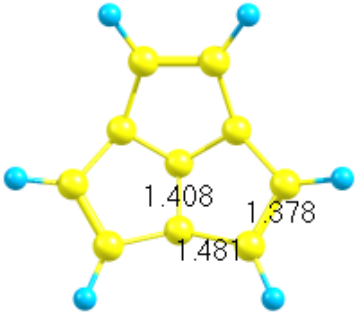
Electronic Supplementary Material (ESI)
for Physical Chemistry Chemical Physics

Supporting Materials for I :

Cartesian coordinates (Å)for optimized structure,
absolute energy for optimized state in **bold,**
CAS MP2 corrected energy and energies for other electronic states.

I (Neutral) CAS(10/10)/cc-pVDZ

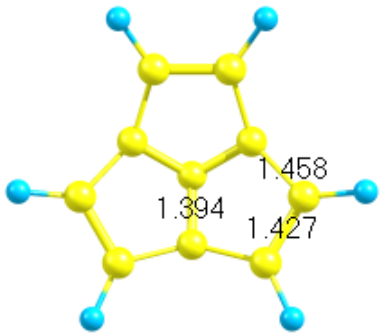
C	6.0	0.8965275490	0.0000226863	0.0000000000
C	6.0	0.4772442752	1.3444454112	0.0000000000
C	6.0	0.4778570721	-0.6723006434	-1.1644370986
C	6.0	0.4778570721	-0.6723006434	1.1644370986
C	6.0	-0.0178758877	1.5891320106	-1.3744091881
C	6.0	-0.0178758877	1.5891320106	1.3744091881
C	6.0	-0.0173474891	0.3954195568	-2.0637081568
C	6.0	-0.0173474891	0.3954195568	2.0637081568
C	6.0	-0.0176117817	-1.9847730299	-0.6892303842
C	6.0	-0.0176117817	-1.9847730299	0.6892303842
H	1.0	-0.3377165507	2.5384976650	-1.7788051828
H	1.0	-0.3377165507	2.5384976650	1.7788051828
H	1.0	-0.3363981949	0.2708590916	-3.0883235912
H	1.0	-0.3363981949	0.2708590916	3.0883235912
H	1.0	-0.3377930801	-2.8094932209	-1.3092828017
H	1.0	-0.3377930801	-2.8094932209	1.3092828017



C_{3v}

Min T_1 -382.13853a.u.
MP2 T_1 -383.34901a.u.
S_0/S_1: -382.13355a.u .
$S_2/2^1A'$: -382.08304 a.u .
SOC $T_1/1^1A''$ 0.42cm-1
MP2 S_0/S_1: -383.34121a.u .

C	6.0	0.7615141090	-0.0000735727	0.0000000000
C	6.0	0.4077648153	1.3481440845	0.0000000000
C	6.0	0.4076207339	-0.6741565764	-1.1675879663
C	6.0	0.4076207339	-0.6741565764	1.1675879663
C	6.0	0.0045853953	1.6175776755	-1.3744762956
C	6.0	0.0045853953	1.6175776755	1.3744762956
C	6.0	0.0044325951	0.3815078475	-2.0880978972
C	6.0	0.0044325951	0.3815078475	2.0880978972
C	6.0	0.0045942737	-1.9992580546	-0.7136636127
C	6.0	0.0045942737	-1.9992580546	0.7136636127
H	1.0	-0.3018431791	2.5637909502	-1.7946161071
H	1.0	-0.3018431791	2.5637909502	1.7946161071
H	1.0	-0.3022444277	0.2723439359	-3.1175328945
H	1.0	-0.3022444277	0.2723439359	3.1175328945
H	1.0	-0.3017848534	-2.8362655557	-1.3229680990
H	1.0	-0.3017848534	-2.8362655557	1.3229680990



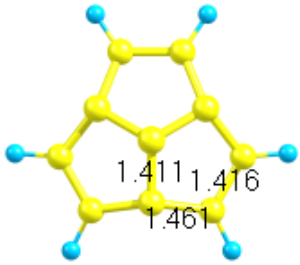
C_{3v}

Min $S_2/2^1A'$ -382.09196 a.u.
S_0/S_1: -382.13361 a.u
T_1: -382.13038a.u
MP2 $S_2/2^1A'$ -383.33033a.u
S_0/S_1: -383.34539a.u.
T_1: -383.34766 a.u

