The Cope Rearrangement of 1,5-Hexadiene: Full Geometry Optimizations Using Analytic MR-CISD and MR-AQCC Gradient Methods

Elizete Ventura, Silmar Andrade do Monte, Michal Dallos, and Hans Lischka

Cartesian coordinates [a.u] and total energies [a.u] for optimized chair, boat and hexadiene structures at MR-AQCC level.

a) Chair form

Ref. space: CAS(4,4) Basis: 6-31G* E=-233.750157

atom	x	y	z
C	0.184902	2.702914	0.000000
C	-0.184902	-2.702914	0.000000
C	-0.596044	1.471196	2.337233
C	0.596044	-1.471196	2.337233
C	-0.596044	1.471196	-2.337233
C	0.596044	-1.471196	-2.337233
H	0.086927	2.403580	4.054203
H	-0.086927	-2.403580	4.054203
H	0.086927	2.403580	-4.054203
H	-0.086927	-2.403580	-4.054203
H	-2.643185	1.206402	2.482108
H	2.643185	-1.206402	2.482108
H	-2.643185	1.206402	-2.482108
H	2.643185	-1.206402	-2.482108
H	-1.993220	-3.693672	0.000000
H	1.993220	3.693672	0.000000

Ref. space: CAS(6,6) Basis: 6-31G* E=-233.754902

atom	x	y	z
C	0.186665	2.708259	0.000000
C	-0.186665	-2.708259	0.000000
C	-0.612194	1.510684	2.325945
C	0.612194	-1.510684	2.325945
C	-0.612194	1.510684	-2.325945
C	0.612194	-1.510684	-2.325945
H	0.081184	2.410658	4.054514
H	-0.081184	-2.410658	4.054514
H	0.081184	2.410658	-4.054514
H	-0.081184	-2.410658	-4.054514
H	-2.651704	1.204702	2.468763
H	2.651704	-1.204702	2.468763
H	-2.651705	1.204702	-2.468763
H	2.651705	-1.204702	-2.468763
H	-2.013142	-3.667001	0.000000
H	2.013142	3.667001	0.000000

Ref. space: CAS(4,4) Basis: 6-31G** E=-233.831372

atom	x	y	z
C	0.185149	2.702992	0.000000
C	-0.185149	-2.702992	0.000000
C	-0.595267	1.470504	2.335145
C	0.595267	-1.470504	2.335145
C	-0.595267	1.470504	-2.335145
C	0.595267	-1.470504	-2.335145
H	0.085473	2.394456	4.044621
H	-0.085473	-2.394456	4.044621
H	0.085473	2.394456	-4.044621
H	-0.085473	-2.394456	-4.044621
H	-2.631890	1.202674	2.476747
H	2.631890	-1.202674	2.476747
H	-2.631890	1.202674	-2.476747
H	2.631890	-1.202674	-2.476747
H	-1.985470	-3.686478	0.000000
H	1.985470	3.686478	0.000000

Ref. space: CAS(6,6) Basis: 6-31G** E=-233.836352

atom	x	y	z
C	0.186654	2.709112	0.000000
C	-0.186654	-2.709112	0.000000
C	-0.612109	1.511724	2.323353
C	0.612109	-1.511724	2.323353
C	-0.612109	1.511724	-2.323353
C	0.612109	-1.511724	-2.323353
H	0.079414	2.402309	4.044691
H	-0.079414	-2.402309	4.044691
H	0.079414	2.402309	-4.044691
H	-0.079414	-2.402309	-4.044691
H	-2.640808	1.201346	2.462161
H	2.640808	-1.201346	2.462161
H	-2.640808	1.201346	-2.462161
H	2.640808	-1.201346	-2.462161
H	-2.007279	-3.656471	0.000000
H	2.007279	3.656471	0.000000

Ref. space: CAS(4,4) Basis: 6-311G** E=-233.915927

atom	x	y	z
C	0.189720	2.704433	0.000000
C	-0.189720	-2.704433	0.000000
C	-0.610468	1.495770	2.331242
C	0.610468	-1.495770	2.331242
C	-0.610468	1.495770	-2.331242
C	0.610468	-1.495770	-2.331242
H	0.081982	2.401205	4.053765
H	-0.081982	-2.401205	4.053765
H	0.081982	2.401205	-4.053765
H	-0.081982	-2.401205	-4.053765
H	-2.649108	1.197125	2.464368
H	2.649108	-1.197125	2.464368
H	-2.649108	1.197125	-2.464368
H	2.649108	-1.197125	-2.464368
H	-2.015793	-3.656529	0.000000
H	2.015793	3.656529	0.000000

