

# Calculation of absorption and emission spectra of [*n*]cycloparaphenylenes: the reason for the large Stokes shift

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(Dated: December 22, 2009)

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Table I: The excitation energies (EE in eV), wave length ( $\lambda$  in nm), and the oscillator strengths for a few strong bands of [6]CP calculated at the B3LYP/def2-TZVP level using the BP86/def2-TZVP optimised structures of the ground state and the first excited state. The excitation energy of the first excited state and the ionisation potential (IP in eV) obtained from Koopmans' theorem are also given. The order of the excited state is given within parenthesis.

State	Ground state			Excited state			
	EE	$\lambda$	Osc.	State	EE	$\lambda$	Osc.
$1^1A_{2g}(1)$	2.284	542	0.000	$1^1A_{2g}(1)$	1.207	1028	0.000
$2^1E_u(4)$	3.619	343	1.657	$2^1E_{1u}(4)$	3.145	394	2.198
$3^1E_u(5)$	3.850	322	0.142	$1^1A_{2u}(11)$	4.046	306	0.030
$4^1E_u(10)$	4.310	288	0.037				
$5^1E_u(14)$	4.630	268	0.022				
$2^1A_{2u}(16)$	4.789	259	0.076				
$6^1E_u(21)$	5.082	244	0.017				
IP <sup>a</sup>	5.107				4.554		

<sup>a</sup> The ionisation potential is calculated using Koopmans' theorem. Excited states above the DFT ionisation limit are unbound. Their energies are completely dependent on the size of the employed basis sets.

Table II: The excitation energies (EE in eV), wave length ( $\lambda$  in nm), and the oscillator strengths for a few strong bands of [6]CP calculated at the BP86/def2-TZVP level using the optimised structures of the ground state and the first excited state. The excitation energy of the first excited state and the ionisation potential (IP in eV) obtained from Koopmans' theorem are also given. The order of the excited state is given within parenthesis.

State	Ground state			Excited state			
	EE	$\lambda$	Osc.	State	EE	$\lambda$	Osc.
$1^1A_{2g}(1)$	1.905	650	0.000	$1^1A_{2g}(1)$	0.988	1255	0.000
$2^1E_u(4)$	3.232	384	0.458	$2^1E_{1u}(5)$	2.982	416	2.062
$3^1E_u(5)$	3.378	367	1.063	$1^1A_{2u}(12)$	3.455	359	0.018
$4^1E_u(8)$	3.594	345	0.057	$2^1A_{2u}(16)$	3.983	311	0.018
$5^1E_u(14)$	3.910	317	0.042				
$2^1A_{2u}(16)$	3.980	312	0.018				
$4^1A_{2u}(33)$	4.684	265	0.025				
IP <sup>a</sup>	4.767				4.299		

<sup>a</sup> See footnote *a* of Table I.

Table III: The excitation energies (EE in eV), wave length ( $\lambda$  in nm), and the oscillator strengths for a few strong bands of [7]CP calculated at the BP86/def2-TZVP level using the optimised structures of the ground state and the first excited state. The excitation energy of the first excited state and the ionisation potential (IP in eV) obtained from Koopmans' theorem are also given. The order of the excited state is given within parenthesis.

State	Ground state			Excited state			
	EE	$\lambda$	Osc.	State	EE	$\lambda$	Osc.
$1^1B(1)$	1.949	636	0.004	$1^1B(1)$	1.183	1048	0.000
$3^1B(4)$	3.073	403	0.292	$4^1B(6)$	2.841	436	1.293
$2^1B(5)$	3.141	395	0.526	$3^1A(7)$	2.842	436	1.297
$4^1B(6)$	3.146	394	0.602	$12^1B(22)$	3.499	354	0.017
$3^1B(7)$	3.198	388	0.364	$17^1B(32)$	4.003	309	0.011
$4^1B(8)$	3.271	379	0.023				
$5^1B(9)$	3.341	371	0.083				
$5^1B(10)$	3.374	367	0.028				
$7^1B(13)$	3.467	358	0.013				
IP <sup>a</sup>	4.811				4.429		

<sup>a</sup> See footnote *a* of Table I.