Electronic Supplementary Material (ESI)
for Physical Chemistry Chemical Physics

I^{-2} (Dianion)
CAS(12/10)/cc-pVDZ

C	6.0	0.6562117423	-0.0000562218	0.0000000000
C	6.0	0.3755435877	1.3827402387	0.0000000000
C	6.0	0.3754291365	-0.6914453919	-1.1975477557
C	6.0	0.3754291365	-0.6914453919	1.1975477557
C	6.0	-0.0369617590	1.6154099738	-1.3821557157
C	6.0	-0.0369617590	1.6154099738	1.3821557157
C	6.0	-0.0370549394	0.3892390207	- 2.0901073563
C	6.0	-0.0370549394	0.3892390207	2.0901073563
C	6.0	-0.0370254803	-2.0048210314	-0.7079396939
C	6.0	-0.0370254803	-2.0048210314	0.7079396939
H	1.0	-0.2266847713	2.5803964465	-1.8647371965
H	1.0	-0.2266847713	2.5803964465	1.8647371965
H	1.0	-0.2269705182	0.3247083339	-3.1670329143
H	1.0	-0.2269705182	0.3247083339	3.1670329143
H	1.0	-0.2266093334	-2.9052538814	-1.3023014092
H	1.0	-0.2266093334	-2.9052538814	1.3023014092

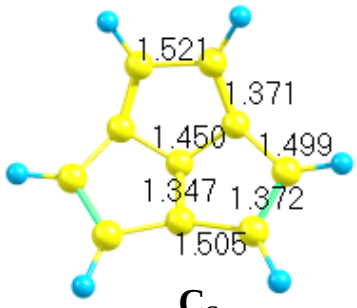


Dianion C_{3V}

Min S_0 -381.96217a.u.
MP2 -383.26200a.u
AnionRadical D_0/D_1 :
$1^2A'/1^2A''$ -382. 13260a.u.
MP2 -383.39300a.u.
Neutral $C_{10}H_6$:
S_0/S_1: -382.12895 a.u
S_2: -382.08331 a.u
T_1: - 382.12469 a.u
MP2
S_0/S_1: -383.34189a.u.
T_1: -383.34214a.u

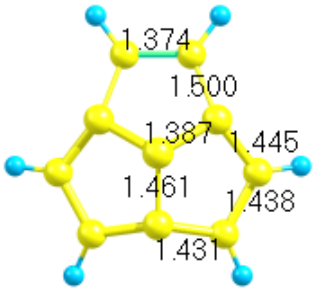
I (Neutral , GS)
CAS(10/10)/cc-pVDZ

C	6.0	0.8262180243	0.0188712069	0.0000000000
C	6.0	0.3342899419	1.2731946704	0.0000000000
C	6.0	0.4866882706	-0.7073903596	-1.2079447458
C	6.0	0.4866882706	-0.7073903596	1.2079447458
C	6.0	-0.0762920311	1.5369356912	-1.4235383816
C	6.0	-0.0762920311	1.5369356912	1.4235383816
C	6.0	0.0533913414	0.3784589971	-2.1466882698
C	6.0	0.0533913414	0.3784589971	2.1466882698
C	6.0	0.0502315386	-1.9280260570	-0.7604003098
C	6.0	0.0502315386	-1.9280260570	0.7604003098
H	1.0	-0.3970176144	2.4851291800	-1.8302751771
H	1.0	-0.3970176144	2.4851291800	1.8302751771
H	1.0	-0.1380576737	0.2804883186	-3.2046693469
H	1.0	-0.1380576737	0.2804883186	3.2046693469
H	1.0	-0.4591978145	-2.6920532304	-1.3314779513
H	1.0	-0.4591978145	-2.6920532304	1.3314779513



C_S
Min S_0 /1^1A'
-382.16504a.u.
MP2 -383.36174a.u

C	6.0	0.7921027344	-0.0210894412	0.0000000000
C	6.0	0.4532772677	1.4001955984	0.0000000000
C	6.0	0.4135721183	-0.6752325306	-1.1632201856
C	6.0	0.4135721183	-0.6752325306	1.1632201856
C	6.0	0.0480368061	1.6478578079	-1.3493916412
C	6.0	0.0480368061	1.6478578079	1.3493916412
C	6.0	-0.0097998451	0.3901735699	-2.0433251067
C	6.0	-0.0097998451	0.3901735699	2.0433251067
C	6.0	-0.0132318327	-2.0323972853	-0.6868225697
C	6.0	-0.0132318327	-2.0323972853	0.6868225697
H	1.0	-0.2870219511	2.5833443235	-1.7717013103
H	1.0	-0.2870219511	2.5833443235	1.7717013103
H	1.0	-0.4165937889	0.2799104241	-3.0384386427
H	1.0	-0.4165937889	0.2799104241	3.0384386427
H	1.0	-0.2576515076	-2.8836339096	-1.3049053968
H	1.0	-0.2576515076	-2.8836339096	1.3049053968

