.209826
C	-1.774585	-1.844054	3.325185
C	4.433365	-0.189818	3.194365
C	2.275389	3.144104	3.262380
C	0.879463	3.365384	3.296991
C	2.878259	1.809542	3.240346
C	1.904343	0.836095	3.248122
C	0.518383	1.055733	3.281776
C	-0.106691	2.282496	3.314214
C	-1.561401	2.121318	3.351251
C	-2.203216	0.861241	3.357755
C	-1.478274	-0.410260	3.327439
C	-0.118531	-0.194547	3.286520
C	4.212289	1.206722	3.208177
C	2.123668	-0.549877	3.232312
H	-2.207098	3.006311	3.370560
H	-3.298677	0.862927	3.380921
H	-2.815942	-2.184891	3.339961
H	-1.115796	-3.885095	3.288257
H	1.930641	-4.367971	3.216941
H	4.073524	-3.276654	3.175075
H	5.475625	-0.526424	3.163712
H	5.099528	1.849291	3.187961
H	2.917546	4.031785	3.245049

H	0.543049	4.408207	3.303570
C	-2.518611	-4.769240	-0.797686
C	-0.026396	-5.297600	-0.882032
C	-4.674262	-2.798574	-0.244003
C	-5.461363	-0.379644	-0.210099
C	-4.882207	2.494349	-0.701024
C	-3.180059	4.389975	-0.764491
C	-0.369926	5.285711	-0.400431
C	2.114852	4.757885	-0.497470
C	4.289218	2.807914	-1.050018
C	5.077676	0.383478	-1.071754
C	4.471022	-2.482589	-0.568516
C	2.773502	-4.374859	-0.506795
C	-5.793235	-1.819423	-0.642147
C	-1.406503	-5.741481	-0.363939
C	4.164844	-3.930477	-0.992137
C	5.383727	1.819462	-0.608670
C	1.011267	5.755632	-0.891069
C	-4.551986	3.926273	-0.242146
H	0.975996	5.796774	-2.003670
H	2.139991	4.713126	0.614680
H	-0.329673	5.245071	0.712497
H	-3.236135	4.415423	-1.876377
H	-4.496150	3.912936	0.870960
H	-4.946691	2.505293	-1.812700
H	-5.389026	-0.374617	0.901944
H	-5.863170	-1.826721	-1.753782
H	-4.603185	-2.787633	0.868236
H	-2.570529	-4.793203	-1.909826
H	-1.364544	-5.720121	0.749920
H	-0.060141	-5.328348	-1.994700
H	2.785879	-4.341164	0.605383
H	4.159531	-3.961123	-2.105732
H	4.471432	-2.455753	0.544264
H	5.078133	0.379941	-2.185570
H	5.389035	1.809959	0.505106
H	4.282457	2.829907	-2.163473
C	4.601285	4.234607	-0.558724
C	3.502167	5.230112	-0.970434
C	-1.477118	6.284877	-0.785486
C	-2.855304	5.817444	-0.284331
C	-6.251663	2.038002	-0.162665
C	-6.582774	0.600707	-0.602753
C	-5.007247	-4.241276	-0.669103
C	-3.890708	-5.218428	-0.259883
C	1.078071	-6.269391	-0.424755

C	2.465652	-5.825660	-0.921701
C	5.868115	-2.038105	-1.039371
C	6.172506	-0.594066	-0.602951
H	-2.812333	5.790503	0.829051
H	-1.519774	6.321664	-1.897945
H	3.482358	5.267420	-2.083560
H	4.618970	4.202979	0.555560
H	6.172736	-0.577482	0.511387
H	5.869456	-2.059980	-2.153132
H	2.449862	-5.859613	-2.035020
H	1.100758	-6.243164	0.689540
H	-3.830667	-5.206473	0.852939
H	-5.072772	-4.253854	-1.780994
H	-6.652281	0.598490	-1.714479
H	-6.188069	2.038736	0.949937
C	3.566158	-6.797043	-0.447763
C	5.261246	-4.901156	-0.510997
C	6.963551	-3.012015	-0.559014
C	7.572158	-0.143926	-1.068578
C	6.780480	2.278297	-1.070550
C	5.994807	4.702510	-1.025542
C	3.818272	6.653974	-0.468455
C	1.330986	7.177378	-0.388668
C	-1.154642	7.710057	-0.291161
C	-3.966629	6.813106	-0.675689
C	-5.667371	4.915895	-0.632949
C	-7.371172	3.022777	-0.558050
C	-7.951787	0.146283	-0.056475
C	-7.160704	-2.272072	-0.093611
C	-6.377400	-4.692820	-0.123323
C	-4.218896	-6.664434	-0.685016
C	-1.727001	-7.190089	-0.782049
C	0.764828	-7.720917	-0.842361
C	7.858638	1.290316	-0.611321
C	7.073264	3.704393	-0.590781
C	6.297134	6.124627	-0.531632
C	5.202731	7.113241	-0.946849
C	2.711130	7.631857	-0.875798
C	0.223823	8.159137	-0.787690
C	-3.635132	8.231581	-0.189964
C	-5.328684	6.334554	-0.161116
C	-7.026520	4.445147	-0.102945
C	-9.059740	1.129816	-0.459298
C	-8.263771	-1.287714	-0.498062
C	-6.697416	-6.129805	-0.558914
C	-3.100802	-7.620800	-0.255635

C	-0.616415	-8.146188	-0.332148
C	1.869236	-8.681175	-0.377539
C	4.943876	-6.338635	-0.937508
C	6.643514	-4.446687	-0.991759
C	8.351549	-2.559683	-1.033708
H	-3.066206	-7.659474	0.853381
H	-3.330399	-8.649958	-0.594677
H	-0.596546	-8.178619	0.777454
H	-0.844388	-9.176657	-0.668315
C	3.250187	-8.238230	-0.872179
H	1.869452	-8.714637	0.731215
H	1.642274	-9.708327	-0.720689
H	4.036125	-8.921205	-0.497662
H	3.282823	-8.300087	-1.978993
H	5.727565	-7.026910	-0.564484
H	4.974658	-6.402574	-2.045186
H	7.422378	-5.139245	-0.616513
H	6.679857	-4.507706	-2.099425
C	8.655476	-1.123552	-0.594927
H	9.123859	-3.255465	-0.654380
H	8.389090	-2.623024	-2.140278
H	9.644495	-0.800537	-0.971580
H	8.713769	-1.082436	0.512179
H	8.852081	1.615117	-0.978140
H	7.915253	1.309619	0.497549
H	8.065280	4.032342	-0.958628
H	7.137427	3.704839	0.517867
H	7.283871	6.451657	-0.910737
H	6.376736	6.108599	0.574717
H	5.420189	8.124219	-0.553065
H	5.187295	7.204034	-2.052038
H	2.936184	8.644055	-0.486195
H	2.694285	7.720353	-1.982078
H	0.455635	9.170405	-0.399691
H	0.199727	8.247805	-1.893832
C	-2.262764	8.695204	-0.689506
H	-2.026470	9.703720	-0.300397
H	-2.282751	8.782644	-1.794902
H	-3.644586	8.240212	0.919165
H	-4.426546	8.933560	-0.514291
H	-5.321581	6.353248	0.948902
H	-6.122814	7.038681	-0.477971
H	-7.011068	4.474817	1.006732
H	-7.821047	5.148315	-0.420917
C	-8.731810	2.559963	-0.017567
C	-7.476678	-3.706402	-0.532080

C	-5.588299	-7.103313	-0.146620
H	-8.710449	2.606708	1.090421
H	-9.523218	3.260774	-0.344377
H	-9.178525	1.102405	-1.561632
H	-10.026428	0.801706	-0.032472
H	-8.381781	-1.309530	-1.601543
H	-9.234704	-1.612112	-0.075080
H	-7.593213	-3.730508	-1.635667
H	-8.449423	-4.026045	-0.109636
H	-7.669599	-6.443419	-0.133676
H	-6.816048	-6.151244	-1.661394
H	-5.537023	-7.154408	0.960221
H	-5.817814	-8.127753	-0.496082
H	-1.765362	-7.209208	-1.893221
H	0.741230	-7.742882	-1.954091
H	3.572359	-6.764978	0.664566
H	5.260813	-4.868733	0.601502
H	6.960047	-2.983103	0.553570
H	7.566518	-0.154805	-2.180740
H	6.773856	2.285568	-2.182545
H	5.976606	4.725494	-2.137346
H	3.841567	6.610140	0.643288
H	1.361098	7.132274	0.722659
H	-1.120145	7.670221	0.820221
H	-4.008603	6.835560	-1.786895
H	-5.719438	4.928425	-1.743690
H	-7.428944	3.022910	-1.668800
H	-7.879563	0.153195	1.053676
H	-7.087747	-2.263990	1.016350
H	-6.306405	-4.683253	0.986921
H	-4.271231	-6.674732	-1.795954

Graphane-catalyzed corannulene product

C	1.220808	1.103443	-0.539065
C	1.734522	-0.285527	-0.961421
C	0.736082	-1.386795	-0.560887
C	-0.674666	-1.117927	-1.120954
C	-1.172004	0.277097	-0.699494
C	-0.187065	1.392636	-1.095456
H	1.830280	-0.294387	-2.070929
H	1.133078	1.092534	0.568906
H	-0.617402	-1.147793	-2.232820
H	-1.212189	0.274904	0.406281
H	-0.121312	1.423324	-2.206730
H	0.654664	-1.359759	0.546930
C	-2.604707	0.562198	-1.186615

C	1.243750	-2.789928	-0.939270
C	3.129294	-0.561631	-0.366845
C	2.217680	2.219043	-0.900791
C	-1.658299	-2.212114	-0.662212
C	-0.688601	2.765447	-0.606493
C	-2.116821	3.066061	-1.097083
C	-3.085712	1.940755	-0.692885
C	2.644037	-3.054900	-0.354100
C	3.645560	-1.958304	-0.758719
C	3.617217	1.931010	-0.324682
C	-3.091050	-1.943956	-1.159239
C	1.706583	3.595187	-0.434869
C	-1.167001	-3.619416	-1.044791
C	4.132657	0.543006	-0.745351
C	0.293906	3.893124	-0.970060
H	3.742221	-1.982530	-1.867845
H	2.548273	-3.021196	0.755285
H	-1.118860	-3.675504	-2.155968
H	-3.081166	-1.975824	-2.272491
H	-3.091939	1.903200	0.418124
H	-2.094937	3.118057	-2.209294
H	-0.732002	2.716035	0.503197
H	2.308603	2.248133	-2.010269
H	3.021233	-0.547925	0.741618
H	1.327006	-2.835259	-2.048862
H	-1.690005	-2.173633	0.447332
H	-2.599127	0.576491	-2.300244
C	0.248643	-3.879457	-0.497340
H	0.182496	-3.831601	0.613137
C	-3.571473	-0.546489	-0.727305
H	-3.574033	-0.534546	0.383703
H	0.355290	3.946262	-2.080660
H	1.635084	3.558637	0.676180
H	4.230786	0.542102	-1.854586
H	3.520647	1.924945	0.785231
C	-4.458129	-1.317162	3.398893
C	-4.737648	0.056664	3.421721
C	-2.501936	-3.112741	3.443786
C	-3.124271	-1.834170	3.146516
C	-2.219560	-0.858508	2.741320
C	-3.713676	1.061779	3.194004
C	-1.110316	-3.273066	3.505200
C	-3.637937	2.471335	3.537752
C	0.217418	2.856726	3.729081
C	1.250178	1.908757	3.752491
C	-1.143737	2.514304	3.352868