Ref. space: CAS(4,4) Basis: 6-311G(2d,1p) E=-233.953691

atom	x	y	z
C	0.193288	2.704088	0.000000
C	-0.193288	-2.704088	0.000000
C	-0.639197	1.570935	2.308548
C	0.639197	-1.570935	2.308548
C	-0.639197	1.570935	-2.308548
C	0.639197	-1.570935	-2.308548
H	0.071788	2.421141	4.043714
H	-0.071788	-2.421141	4.043714
H	0.071788	2.421141	-4.043714
H	-0.071788	-2.421141	-4.043714
H	-2.659071	1.202353	2.439301
H	2.659071	-1.202353	2.439301
H	-2.659071	1.202353	-2.439301
H	2.659071	-1.202353	-2.439301
H	-2.030514	-3.627525	0.000000
H	2.030514	3.627525	0.000000

Ref. space: CAS(6,6) Basis: 6-311G(2d,1p) E=-233.960786

atom	x	y	z
C	0.193862	2.722010	0.000000
C	-0.193862	-2.722010	0.000000
C	-0.672391	1.666940	2.300741
C	0.672391	-1.666940	2.300741
C	-0.672391	1.666940	-2.300741
C	0.672391	-1.666940	-2.300741
H	0.066440	2.460889	4.047991
H	-0.066440	-2.460889	4.047991
H	0.066440	2.460889	-4.047991
H	-0.066440	-2.460889	-4.047991
H	-2.673741	1.219708	2.425767
H	2.673741	-1.219708	2.425767
H	-2.673741	1.219708	-2.425767
H	2.673741	-1.219708	-2.425767
H	-2.038930	-3.631480	0.000000
H	2.038930	3.631480	0.000000

b) Boat form

Ref. space: CAS(4,4) Basis: 6-31G* E=-233.730412

atom	x	y	z
C	0.000000	2.690453	-0.792560
C	0.000000	-2.690453	-0.792560
C	2.306597	-2.069554	0.340040
C	-2.306597	-2.069554	0.340040
C	2.306597	2.069554	0.340040
C	-2.306597	2.069554	0.340040
H	-4.064278	-2.500675	-0.636456
H	4.064278	-2.500675	-0.636456
H	-4.064278	2.500675	-0.636456
H	4.064278	2.500675	-0.636456
H	-2.434759	-2.120335	2.391953
H	2.434759	-2.120335	2.391953
H	-2.434759	2.120335	2.391953
H	2.434759	2.120335	2.391953
H	0.000000	3.002367	-2.832118
H	0.000000	-3.002367	-2.832118

Ref. space: CAS(6,6) Basis: 6-31G* E=-233.737004

atom	x	y	z
C	0.000000	2.692814	-0.793255
C	0.000000	-2.692814	-0.793255
C	2.307847	-2.069752	0.340304
C	-2.307847	-2.069752	0.340304
C	2.307847	2.069752	0.340304
C	-2.307847	2.069752	0.340304
H	-4.065905	-2.501032	-0.636357
H	4.065905	-2.501032	-0.636357
H	-4.065905	2.501032	-0.636357
H	4.065905	2.501032	-0.636357
H	-2.435752	-2.120362	2.392675
H	2.435752	-2.120362	2.392675
H	-2.435752	2.120362	2.392675
H	2.435752	2.120362	2.392675
H	0.000000	3.005359	-2.833261
H	0.000000	-3.005359	-2.833261

Ref. space: CAS(4,4) Basis: 6-31G** E=-233.812009

atom	x	y	z
C	0.000000	2.693782	-0.792466
C	0.000000	-2.693782	-0.792466
C	2.303908	-2.072154	0.339553
C	-2.303908	-2.072154	0.339553
C	2.303908	2.072154	0.339553
C	-2.303908	2.072154	0.339553
H	-4.053776	-2.498446	-0.630977
H	4.053776	-2.498446	-0.630977
H	-4.053776	2.498446	-0.630977
H	4.053776	2.498446	-0.630977
H	-2.426322	-2.108346	2.381625
H	2.426322	-2.108346	2.381625
H	-2.426322	2.108346	2.381625
H	2.426322	2.108346	2.381625
H	0.000000	3.010884	-2.820401
H	0.000000	-3.010884	-2.820401

c) Hexadiene (C_{2h} symmetry)

