

The Cartesian Coordinates of Special Points as Well as Along BLA of *s-trans*-Butadiene and *s-trans*-Hexatriene

August 17, 2021

1 Input Example

GAMESS input example for delta-CR-EOMCC(2,3)

```
$CONTRL SCFTYP=RHF RUNTYP=ENERGY ICHARG=0 CCTYP=CR-  
EOML MAXIT=200 MULT=1 ISPHER=1 NUMGRD=.T. EXETYP=RUN  
$END  
$SCF DIRSCF=.T. diis=.t. soscf=.f. $END  
$BASIS GBASIS=cct $END  
$SYSTEM TIMLIM=999999100 MWORDS=1500 $END  
$EOMINP nstate(1)=1,0,0,1 MTRIP=4 $END  
$DATA  
Comment  
Cnh 2  
  
C 6.0 -0.816836949 -1.714214126 0.000000000  
C 6.0 -0.625372622 -0.315539853 0.000000000  
H 1.0 -1.810048497 -2.137287676 0.000000000  
H 1.0 -1.505828614 0.318385932 0.000000000  
H 1.0 0.032516917 -2.385520489 0.000000000  
$END
```

2 Cartesian Coordinates of *s-trans*-Butadiene

2.1 Optimized Geometries of $\text{FC} = \text{S}_{0,\text{min}}$, $1^1B_{u,\text{min}}^+$ and $2^1A_{g,\text{min}}^-$

Table 1: Cartesian coordinates of the optimized geometry of $\text{FC} = \text{S}_{0,\text{min}}$

Atom	X	Y	Z
C	-0.410990219	-1.798958603	0.000000000
C	-0.559475119	-0.470573512	0.000000000
C	0.410990219	1.798958603	0.000000000
C	0.559475119	0.470573512	0.000000000
H	-1.263114858	-2.463113554	0.000000000
H	0.571968115	-2.252448386	0.000000000
H	1.263114858	2.463113554	0.000000000
H	-1.554995711	-0.040726039	0.000000000
H	-0.571968115	2.252448386	0.000000000
H	1.554995711	0.040726039	0.000000000

Table 2: Cartesian coordinates of the optimized geometry of $1^1B_{u,\text{min}}^+$

Atom	X	Y	Z
C	0.691031929	1.768679605	0.000000000
C	-0.197855389	0.671944611	0.000000000
C	-0.691031929	-1.768679605	0.000000000
C	0.197855389	-0.671944611	0.000000000
H	0.319875581	2.782436663	0.000000000
H	1.761762911	1.608712776	0.000000000
H	-0.319875581	-2.782436663	0.000000000
H	-1.262611958	0.880170699	0.000000000
H	-1.761762911	-1.608712776	0.000000000
H	1.262611958	-0.880170699	0.000000000

Table 3: Cartesian coordinates of the optimized geometry of $2^1A_{g,min}^-$

Atom	X	Y	Z
C	1.795960445	0.695868654	0.000000000
C	0.330095456	0.624082465	0.000000000
C	-1.795960445	-0.695868654	0.000000000
C	-0.330095456	-0.624082465	0.000000000
H	2.312673282	1.642001294	0.000000000
H	2.377075070	-0.214004277	0.000000000
H	-2.312673282	-1.642001294	0.000000000
H	-0.252552227	1.533990884	0.000000000
H	-2.377075070	0.214004277	0.000000000
H	0.252552227	-1.533990884	0.000000000

2.2 Geodesic Interpolated Geometries along the PATH of $\text{FC} \rightarrow 1^1B_{u,min}^+ \rightarrow 2^1A_{g,min}^-$

Table 4: XYZ coordinates of Butadiene from $\text{FC} \rightarrow 1^1B_{u,min}^+ \rightarrow 2^1A_{g,min}^-$.

Atoms	x	y	z
		FC, BLA : -0.125466	
C	-0.410990219	-1.798958603	0.000000000
C	-0.559475119	-0.470573512	0.000000000
C	0.410990219	1.798958603	0.000000000
C	0.559475119	0.470573512	0.000000000
H	-1.263114858	-2.463113554	0.000000000
H	0.571968115	-2.252448386	0.000000000
H	1.263114858	2.463113554	0.000000000
H	-1.554995711	-0.040726039	0.000000000
H	-0.571968115	2.252448386	0.000000000
H	1.554995711	0.040726039	0.000000000
		point 1, BLA : -0.110464	
C	1.847243495	0.119160713	0.000000000
C	0.607180620	-0.400874115	0.000000000
C	-1.847243495	-0.119160713	0.000000000
C	-0.607180620	0.400874115	0.000000000
H	2.723768680	-0.512267421	0.000000000
H	2.003837433	1.190303772	0.000000000
H	-2.723768680	0.512267421	0.000000000
H	0.479324426	-1.477730117	0.000000000
H	-2.003837433	-1.190303772	0.000000000
H	-0.479324426	1.477730117	0.000000000
		point 2, BLA : -0.0954646	
C	1.855444943	0.072294551	0.000000000
C	0.593459440	-0.414907410	0.000000000
C	-1.855444943	-0.072294551	0.000000000
C	-0.593459440	0.414907410	0.000000000
H	2.712582436	-0.585060134	0.000000000
H	2.041283165	1.138751496	0.000000000
H	-2.712582436	0.585060134	0.000000000
H	0.438622158	-1.488258687	0.000000000
H	-2.041283165	-1.138751496	0.000000000
H	-0.438622158	1.488258687	0.000000000
		point 3, BLA : -0.0803673	
C	1.859493493	0.109998987	0.000000000
C	0.598371098	-0.401623638	0.000000000
C	-1.859493493	-0.109998987	0.000000000
C	-0.598371098	0.401623638	0.000000000