C	-1.269122	1.228266	2.838501
C	-0.224205	0.268824	2.863103
C	1.033851	0.515176	3.402493
C	1.779506	-0.693836	3.707523
C	1.198724	-1.968685	3.647181
C	-0.190828	-2.172052	3.275657
C	-0.811932	-1.020695	2.803164
C	-2.418957	3.160115	3.613224
C	-2.502379	0.531212	2.763020
H	2.808941	-0.614215	4.074291
H	1.801833	-2.824915	3.969197
H	-0.717517	-4.248470	3.813205
H	-3.130987	-3.970386	3.707075
H	-5.265135	-2.011140	3.659108
H	-5.749935	0.371336	3.698824
H	-4.549796	3.005581	3.826989
H	-2.436097	4.199914	3.958330
H	0.439986	3.868938	4.084698
H	2.230885	2.225243	4.124822
C	4.616493	3.042237	-0.696282
C	2.696010	4.717199	-0.800076
C	5.528949	0.265191	-0.157431
C	5.041404	-2.230414	-0.166960
C	3.155774	-4.456878	-0.733318
C	0.748936	-5.287263	-0.869382
C	-2.147936	-4.704383	-0.561718
C	-4.059730	-3.035509	-0.665053
C	-5.015821	-0.268150	-1.180475
C	-4.528123	2.236240	-1.142598
C	-2.604959	4.430037	-0.572371
C	-0.205802	5.259591	-0.464143
C	6.043080	-1.129191	-0.558266
C	4.106027	4.425811	-0.254758
C	-1.633131	5.560278	-0.955236
C	-5.488698	1.116693	-0.701638
C	-3.578160	-4.441117	-1.065977
C	2.158793	-5.550496	-0.309487
H	-3.558578	-4.486974	-2.178815
H	-4.061364	-2.991360	0.447557
H	-2.174581	-4.649070	0.550411
H	0.814370	-5.335904	-1.979967
H	2.084868	-5.517745	0.802003
H	3.240269	-4.491467	-1.843158
H	4.940777	-2.209918	0.942311
H	6.140104	-1.144048	-1.667842
H	5.429563	0.276276	0.952120

H	4.702322	3.054407	-1.806476
H	4.034541	4.412496	0.857150
H	2.766059	4.750894	-1.910939
H	-0.244063	5.204079	0.647984
H	-1.602580	5.614923	-2.067396
H	-2.621312	4.366231	0.539633
H	-4.536547	2.271857	-2.255672
H	-5.481285	1.096865	0.412252
H	-5.029936	-0.266869	-2.294058
C	-5.978006	-1.371998	-0.700652
C	-5.501910	-2.769196	-1.135411
C	-1.660806	-6.114866	-0.943110
C	-0.239437	-6.378041	-0.414421
C	4.557883	-4.727086	-0.154780
C	5.557669	-3.628437	-0.557046
C	6.532142	1.369389	-0.541345
C	6.020175	2.760427	-0.127112
C	2.193382	6.093921	-0.325319
C	0.772333	6.389605	-0.837464
C	-4.042223	4.734571	-1.034768
C	-5.007629	3.607400	-0.628250
H	-0.287574	-6.336663	0.698255
H	-1.621074	-6.165774	-2.055169
H	-5.503708	-2.796430	-2.249056
H	-5.969974	-1.351882	0.413453
H	-5.009735	3.558641	0.485185
H	-4.033746	4.786267	-2.147510
H	0.818231	6.435975	-1.949463
H	2.144252	6.062124	0.787465
H	5.934906	2.765620	0.983881
H	6.625743	1.362987	-1.651322
H	5.652301	-3.651020	-1.666732
H	4.468844	-4.705004	0.955742
C	0.275625	7.762984	-0.340952
C	-2.123906	6.928295	-0.441757
C	-4.526718	6.103676	-0.515129
C	-6.452100	3.907032	-1.078742
C	-6.936003	1.405829	-1.145950
C	-7.425664	-1.095788	-1.155640
C	-6.469541	-3.866554	-0.646934
C	-4.552230	-5.531454	-0.577897
C	-2.642950	-7.205352	-0.468357
C	0.256624	-7.786904	-0.799877
C	2.663946	-6.955246	-0.693827
C	5.069889	-6.128738	-0.545533
C	6.958585	-3.901350	0.028163

C	7.442093	-1.403977	0.027809
C	7.934227	1.091740	0.038815
C	7.019549	3.869643	-0.514984
C	5.098756	5.541478	-0.636911
C	3.178319	7.217537	-0.708825
C	-7.396341	2.780168	-0.647388
C	-7.881571	0.290153	-0.687356
C	-8.379167	-2.201295	-0.679874
C	-7.902926	-3.589067	-1.120540
C	-5.976286	-5.253721	-1.070406
C	-4.058608	-6.924479	-0.982717
C	-0.732336	-8.867857	-0.340030
C	1.667134	-8.033205	-0.253324
C	4.065405	-7.207511	-0.126384
C	7.461311	-5.295860	-0.371286
C	7.939977	-2.796092	-0.375784
C	8.923132	2.196688	-0.358831
C	6.496734	5.243918	-0.082645
C	4.583505	6.910792	-0.179125
C	2.672129	8.585622	-0.228852
C	-1.146949	8.040577	-0.837775
C	-3.551253	7.213293	-0.920465
C	-5.960871	6.394861	-0.978467
H	6.460074	5.282289	1.026286
H	7.204859	6.035564	-0.396940
H	4.562517	6.934383	0.930645
H	5.288997	7.705090	-0.492681
C	1.255675	8.876842	-0.735504
H	2.674616	8.597084	0.880316
H	3.373171	9.378936	-0.550679
H	0.895498	9.848985	-0.348596
H	1.269676	8.965365	-1.840917
H	-1.501811	9.014444	-0.446928
H	-1.133996	8.134660	-1.943677
H	-3.897041	8.187567	-0.522481
H	-3.551271	7.310518	-2.026176
C	-6.921894	5.275670	-0.565416
H	-6.296786	7.367929	-0.572408
H	-5.966616	6.497294	-2.082756
H	-7.945129	5.482937	-0.932187
H	-6.987729	5.238071	0.541347
H	-8.424516	2.987953	-1.003521
H	-7.449362	2.760633	0.461603
H	-8.910053	0.493597	-1.045129
H	-7.931225	0.295084	0.421957
H	-9.401593	-2.001340	-1.052888

H	-8.438052	-2.168791	0.427463
H	-8.583388	-4.374483	-0.740061
H	-7.933993	-3.656586	-2.227083
H	-6.666697	-6.033997	-0.693894
H	-5.998752	-5.325454	-2.177813
H	-4.758099	-7.698385	-0.609950
H	-4.066005	-7.004764	-2.089747
C	-2.147133	-8.602917	-0.865347
H	-2.851202	-9.371423	-0.493622
H	-2.151250	-8.683002	-1.971479
H	-0.749986	-8.886090	0.768957
H	-0.375505	-9.864316	-0.662788
H	1.625048	-8.052693	0.855969
H	2.026879	-9.032669	-0.567369
H	4.006414	-7.233528	0.981969
H	4.427214	-8.205992	-0.441119
C	6.467790	-6.389629	0.033683
C	8.426994	-0.299864	-0.371823
C	8.415859	3.581849	0.055486
H	6.394443	-6.428290	1.139795
H	6.828259	-7.384334	-0.290286
H	7.610267	-5.321219	-1.470017
H	8.453057	-5.481679	0.082932
H	8.085208	-2.824401	-1.475887
H	8.933887	-2.987881	0.073997
H	8.571102	-0.323687	-1.472180
H	9.420515	-0.497778	0.076148
H	9.913755	1.993756	0.090452
H	9.066289	2.169738	-1.458287
H	8.367822	3.639475	1.162142
H	9.122494	4.369612	-0.267705
H	5.166125	5.554248	-1.746814
H	3.228033	7.243565	-1.819620
H	0.244661	7.716606	0.770258
H	-2.143777	6.872482	0.669214
H	-4.535040	6.046308	0.596064
H	-6.447539	3.944542	-2.190340
H	-6.941870	1.424929	-2.257790
H	-7.427129	-1.101044	-2.267861
H	-6.467986	-3.830333	0.465383
H	-4.563167	-5.485075	0.533815
H	-2.669875	-7.158564	0.643024
H	0.307712	-7.822977	-1.910324
H	2.733628	-6.986242	-1.803226
H	5.152526	-6.149249	-1.654527
H	6.859694	-3.881340	1.136100

H	7.342613	-1.386476	1.135574
H	7.838020	1.105818	1.147079
H	7.098153	3.865627	-1.624442

Graphane-catalyzed sumanene reactant

C	1.713829	-0.049008	-0.465014
C	0.959969	-1.297043	-0.957716
C	-0.527685	-1.247235	-0.561976
C	-1.197172	0.048272	-1.055678
C	-0.443141	1.294940	-0.558116
C	1.044242	1.247109	-0.955237
H	1.010965	-1.307249	-2.070394
H	1.658172	-0.048319	0.644558
H	-1.145220	0.048338	-2.168420
H	-0.494776	1.293347	0.554157
H	1.094802	1.255689	-2.067934
H	-0.579983	-1.246183	0.550281
C	-1.112147	2.591372	-1.051640
C	-1.280404	-2.494746	-1.061076
C	1.629091	-2.587288	-0.450031
C	3.203132	-0.098192	-0.854710
C	-2.685052	0.096713	-0.663045
C	1.798252	2.489254	-0.446549
C	1.129330	3.793142	-0.919118
C	-0.362069	3.834657	-0.539473
C	-0.615637	-3.786827	-0.552076
C	0.876354	-3.842896	-0.927411
C	3.871985	-1.391140	-0.352578
C	-3.355033	1.392364	-1.157397
C	3.956479	1.147313	-0.352246
C	-3.438866	-1.149298	-1.164335
C	3.119174	-2.644624	-0.833187
C	3.288328	2.448305	-0.831649
H	0.939068	-3.865493	-2.038984
H	-0.682962	-3.772631	0.559016
H	-3.392949	-1.143673	-2.277266
H	-3.310948	1.389276	-2.270416
H	-0.426541	3.820619	0.571917
H	1.190436	3.814366	-2.030790
H	1.747061	2.468556	0.665261
H	3.261907	-0.099927	-1.966908
H	1.576861	-2.565195	0.661646
H	-1.219242	-2.500913	-2.173295
H	-2.735280	0.095578	0.449270
H	-1.052522	2.597618	-2.163936
C	-2.769095	-2.444671	-0.673638