Ref. space: CAS(4,4) Basis: 6-31G* E=-233.809517

atom	x	y	z
C	0.691330	4.991530	0.000000
C	-0.691330	-4.991530	0.000000
C	-1.332590	3.455049	0.000000
C	1.332590	-3.455049	0.000000
C	-1.311571	0.601869	0.000000
C	1.311571	-0.601869	0.000000
H	0.468391	7.034459	0.000000
H	-0.468391	-7.034459	0.000000
H	2.621783	4.288091	0.000000
H	-2.621783	-4.288091	0.000000
H	-3.211101	4.310152	0.000000
H	3.211101	-4.310152	0.000000
H	-2.378915	-0.066147	1.655204
H	2.378915	0.066147	1.655204
H	-2.378915	-0.066147	-1.655204
H	2.378915	0.066147	-1.655204

Ref. space: CAS(6,6) Basis: 6-31G* E=-233.812039

atom	x	y	z
C	0.691227	4.991263	0.000000
C	-0.691227	-4.991263	0.000000
C	-1.334173	3.456163	0.000000
C	1.334173	-3.456163	0.000000
C	-1.315373	0.603640	0.000000
C	1.315373	-0.603640	0.000000
H	0.469223	7.034386	0.000000
H	-0.469223	-7.034386	0.000000
H	2.621229	4.286454	0.000000
H	-2.621229	-4.286454	0.000000
H	-3.212084	4.312891	0.000000
H	3.212084	-4.312891	0.000000
H	-2.380109	-0.066397	1.656099
H	2.380109	0.066397	1.656099
H	-2.380109	-0.066397	-1.656099
H	2.380109	0.066397	-1.656099

Ref. space: CAS(4,4) Basis: 6-31G** E=-233.890860

atom	x	y	z
C	0.690771	4.982086	0.000000
C	-0.690771	-4.982086	0.000000
C	-1.334905	3.451111	0.000000
C	1.334905	-3.451111	0.000000
C	-1.311656	0.599429	0.000000
C	1.311656	-0.599429	0.000000
H	0.471952	7.014630	0.000000
H	-0.471952	-7.014630	0.000000
H	2.607668	4.271781	0.000000
H	-2.607668	-4.271781	0.000000
H	-3.202840	4.303286	0.000000
H	3.202840	-4.303286	0.000000
H	-2.371024	-0.066186	1.648148
H	2.371024	0.066186	1.648148
H	-2.371024	-0.066186	-1.648148
H	2.371024	0.066186	-1.648148

Ref. space: CAS(6,6) Basis: 6-31G** E=-233.893422

atom	x	y	z
C	0.690455	4.982061	0.000000
C	-0.690455	-4.982061	0.000000
C	-1.336582	3.452349	0.000000
C	1.336582	-3.452349	0.000000
C	-1.315411	0.601249	0.000000
C	1.315411	-0.601249	0.000000
H	0.472987	7.014833	0.000000
H	-0.472987	-7.014833	0.000000
H	2.606849	4.270214	0.000000
H	-2.606849	-4.270214	0.000000
H	-3.203944	4.306073	0.000000
H	3.203944	-4.306073	0.000000
H	-2.372588	-0.066259	1.648846
H	2.372588	0.066259	1.648846
H	-2.372588	-0.066259	-1.648846
H	2.372588	0.066259	-1.648846

Ref. space: CAS(4,4) Basis: 6-311G** E=-233.974823

atom	x	y	z
C	0.691175	4.989777	0.000000
C	-0.691175	-4.989777	0.000000
C	-1.335898	3.458148	0.000000
C	1.335898	-3.458148	0.000000
C	-1.313544	0.601261	0.000000
C	1.313544	-0.601261	0.000000
H	0.464979	7.029687	0.000000
H	-0.464979	-7.029687	0.000000
H	2.614038	4.272419	0.000000
H	-2.614038	-4.272419	0.000000
H	-3.210283	4.314412	0.000000
H	3.210283	-4.314412	0.000000
H	-2.375444	-0.062374	1.656546
H	2.375444	0.062374	1.656546
H	-2.375444	-0.062374	-1.656546
H	2.375444	0.062374	-1.656546