H	2.726774916	-0.533828464	0.000000000
H	2.025822296	1.179699526	0.000000000
H	-2.726774916	0.533828464	0.000000000
H	0.465617945	-1.478054215	0.000000000
H	-2.025822296	-1.179699526	0.000000000
H	-0.465617945	1.478054215	0.000000000
point 4, BLA : -0.0652275			
C	-1.867836681	0.057291882	0.000000000
C	-0.556747017	0.452194009	0.000000000
C	1.867836681	-0.057291882	0.000000000
C	0.556747017	-0.452194009	0.000000000
H	-2.670626670	0.779762399	0.000000000
H	-2.131441721	-0.992690690	0.000000000
H	2.670626670	-0.779762399	0.000000000
H	-0.328532979	1.512549960	0.000000000
H	2.131441721	0.992690690	0.000000000
H	0.328532979	-1.512549960	0.000000000
point 5, BLA : -0.0500952			
C	1.865569597	-0.184425239	0.000000000
C	0.606981017	0.375706299	0.000000000
C	-1.865569597	0.184425239	0.000000000
C	-0.606981017	-0.375706299	0.000000000
H	2.752000045	0.432425961	0.000000000
H	1.993733974	-1.259373539	0.000000000
H	-2.752000045	-0.432425961	0.000000000
H	0.517711060	1.456709308	0.000000000
H	-1.993733974	1.259373539	0.000000000
H	-0.517711060	-1.456709308	0.000000000
point 6, BLA : -0.0349265			
C	-1.860215598	0.276521292	0.000000000
C	-0.621238252	-0.344697576	0.000000000
C	1.860215598	-0.276521292	0.000000000
C	0.621238252	0.344697576	0.000000000
H	-2.773264707	-0.299985529	0.000000000
H	-1.937551709	1.356331940	0.000000000
H	2.773264707	0.299985529	0.000000000
H	-0.585510637	-1.428860560	0.000000000
H	1.937551709	-1.356331940	0.000000000
H	0.585510637	1.428860560	0.000000000
point 7, BLA : -0.0198214			
C	-1.883401320	0.110201947	0.000000000
C	-0.584746829	-0.397590134	0.000000000
C	1.883401320	-0.110201947	0.000000000

C	0.584746829	0.397590134	0.000000000
H	-2.738660775	-0.548846331	0.000000000
H	-2.058332571	1.178540408	0.000000000
H	2.738660775	0.548846331	0.000000000
H	-0.453082383	-1.474391779	0.000000000
H	2.058332571	-1.178540408	0.000000000
H	0.453082383	1.474391779	0.000000000

point 8, BLA : -0.00452051

C	1.891637480	-0.065084923	0.000000000
C	0.571657332	0.410510539	0.000000000
C	-1.891637480	0.065084923	0.000000000
C	-0.571657332	-0.410510539	0.000000000
H	2.727845205	0.617857190	0.000000000
H	2.094075448	-1.128588052	0.000000000
H	-2.727845205	-0.617857190	0.000000000
H	0.414558954	1.483941435	0.000000000
H	-2.094075448	1.128588052	0.000000000
H	-0.414558954	-1.483941435	0.000000000

$1^1B_{u,min}^+$, BLA : 0.0107809

C	0.691031929	1.768679605	0.000000000
C	-0.197855389	0.671944611	0.000000000
C	-0.691031929	-1.768679605	0.000000000
C	0.197855389	-0.671944611	0.000000000
H	0.319875581	2.782436663	0.000000000
H	1.761762911	1.608712776	0.000000000
H	-0.319875581	-2.782436663	0.000000000
H	-1.262611958	0.880170699	0.000000000
H	-1.761762911	-1.608712776	0.000000000
H	1.262611958	-0.880170699	0.000000000