Table IV: The excitation energies (EE in eV), wave length ( $\lambda$  in nm), and the oscillator strengths for a few strong bands of [8]CP calculated at the BP86/def2-TZVP level using the optimised structures of the ground state and the first excited state. The excitation energy of the first excited state and the ionisation potential (IP in eV) obtained from Koopmans' theorem are also given. The order of the excited state is given within parenthesis.

State	Ground state			Excited state			
	EE	$\lambda$	Osc.	State	EE	$\lambda$	Osc.
$1^1A_2(1)$	2.143	579	0.000	$1^1A_2(1)$	1.396	888	0.000
$2^1E_1(3)$	3.063	405	2.001	$2^1E_1(3)$	2.733	454	2.917
$3^1E_1(8)$	3.382	367	0.029	$1^1B_2(16)$	3.558	348	0.015
$4^1E_1(12)$	3.648	340	0.012	$8^1E_1(28)$	3.990	311	0.388
$5^1E_1(15)$	3.788	327	0.013	$9^1E_1(30)$	4.046	306	0.122
$2^1B_2(21)$	3.964	313	0.010	$3^1B_2(38)$	4.265	291	0.029
$6^1E_1(23)$	4.003	310	0.024				
$7^1E_1(24)$	4.076	304	0.284				
$8^1E_1(28)$	4.144	299	0.042				
$9^1E_1(36)$	4.299	288	0.671				
IP <sup>a</sup>	4.924				4.553		

<sup>a</sup> See footnote *a* of Table I.

Table V: The excitation energies (EE in eV), wave length ( $\lambda$  in nm), and the oscillator strengths for a few strong bands of [9]CP calculated at the BP86/def2-TZVP level using the optimised structures of the ground state and the first excited state. The excitation energy of the first excited state and the ionisation potential (IP in eV) obtained from Koopmans' theorem are also given. The order of the excited state is given within parenthesis.

State	Ground state			Excited state			
	EE	$\lambda$	Osc.	State	EE	$\lambda$	Osc.
$1^1B(1)$	2.150	577	0.005	$1^1A$	1.502	825	0.000
$3^1B(4)$	2.917	425	1.080	$4^1A$	2.612	475	1.575
$2^1B(5)$	2.933	423	0.932	$5^1A$	2.618	474	1.394
$3^1B(6)$	2.965	418	0.020	$6^1A$	2.624	473	0.173
$4^1B(7)$	3.027	410	0.060	$7^1A$	2.712	457	0.027
$4^1B(8)$	3.100	400	0.109	$34^1A$	3.582	346	0.014
$5^1B(9)$	3.122	397	0.026	$35^1A$	3.651	340	0.011
$11^1B(22)$	3.694	336	0.011	$37^1A$	3.684	337	0.096
$16^1B(31)$	3.781	328	0.020	$38^1A$	3.694	336	0.112
$16^1B(32)$	3.798	326	0.011	$40^1A$	3.722	333	0.033
$18^1B(34)$	3.816	325	0.015				
$19^1B(35)$	3.830	324	0.015				
$20^1B(38)$	3.854	322	0.147				
$19^1B(39)$	3.876	320	0.161				
IP <sup>a</sup>	4.939				4.629		

<sup>a</sup> See footnote *a* of Table I.

Table VI: The excitation energies (EE in eV), wave length ( $\lambda$  in nm), and the oscillator strengths for a few strong bands of [10]CP calculated at the BP86/def2-TZVP level using the optimised structures of the ground state and the first excited state. The excitation energy of the first excited state and the ionisation potential (IP in eV) obtained from Koopmans' theorem are also given. The order of the excited state is given within parenthesis.