H	-2.819109	-2.440243	0.435954
C	-2.600235	2.638072	-0.661465
H	-2.648322	2.630539	0.448052
H	3.347849	2.466627	-1.943387
H	3.901244	1.139081	0.760055
H	3.178583	-2.666013	-1.944902
H	3.817232	-1.379279	0.759622
C	5.362207	-1.445496	-0.735081
C	5.446900	1.102583	-0.735211
C	3.784598	-3.930326	-0.307775
C	1.539492	-5.129537	-0.401473
C	-1.364271	-5.041041	-1.038877
C	-3.523426	-3.692941	-1.167974
C	-4.924073	-1.103773	-0.761356
C	-4.839569	1.442467	-0.752303
C	-3.271483	3.936121	-1.146938
C	-1.027594	5.137494	-1.019221
C	1.877642	5.031608	-0.391812
C	4.038232	3.686388	-0.305632
C	3.031315	-5.188087	-0.777229
C	6.113908	-0.195007	-0.243605
C	3.369061	4.992030	-0.771689
C	-2.518806	5.179817	-0.639984
C	-5.600367	0.194879	-1.236757
C	-2.856414	-4.986076	-0.664976
H	-5.569208	0.197889	-2.350229
H	-4.875190	1.447111	0.360694
H	-4.961517	-1.114677	0.351493
H	-3.471887	-3.699666	-2.280566
H	-2.919310	-4.978794	0.447459
H	-1.298198	-5.058629	-2.150362
H	1.476097	-5.106281	0.710961
H	3.092837	-5.217613	-1.889048
H	3.726382	-3.902743	0.804546
H	5.420884	-1.457633	-1.846967
H	6.061482	-0.193170	0.869425
H	5.505808	1.110523	-1.847122
H	3.979980	3.660963	0.806705
H	3.429644	5.019256	-1.883613
H	1.815781	5.009353	0.720689
H	-0.964512	5.154470	-2.130888
H	-2.578476	5.172008	0.472761
H	-3.222925	3.945387	-2.259642
C	-4.758695	3.985364	-0.748191
C	-5.518309	2.738277	-1.234226
C	-5.686186	-2.348477	-1.253241

C	-5.011906	-3.646110	-0.773825
C	-0.703387	-6.330243	-0.514662
C	0.790862	-6.388141	-0.879537
C	5.275607	-3.991627	-0.690365
C	6.030294	-2.734944	-0.220517
C	6.199528	2.344842	-0.221277
C	5.529490	3.648946	-0.690276
C	1.212522	6.338290	-0.864301
C	-0.280897	6.378397	-0.493664
H	-5.059636	-3.652242	0.339593
H	-5.651149	-2.343373	-2.366569
H	-5.485404	2.738365	-2.347643
H	-4.802729	3.987441	0.365476
H	-0.349507	6.360794	0.618553
H	1.280840	6.362175	-1.975892
H	5.586767	3.674048	-1.802449
H	6.148161	2.326331	0.891596
H	5.979326	-2.713020	0.892319
H	5.332419	-4.020232	-1.802482
H	0.861694	-6.413885	-1.990928
H	-0.775095	-6.311459	0.597375
C	-2.202667	3.284949	3.126993
C	-3.471326	2.610844	3.067559
C	-3.628624	1.302576	3.559596
C	-1.068787	2.663083	3.680046
C	0.467706	2.809746	3.498525
C	-2.432571	-3.205711	3.114407
C	-1.257532	-2.667654	3.669537
C	0.264884	-2.922137	3.487963
C	-3.650169	-2.443112	3.057257
C	-3.714631	-1.128780	3.554235
C	-2.570111	-0.671432	4.231294
C	-1.389405	-1.410906	4.286436
C	-0.123510	-0.737973	4.346282
C	0.888883	-1.527050	3.772012
C	2.030109	-0.834321	3.328831
C	2.080999	0.602671	3.331280
C	0.991595	1.372914	3.777181
C	-0.074111	0.655412	4.348924
C	-1.289242	1.416487	4.292294
C	-2.519319	0.762625	4.234465
C	-4.591313	0.120153	3.258613
H	-4.488190	-2.874445	2.497898
H	-2.418361	-4.170852	2.595293
H	-4.276588	3.102436	2.509740
H	-2.120238	4.247885	2.610191

H	2.947188	1.076230	2.855269
H	2.860630	-1.366658	2.851400
H	0.643503	-3.697057	4.182529
H	0.499426	-3.273306	2.468101
H	-4.936423	0.134968	2.210319
H	-5.500276	0.150862	3.890326
H	0.725619	3.146883	2.479591
H	0.900683	3.553565	4.195330
C	-1.451185	-7.588551	-1.001110
C	1.452602	-7.676118	-0.347983
C	3.696356	-6.473663	-0.247149
C	5.943648	-5.278274	-0.163428
C	7.521853	-2.792695	-0.609476
C	7.604975	-0.244725	-0.631171
C	7.691312	2.303217	-0.611418
C	6.282240	4.888125	-0.163786
C	4.119266	6.229748	-0.241372
C	1.960080	7.578235	-0.332289
C	-0.945735	7.684933	-0.973361
C	-3.187434	6.482683	-1.120092
C	-5.434667	5.284859	-1.230783
C	-7.002529	2.787582	-0.817266
C	-7.083515	0.242224	-0.819628
C	-7.171178	-2.302681	-0.838627
C	-5.770699	-4.895289	-1.266135
C	-3.607821	-6.239898	-1.153137
C	-0.786423	-8.865649	-0.467583
C	2.937862	-7.717425	-0.724328
C	5.178793	-6.519936	-0.634877
C	7.426782	-5.329298	-0.557408
C	8.178767	-4.079208	-0.088536
C	8.256898	-1.537319	-0.126424
C	8.341557	1.002105	-0.127762
C	7.764843	4.840681	-0.560130
C	5.600512	6.178134	-0.632918
C	3.443449	7.521916	-0.714084
C	-0.195570	8.913691	-0.439567
C	-2.430813	7.708504	-0.595579
C	-4.668553	6.512674	-0.726160
C	-7.669354	4.081549	-1.305270
C	-7.745327	1.537932	-1.302000
C	-7.829095	-1.002703	-1.313451
C	-5.089372	-6.173622	-0.765347
C	-2.936290	-7.514913	-0.629998
C	0.700462	-8.923703	-0.833266
C	8.432827	3.543517	-0.091911

C	1.290345	8.874121	-0.811623
C	-6.913806	5.323109	-0.820124
C	-7.920869	-3.545915	-1.338059
C	-7.250569	-4.838197	-0.860161
H	-8.975304	-3.507647	-1.005061
H	-7.941556	-3.529000	-2.446764
H	-7.319357	-4.900468	0.245176
H	-7.782611	-5.723751	-1.256172
H	-5.174188	-6.216763	0.340822
H	-5.622130	-7.064327	-1.151893
H	-3.034031	-7.546065	0.475441
H	-3.467668	-8.407747	-1.013546
H	-0.895673	-8.891019	0.635840
H	-1.318270	-9.755284	-0.854672
H	0.805888	-8.998244	-1.934792
H	1.170595	-9.832458	-0.412203
H	3.408775	-8.630026	-0.309534
H	3.028651	-7.794555	-1.827938
H	5.649346	-7.434020	-0.222940
H	5.261130	-6.598008	-1.739086
H	7.893681	-6.243119	-0.143757
H	7.500660	-5.411786	-1.660944
H	9.236754	-4.116711	-0.410123
H	8.189387	-4.050647	1.020142
H	9.317854	-1.574213	-0.442126
H	8.262976	-1.528055	0.983593
H	9.402467	0.968143	-0.443949
H	8.347552	0.993351	0.982261
H	8.443037	3.514669	1.016765
H	9.490533	3.510589	-0.414914
H	8.291989	5.721553	-0.147390
H	7.842352	4.917915	-1.663796
H	6.131610	7.058677	-0.221529
H	5.685212	6.251405	-1.737274
H	3.975217	8.400529	-0.299457
H	3.535339	7.594894	-1.817885
H	1.821378	9.748671	-0.390532
H	1.395892	8.944303	-1.913426
H	-0.668971	9.837652	-0.822108
H	-0.298208	8.943200	0.664386
H	-2.903624	8.635892	-0.973764
H	-2.521435	7.742072	0.510380
H	-5.142749	7.438611	-1.106130
H	-4.746023	6.555577	0.380540
H	-6.975213	5.381757	0.285834
H	-7.387179	6.244754	-1.208182

H	-7.693806	4.074399	-2.414010
H	-8.723207	4.110596	-0.969515
H	-7.769229	1.539322	-2.411717
H	-8.800963	1.570918	-0.968475
H	-7.851663	-0.993103	-2.423152
H	-8.885007	-0.968649	-0.980909
H	-7.199684	-2.313215	0.273711
H	-5.721379	-4.891898	-2.377212
H	-3.544190	-6.249604	-2.263270
H	-1.376148	-7.604662	-2.110724
H	1.381204	-7.646710	0.761720
H	3.634681	-6.441224	0.862872
H	5.888394	-5.244200	0.947050
H	7.569732	-2.812183	-1.720539
H	7.655334	-0.246964	-1.742072
H	7.739530	2.318666	-1.722527
H	6.226695	4.857017	0.946770
H	4.058529	6.199412	0.868765
H	1.890972	7.550749	0.777610
H	-0.874698	7.699350	-2.083266
H	-3.127923	6.492525	-2.230462
H	-5.389283	5.284350	-2.342050
H	-7.028967	2.790696	0.295157
H	-7.111987	0.238202	0.292824

Graphane-catalyzed sumanene inversion TS

C	-1.716933	0.002555	-0.458304
C	-1.008678	1.274950	-0.957739
C	0.480898	1.269539	-0.568528
C	1.193575	-0.001472	-1.066353
C	0.477307	-1.270636	-0.568893
C	-1.012393	-1.271900	-0.957669
H	-1.070007	1.286755	-2.069774
H	-1.648432	0.002542	0.650582
H	1.150622	-0.001243	-2.179326
H	0.527128	-1.260220	0.541668
H	-1.074080	-1.283740	-2.069687
H	0.530375	1.258543	0.542041
C	1.191234	-2.549129	-1.044544
C	1.198659	2.546191	-1.043438
C	-1.713962	2.540483	-0.435914
C	-3.212503	0.004549	-0.824861
C	2.677005	-0.003620	-0.653436
C	-1.721072	-2.535384	-0.435394
C	-1.013246	-3.819600	-0.905322
C	0.477936	-3.810455	-0.523267