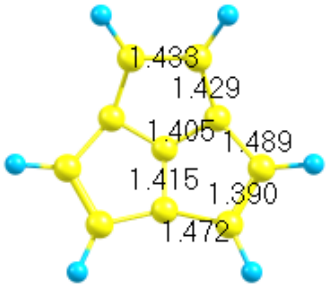


C_S
TS S_0 /1^1A"
-382.14683a.u.
MP2 -383. 35239a.u

Electronic Supplementary Material (ESI)
for Physical Chemistry Chemical Physics

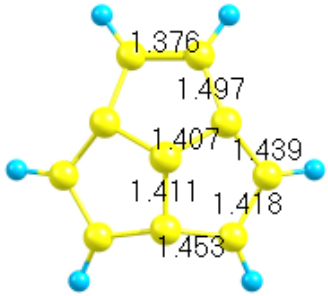
I^{-1} (AnionRadical)
CAS(11/10)/cc-pVDZ

C	6.0	0.8016467300	-0.0151123359	0.0000000000
C	6.0	0.3777745416	1.3349347175	0.0000000000
C	6.0	0.4671945715	-0.7024936836	-1.1787311138
C	6.0	0.4671945715	-0.7024936836	1.1787311138
C	6.0	-0.0454111078	1.5888255743	-1.3864761286
C	6.0	-0.0454111078	1.5888255743	1.3864761286
C	6.0	0.0135934414	0.3886649819	-2.0847497938
C	6.0	0.0135934414	0.3886649819	2.0847497938
C	6.0	-0.0190494139	-1.9644973556	-0.7164308063
C	6.0	-0.0190494139	-1.9644973556	0.7164308063
H	1.0	-0.3206371358	2.5434269522	1.8215503228
H	1.0	-0.3206371358	2.5434269522	1.8215503228
H	1.0	-0.2480505708	0.2954824016	-3.1347590140
H	1.0	-0.2480505708	0.2954824016	3.1347590140
H	1.0	-0.3373504206	-2.8097445832	-1.3204978180
H	1.0	-0.3373504206	-2.8097445832	1.3204978180



AnionRadical C_S
D_0 /1^2A'
-382.14052a.u.
MP2 -383.40032a.u.

C	6.0	0.8081543343	0.0074619404	0.0000000000
C	6.0	0.5238763367	1.3891503105	0.0000000000
C	6.0	0.4008671933	-0.6599420655	-1.1703602599
C	6.0	0.4008671933	-0.6599420655	1.1703602599
C	6.0	0.0172756547	1.6146411004	-1.3427860316
C	6.0	0.0172756547	1.6146411004	1.3427860316
C	6.0	-0.0532603852	0.3862098186	-2.0480425588
C	6.0	-0.0532603852	0.3862098186	2.0480425588
C	6.0	-0.0152026206	-2.0147783591	-0.6880647514
C	6.0	-0.0152026206	-2.0147783591	0.6880647514
H	1.0	-0.2823225625	2.5657889866	-1.7753289088
H	1.0	-0.2823225625	2.5657889866	1.7753289088
H	1.0	-0.3771537451	0.2871426834	-3.0792826927
H	1.0	-0.3771537451	0.2871426834	3.0792826927
H	1.0	-0.2562188700	-2.8777928114	-1.2996713255
H	1.0	-0.2562188700	-2.8777928114	1.2996713255



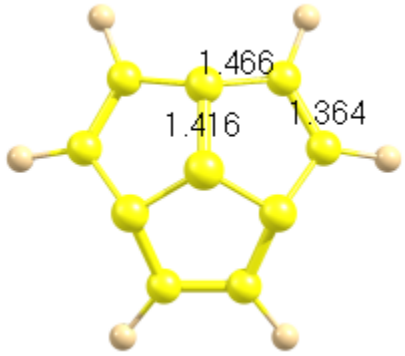
AnionRadical C_S
D_0 /1^2A"
-382.14061a.u.
MP2 -383.40151a.u.