State	Ground state			Excited state			
	EE	$\lambda$	Osc.	State	EE	$\lambda$	Osc.
$1^1A''(1)$	2.183	568	0.009	$1^1A$	1.598	776	0.001
$3^1A''(4)$	2.823	439	1.017	$4^1A$	2.514	493	0.043
$2^1A'(5)$	2.847	435	1.108	$5^1A$	2.516	493	1.547
$4^1A''(7)$	2.957	419	0.142	$6^1A$	2.526	491	1.600
$5^1A''(9)$	2.987	415	0.038	$7^1A$	2.601	477	0.099
$9^1A'(18)$	3.545	350	0.012	$9^1A$	2.651	468	0.019
$10^1A'(19)$	3.590	345	0.012	$27^1A$	3.418	363	0.015
$11^1A''(21)$	3.609	344	0.016	$28^1A$	3.460	358	0.022
$14^1A'(26)$	3.653	339	0.038	$29^1A$	3.469	358	0.079
$13^1A''(27)$	3.660	339	0.013	$30^1A$	3.478	356	0.053
$15^1A'(28)$	3.673	338	0.110	$31^1A$	3.489	355	0.014
$14^1A''(29)$	3.691	336	0.036	$32^1A$	3.508	353	0.321
$15^1A''(31)$	3.711	334	0.091	$33^1A$	3.515	353	0.554
$16^1A''(32)$	3.718	333	0.049	$34^1A$	3.522	352	0.012
$17^1A'(33)$	3.736	332	0.011	$35^1A$	3.529	351	0.144
$17^1A''(34)$	3.744	331	0.055	$36^1A$	3.545	350	0.092
$18^1A'(35)$	3.748	331	0.228	$37^1A$	3.555	349	0.027
$18^1A''(36)$	3.760	330	0.264				
$19^1A''(37)$	3.769	329	0.217				
IP <sup>a</sup>	4.963				4.689		

<sup>a</sup> See footnote *a* of Table I.



Table VII: The excitation energies (EE in eV), wave length ( $\lambda$  in nm), and the oscillator strengths for a few strong bands of [11]CP calculated at the BP86/def2-TZVP level using the optimised structures of the ground state and the first excited state. The excitation energy of the first excited state and the ionisation potential (IP in eV) obtained from Koopmans' theorem are also given. The order of the excited state is given within parenthesis.

State	Ground state			Excited state			
	EE	$\lambda$	Osc.	State	EE	$\lambda$	Osc.
$1^1A$	2.200	564	0.001	$1^1A$	1.670	742	0.000
$4^1A$	2.746	452	1.160	$5^1A$	2.441	508	1.690
$5^1A$	2.770	448	0.780	$6^1A$	2.450	506	1.615
$6^1A$	2.775	447	0.271	$7^1A$	2.497	497	0.039
$7^1A$	2.821	440	0.144	$9^1A$	2.566	483	0.018
$8^1A$	2.877	431	0.039	$20^1A$	3.300	376	0.062
$9^1A$	2.919	425	0.032	$21^1A$	3.303	375	0.037
$20^1A$	3.504	354	0.053	$22^1A$	3.321	373	0.166
$21^1A$	3.518	352	0.028	$23^1A$	3.325	373	0.013
$22^1A$	3.543	350	0.137	$24^1A$	3.328	373	0.605
$23^1A$	3.553	349	0.428	$25^1A$	3.337	372	0.607
$24^1A$	3.575	347	0.353	$26^1A$	3.347	370	0.063
$25^1A$	3.582	346	0.084	$28^1A$	3.358	369	0.049
$26^1A$	3.596	345	0.232	$29^1A$	3.370	368	0.045
$27^1A$	3.602	344	0.076	$30^1A$	3.377	367	0.143
$29^1A$	3.624	342	0.094	$32^1A$	3.395	365	0.010
$30^1A$	3.630	342	0.130	$33^1A$	3.399	365	0.017
$31^1A$	3.639	341	0.024				
$32^1A$	3.643	340	0.181				
$33^1A$	3.657	339	0.204				
IP <sup>a</sup>	4.981				4.733		

<sup>a</sup> See footnote *a* of Table I.