point 1, BLA : 0.0138626

C	1.876542852	0.302466832	0.000000000
C	0.614056669	-0.337842238	0.000000000
C	-1.876542852	-0.302466832	0.000000000
C	-0.614056669	0.337842238	0.000000000
H	2.790108765	-0.272499683	0.000000000
H	1.944084016	1.382743195	0.000000000
H	-2.790108765	0.272499683	0.000000000
H	0.591266501	-1.422207552	0.000000000
H	-1.944084016	-1.382743195	0.000000000
H	-0.591266501	1.422207552	0.000000000

point 2, BLA : 0.0200338

C	-1.901080641	0.114577198	0.000000000
---	--------------	-------------	-------------

C	-0.574900598	-0.402237631	0.000000000
C	1.901080641	-0.114577198	0.000000000
C	0.574900598	0.402237631	0.000000000
H	-2.755248674	-0.545115910	0.000000000
H	-2.071562576	1.183086840	0.000000000
H	2.755248674	0.545115910	0.000000000
H	-0.441348756	-1.477941036	0.000000000
H	2.071562576	-1.183086840	0.000000000
H	0.441348756	1.477941036	0.000000000

point 3, BLA : 0.0230615

C	-1.638949321	0.973840681	0.000000000
C	-0.695358816	-0.096974717	0.000000000
C	1.638949321	-0.973840681	0.000000000
C	0.695358816	0.096974717	0.000000000
H	-2.700656745	0.780732554	0.000000000
H	-1.299053299	2.000820445	0.000000000
H	2.700656745	-0.780732554	0.000000000
H	-1.067825260	-1.114588979	0.000000000
H	1.299053299	-2.000820445	0.000000000
H	1.067825260	1.114588979	0.000000000

point 4, BLA : 0.0262975

C	0.154448808	1.902112913	0.000000000
C	0.483781206	0.509311942	0.000000000
C	-0.154448808	-1.902112913	0.000000000
C	-0.483781206	-0.509311942	0.000000000
H	0.925047967	2.657388500	0.000000000
H	-0.880163696	2.217305577	0.000000000
H	-0.925047967	-2.657388500	0.000000000
H	1.528509312	0.222728355	0.000000000
H	0.880163696	-2.217305577	0.000000000
H	-1.528509312	-0.222728355	0.000000000

point 5, BLA : 0.0295307

C	1.909919246	-0.039278780	0.000000000
C	0.536092842	-0.454518220	0.000000000
C	-1.909919246	0.039278780	0.000000000
C	-0.536092842	0.454518220	0.000000000
H	2.711483404	-0.761439949	0.000000000
H	2.160019101	1.012726267	0.000000000
H	-2.711483404	0.761439949	0.000000000
H	0.311601354	-1.513991884	0.000000000
H	-2.160019101	-1.012726267	0.000000000
H	-0.311601354	1.513991884	0.000000000

point 6, BLA : 0.0327402

C	-1.774014226	0.713888354	0.000000000
C	-0.338111782	0.616610356	0.000000000
C	1.774014226	-0.713888354	0.000000000
C	0.338111782	-0.616610356	0.000000000
H	-2.269388804	1.672203954	0.000000000
H	-2.378718337	-0.182275532	0.000000000
H	2.269388804	-1.672203954	0.000000000
H	0.248241642	1.526785658	0.000000000
H	2.378718337	0.182275532	0.000000000
H	-0.248241642	-1.526785658	0.000000000
point 7, BLA : 0.0359374			
C	1.435016296	1.266886802	0.000000000
C	0.109963128	0.694987234	0.000000000
C	-1.435016296	-1.266886802	0.000000000
C	-0.109963128	-0.694987234	0.000000000
H	1.583418329	2.335334762	0.000000000
H	2.303011818	0.622706302	0.000000000
H	-1.583418329	-2.335334762	0.000000000
H	-0.747577042	1.355399111	0.000000000
H	-2.303011818	-0.622706302	0.000000000
H	0.747577042	-1.355399111	0.000000000
point 8, BLA : 0.0390515			
C	1.914422787	-0.080036463	0.000000000
C	0.521652376	-0.472777286	0.000000000
C	-1.914422787	0.080036463	0.000000000
C	-0.521652376	0.472777286	0.000000000
H	2.703510863	-0.815270148	0.000000000
H	2.180932033	0.967306641	0.000000000
H	-2.703510863	0.815270148	0.000000000
H	0.270300514	-1.525172426	0.000000000
H	-2.180932033	-0.967306641	0.000000000
H	-0.270300514	1.525172426	0.000000000
point 9, BLA : 0.0423162			
C	1.916995242	0.065368701	0.000000000
C	0.554562793	-0.434395935	0.000000000
C	-1.916995242	-0.065368701	0.000000000
C	-0.554562793	0.434395935	0.000000000
H	2.760515228	-0.606515801	0.000000000
H	2.101350430	1.130009481	0.000000000
H	-2.760515228	0.606515801	0.000000000
H	0.382204838	-1.502220041	0.000000000
H	-2.101350430	-1.130009481	0.000000000
H	-0.382204838	1.502220041	0.000000000