C	0.488724	3.809347	-0.522085
C	-1.002103	3.822685	-0.905359
C	-3.913490	1.275365	-0.309609
C	3.396907	-1.278733	-1.128983
C	-3.917035	-1.263986	-0.308785
C	3.400593	1.269745	-1.128150
C	-3.208643	2.551697	-0.803442
C	-3.215989	-2.542560	-0.802170
H	-1.062836	3.852089	-2.016839
H	0.550482	3.779828	0.588287
H	3.377383	1.279025	-2.241661
H	3.373620	-1.287209	-2.242500
H	0.540719	-3.781414	0.587030
H	-1.074972	-3.848963	-2.016749
H	-1.658974	-2.503899	0.674675
H	-3.289626	0.004291	-1.936059
H	-1.652694	2.508845	0.674197
H	1.154056	2.567397	-2.156160
H	2.707257	-0.003988	0.457933
H	1.146149	-2.569830	-2.157252
C	2.681315	2.535697	-0.629529
H	2.712089	2.515533	0.480925
C	2.674052	-2.542970	-0.631114
H	2.705266	-2.523587	0.479333
H	-3.291042	-2.561415	-1.913039
H	-3.840020	-1.252954	0.801976
H	-3.283139	2.570119	-1.914351
H	-3.836793	1.264758	0.801186
C	-5.410046	1.281687	-0.670900
C	-5.413683	-1.266454	-0.669779
C	-3.908908	3.815508	-0.270044
C	-1.706433	5.084065	-0.371298
C	1.204454	5.093012	-0.979998
C	3.406516	3.815239	-1.085538
C	4.876719	1.265517	-0.690156
C	4.873058	-1.278967	-0.691040
C	3.395357	-3.824304	-1.088149
C	1.189586	-5.096051	-0.981928
C	-1.720775	-5.078927	-0.370535
C	-3.919603	-3.804131	-0.267810
C	-3.199801	5.097013	-0.743873
C	-6.114939	0.008839	-0.167821
C	-3.214555	-5.087821	-0.741668
C	2.674435	-5.084783	-0.576333
C	5.603910	-0.007604	-1.159141
C	2.688993	5.077474	-0.573397

H	5.596605	-0.007165	-2.272989
H	4.879394	-1.280808	0.421479
H	4.882929	1.266554	0.422339
H	3.379917	3.840964	-2.198829
H	2.726309	5.048157	0.539579
H	1.159357	5.124854	-2.092254
H	-1.643863	5.055309	0.741615
H	-3.266095	5.124772	-1.855383
H	-3.838201	3.788481	0.841649
H	-5.484684	1.288871	-1.781986
H	-6.046423	0.009254	0.944410
H	-5.488542	-1.274530	-1.780846
H	-3.848048	-3.776846	0.843819
H	-3.281957	-5.115927	-1.853105
H	-1.657063	-5.050231	0.742312
H	1.143568	-5.127666	-2.094149
H	2.712584	-5.056068	0.536636
H	3.368270	-3.849323	-2.201443
C	4.874746	-3.819762	-0.658303
C	5.603283	-2.555444	-1.147614
C	5.610746	2.540262	-1.145470
C	4.885760	3.806229	-0.655215
C	0.495255	6.354249	-0.450706
C	-0.995046	6.369313	-0.834570
C	-5.405148	3.828844	-0.635939
C	-6.112990	2.550568	-0.151783
C	-6.120080	-2.532878	-0.149342
C	-5.416130	-3.813557	-0.632762
C	-1.013569	-6.366223	-0.834362
C	0.477191	-6.355315	-0.452102
H	4.903358	3.787304	0.458551
H	5.600948	2.555297	-2.259261
H	5.593183	-2.569401	-2.261419
H	4.892770	-3.801796	0.455463
H	0.534868	-6.324825	0.660589
H	-1.074635	-6.397277	-1.946118
H	-5.487502	-3.835989	-1.744169
H	-6.053359	-2.516525	0.962859
H	-6.046765	2.534954	0.960461
H	-5.475817	3.850489	-1.747405
H	-1.054825	6.400335	-1.946396
H	0.551639	6.323556	0.662044
C	2.439178	-3.418136	3.211750
C	3.702866	-2.687311	3.164709
C	3.772538	-1.264328	3.177599
C	1.173190	-2.767610	3.274526

C	-0.406577	-2.982028	3.342741
C	2.436486	3.413906	3.214040
C	1.171004	2.762332	3.276200
C	-0.408897	2.975475	3.344478
C	3.700743	2.684103	3.166521
C	3.771564	1.261159	3.178405
C	2.507620	0.699503	3.236363
C	1.318562	1.385903	3.281157
C	0.104361	0.683830	3.326058
C	-1.014233	1.498785	3.357337
C	-2.211099	0.726266	3.387343
C	-2.210514	-0.734310	3.386981
C	-1.013036	-1.505839	3.356587
C	0.104894	-0.689966	3.325766
C	1.319640	-1.391066	3.280424
C	2.508158	-0.703712	3.235938
C	4.747381	-0.001218	3.150767
H	4.604393	3.301734	3.114595
H	2.517208	4.506515	3.192680
H	4.607020	-3.304168	3.112317
H	2.520759	-4.510660	3.189532
H	-3.197504	-1.209988	3.405877
H	-3.198484	1.201108	3.406522
H	-0.699225	3.535601	4.251208
H	-0.778001	3.559385	2.482655
H	5.387713	-0.000722	2.250843
H	5.427790	-0.001218	4.020955
H	-0.775373	-3.565576	2.480546
H	-0.696395	-3.543011	4.249104
C	1.212145	7.640497	-0.909760
C	-1.701777	7.632347	-0.301221
C	-3.903358	6.360472	-0.210351
C	-6.108544	5.095561	-0.106816
C	-7.610534	2.558777	-0.521471
C	-7.612052	0.010696	-0.534846
C	-7.617783	-2.537336	-0.518470
C	-6.122868	-5.077835	-0.102166
C	-3.921285	-6.349026	-0.206912
C	-1.723384	-7.627137	-0.299986
C	1.189798	-7.643609	-0.911944
C	3.393866	-6.370438	-1.028546
C	5.602043	-5.102534	-1.109844
C	7.079349	-2.552583	-0.699762
C	7.078804	-0.009910	-0.710640
C	7.086686	2.532742	-0.697262
C	5.617049	5.087239	-1.105451

C	3.412554	6.361224	-1.024591
C	0.497509	8.892590	-0.381433
C	-3.185002	7.627935	-0.686664
C	-5.388264	6.359012	-0.590201
C	-7.596800	5.097100	-0.483933
C	-8.302332	3.826186	0.000926
C	-8.298211	1.282653	-0.023567
C	-8.301723	-1.258688	-0.021920
C	-7.611405	-5.075600	-0.478210
C	-5.406584	-6.343664	-0.585211
C	-3.207071	-7.618677	-0.683574
C	0.472172	-8.893625	-0.382715
C	2.667808	-7.616014	-0.507862
C	4.866499	-6.348207	-0.604120
C	7.797833	-3.829113	-1.158692
C	7.791059	-1.283222	-1.179243
C	7.794781	1.261802	-1.177900
C	4.884832	6.334626	-0.599196
C	2.689638	7.608677	-0.504121
C	-0.984204	8.905504	-0.771395
C	-8.312962	-3.802163	0.005719
C	-1.010043	-8.902403	-0.770862
C	7.073389	-5.087995	-0.670858
C	7.809080	3.807619	-1.154691
C	7.088170	5.068152	-0.665929
H	8.856748	3.794396	-0.798761
H	7.854572	3.814805	-2.262748
H	7.129560	5.108508	0.441923
H	7.601053	5.978205	-1.030751
H	4.939661	6.359329	0.509540
H	5.399316	7.248468	-0.955771
H	2.759354	7.629957	0.603804
H	3.202179	8.521995	-0.864714
H	0.586698	8.915157	0.723953
H	1.007580	9.800869	-0.754396
H	-1.074887	8.980857	-1.874165
H	-1.489780	9.797050	-0.354428
H	-3.686800	8.525127	-0.274271
H	-3.273013	7.701476	-1.790702
H	-5.885207	7.259563	-0.179256
H	-5.479995	6.428929	-1.694183
H	-8.088093	5.997970	-0.069976
H	-7.686054	5.170441	-1.586970
H	-9.364940	3.827616	-0.307510
H	-8.298266	3.803760	1.109851
H	-9.364369	1.284401	-0.323775

H	-8.287713	1.276938	1.086511
H	-9.367943	-1.257814	-0.321906
H	-8.290965	-1.251729	1.088147
H	-8.308159	-3.778597	1.114616
H	-9.375744	-3.800877	-0.302102
H	-8.104863	-5.974664	-0.062898
H	-7.701658	-5.149964	-1.581100
H	-5.905545	-7.242545	-0.173062
H	-5.499640	-6.414234	-1.689046
H	-3.710796	-8.514344	-0.270227
H	-3.296660	-7.692417	-1.787476
H	-1.517568	-9.792481	-0.353146
H	-1.102277	-8.977667	-1.873512
H	0.979277	-9.803353	-0.756211
H	0.562646	-8.916345	0.722563
H	3.177479	-8.530629	-0.869242
H	2.738576	-7.637826	0.599986
H	5.378267	-7.263214	-0.961616
H	4.921923	-6.373797	0.504565
H	7.115021	-5.129389	0.436945
H	7.583602	-5.999164	-1.036624
H	7.842902	-3.835293	-2.266772
H	8.845671	-3.819302	-0.803141
H	7.832669	-1.287237	-2.288363
H	8.841750	-1.281016	-0.828434
H	7.836530	1.266879	-2.287011
H	8.845419	1.256247	-0.826973
H	7.088565	2.523326	0.415633
H	5.594392	5.104217	-2.217360
H	3.377922	6.384903	-2.135883
H	1.161907	7.664209	-2.020618
H	-1.637985	7.598390	0.809006
H	-3.836369	6.328793	0.899567
H	-6.040191	5.067992	1.003223
H	-7.673124	2.570765	-1.631910
H	-7.677239	0.010047	-1.644996
H	-7.680794	-2.550556	-1.628874
H	-6.053586	-5.049633	1.007795
H	-3.853003	-6.317111	0.902916
H	-1.658090	-7.593183	0.810152
H	1.138256	-7.667223	-2.022742
H	3.358346	-6.393630	-2.139817
H	5.578874	-5.118586	-2.221755
H	7.081530	-2.544260	0.413138
H	7.083718	-0.010487	0.402862

Graphane-catalyzed sumanene product

C	-1.300427	0.543747	-0.824390
C	-0.107691	1.432432	-1.225015
C	1.207358	0.865209	-0.658121
C	1.435860	-0.604542	-1.057979
C	0.227618	-1.471055	-0.656752
C	-1.098185	-0.930309	-1.224082
H	-0.036960	1.443367	-2.336440
H	-1.348645	0.564476	0.283284
H	1.550476	-0.654635	-2.164606
H	0.147581	-1.404467	0.446274
H	-1.054872	-0.990862	-2.335215
H	1.104882	0.877725	0.446754
C	0.440422	-2.959279	-0.986697
C	2.418457	1.755986	-0.988967
C	-0.324946	2.880682	-0.741771
C	-2.641451	1.107158	-1.327204
C	2.728988	-1.146593	-0.414702
C	-2.285250	-1.789791	-0.743428
C	-2.089961	-3.275920	-1.092939
C	-0.761247	-3.807237	-0.525715
C	2.182381	3.206488	-0.525843
C	0.871849	3.785063	-1.088839
C	-2.840038	2.562781	-0.863073
C	2.961474	-2.628648	-0.761551
C	-3.820315	0.227169	-0.867846
C	3.948914	-0.275606	-0.764590
C	-1.653668	3.461083	-1.258625
C	-3.627580	-1.247111	-1.266106
H	0.962700	3.820714	-2.198162
H	2.074206	3.181409	0.582515
H	4.089550	-0.310740	-1.868858
H	3.084901	-2.706378	-1.865527
H	-0.821166	-3.714327	0.582798
H	-2.045364	-3.362904	-2.202274
H	-2.312819	-1.716737	0.366071
H	-2.625320	1.101785	-2.440529
H	-0.395159	2.846304	0.367451
H	2.548813	1.766589	-2.094644
H	2.594785	-1.086902	0.687772
H	0.525592	-3.060630	-2.092359
C	3.709755	1.191490	-0.365394
H	3.572096	1.207411	0.739988
C	1.746566	-3.485558	-0.361315
H	1.639550	-3.397626	0.744056
H	-3.607280	-1.300203	-2.378233