Electronic Supplementary Material (ESI)
for Physical Chemistry Chemical Physics

Supporting Materials for I I:
Cartesian coordinates (Å)for optimized structure,
absolute energy for optimized state in **bold,**
CAS MP2 corrected energy and energies for other electronic states.

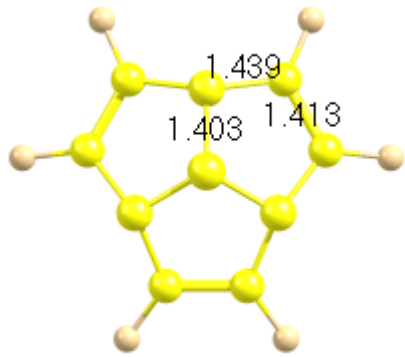
II (Neutral) CAS(10/10)/cc-pVDZ

C	6.0	0.9672674644	-0.0000232400	0.0000000000
C	6.0	0.5483932847	-1.3530364114	0.0000000000
C	6.0	0.5484136403	0.6765028097	-1.1717519575
C	6.0	0.5484136403	0.6765028097	1.1717519575
C	6.0	0.0233435534	-1.5681225778	-1.3519543030
C	6.0	0.0233435534	-1.5681225778	1.3519543030
C	6.0	0.0233747340	-0.3867333794	-2.0339829544
C	6.0	0.0233747340	-0.3867333794	2.0339829544
C	6.0	0.0234083521	1.9548193246	-0.6821147836
C	6.0	0.0234083521	1.9548193246	0.6821147836
F	9.0	-0.3583488221	-2.7283566141	-1.8300660853
F	9.0	-0.3583488221	-2.7283566141	1.8300660853
F	9.0	-0.3583414747	-0.2206678731	-3.2778301201
F	9.0	-0.3583414747	-0.2206678731	3.2778301201
F	9.0	-0.3583213575	2.9490406361	-1.4478230333
F	9.0	-0.3583213575	2.9490406361	1.4478230333



C_{3v}
Min T_1 -975.23641a.u.
S_0/S_1: -975.23073a.u .
$S_2/2^1A'$: -975.17895a.u .
SOC $T_1/1^1A''$ 0.80cm-1
MP2 T_1 -977.52947a.u.
MP2 S_0/S_1: -977.52251a.u .

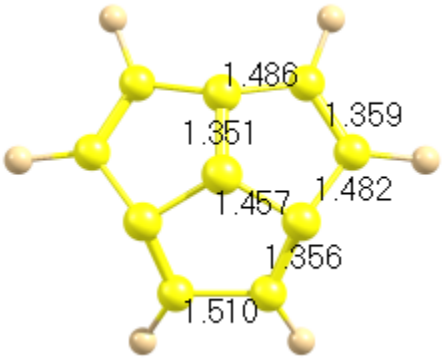
C	6.0	0.7984707194	0.0000044715	0.0000000000
C	6.0	0.4547491405	-1.3598915685	0.0000000000
C	6.0	0.4548378641	0.6799576188	-1.1776928256
C	6.0	0.4548378641	0.6799576188	1.1776928256
C	6.0	0.0364225958	-1.5990025867	-1.3560420040
C	6.0	0.0364225958	-1.5990025867	1.3560420040
C	6.0	0.0364886306	-0.3748860103	-2.0627507285
C	6.0	0.0364886306	-0.3748860103	2.0627507285
C	6.0	0.0364452545	1.9738471027	-0.7067329363
C	6.0	0.0364452545	1.9738471027	0.7067329363
F	9.0	-0.2964995550	-2.7473685295	-1.8875997889
F	9.0	-0.2964995550	-2.7473685295	1.8875997889
F	9.0	-0.2964707440	-0.2610366245	-3.3231328995
F	9.0	-0.2964707440	-0.2610366245	3.3231328995
F	9.0	-0.2964749759	3.0083850787	-1.4355043491
F	9.0	-0.2964749759	3.0083850787	1.4355043491



C_{3v}
Min $S_2/2^1A'$ -975.18866 a.u.
S_0/S_1: -975.23094a.u
T_1: -975.22634a.u
MP2
$S_2/2^1A'$ -977.52086 a.u.
S_0/S_1: -977.53010 a.u
T_1: -977.53173 a.u