		point 10, BLA : 0.0457886	
C	-1.756020123	-0.776680094	0.000000000
C	-0.307684524	-0.634065555	0.000000000
C	1.756020123	0.776680094	0.000000000
C	0.307684524	0.634065555	0.000000000
H	-2.224182491	-1.748035366	0.000000000
H	-2.383922290	0.102350408	0.000000000
H	2.224182491	1.748035366	0.000000000
H	0.313502526	-1.519211532	0.000000000
H	2.383922290	-0.102350408	0.000000000
H	-0.313502526	1.519211532	0.000000000
		point 11, BLA : 0.0490522	
C	-1.921475764	-0.048743313	0.000000000
C	-0.547782842	0.444097393	0.000000000
C	1.921475764	0.048743313	0.000000000
C	0.547782842	-0.444097393	0.000000000
H	-2.760905465	0.627943105	0.000000000
H	-2.111385812	-1.111952530	0.000000000
H	2.760905465	-0.627943105	0.000000000
H	-0.363182947	1.509282482	0.000000000
H	2.111385812	1.111952530	0.000000000
H	0.363182947	-1.509282482	0.000000000
		point 12, BLA : 0.0523145	
C	-1.921512445	-0.099052337	0.000000000
C	-0.557799536	0.432118495	0.000000000
C	1.921512445	0.099052337	0.000000000
C	0.557799536	-0.432118495	0.000000000
H	-2.779124384	0.554268233	0.000000000
H	-2.081720326	-1.166917949	0.000000000
H	2.779124384	-0.554268233	0.000000000
H	-0.399574898	1.501245192	0.000000000
H	2.081720326	1.166917949	0.000000000
H	0.399574898	-1.501245192	0.000000000
		$2^1 A_{g,min}^-$, BLA : 0.0556133	
C	1.795960445	0.695868654	0.000000000
C	0.330095456	0.624082465	0.000000000
C	-1.795960445	-0.695868654	0.000000000
C	-0.330095456	-0.624082465	0.000000000
H	2.312673282	1.642001294	0.000000000
H	2.377075070	-0.214004277	0.000000000
H	-2.312673282	-1.642001294	0.000000000
H	-0.252552227	1.533990884	0.000000000
H	-2.377075070	0.214004277	0.000000000

H	0.252552227	-1.533990884	0.000000000
---	-------------	--------------	-------------

3 Cartesian Coordinates of *s-trans*-Hexatriene

3.1 Optimized Geometries of $\text{FC} = \text{S}_{0,\text{min}}$, $1^1B_{u,\text{min}}^+$ and $2^1A_{g,\text{min}}^-$

Table 5: Cartesian coordinates of the optimized geometry of $\text{FC} = \text{S}_{0,\text{min}}$

Atom	X	Y	Z
C	-2.599190241	-1.632087481	0.000000000
C	2.599190241	1.632087481	0.000000000
C	-1.838677149	-0.531510131	0.000000000
C	1.838677149	0.531510131	0.000000000
C	-0.381291693	-0.552694421	0.000000000
C	0.381291693	0.552694421	0.000000000
H	-3.677898676	-1.572919256	0.000000000
H	3.677898676	1.572919256	0.000000000
H	-2.155752736	-2.619601234	0.000000000
H	2.155752736	2.619601234	0.000000000
H	-2.310234599	0.444966297	0.000000000
H	2.310234599	-0.444966297	0.000000000
H	0.096257532	-1.527272287	0.000000000
H	-0.096257532	1.527272287	0.000000000

Table 6: Cartesian coordinates of the optimized geometry of $1^1B_{u,\text{min}}^+$

Atom	X	Y	Z
C	-1.589263721	-2.672091585	0.000000000
C	1.589263721	2.672091585	0.000000000
C	-1.367089916	-1.310674401	0.000000000
C	1.367089916	1.310674401	0.000000000
C	-0.099223468	-0.700142664	0.000000000
C	0.099223468	0.700142664	0.000000000
H	-2.592178488	-3.073386618	0.000000000
H	2.592178488	3.073386618	0.000000000
H	-0.762604915	-3.371669028	0.000000000
H	0.762604915	3.371669028	0.000000000
H	-2.228302232	-0.649587800	0.000000000
H	2.228302232	0.649587800	0.000000000
H	0.779988971	-1.336628376	0.000000000
H	-0.779988971	1.336628376	0.000000000

Table 7: Cartesian coordinates of the optimized geometry of $2^1A_{g,min}^-$

Atom	X	Y	Z
C	1.586707311	2.715957152	0.000000000
C	-1.586707311	-2.715957152	0.000000000
C	1.369450642	1.293845073	0.000000000
C	-1.369450642	-1.293845073	0.000000000
C	0.111086292	0.710462149	0.000000000
C	-0.111086292	-0.710462149	0.000000000
H	2.583389424	3.127275187	0.000000000
H	-2.583389424	-3.127275187	0.000000000
H	0.748432850	3.397366647	0.000000000
H	-0.748432850	-3.397366647	0.000000000
H	2.237343342	0.645223607	0.000000000
H	-2.237343342	-0.645223607	0.000000000
H	-0.759559980	1.356768452	0.000000000
H	0.759559980	-1.356768452	0.000000000

3.2 Geodesic Interpolated Geometries along the PATH of $\text{FC} \rightarrow 1^1B_{u,min}^+ \rightarrow 2^1A_{g,min}^-$

Table 8: XYZ coordinates of Hexatriene from from $\text{FC} \rightarrow 1^1B_{u,min}^+ \rightarrow 2^1A_{g,min}^-$.