Ref. space: CAS(4,4) Basis: 6-311G(2d,1p) E=-234.014643

atom	x	y	z
C	0.686451	4.975051	0.000000
C	-0.686451	-4.975051	0.000000
C	-1.331669	3.450582	0.000000
C	1.331669	-3.450582	0.000000
C	-1.310480	0.599619	0.000000
C	1.310480	-0.599619	0.000000
H	0.464516	7.012263	0.000000
H	-0.464516	-7.012263	0.000000
H	2.605597	4.255600	0.000000
H	-2.605597	-4.255600	0.000000
H	-3.200642	4.311135	0.000000
H	3.200642	-4.311135	0.000000
H	-2.374319	-0.062715	1.651599
H	2.374319	0.062715	1.651599
H	-2.374319	-0.062715	-1.651599
H	2.374319	0.062715	-1.651599

Ref. space: CAS(6,6) Basis: 6-311G(2d,1p) E=-234.017550

atom	x	y	z
C	0.686110	4.975247	0.000000
C	-0.686110	-4.975247	0.000000
C	-1.333396	3.451973	0.000000
C	1.333396	-3.451973	0.000000
C	-1.314611	0.601438	0.000000
C	1.314611	-0.601438	0.000000
H	0.465663	7.012761	0.000000
H	-0.465663	-7.012761	0.000000
H	2.604649	4.253878	0.000000
H	-2.604649	-4.253878	0.000000
H	-3.201985	4.313696	0.000000
H	3.201985	-4.313696	0.000000
H	-2.376792	-0.062358	1.652193
H	2.376792	0.062358	1.652193
H	-2.376792	-0.062358	-1.652193
H	2.376792	0.062358	-1.652193

d) Hexadiene (C_i symmetry)

Ref. space: CAS(4,4) Basis: 6-31G* E=-233.811384

atom	x	y	z
C	-2.524305	-0.963429	2.459426
C	2.524305	0.963429	-2.459426
C	-2.490143	-1.047591	4.998036
C	2.490144	1.047591	-4.998036
C	-0.223919	-1.195186	0.799907
C	0.223919	1.195186	-0.799907
H	-4.206174	-0.851400	6.112030
H	4.206174	0.851400	-6.112030
H	-0.738993	-1.324030	6.044004
H	0.738993	1.324030	-6.044003
H	4.323165	0.679764	-1.485758
H	-4.323165	-0.679763	1.485758
H	1.446263	-1.572751	1.975938
H	-1.446263	1.572751	-1.975938
H	-0.435379	-2.819766	-0.479705
H	0.435379	2.819766	0.479705

Ref. space: CAS(6,6) Basis: 6-31G* E=-233.814280

atom	x	y	z
C	-2.525367	-0.970440	2.456449
C	2.525367	0.970440	-2.456449
C	-2.487886	-1.041819	4.995874
C	2.487886	1.041819	-4.995874
C	-0.227555	-1.203246	0.796677
C	0.227555	1.203246	-0.796678
H	-4.202902	-0.842765	6.111001
H	4.202902	0.842765	-6.111000
H	-0.734684	-1.309621	6.040791
H	0.734684	1.309621	-6.040791
H	4.326273	0.694437	-1.484094
H	-4.326273	-0.694437	1.484094
H	1.444487	-1.587551	1.967912
H	-1.444487	1.587551	-1.967912
H	-0.442848	-2.817143	-0.495515
H	0.442848	2.817143	0.495515

Ref. space: CAS(4,4) Basis: 6-31G** E=-233.892684

atom	x	y	z
C	-2.525647	-0.962655	2.457517
C	2.525647	0.962655	-2.457517
C	-2.487651	-1.047305	4.994168
C	2.487651	1.047305	-4.994168
C	-0.225251	-1.193025	0.800433
C	0.225251	1.193025	-0.800433
H	-4.194415	-0.853312	6.103105
H	4.194415	0.853312	-6.103105
H	-0.741195	-1.321586	6.027572
H	0.741195	1.321586	-6.027572
H	4.316052	0.681313	-1.490436
H	-4.316052	-0.681313	1.490436
H	1.436043	-1.565327	1.972093
H	-1.436043	1.565327	-1.972093
H	-0.435163	-2.810059	-0.472045
H	0.435163	2.810059	0.472045