H	-3.839929	0.261051	0.245381
H	-1.604786	3.490532	-2.370765
H	-2.877585	2.548026	0.250240
C	-4.178841	3.136395	-1.362145
C	-5.165523	0.782486	-1.370203
C	-1.866263	4.903322	-0.761251
C	0.648098	5.225691	-0.591260
C	3.388571	4.106797	-0.850898
C	4.927304	2.076478	-0.690655
C	5.232915	-0.821392	-0.110797
C	4.250345	-3.163010	-0.108461
C	1.967728	-4.974212	-0.686404
C	-0.557708	-5.297773	-0.852551
C	-3.278081	-4.127330	-0.605424
C	-4.809076	-2.107946	-0.779321
C	-0.673853	5.807120	-1.122938
C	-5.363191	2.247341	-0.940815
C	-4.614824	-3.589565	-1.146028
C	0.759720	-5.827679	-0.258368
C	5.468622	-2.297613	-0.476100
C	4.690521	3.535410	-0.260678
H	5.601071	-2.354042	-1.580761
H	4.113956	-3.091705	0.994609
H	5.087111	-0.772246	0.992376
H	5.059892	2.068747	-1.796178
H	4.577408	3.537344	0.848960
H	3.501211	4.127293	-1.958482
H	0.568182	5.180847	0.518894
H	-0.603797	5.842589	-2.234181
H	-1.926250	4.861367	0.350262
H	-4.144731	3.144636	-2.475059
H	-5.405676	2.260588	0.173637
H	-5.142067	0.757960	-2.483126
H	-4.829010	-2.040799	0.332443
H	-4.580739	-3.660033	-2.257276
H	-3.309569	-4.042856	0.504937
H	-0.488175	-5.390225	-1.960015
H	0.677407	-5.748663	0.851148
H	2.067012	-5.063185	-1.791872
C	3.269989	-5.507361	-0.059065
C	4.483576	-4.646423	-0.451898
C	6.455287	0.050734	-0.455350
C	6.220049	1.519856	-0.063841
C	3.159808	5.555827	-0.380590
C	1.845175	6.133033	-0.933868
C	-3.195773	5.486296	-1.276390

C	-4.386061	4.588980	-0.893197
C	-6.349661	-0.090587	-0.912198
C	-6.152738	-1.565767	-1.302221
C	-3.083697	-5.615141	-0.952337
C	-1.755152	-6.150850	-0.390661
H	6.091007	1.550490	1.042677
H	6.591138	0.014557	-1.560413
H	4.603699	-4.718597	-1.557021
H	3.158461	-5.435736	1.047467
H	-1.808532	-6.072167	0.719695
H	-3.036260	-5.696029	-2.062369
H	-6.124437	-1.619726	-2.414503
H	-6.383935	-0.044907	0.200731
H	-4.442955	4.571569	0.219640
H	-3.140296	5.513375	-2.388651
H	1.931984	6.165983	-2.043983
H	3.068786	5.532212	0.729880
C	3.119319	-0.505754	4.128817
C	2.565342	-1.834119	4.135043
C	1.296530	-2.105552	3.585510
C	2.416925	0.582322	3.573779
C	2.406422	2.129602	3.762271
C	-3.345853	-1.352394	3.708376
C	-2.880960	-0.111680	3.228516
C	-3.291244	1.383044	3.391917
C	-2.476014	-2.494629	3.806313
C	-1.120782	-2.422104	3.427413
C	-0.728427	-1.217766	2.823926
C	-1.570049	-0.113007	2.728468
C	-1.018205	1.208938	2.724973
C	-1.940937	2.142688	3.221397
C	-1.385930	3.349848	3.690841
C	0.038373	3.537046	3.782821
C	0.939916	2.520631	3.408262
C	0.358227	1.390172	2.815153
C	1.224556	0.253052	2.912090
C	0.689044	-1.032019	2.917100
C	0.190453	-3.185524	3.784588
H	-2.873887	-3.386724	4.302692
H	-4.350119	-1.449093	4.135715
H	3.112933	-2.602767	4.691652
H	4.052539	-0.349031	4.681113
H	0.393167	4.451881	4.270337
H	-2.023120	4.134326	4.114197
H	-4.031862	1.690117	2.626553
H	-3.751288	1.577730	4.375816

H	0.173550	-3.571239	4.818285
H	0.347889	-4.058359	3.120118
H	2.671716	2.420000	4.793272
H	3.134984	2.628543	3.092435
C	4.364180	6.457237	-0.722857
C	1.622112	7.579790	-0.448382
C	-0.892301	7.251370	-0.631356
C	-3.409795	6.934996	-0.792709
C	-5.719988	5.164772	-1.411943
C	-6.702250	2.811782	-1.455133
C	-7.691461	0.461324	-1.435809
C	-7.340340	-2.430820	-0.831648
C	-5.803092	-4.447999	-0.668746
C	-4.277203	-6.471435	-0.480836
C	-1.552704	-7.640364	-0.736111
C	0.972335	-7.316610	-0.595712
C	3.493986	-6.994313	-0.403049
C	5.780150	-5.184137	0.187329
C	6.758925	-2.839086	0.170003
C	7.747121	-0.498019	0.184343
C	7.438725	2.401081	-0.408042
C	5.902264	4.427409	-0.596555
C	4.129739	7.899522	-0.250960
C	0.303757	8.138491	-0.993121
C	-2.212830	7.815576	-1.165902
C	-4.733777	7.502477	-1.323444
C	-5.920596	6.612353	-0.940745
C	-6.892152	4.264905	-1.005769
C	-7.873839	1.924622	-1.019094
C	-8.669456	-1.880949	-1.367866
C	-7.126468	-3.899052	-1.211940
C	-5.594187	-5.920401	-1.036467
C	-2.750321	-8.484821	-0.276261
C	-0.232345	-8.155555	-0.153330
C	2.280847	-7.833856	0.012451
C	6.000274	-6.660424	-0.171304
C	6.978046	-4.310131	-0.198086
C	7.962206	-1.965196	-0.199608
C	7.188878	3.854427	0.008204
C	5.658453	5.872466	-0.147502
C	2.820336	8.471361	-0.803700
C	-8.868060	-0.412815	-0.978075
C	-4.070363	-7.949358	-0.839976
C	4.794274	-7.519683	0.222562
C	8.955134	0.378280	-0.176103
C	8.724577	1.840865	0.216964

H	9.866112	-0.017630	0.311496
H	9.131091	0.313198	-1.269183
H	8.647328	1.916533	1.320927
H	9.587904	2.466476	-0.079122
H	7.119258	3.903691	1.115216
H	8.053633	4.485524	-0.276038
H	5.603245	5.899207	0.961097
H	6.520692	6.507800	-0.429948
H	4.095499	7.910222	0.857700
H	4.988022	8.534006	-0.542766
H	2.889729	8.553919	-1.907512
H	2.651092	9.496757	-0.423669
H	0.141613	9.166508	-0.613693
H	0.372516	8.221488	-2.097911
H	-2.366490	8.845145	-0.787180
H	-2.152491	7.896021	-2.271365
H	-4.880200	8.531922	-0.945009
H	-4.672424	7.580448	-2.428065
H	-6.862725	7.015286	-1.358428
H	-6.041110	6.614769	0.161946
H	-7.839519	4.666809	-1.415457
H	-6.997311	4.288378	0.099296
H	-8.822759	2.321361	-1.430240
H	-7.969947	1.973580	0.085954
H	-8.961623	-0.335740	0.124547
H	-9.812847	-0.020367	-1.399651
H	-9.508462	-2.499493	-0.996451
H	-8.676357	-1.974647	-2.472949
H	-7.971119	-4.513351	-0.842834
H	-7.132574	-3.993073	-2.317958
H	-6.444565	-6.527555	-0.668702
H	-5.593427	-6.022115	-2.141823
H	-4.924040	-8.548856	-0.470861
H	-4.069065	-8.052475	-1.944217
H	-2.598973	-9.540890	-0.569935
H	-2.791687	-8.470992	0.832128
H	-0.079677	-9.215556	-0.436197
H	-0.296362	-8.135910	0.954934
H	2.437162	-8.893438	-0.269950
H	2.194692	-7.816806	1.119256
H	4.685921	-7.515311	1.326492
H	4.952576	-8.574619	-0.071401
H	6.170704	-6.741274	-1.264205
H	6.920817	-7.032597	0.317141
H	7.148778	-4.389108	-1.292053
H	7.897718	-4.689883	0.288795

H	8.137660	-2.032464	-1.293609
H	8.877989	-2.354412	0.287088
H	7.611502	-0.450914	1.287620
H	7.558733	2.376057	-1.513455
H	6.012513	4.426191	-1.703026
H	4.456238	6.472796	-1.831154
H	1.543938	7.543535	0.660814
H	-0.963360	7.212132	0.478013
H	-3.475612	6.902203	0.317400
H	-5.662687	5.173442	-2.522636
H	-6.657584	2.798879	-2.566085
H	-7.650384	0.421725	-2.546512
H	-7.370673	-2.368165	0.278748
H	-5.834690	-4.375747	0.440827
H	-4.316682	-6.394225	0.628340
H	-1.490867	-7.713529	-1.844189
H	1.054845	-7.392420	-1.702023
H	3.596362	-7.062023	-1.508485
H	5.652280	-5.118390	1.290543
H	6.622583	-2.780874	1.272422

Graphane-catalyzed 2,2prime-dimethylbiphenyl reactant

C	0.145017	-1.410432	-0.411901
C	-1.159728	-0.739338	-0.881696
C	-1.242969	0.716830	-0.386409
C	-0.014036	1.528480	-0.839067
C	1.293147	0.862049	-0.368214
C	1.388125	-0.603270	-0.831160
H	-1.147621	-0.716343	-1.995220
H	0.124650	-1.424334	0.701336
H	-0.009344	1.533880	-1.952979
H	1.274919	0.846887	0.742416
H	1.431590	-0.604892	-1.944216
H	-1.237689	0.683598	0.726676
C	2.534020	1.666627	-0.799375
C	-2.560281	1.389051	-0.817006
C	-2.390143	-1.554770	-0.443000
C	0.241791	-2.869870	-0.895665
C	-0.095714	2.993859	-0.370056
C	2.677600	-1.265618	-0.308163
C	3.930268	-0.465147	-0.712130
C	3.828242	1.009900	-0.281416
C	-3.779943	0.571750	-0.350195
C	-3.707964	-0.878607	-0.864646
C	-1.000766	-3.687608	-0.496970
C	1.134125	3.800696	-0.827793