Atoms	x	y	z
FC = S_{0,min}, BLA : -0.118049			
C	-2.599190241	-1.632087481	0.000000000
C	2.599190241	1.632087481	0.000000000
C	-1.838677149	-0.531510131	0.000000000
C	1.838677149	0.531510131	0.000000000
C	-0.381291693	-0.552694421	0.000000000
C	0.381291693	0.552694421	0.000000000
H	-3.677898676	-1.572919256	0.000000000
H	3.677898676	1.572919256	0.000000000
H	-2.155752736	-2.619601234	0.000000000
H	2.155752736	2.619601234	0.000000000
H	-2.310234599	0.444966297	0.000000000
H	2.310234599	-0.444966297	0.000000000
H	0.096257532	-1.527272287	0.000000000
H	-0.096257532	1.527272287	0.000000000
point 1, BLA : -0.106751			
C	3.055546058	-0.332133522	0.000000000
C	-3.055546058	0.332133522	0.000000000
C	1.884127654	0.323270269	0.000000000
C	-1.884127654	-0.323270269	0.000000000
C	0.588335523	-0.331440407	0.000000000
C	-0.588335523	0.331440407	0.000000000
H	3.997513991	0.196831997	0.000000000
H	-3.997513991	-0.196831997	0.000000000
H	3.092050002	-1.414072942	0.000000000
H	-3.092050002	1.414072942	0.000000000
H	1.880444472	1.407782910	0.000000000
H	-1.880444472	-1.407782910	0.000000000
H	0.583116810	-1.416746405	0.000000000
H	-0.583116810	1.416746405	0.000000000
point 2, BLA : -0.0954534			
C	3.039958405	0.482080033	0.000000000
C	-3.039958405	-0.482080033	0.000000000
C	1.895673827	-0.228238269	0.000000000
C	-1.895673827	0.228238269	0.000000000
C	0.575139523	0.361047436	0.000000000
C	-0.575139523	-0.361047436	0.000000000
H	4.004573113	-0.004404560	0.000000000

H	-4.004573113	0.004404560	0.000000000
H	3.027029210	1.564617846	0.000000000
H	-3.027029210	-1.564617846	0.000000000
H	1.944195559	-1.311825866	0.000000000
H	-1.944195559	1.311825866	0.000000000
H	0.515020535	1.444735600	0.000000000
H	-0.515020535	-1.444735600	0.000000000

point 3, BLA : -0.0841844

C	-3.052930293	0.425096429	0.000000000
C	3.052930293	-0.425096429	0.000000000
C	-1.889065999	-0.261734985	0.000000000
C	1.889065999	0.261734985	0.000000000
C	-0.585634159	0.351399148	0.000000000
C	0.585634159	-0.351399148	0.000000000
H	-4.005932896	-0.083656083	0.000000000
H	4.005932896	0.083656083	0.000000000
H	-3.063883123	1.507704432	0.000000000
H	3.063883123	-1.507704432	0.000000000
H	-1.916126259	-1.346192427	0.000000000
H	1.916126259	1.346192427	0.000000000
H	-0.544282590	1.435982621	0.000000000
H	0.544282590	-1.435982621	0.000000000

point 4, BLA : -0.0729035

C	-3.069563904	-0.326188337	0.000000000
C	3.069563904	0.326188337	0.000000000
C	-1.877725281	0.320580296	0.000000000
C	1.877725281	-0.320580296	0.000000000
C	-0.600579087	-0.333474027	0.000000000
C	0.600579087	0.333474027	0.000000000
H	-4.003228437	0.217211761	0.000000000
H	4.003228437	-0.217211761	0.000000000
H	-3.119121040	-1.407730325	0.000000000
H	3.119121040	1.407730325	0.000000000
H	-1.868707698	1.405508935	0.000000000
H	1.868707698	-1.405508935	0.000000000
H	-0.592646304	-1.418763893	0.000000000
H	0.592646304	1.418763893	0.000000000

point 5, BLA : -0.0615574

C	3.086382055	0.171879352	0.000000000
C	-3.086382055	-0.171879352	0.000000000
C	1.857466995	-0.411943502	0.000000000
C	-1.857466995	0.411943502	0.000000000
C	0.620455245	0.303755144	0.000000000