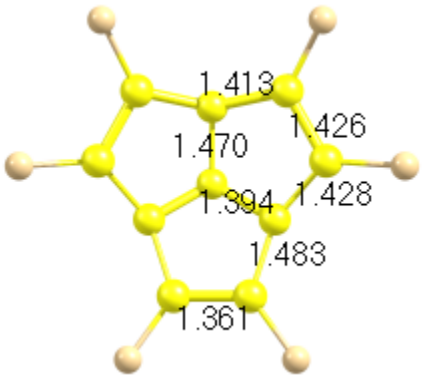
II (Neutral) CAS(10/10)/cc-pVDZ

C	6.0	0.8440545256	-0.0140794178	0.0000000000
C	6.0	0.3856458954	-1.2853506684	0.0000000000
C	6.0	0.5156841706	0.7073246350	-1.2224741422
C	6.0	0.5156841706	0.7073246350	1.2224741422
C	6.0	-0.0406171416	-1.5281234308	-1.4028472918
C	6.0	-0.0406171416	-1.5281234308	1.4028472918
C	6.0	0.0738345025	-0.3819614383	-2.1249133329
C	6.0	0.0738345025	-0.3819614383	2.1249133329
C	6.0	0.1122145321	1.9144994748	-0.7549707467
C	6.0	0.1122145321	1.9144994748	0.7549707467
F	9.0	-0.3845151448	-2.7018680138	-1.8821368270
F	9.0	-0.3845151448	-2.7018680138	1.8821368270
F	9.0	-0.1293434638	-0.2605078754	-3.4155050005
F	9.0	-0.1293434638	-0.2605078754	3.4155050005
F	9.0	-0.4607486654	2.9003041914	-1.3928528398
F	9.0	-0.4607486654	2.9003041914	1.3928528398



C_S
Min S_0 /1^1A'
-975.26662a.u
MP2 -977.54843a.u

C	6.0	0.8212836142	0.0186427565	0.0000000000
C	6.0	0.4857988830	-1.4122188873	0.0000000000
C	6.0	0.4569662928	0.6829663894	-1.1705267213
C	6.0	0.4569662928	0.6829663894	1.1705267213
C	6.0	0.0911246913	-1.6304128023	-1.3389429051
C	6.0	0.0911246913	-1.6304128023	1.3389429051
C	6.0	0.0371623274	-0.3815100990	-2.0245944303
C	6.0	0.0371623274	-0.3815100990	2.0245944303
C	6.0	0.0102119068	2.0096723502	-0.6802629252
C	6.0	0.0102119068	2.0096723502	0.6802629252
F	9.0	-0.2886877167	-2.7599067553	-1.8861718010
F	9.0	-0.2886877167	-2.7599067553	1.8861718010
F	9.0	-0.4104859521	-0.2687570283	-3.2488616786
F	9.0	-0.4104859521	-0.2687570283	3.2488616786
F	9.0	-0.2484737980	3.0446885105	-1.4463529692
F	9.0	-0.2484737980	3.0446885105	1.4463529692

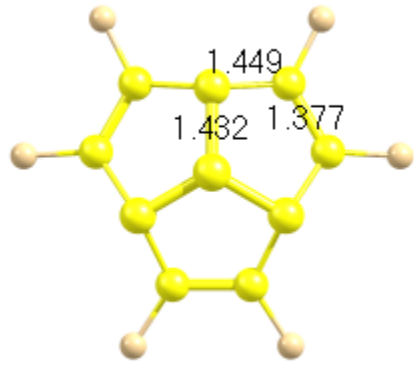


C_S
TS S_0 /1^1A"
-975.24566 a.u
MP2 -977.53810a.u

Electronic Supplementary Material (ESI)
for Physical Chemistry Chemical Physics

II^{-2} (Dianion)
CAS(12/10)/cc-pVDZ

C	6.0	0.7882320095	-0.0000134620	0.0000000000
C	6.0	0.4908908203	-1.4011553261	0.0000000000
C	6.0	0.4909216053	0.7005617648	-1.2134110477
C	6.0	0.4909216053	0.7005617648	1.2134110477
C	6.0	-0.0291176406	-1.5694591735	-1.3416079045
C	6.0	-0.0291176406	-1.5694591735	1.3416079045
C	6.0	-0.0291014221	-0.3771638077	-2.0299853841
C	6.0	-0.0291014221	-0.3771638077	2.0299853841
C	6.0	-0.0291104664	1.9465907658	-0.6883658015
C	6.0	-0.0291104664	1.9465907658	0.6883658015
F	9.0	-0.2472913958	-2.7703667269	-1.9675880720
F	9.0	-0.2472913958	-2.7703667269	1.9675880720
F	9.0	-0.2472749334	-0.3187582028	-3.3830142523
F	9.0	-0.2472749334	-0.3187582028	3.3830142523
F	9.0	-0.2472281618	3.0891322741	-1.4154289133
F	9.0	-0.2472281618	3.0891322741	1.4154289133