C	1.531125	-3.541570	-0.384553
C	-1.414422	3.660125	-0.804215
C	-2.307773	-3.008095	-0.948419
C	2.784853	-2.732416	-0.765480
H	-3.730590	-0.842021	-1.977705
H	-3.749607	0.533752	0.761995
H	-1.437290	3.673336	-1.917574
H	1.140786	3.803251	-1.941407
H	3.782802	1.026679	0.831303
H	3.994622	-0.483422	-1.824026
H	2.621939	-1.262910	0.803576
H	0.289454	-2.850194	-2.008259
H	-2.383020	-1.580554	0.667627
H	-2.577845	1.412128	-1.930522
H	-0.088543	2.988571	0.741279
H	2.572335	1.656013	-1.912427
C	-2.632394	2.847157	-0.324914
H	-2.602798	2.824066	0.788587
C	2.442237	3.138729	-0.354568
H	2.430217	3.148961	0.759475
H	2.855224	-2.730777	-1.877164
H	1.474255	-3.561880	0.728013
H	-2.304517	-2.974995	-2.061757
H	-1.018756	-3.734193	0.613148
C	-0.906697	-5.139003	-1.002645
C	1.640197	-4.998985	-0.871916
C	-3.536106	-3.830718	-0.514118
C	-4.926391	-1.701135	-0.402924
C	-5.103810	1.246021	-0.755975
C	-3.956543	3.517434	-0.737866
C	-1.486749	5.121243	-0.320999
C	1.053669	5.265932	-0.358899
C	3.681086	3.939004	-0.798529
C	5.077816	1.804121	-0.705531
C	5.212850	-1.119631	-0.163359
C	4.063495	-3.398085	-0.221352
C	-4.854862	-3.149014	-0.923552
C	0.386182	-5.816110	-0.508267
C	5.322413	-2.593754	-0.596633
C	4.979350	3.283894	-0.289069
C	-0.265282	5.930587	-0.796848
C	-5.171360	2.701626	-0.256346
H	-0.283429	5.940245	-1.910614
H	1.064273	5.257089	0.755136
H	-1.460000	5.103196	0.792498
H	-3.987609	3.534808	-1.851137

H	-5.136335	2.675101	0.856962
H	-5.136798	1.275447	-1.869038
H	-4.892492	-1.744093	0.709823
H	-4.878830	-3.104520	-2.036330
H	-3.526379	-3.881462	0.599284
H	-0.869830	-5.107521	-2.115154
H	0.329679	-5.858495	0.603809
H	1.711444	-4.972174	-1.983030
H	3.986592	-3.402700	0.889855
H	5.404533	-2.606198	-1.707702
H	5.144140	-1.100332	0.948581
H	5.129674	1.772758	-1.817554
H	4.948007	3.314093	0.824597
H	3.708374	3.921804	-1.911652
C	3.593764	5.413617	-0.358159
C	2.281679	6.073131	-0.823788
C	-2.810774	5.791322	-0.737222
C	-4.027063	4.979047	-0.253392
C	-6.320353	0.426995	-0.281349
C	-6.253894	-1.023901	-0.794557
C	-3.456720	-5.278793	-1.035700
C	-2.146688	-5.961146	-0.598848
C	2.919398	-5.675947	-0.340810
C	4.180376	-4.862436	-0.688375
C	6.471367	-0.326488	-0.566820
C	6.366941	1.156054	-0.162373
H	-3.996052	4.962942	0.860167
H	-2.841493	5.807658	-1.850715
H	2.280088	6.071452	-1.937728
H	3.591519	5.426498	0.756091
H	6.313820	1.196453	0.949988
H	6.542632	-0.363207	-1.678039
H	4.271315	-4.848307	-1.798696
H	2.838783	-5.709168	0.769906
H	-2.158718	-6.013457	0.514305
H	-3.459172	-5.232153	-2.148608
H	-6.292744	-0.984792	-1.907251
H	-6.283209	0.390949	0.831976
C	5.453925	-5.534596	-0.132947
C	6.598707	-3.253331	-0.036070
C	7.753625	-0.975470	-0.003884
C	7.623034	1.943518	-0.591159
C	6.226194	4.074882	-0.733542
C	4.830224	6.212222	-0.821906
C	2.203348	7.544663	-0.366140
C	-0.337789	7.396223	-0.323404

C	-2.879771	7.255597	-0.255397
C	-5.355168	5.648260	-0.665260
C	-6.499289	3.372983	-0.660706
C	-7.650394	1.102327	-0.676114
C	-7.468939	-1.849985	-0.322658
C	-6.073839	-3.977192	-0.469641
C	-4.685528	-6.107580	-0.605878
C	-2.055436	-7.409704	-1.123259
C	0.494779	-7.267796	-1.016509
C	3.038351	-7.132523	-0.836748
C	7.504703	3.420210	-0.193274
C	6.119335	5.548439	-0.319610
C	4.737371	7.683067	-0.386365
C	3.428812	8.334548	-0.850432
C	0.883276	8.185897	-0.812661
C	-1.660829	8.045270	-0.749707
C	-5.413639	7.105463	-0.181885
C	-6.551320	4.825355	-0.169663
C	-7.696852	2.549451	-0.169594
C	-8.789513	-1.165523	-0.707626
C	-7.385971	-3.284956	-0.859037
C	-4.596190	-7.540577	-1.152236
C	-0.757137	-8.074432	-0.646550
C	1.775219	-7.931937	-0.492509
C	4.307890	-7.798987	-0.283835
C	6.701077	-4.715652	-0.489685
C	7.845930	-2.448093	-0.423663
C	9.002612	-0.182733	-0.420083
H	-0.797874	-8.186831	0.457345
H	-0.681828	-9.099376	-1.059676
H	1.701717	-8.031134	0.610934
H	1.858637	-8.961811	-0.891628
C	5.566058	-6.988579	-0.617863
H	4.210813	-7.891455	0.817266
H	4.393202	-8.829541	-0.677509
H	6.463185	-7.463162	-0.177126
H	5.720855	-6.986219	-1.716191
H	7.602004	-5.186303	-0.049535
H	6.844014	-4.740135	-1.590437
H	8.748834	-2.912433	0.019103
H	7.978258	-2.499561	-1.524804
C	8.896760	1.295433	-0.026415
H	9.904472	-0.641415	0.027703
H	9.124260	-0.262176	-1.519711
H	9.787251	1.854434	-0.371087
H	8.880909	1.382517	1.079284

H	8.394097	3.979146	-0.544546
H	7.506676	3.496756	0.914396
H	7.002098	6.108377	-0.685668
H	6.147302	5.613886	0.788418
H	5.610271	8.243378	-0.771453
H	4.797909	7.731434	0.720167
H	3.367475	9.380031	-0.493446
H	3.410560	8.379886	-1.958517
H	0.828772	9.231178	-0.450350
H	0.860926	8.238260	-1.921377
H	-1.707617	9.087579	-0.377852
H	-1.694639	8.107482	-1.857643
C	-4.204843	7.912465	-0.671493
H	-4.246748	8.949089	-0.286898
H	-4.235633	7.987112	-1.777755
H	-5.437189	7.113980	0.927078
H	-6.357521	7.574680	-0.518295
H	-6.560951	4.833121	0.940527
H	-7.498501	5.300204	-0.492602
H	-7.703329	2.545437	0.940689
H	-8.643158	3.031125	-0.484866
C	-8.852219	0.277200	-0.191452
C	-5.988509	-5.409098	-1.014113
C	-3.294008	-8.226207	-0.721194
H	-8.859444	0.272362	0.917794
H	-9.794286	0.763333	-0.508307
H	-8.882429	-1.164334	-1.812918
H	-9.643152	-1.755097	-0.322974
H	-7.469308	-3.261650	-1.965834
H	-8.248080	-3.877262	-0.494624
H	-6.053725	-5.379058	-2.121933
H	-6.858880	-5.999596	-0.666838
H	-5.472900	-8.126508	-0.817077
H	-4.647238	-7.505047	-2.259619
H	-3.294490	-8.352211	0.380904
H	-3.227679	-9.243454	-1.151322
H	0.559569	-7.223927	-2.125837
H	3.128694	-7.094532	-1.944732
H	5.358874	-5.551065	0.975217
H	6.514007	-3.242713	1.072955
H	7.679924	-0.937857	1.105471
H	7.678439	1.891545	-1.700900
H	6.262628	4.033165	-1.844306
H	4.839574	6.186135	-1.933816
H	2.220164	7.542498	0.746278
H	-0.310098	7.383121	0.788601

H	-2.845997	7.236602	0.856415
H	-5.385774	5.658969	-1.777210
H	-6.532710	3.389986	-1.772423
H	-7.685684	1.130009	-1.787651
H	-7.421993	-1.896428	0.788013
H	-6.036517	-4.032841	0.640997
H	-4.666319	-6.167464	0.504962
H	-2.028268	-7.355410	-2.233795
C	0.261969	-0.516940	4.177343
C	0.812840	-1.731172	4.643415
C	2.184419	-1.998294	4.581699
C	3.050379	-1.036661	4.047017
C	2.528393	0.189856	3.621114
C	1.152496	0.483278	3.687959
C	-1.220182	-0.326549	4.166829
C	-2.102477	-1.307112	3.625929
C	-3.476499	-1.008023	3.541572
C	-4.004832	0.203166	4.001484
C	-3.147965	1.143214	4.587447
C	-1.778418	0.871729	4.664865
H	0.143119	-2.480336	5.074332
H	2.570929	-2.955418	4.946509
H	4.124654	-1.233499	3.967299
H	3.204480	0.952526	3.217159
H	-4.145077	-1.754004	3.095985
H	-5.076855	0.405694	3.907232
H	-3.540515	2.086954	4.979628
H	-1.115707	1.603990	5.133831
C	-1.643795	-2.660930	3.132217
H	-0.661867	-2.618985	2.633908
H	-1.552617	-3.387740	3.960445
H	-2.375219	-3.079151	2.421685
C	0.698542	1.850850	3.228539
H	-0.265621	1.818003	2.696027
H	0.573936	2.549601	4.076007
H	1.449256	2.297058	2.556425

Graphane-catalyzed 2,2prime-dimethylbiphenyl rotation TS

C	-0.809800	-1.038689	-0.251658
C	-1.373141	0.286724	-0.798130
C	-0.440807	1.466579	-0.461725
C	0.995142	1.215533	-0.960651
C	1.551514	-0.112428	-0.412550
C	0.626488	-1.298794	-0.744458
H	-1.425519	0.203805	-1.907778
H	-0.764247	-0.942706	0.854842