C	-0.620455245	-0.303755144	0.000000000
H	3.989145147	-0.421664900	0.000000000
H	-3.989145147	0.421664900	0.000000000
H	3.193560497	1.249423253	0.000000000
H	-3.193560497	-1.249423253	0.000000000
H	1.793354735	-1.495087553	0.000000000
H	-1.793354735	1.495087553	0.000000000
H	0.665300125	1.388204221	0.000000000
H	-0.665300125	-1.388204221	0.000000000

point 6, BLA : -0.0502279

C	1.334373465	-2.793295745	0.000000000
C	-1.334373465	2.793295745	0.000000000
C	0.326769297	-1.872110005	0.000000000
C	-0.326769297	1.872110005	0.000000000
C	0.519473275	-0.461562375	0.000000000
C	-0.519473275	0.461562375	0.000000000
H	1.124078683	-3.853051565	0.000000000
H	-1.124078683	3.853051565	0.000000000
H	2.372631016	-2.485895754	0.000000000
H	-2.372631016	2.485895754	0.000000000
H	-0.699818685	-2.223743264	0.000000000
H	0.699818685	2.223743264	0.000000000
H	1.538859642	-0.088975479	0.000000000
H	-1.538859642	0.088975479	0.000000000

point 7, BLA : -0.0388971

C	3.039727301	-0.608986997	0.000000000
C	-3.039727301	0.608986997	0.000000000
C	1.692777390	-0.858955949	0.000000000
C	-1.692777390	0.858955949	0.000000000
C	0.685032343	0.138876049	0.000000000
C	-0.685032343	-0.138876049	0.000000000
H	3.758097795	-1.415918538	0.000000000
H	-3.758097795	1.415918538	0.000000000
H	3.419369593	0.405100906	0.000000000
H	-3.419369593	-0.405100906	0.000000000
H	1.357362166	-1.891180941	0.000000000
H	-1.357362166	1.891180941	0.000000000
H	0.996607077	1.178574640	0.000000000
H	-0.996607077	-1.178574640	0.000000000

point 8, BLA : -0.0275243

C	3.100076095	0.167080056	0.000000000
C	-3.100076095	-0.167080056	0.000000000
C	1.851581005	-0.408291253	0.000000000

C	-1.851581005	0.408291253	0.000000000
C	0.632878865	0.306162896	0.000000000
C	-0.632878865	-0.306162896	0.000000000
H	3.994208051	-0.439136539	0.000000000
H	-3.994208051	0.439136539	0.000000000
H	3.218230375	1.243497399	0.000000000
H	-3.218230375	-1.243497399	0.000000000
H	1.782712599	-1.491631397	0.000000000
H	-1.782712599	1.491631397	0.000000000
H	0.674022013	1.390782116	0.000000000
H	-0.674022013	-1.390782116	0.000000000

$1^1B_{u,min}^+$, BLA : -0.0161645

C	-1.589263721	-2.672091585	0.000000000
C	1.589263721	2.672091585	0.000000000
C	-1.367089916	-1.310674401	0.000000000
C	1.367089916	1.310674401	0.000000000
C	-0.099223468	-0.700142664	0.000000000
C	0.099223468	0.700142664	0.000000000
H	-2.592178488	-3.073386618	0.000000000
H	2.592178488	3.073386618	0.000000000
H	-0.762604915	-3.371669028	0.000000000
H	0.762604915	3.371669028	0.000000000
H	-2.228302232	-0.649587800	0.000000000
H	2.228302232	0.649587800	0.000000000
H	0.779988971	-1.336628376	0.000000000
H	-0.779988971	1.336628376	0.000000000

point 1, BLA : -0.0113935

C	3.110350622	0.085500452	0.000000000
C	-3.110350622	-0.085500452	0.000000000
C	1.837331499	-0.456311110	0.000000000
C	-1.837331499	0.456311110	0.000000000
C	0.645951527	0.289812356	0.000000000
C	-0.645951527	-0.289812356	0.000000000
H	3.985535348	-0.547436910	0.000000000
H	-3.985535348	0.547436910	0.000000000
H	3.258666374	1.158020472	0.000000000
H	-3.258666374	-1.158020472	0.000000000
H	1.739515205	-1.537398628	0.000000000
H	-1.739515205	1.537398628	0.000000000
H	0.715239486	1.372925953	0.000000000
H	-0.715239486	-1.372925953	0.000000000

point 2, BLA : -0.00662567

C	2.715219264	-1.524801466	0.000000000
---	-------------	--------------	-------------

C	-2.715219264	1.524801466	0.000000000
C	1.340544398	-1.335746331	0.000000000
C	-1.340544398	1.335746331	0.000000000
C	0.703837000	-0.084120918	0.000000000
C	-0.703837000	0.084120918	0.000000000
H	3.141379202	-2.517079033	0.000000000
H	-3.141379202	2.517079033	0.000000000
H	3.392220050	-0.680105106	0.000000000
H	-3.392220050	0.680105106	0.000000000
H	0.701929179	-2.213358425	0.000000000
H	-0.701929179	2.213358425	0.000000000
H	1.320485453	0.808912218	0.000000000
H	-1.320485453	-0.808912218	0.000000000