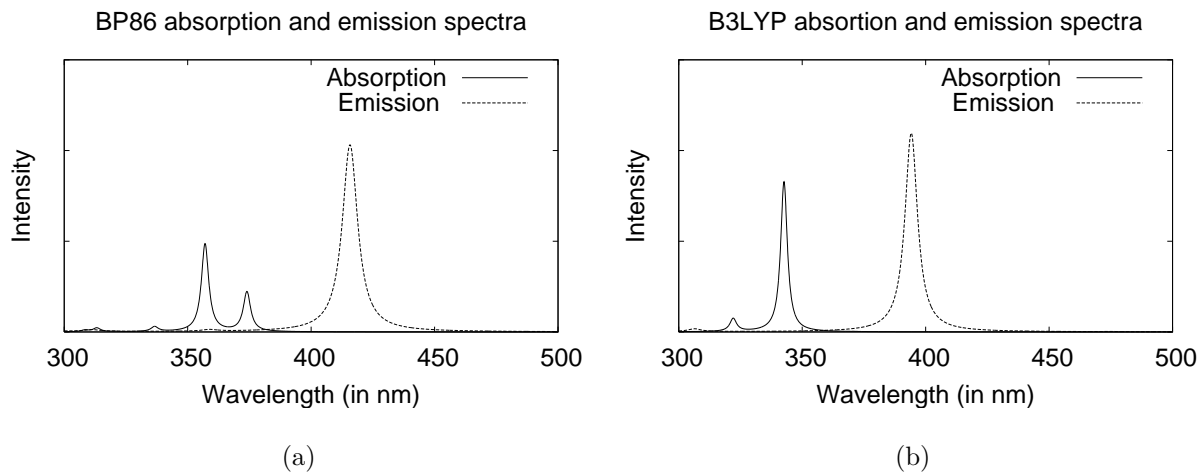


Figure 1: The calculated absorption and emission spectra for [6]CP at the (a) BP86/def2-TZVP level, (b) B3LYP/def2-TZVP level.

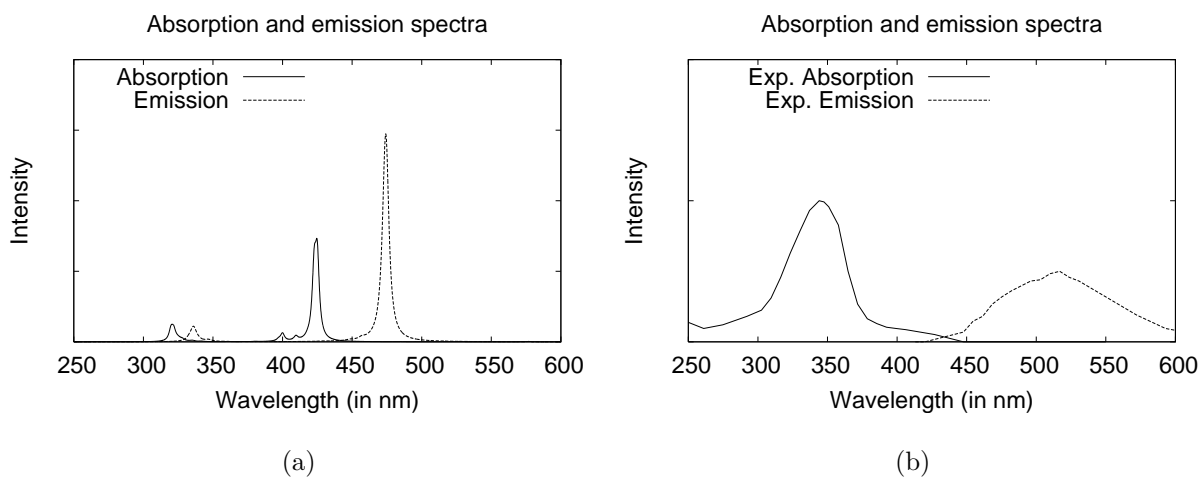


Figure 2: The absorption and emission spectra for [9]CP. (a) Calculated at the BP86/def2-TZVP level, (b) experimental spectrum from R. Jasti, J. Bhattacharjee, J. B. Neaton, and C. R. Bertozzi, *J. Am. Chem. Soc.*, 2008, **130**, 17646-17647.

## I. MOLECULAR STRUCTURES

The molecular structures of the ground and first excited states of [n]CP, n=6,11 optimised at the BP86/def2-TZVP level.