H	0.955466	1.132476	-2.070535
H	1.582338	-0.029858	0.695331
H	0.593572	-1.405064	-1.852864
H	-0.401520	1.541439	0.648784
C	2.994875	-0.367463	-0.886191
C	-1.002587	2.801140	-0.987434
C	-2.799664	0.539763	-0.274248
C	-1.740176	-2.225161	-0.567982
C	1.923028	2.397746	-0.618610
C	1.181650	-2.610754	-0.157791
C	2.626169	-2.876226	-0.623188
C	3.546440	-1.683003	-0.303810
C	-2.429534	3.050835	-0.463095
C	-3.368200	1.874613	-0.792589
C	-3.170831	-1.963957	-0.059646
C	3.363405	2.145731	-1.103035
C	-1.179796	-3.540238	0.007762
C	1.364941	3.729593	-1.154983
C	-3.738757	-0.637648	-0.598281
C	0.260505	-3.805549	-0.469103
H	-3.441354	1.804040	-1.901984
H	-2.366171	3.120469	0.646463
H	1.320205	3.651074	-2.264888
H	3.333093	2.056641	-2.212652
H	3.563775	-1.570019	0.803139
H	2.608457	-3.001688	-1.730039
H	1.205792	-2.490421	0.946349
H	-1.787607	-2.334151	-1.675472
H	-2.734638	0.614494	0.832403
H	-1.059447	2.727546	-2.097254
H	1.960787	2.481738	0.491602
H	2.974906	-0.469751	-1.995063
C	-0.068448	3.979032	-0.649211
H	-0.019369	4.054716	0.461560
C	3.916282	0.820165	-0.546340
H	3.940773	0.912436	0.564210
H	0.231776	-3.933206	-1.575399
H	-1.137618	-3.422821	1.114510
H	-3.810418	-0.722052	-1.706743
H	-3.110954	-1.859327	1.045358
C	-4.106758	-3.148597	-0.364770
C	-2.105293	-4.732958	-0.298070
C	-5.157490	-0.384203	-0.052836
C	-4.786688	2.126849	-0.246514
C	-2.997825	4.386222	-0.979969
C	-0.630679	5.312962	-1.177149

C	2.293995	4.909694	-0.810938
C	4.288625	3.328601	-0.758165
C	5.360370	0.565316	-1.018796
C	4.992250	-1.945841	-0.764946
C	3.178017	-4.180205	-0.014905
C	0.812686	-5.110347	0.137105
C	-5.731026	0.951542	-0.561375
C	-3.542411	-4.470562	0.189613
C	2.259355	-5.378397	-0.318168
C	5.912818	-0.752895	-0.444400
C	3.731820	4.657757	-1.302639
C	-2.058722	5.563944	-0.657285
H	3.696469	4.575612	-2.413029
H	4.319823	3.411850	0.352398
H	2.331978	4.988687	0.299646
H	-0.687241	5.233318	-2.286528
H	-1.997983	5.646684	0.452397
H	-3.069304	4.310498	-2.088826
H	-4.702623	2.196828	0.861213
H	-5.820455	0.880078	-1.669643
H	-5.071094	-0.306587	1.053793
H	-4.170439	-3.248894	-1.472105
H	-3.501541	-4.373050	1.299175
H	-2.142207	-4.851313	-1.404797
H	0.832062	-4.975197	1.242268
H	2.242827	-5.516734	-1.423581
H	3.192739	-4.045266	1.090037
H	4.973797	-2.066206	-1.872016
H	5.941375	-0.644404	0.664503
H	5.334026	0.462729	-2.127410
C	6.285930	1.752398	-0.686508
C	5.730503	3.077531	-1.241330
C	1.736454	6.242682	-1.347890
C	0.302284	6.494553	-0.846073
C	-4.419135	4.640377	-0.440537
C	-5.362793	3.463750	-0.752221
C	-6.103485	-1.560713	-0.360462
C	-5.532658	-2.892428	0.161749
C	-1.551077	-6.045108	0.291385
C	-0.105147	-6.310140	-0.167445
C	4.625817	-4.451113	-0.468056
C	5.545902	-3.253647	-0.165623
H	0.348804	6.580325	0.263884
H	1.694191	6.162894	-2.458234
H	5.699631	2.989332	-2.351407
H	6.320820	1.845719	0.423333

H	5.571239	-3.125136	0.941283
H	4.609134	-4.589049	-1.573434
H	-0.123776	-6.443052	-1.273376
H	-1.531072	-5.926416	1.399581
H	-5.464525	-2.810264	1.271584
H	-6.187804	-1.642766	-1.468263
H	-5.451428	3.391136	-1.860366
H	-4.342636	4.721150	0.668393
C	0.444919	-7.616518	0.443033
C	2.809854	-6.679639	0.299682
C	5.178739	-5.753161	0.149039
C	6.993016	-3.523198	-0.629383
C	7.357287	-1.015042	-0.916503
C	7.728833	1.495658	-1.170099
C	6.658105	4.262926	-0.900882
C	4.659723	5.840574	-0.959304
C	2.667073	7.425905	-1.008080
C	-0.260880	7.826691	-1.384849
C	-2.627240	6.896683	-1.185559
C	-4.994164	5.975568	-0.958998
C	-6.778861	3.717409	-0.193613
C	-7.145284	1.203259	-0.000826
C	-7.522179	-1.308086	0.191913
C	-6.474168	-4.073841	-0.153272
C	-4.472971	-5.659194	-0.124391
C	-2.472393	-7.242181	-0.024678
C	7.895743	-2.322192	-0.320743
C	8.265131	0.178902	-0.594506
C	8.644710	2.683761	-0.837575
C	8.089760	4.000956	-1.392749
C	6.087559	5.575231	-1.452996
C	4.092257	7.156421	-1.506687
C	0.675144	8.999049	-1.052534
C	-1.683687	8.062296	-0.862550
C	-4.042655	7.136798	-0.644949
C	-7.346133	5.049641	-0.707573
C	-7.706440	2.537377	-0.508380
C	-8.457051	-2.483832	-0.129940
C	-5.894564	-5.388026	0.384384
C	-3.904572	-6.964059	0.448057
C	-1.915390	-8.543134	0.574031
C	1.887977	-7.865024	-0.012313
C	4.251477	-6.935661	-0.156952
C	6.620057	-6.016060	-0.313504
H	-5.875927	-5.344404	1.493912
H	-6.559594	-6.233046	0.118702

H	-3.910969	-6.901998	1.556782
H	-4.563938	-7.813237	0.181511
C	-0.474008	-8.805184	0.122160
H	-1.945722	-8.467660	1.680374
H	-2.570356	-9.392151	0.301073
H	-0.078688	-9.724150	0.594990
H	-0.457337	-8.983840	-0.972386
H	2.281458	-8.786162	0.460662
H	1.895016	-8.049451	-1.107069
H	4.641656	-7.856777	0.318791
H	4.255716	-7.124279	-1.251011
C	7.536305	-4.823162	-0.016391
H	7.007278	-6.934136	0.167683
H	6.614135	-6.213096	-1.405015
H	8.559919	-5.015310	-0.390006
H	7.623426	-4.690594	1.081511
H	8.921447	-2.513632	-0.692492
H	7.980122	-2.208049	0.780505
H	9.288641	-0.011651	-0.972667
H	8.354005	0.277653	0.507845
H	9.662139	2.493482	-1.228567
H	8.742278	2.761731	0.264623
H	8.744025	4.848051	-1.112388
H	8.085593	3.961508	-2.501226
H	6.747003	6.421182	-1.176668
H	6.085178	5.531039	-2.562317
H	4.756210	7.998852	-1.230384
H	4.086431	7.114784	-2.616094
C	2.101833	8.746001	-1.554163
H	2.767668	9.583985	-1.273607
H	2.101295	8.703564	-2.662529
H	0.692208	9.141573	0.047397
H	0.270828	9.934923	-1.482524
H	-1.644872	8.200994	0.238394
H	-2.089967	9.004388	-1.280013
H	-3.989749	7.272772	0.455775
H	-4.449557	8.081768	-1.055290
C	-6.405220	6.221308	-0.402866
C	-8.076556	0.027071	-0.319430
C	-7.890003	-3.812505	0.383645
H	-6.336275	6.362340	0.695270
H	-6.811772	7.164714	-0.813987
H	-7.496632	4.973984	-1.803869
H	-8.345225	5.227445	-0.266508
H	-7.850028	2.474069	-1.607418
H	-8.709359	2.716813	-0.073630

H	-8.215655	-0.036039	-1.419047
H	-9.080528	0.210787	0.111101
H	-9.459179	-2.296006	0.300008
H	-8.593278	-2.540958	-1.229186
H	-7.851955	-3.791279	1.492190
H	-8.556002	-4.652780	0.110396
H	-4.516741	-5.759424	-1.231056
H	-2.491572	-7.357250	-1.130795
H	0.453673	-7.482617	1.547647
H	2.821855	-6.538275	1.403304
H	5.196911	-5.609804	1.252370
H	6.963484	-3.654522	-1.733521
H	7.325061	-1.130940	-2.022163
H	7.690488	1.395748	-2.277279
H	6.690514	4.345284	0.208101
H	4.692826	5.920270	0.149747
H	2.703233	7.506024	0.100942
H	-0.312371	7.736581	-2.492327
H	-2.694382	6.808809	-2.292239
H	-5.075098	5.889238	-2.064998
H	-6.684947	3.792609	0.912637
H	-7.050619	1.272506	1.105867
H	-7.433350	-1.238347	1.299096
H	-6.539046	-4.154162	-1.260692
C	-0.014855	-1.041407	3.612673
C	0.004141	-2.455120	3.748031
C	1.159505	-3.240434	3.744370
C	2.404798	-2.631172	3.599322
C	2.436286	-1.241599	3.471899
C	1.286212	-0.422876	3.478115
C	-1.344202	-0.317242	3.604983
C	-2.647490	-0.939613	3.693839
C	-3.799774	-0.126294	3.634946
C	-3.767915	1.263390	3.507194
C	-2.519449	1.879362	3.441006
C	-1.362202	1.098267	3.490532
H	-0.925914	-2.992251	3.863330
H	1.069527	-4.326668	3.848952
H	3.331472	-3.213366	3.581467
H	3.407491	-0.747746	3.357947
H	-4.773571	-0.624646	3.693711
H	-4.697150	1.839949	3.460877
H	-2.428711	2.966290	3.344507
H	-0.429818	1.640876	3.436716
C	-2.974856	-2.414592	3.859970
H	-2.611742	-3.036209	3.022701

H	-2.576768	-2.838783	4.799012
H	-4.068970	-2.544491	3.890005
C	1.613477	1.054851	3.340820
H	1.163741	1.515792	2.443992
H	1.304022	1.646455	4.221015
H	2.703921	1.179806	3.239737