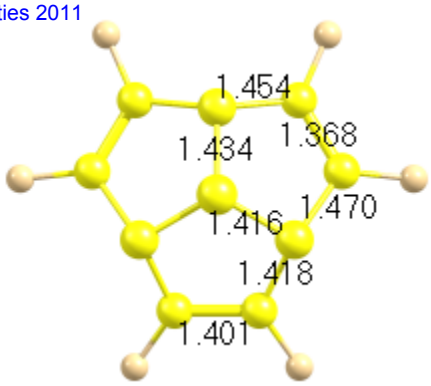
Dianion C_{3V}

Min S_0	**-975.17752a.u.**
MP2	-977.52581a.u
D_0/D_1:	-975.28260a.u .
MP2 D_0/D_1	-977.61891a.u .
Neutral	
S_0/S_1:	-975.20066a.u
S_2:	-975.15204a.u
T_1:	-975.20218a.u
MP2	
S_0/S_1:	-977.51137 a.u
T_1:	-977.51275 a.u

Electronic Supplementary Material (ESI)
for Physical Chemistry Chemical Physics

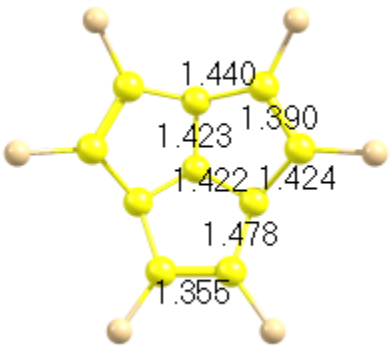
II^{-1} (AnionRadical)
CAS(11/10)/cc-pVDZ

C	6.0	0.8812471448	0.0150507565	0.0000000000
C	6.0	0.4339586383	-1.3473861923	0.0000000000
C	6.0	0.5500961915	0.7040972703	-1.1915680332
C	6.0	0.5500961915	0.7040972703	1.1915680332
C	6.0	-0.0331385539	-1.5568915788	-1.3604904470
C	6.0	-0.0331385539	-1.5568915788	1.3604904470
C	6.0	0.0487436662	-0.3787444222	-2.0507866632
C	6.0	0.0487436662	-0.3787444222	2.0507866632
C	6.0	0.0104714196	1.9201259753	-0.7005347393
C	6.0	0.0104714196	1.9201259753	0.7005347393
F	9.0	-0.3377440581	-2.7418535034	-1.9053166372
F	9.0	-0.3377440581	-2.7418535034	1.9053166372
F	9.0	-0.2308998832	-0.2648332035	-3.3486343148
F	9.0	-0.2308998832	-0.2648332035	3.3486343148
F	9.0	-0.3637726733	2.9842196795	-1.4285149458
F	9.0	-0.3637726733	2.9842196795	1.4285149458



AnionRadical C_S
$S_0/1^1A'$
-975.29741a.u.

C	6.0	0.8885116563	-0.0062144056	0.0000000000
C	6.0	0.6227034854	-1.4046379980	0.0000000000
C	6.0	0.4633808947	0.6701176860	-1.1758698205
C	6.0	0.4633808947	0.6701176860	1.1758698205
C	6.0	0.0570182764	-1.5869917165	-1.3121151189
C	6.0	0.0570182764	-1.5869917165	1.3121151189
C	6.0	-0.0372682137	-0.3806488058	-1.9967906521
C	6.0	-0.0372682137	-0.3806488058	1.9967906521
C	6.0	0.0049642327	1.9837039401	-0.6776129726
C	6.0	0.0049642327	1.9837039401	0.6776129726
F	9.0	-0.2760704560	-2.7556592271	-1.8694642023
F	9.0	-0.2760704560	-2.7556592271	1.8694642023
F	9.0	-0.4265549632	-0.2755637125	-3.2774376248
F	9.0	-0.4265549632	-0.2755637125	3.2774376248
F	9.0	-0.2397183420	3.0504205369	-1.4412847423
F	9.0	-0.2397183420	3.0504205369	1.4412847423



AnionRadical C_S
$S_0/1^1A''$
-975.29801a.u.