point 3, BLA : -0.00191423

C	-3.078919190	0.483150493	0.000000000
C	3.078919190	-0.483150493	0.000000000
C	-1.878718666	-0.221373764	0.000000000
C	1.878718666	0.221373764	0.000000000
C	-0.606179163	0.369043068	0.000000000
C	0.606179163	-0.369043068	0.000000000
H	-4.027709582	-0.032280819	0.000000000
H	4.027709582	0.032280819	0.000000000
H	-3.087014831	1.565426156	0.000000000
H	3.087014831	-1.565426156	0.000000000
H	-1.920640521	-1.305819289	0.000000000
H	1.920640521	1.305819289	0.000000000
H	-0.539223334	1.452160483	0.000000000
H	0.539223334	-1.452160483	0.000000000

point 4, BLA : 0.00281702

C	3.112200384	0.208137449	0.000000000
C	-3.112200384	-0.208137449	0.000000000
C	1.850581847	-0.389034646	0.000000000
C	-1.850581847	0.389034646	0.000000000
C	0.637786990	0.313146484	0.000000000
C	-0.637786990	-0.313146484	0.000000000
H	4.011545584	-0.389211163	0.000000000
H	-4.011545584	0.389211163	0.000000000
H	3.215414400	1.285316315	0.000000000
H	-3.215414400	-1.285316315	0.000000000
H	1.796491505	-1.472787637	0.000000000
H	-1.796491505	1.472787637	0.000000000
H	0.668783294	1.397886579	0.000000000
H	-0.668783294	-1.397886579	0.000000000

point 5, BLA : 0.00766337

C	0.323112579	3.104941249	0.000000000
C	-0.323112579	-3.104941249	0.000000000
C	-0.322410809	1.862550440	0.000000000
C	0.322410809	-1.862550440	0.000000000
C	0.335852760	0.627031914	0.000000000
C	-0.335852760	-0.627031914	0.000000000
H	-0.240367635	4.025726239	0.000000000
H	0.240367635	-4.025726239	0.000000000
H	1.403254949	3.167467377	0.000000000
H	-1.403254949	-3.167467377	0.000000000
H	-1.407214935	1.848938366	0.000000000
H	1.407214935	-1.848938366	0.000000000
H	1.420744883	0.619590360	0.000000000
H	-1.420744883	-0.619590360	0.000000000

point 6, BLA : 0.0124738

C	3.114526179	0.246691250	0.000000000
C	-3.114526179	-0.246691250	0.000000000
C	1.852940226	-0.370043947	0.000000000
C	-1.852940226	0.370043947	0.000000000
C	0.636381074	0.319692617	0.000000000
C	-0.636381074	-0.319692617	0.000000000
H	4.021088653	-0.339115891	0.000000000
H	-4.021088653	0.339115891	0.000000000
H	3.202787498	1.324808632	0.000000000
H	-3.202787498	-1.324808632	0.000000000
H	1.813058069	-1.454087316	0.000000000
H	-1.813058069	1.454087316	0.000000000
H	0.657193529	1.404379726	0.000000000
H	-0.657193529	-1.404379726	0.000000000

point 7, BLA : 0.017367

C	3.123660618	0.142316934	0.000000000
C	-3.123660618	-0.142316934	0.000000000
C	1.791300055	0.599062573	0.000000000
C	-1.791300055	-0.599062573	0.000000000
C	0.672397219	-0.237395923	0.000000000
C	-0.672397219	0.237395923	0.000000000
H	3.950419526	0.835951016	0.000000000
H	-3.950419526	-0.835951016	0.000000000
H	3.344286477	-0.916512575	0.000000000
H	-3.344286477	0.916512575	0.000000000
H	1.617474922	1.669646147	0.000000000
H	-1.617474922	-1.669646147	0.000000000
H	0.829284990	-1.310830806	0.000000000