Graphane-catalyzed 2,2prime-dimethylbiphenyl product

C	0.547242	-1.278848	-0.431511
C	-0.929955	-1.195131	-0.862000
C	-1.578971	0.118622	-0.388503
C	-0.776729	1.353260	-0.842393
C	0.698977	1.255338	-0.409087
C	1.348467	-0.050506	-0.904370
H	-0.958506	-1.208398	-1.975460
H	0.570690	-1.276642	0.681460
H	-0.796369	1.380256	-1.955674
H	0.724476	1.222851	0.703175
H	1.326394	-0.038152	-2.018026
H	-1.561448	0.101061	0.721103
C	1.502818	2.496372	-0.839542
C	-3.056161	0.208518	-0.815042
C	-1.725623	-2.415026	-0.358064
C	1.194120	-2.595073	-0.903734
C	-1.427900	2.655967	-0.337446
C	2.820903	-0.143965	-0.462306
C	3.625864	1.093369	-0.903504
C	2.973365	2.391938	-0.392437
C	-3.853028	-1.014866	-0.321476
C	-3.206232	-2.336439	-0.777334
C	0.400382	-3.817508	-0.403733
C	-0.623094	3.898003	-0.765435
C	2.673297	-2.680806	-0.482179
C	-2.901305	2.756294	-0.776674
C	-1.081989	-3.737980	-0.815117
C	3.471866	-1.450947	-0.954485
H	-3.239868	-2.359090	-1.890438
H	-3.825245	-0.998778	0.791934
H	-2.915978	2.783978	-1.889775
H	-0.635620	3.936957	-1.878270
H	2.980672	2.347319	0.720454
H	3.615604	1.126991	-2.017023
H	2.830998	-0.165478	0.648407
H	1.160192	-2.605496	-2.017044
H	-1.691955	-2.392678	0.754790
H	-3.089146	0.207663	-1.928291

H	-1.416780	2.625240	0.776849
H	1.491815	2.535998	-1.952390
C	-3.704850	1.520297	-0.331895
H	-3.691573	1.503846	0.782011
C	0.848779	3.793147	-0.324494
H	0.858941	3.750707	0.789704
H	3.451615	-1.441184	-2.068426
H	2.698603	-2.679305	0.629902
H	-1.120294	-3.760713	-1.928024
H	0.438364	-3.802719	0.709794
C	1.041447	-5.138177	-0.871314
C	3.319520	-3.995214	-0.958633
C	-1.873085	-4.955862	-0.300812
C	-4.001547	-3.552717	-0.265296
C	-5.330373	-0.935018	-0.751357
C	-5.179602	1.613378	-0.766649
C	-3.554384	4.057033	-0.270764
C	-1.275708	5.194851	-0.249101
C	1.654453	5.037989	-0.742367
C	3.780344	3.635167	-0.811684
C	5.095939	0.993092	-0.453510
C	4.945662	-1.545447	-0.515278
C	-3.355926	-4.878431	-0.711300
C	2.525623	-5.220360	-0.466929
C	5.750463	-0.308073	-0.954725
C	3.125107	4.930956	-0.297030
C	-2.746786	5.298706	-0.693952
C	-5.980966	0.384875	-0.295190
H	-2.756278	5.340646	-1.807119
H	-1.266148	5.150435	0.863948
H	-3.546303	4.019756	0.842696
H	-5.198605	1.620741	-1.880041
H	-5.970395	0.391515	0.819110
H	-5.354021	-0.952528	-1.864702
H	-3.970247	-3.523633	0.847603
H	-3.395045	-4.910066	-1.824279
H	-1.832476	-4.931619	0.811966
H	0.997686	-5.152202	-1.984091
H	2.567530	-5.216512	0.646751
H	3.287917	-3.999588	-2.071935
H	4.953816	-1.563635	0.596406
H	5.747115	-0.279777	-2.068518
H	5.095066	0.956905	0.658372
H	3.773913	3.677362	-1.924634
H	3.133833	4.888843	0.816550
H	1.645187	5.080837	-1.855192

C	1.001446	6.335067	-0.225292
C	-0.470184	6.440917	-0.666908
C	-5.025985	4.159682	-0.717573
C	-5.833748	2.922538	-0.282249
C	-6.131868	-2.153322	-0.252034
C	-5.481810	-3.479488	-0.689480
C	-1.233432	-6.281514	-0.758867
C	0.252932	-6.360978	-0.362435
C	4.799622	-4.084970	-0.537441
C	5.599559	-2.853156	-1.001101
C	5.906746	2.234555	-0.872553
C	5.251020	3.531649	-0.362720
H	-5.831527	2.900961	0.831859
H	-5.034267	4.191780	-1.831057
H	-0.482192	6.487610	-1.779895
H	1.013875	6.292821	0.888030
H	5.256038	3.491514	0.751204
H	5.907767	2.275299	-1.985860
H	5.585375	-2.842568	-2.114960
H	4.826529	-4.096059	0.577143
H	0.303007	-6.348202	0.750557
H	-1.283275	-6.306930	-1.871556
H	-5.510311	-3.514173	-1.802663
H	-6.116104	-2.126085	0.861678
C	7.075385	-2.948627	-0.559953
C	7.220861	-0.408823	-0.501273
C	7.376920	2.130466	-0.415143
C	6.061087	4.776958	-0.780543
C	3.932563	6.176253	-0.715845
C	1.808211	7.581773	-0.645636
C	-1.124745	7.738047	-0.146495
C	-3.402707	6.596404	-0.180288
C	-5.683655	5.462449	-0.215442
C	-7.305930	3.017796	-0.735307
C	-7.455174	0.468680	-0.739861
C	-7.609210	-2.078391	-0.692444
C	-6.280829	-4.694314	-0.172412
C	-4.148947	-6.093905	-0.190268
C	-2.022019	-7.501025	-0.236909
C	0.890731	-7.684492	-0.835271
C	3.166319	-6.538992	-0.945309
C	5.447370	-5.398915	-1.023020
C	5.393280	6.057135	-0.263062
C	3.269439	7.458198	-0.196199
C	1.149670	8.867864	-0.123372
C	-0.314282	8.973797	-0.566964

C	-2.587222	7.825935	-0.600326
C	-4.863195	6.686612	-0.640630
C	-7.952602	4.324311	-0.248960
C	-8.093844	1.784296	-0.275596
C	-8.242445	-0.753429	-0.249115
C	-7.751487	-4.613909	-0.610415
C	-5.621011	-6.006870	-0.613500
C	-1.379426	-8.816170	-0.704382
C	2.370552	-7.747911	-0.436740
C	4.643028	-6.610722	-0.535763
C	6.922002	-5.481285	-0.598582
C	7.859413	-1.708606	-1.006353
C	8.013390	0.832807	-0.928115
C	8.176932	3.373307	-0.834080
H	2.444857	-7.788453	0.670356
H	2.824497	-8.685625	-0.812989
H	4.707862	-6.663769	0.571459
H	5.096631	-7.546073	-0.918229
C	7.715885	-4.252758	-1.058638
H	6.971149	-5.556695	0.507105
H	7.374824	-6.409737	-0.995071
H	8.764274	-4.314177	-0.710115
H	7.754412	-4.231436	-2.166884
H	8.908253	-1.777048	-0.656677
H	7.900971	-1.684578	-2.115445
H	9.059193	0.755907	-0.571181
H	8.063754	0.867582	-2.036578
C	7.523774	4.663615	-0.324365
H	9.217304	3.291591	-0.466288
H	8.237353	3.403460	-1.941188
H	8.092750	5.549503	-0.664578
H	7.554422	4.678505	0.784417
H	5.966193	6.944917	-0.595492
H	5.429346	6.060657	0.846670
H	3.844952	8.343859	-0.529744
H	3.307895	7.461331	0.913405
H	1.725052	9.749133	-0.464724
H	1.199960	8.870743	0.984698
H	-0.781770	9.887336	-0.153302
H	-0.358281	9.071634	-1.670961
H	-3.054882	8.745482	-0.197151
H	-2.617356	7.920013	-1.706152
H	-5.328661	7.610461	-0.244814
H	-4.888834	6.773920	-1.747113
C	-7.145024	5.554442	-0.680202
H	-7.606583	6.480073	-0.287255

H	-7.163786	5.639714	-1.785944
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H	-8.148324	1.785902	0.833388
H	-9.138900	1.845467	-0.637467
H	-8.288554	-0.729653	0.859985
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C	-8.399681	-3.292503	-0.180389
C	-3.497985	-7.406946	-0.643897
C	0.101100	-8.894638	-0.313146
H	-8.444085	-3.247591	0.927038
H	-9.445479	-3.237214	-0.537556
H	-7.800434	-4.705751	-1.714739
H	-8.312968	-5.474578	-0.200184
H	-5.683808	-6.088495	-1.718993
H	-6.183785	-6.869502	-0.205947
H	-3.572788	-7.483414	-1.749014
H	-4.059946	-8.269112	-0.234235
H	-1.938528	-9.675566	-0.288263
H	-1.472710	-8.886378	-1.807440
H	0.188796	-8.928135	0.792118
H	0.554756	-9.830382	-0.691144
H	3.119423	-6.542166	-2.056501
H	5.413427	-5.388847	-2.134714
H	7.082341	-2.972046	0.552639
H	7.218292	-0.442599	0.611434
H	7.370789	2.090612	0.696914
H	6.054496	4.813640	-1.892264
H	3.922836	6.214642	-1.827384
H	1.794663	7.621181	-1.757234
H	-1.113720	7.687418	0.964723
H	-3.398005	6.548675	0.930998
H	-5.683309	5.421541	0.896269
H	-7.306081	3.031317	-1.847510
H	-7.463647	0.457639	-1.851923
H	-7.621335	-2.109105	-1.804292
H	-6.254402	-4.654374	0.938937
H	-4.110195	-6.059239	0.920758
H	-1.970437	-7.473363	0.873940
H	0.834810	-7.696124	-1.946179
C	1.500982	-0.268461	3.669157
C	2.167781	-1.481141	3.386112
C	3.541073	-1.523484	3.125713
C	4.279177	-0.332407	3.130777
C	3.627487	0.880075	3.383555
C	2.246069	0.942470	3.653851

C	0.040979	-0.308485	3.981544
C	-0.479139	-1.149662	5.003634
C	-1.870967	-1.174114	5.213964
C	-2.749684	-0.396845	4.450819
C	-2.235147	0.449344	3.460973
C	-0.854600	0.489206	3.239904
H	1.583504	-2.406828	3.363473
H	4.029135	-2.480510	2.913807
H	5.355784	-0.345413	2.931046
H	4.203881	1.812803	3.383714
H	-2.268732	-1.817002	6.008022
H	-3.827501	-0.441845	4.638189
H	-2.901812	1.074251	2.857539
H	-0.454710	1.141676	2.458837
C	0.406367	-1.991137	5.897865
H	0.587684	-2.996775	5.475673
H	1.393644	-1.527924	6.053280
H	-0.070093	-2.137003	6.881888
C	1.620571	2.290522	3.935906
H	1.237701	2.761383	3.010215
H	0.771285	2.215584	4.633422
H	2.366255	2.982311	4.362031

Complete references for quantum chemical software

All geometry optimizations and frequency calculations were carried out using the Gaussian 16 rev. A.03 program suite.[1] All the DHDFT calculations were performed using the ORCA 4.2.0 program suite.[2] All EDA calculations were carried out with the Q-Chem 5.2 program suite.[3,4]

References

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