H	-0.829284990	1.310830806	0.000000000
point 8, BLA : 0.0221922			
C	-3.063149083	0.640887071	0.000000000
C	3.063149083	-0.640887071	0.000000000
C	-1.883201783	-0.135919380	0.000000000
C	1.883201783	0.135919380	0.000000000
C	-0.593391216	0.396970081	0.000000000
C	0.593391216	-0.396970081	0.000000000
H	-4.036574589	0.175299650	0.000000000
H	4.036574589	-0.175299650	0.000000000
H	-3.012066274	1.721105238	0.000000000
H	3.012066274	-1.721105238	0.000000000
H	-1.981901038	-1.215854984	0.000000000
H	1.981901038	1.215854984	0.000000000
H	-0.479441586	1.475756411	0.000000000
H	0.479441586	-1.475756411	0.000000000
point 9, BLA : 0.0270395			
C	2.989891250	-0.933187554	0.000000000
C	-2.989891250	0.933187554	0.000000000
C	1.576817221	-1.037304379	0.000000000
C	-1.576817221	1.037304379	0.000000000
C	0.712575484	0.056601117	0.000000000
C	-0.712575484	-0.056601117	0.000000000
H	3.613184985	-1.813859925	0.000000000
H	-3.613184985	1.813859925	0.000000000
H	3.470606994	0.035265062	0.000000000
H	-3.470606994	-0.035265062	0.000000000
H	1.137337852	-2.028517179	0.000000000
H	-1.137337852	2.028517179	0.000000000
H	1.139831094	1.053576674	0.000000000
H	-1.139831094	-1.053576674	0.000000000
point 10, BLA : 0.0318568			
C	1.054649392	-2.952052601	0.000000000
C	-1.054649392	2.952052601	0.000000000
C	0.118232518	-1.883022781	0.000000000
C	-0.118232518	1.883022781	0.000000000
C	0.473695192	-0.536456836	0.000000000
C	-0.473695192	0.536456836	0.000000000
H	0.726590388	-3.979749969	0.000000000
H	-0.726590388	3.979749969	0.000000000
H	2.117073239	-2.752293831	0.000000000
H	-2.117073239	2.752293831	0.000000000
H	-0.937660331	-2.128815828	0.000000000

H	0.937660331	2.128815828	0.000000000
H	1.527408750	-0.279355082	0.000000000
H	-1.527408750	0.279355082	0.000000000

point 11, BLA : 0.0366486

C	-0.804790263	3.032453917	0.000000000
C	0.804790263	-3.032453917	0.000000000
C	-0.971241186	1.616765949	0.000000000
C	0.971241186	-1.616765949	0.000000000
C	0.085220472	0.711421188	0.000000000
C	-0.085220472	-0.711421188	0.000000000
H	-1.657187349	3.693431885	0.000000000
H	1.657187349	-3.693431885	0.000000000
H	0.183956986	3.469084982	0.000000000
H	-0.183956986	-3.469084982	0.000000000
H	-1.980485195	1.221306771	0.000000000
H	1.980485195	-1.221306771	0.000000000
H	1.098451562	1.098237540	0.000000000
H	-1.098451562	-1.098237540	0.000000000

point 12, BLA : 0.0416372

C	3.136323715	-0.154633877	0.000000000
C	-3.136323715	0.154633877	0.000000000
C	1.782409480	-0.614490448	0.000000000
C	-1.782409480	0.614490448	0.000000000
C	0.679202579	0.230881297	0.000000000
C	-0.679202579	-0.230881297	0.000000000
H	3.960743642	-0.849961812	0.000000000
H	-3.960743642	0.849961812	0.000000000
H	3.356150535	0.903430966	0.000000000
H	-3.356150535	-0.903430966	0.000000000
H	1.606562411	-1.683914651	0.000000000
H	-1.606562411	1.683914651	0.000000000
H	0.847770517	1.302170682	0.000000000
H	-0.847770517	-1.302170682	0.000000000

point 13, BLA : 0.0465198

C	3.142156374	0.063570799	0.000000000
C	-3.142156374	-0.063570799	0.000000000
C	1.798198998	0.564346824	0.000000000
C	-1.798198998	-0.564346824	0.000000000
C	0.673423060	-0.249691351	0.000000000
C	-0.673423060	0.249691351	0.000000000
H	3.986524838	0.734321288	0.000000000
H	-3.986524838	-0.734321288	0.000000000
H	3.330196669	-1.000397370	0.000000000

H	-3.330196669	1.000397370	0.000000000
H	1.653835865	1.638330062	0.000000000
H	-1.653835865	-1.638330062	0.000000000
H	0.812435833	-1.325136397	0.000000000
H	-0.812435833	1.325136397	0.000000000
		$2^1 A_{g,min}^-$, BLA : 0.0514535	
C	1.586707311	2.715957152	0.000000000
C	-1.586707311	-2.715957152	0.000000000
C	1.369450642	1.293845073	0.000000000
C	-1.369450642	-1.293845073	0.000000000
C	0.111086292	0.710462149	0.000000000
C	-0.111086292	-0.710462149	0.000000000
H	2.583389424	3.127275187	0.000000000
H	-2.583389424	-3.127275187	0.000000000
H	0.748432850	3.397366647	0.000000000
H	-0.748432850	-3.397366647	0.000000000
H	2.237343342	0.645223607	0.000000000
H	-2.237343342	-0.645223607	0.000000000
H	-0.759559980	1.356768452	0.000000000
H	0.759559980	-1.356768452	0.000000000