### A. [6]CP ground state

\$coord

-6.57803336983808	5.31805294917168	1.98040404573968	c
-7.89458563757248	3.03771753063567	1.98040404573968	c
-7.80166148280344	1.39662607707279	-0.12390652569301	c
-6.87443064573004	2.45158269244514	-2.38853305346435	c
-5.56034821400076	4.72764022953395	-2.38853305346435	c
-5.11034440373463	6.05812399729797	-0.12390652569301	c
-6.51293023964979	6.42655124780123	3.71909337666655	h
-8.82202175914333	2.42708741671198	3.71909337666655	h
-6.85348354899302	1.31467330480515	-4.10724233868683	h
-4.56528225413495	5.27795420544410	-4.10724233868683	h
-7.80166148280344	-1.39662607707279	0.12390652569301	c
-6.87443064573004	-2.45158269244514	2.38853305346435	c
-7.89458563757248	-3.03771753063567	-1.98040404573968	c
-5.56034821400076	-4.72764022953395	2.38853305346435	c
-6.85348354899302	-1.31467330480515	4.10724233868683	h
-6.57803336983808	-5.31805294917168	-1.98040404573968	c
-8.82202175914333	-2.42708741671198	-3.71909337666655	h
-5.11034440373463	-6.05812399729797	0.12390652569301	c
-4.56528225413495	-5.27795420544410	4.10724233868683	h
-6.51293023964979	-6.42655124780123	-3.71909337666655	h
-2.69131707906887	-7.45475007437079	-0.12390652569301	c
-1.31408243172932	-7.17922292197906	-2.38853305346435	c
-1.31655226773443	-8.35577047980735	1.98040404573968	c
1.31408243172932	-7.17922292197906	-2.38853305346435	c

-2.28820129485805	-6.59262751024916	-4.10724233868683	h
1.31655226773444	-8.35577047980735	1.98040404573968	c
-2.30909151949358	-8.85363866451316	3.71909337666655	h
2.69131707906887	-7.45475007437079	-0.12390652569301	c
2.28820129485806	-6.59262751024916	-4.10724233868683	h
2.30909151949358	-8.85363866451316	3.71909337666655	h
5.11034440373463	-6.05812399729795	0.12390652569301	c
6.57803336983808	-5.31805294917168	-1.98040404573968	c
5.56034821400076	-4.72764022953393	2.38853305346435	c
7.89458563757248	-3.03771753063567	-1.98040404573968	c
6.51293023964979	-6.42655124780123	-3.71909337666655	h
6.87443064573004	-2.45158269244514	2.38853305346435	c
4.56528225413496	-5.27795420544410	4.10724233868683	h
7.80166148280344	-1.39662607707279	0.12390652569301	c
8.82202175914333	-2.42708741671198	-3.71909337666655	h
6.85348354899302	-1.31467330480515	4.10724233868683	h
-2.69131707906887	7.45475007437079	0.12390652569301	c
-1.31408243172932	7.17922292197906	2.38853305346435	c
-1.31655226773443	8.35577047980735	-1.98040404573968	c
1.31408243172932	7.17922292197906	2.38853305346435	c
-2.28820129485805	6.59262751024916	4.10724233868683	h
1.31655226773444	8.35577047980735	-1.98040404573968	c
-2.30909151949358	8.85363866451316	-3.71909337666655	h
2.69131707906887	7.45475007437079	0.12390652569301	c
2.28820129485806	6.59262751024916	4.10724233868683	h
2.30909151949358	8.85363866451316	-3.71909337666655	h
7.80166148280344	1.39662607707279	-0.12390652569301	c
6.87443064573004	2.45158269244514	-2.38853305346435	c
7.89458563757248	3.03771753063567	1.98040404573968	c
5.56034821400076	4.72764022953393	-2.38853305346435	c
6.85348354899302	1.31467330480515	-4.10724233868683	h
6.57803336983808	5.31805294917168	1.98040404573968	c

8.82202175914333	2.42708741671198	3.71909337666655	h
5.11034440373463	6.05812399729795	-0.12390652569301	c
4.56528225413496	5.27795420544410	-4.10724233868683	h
6.51293023964979	6.42655124780123	3.71909337666655	h

\$end

**B. [6]CP excited state**

\$coord

-7.81153166290388	1.30153212824124	2.27525525121400	c
-7.81153166290388	-1.30153212824124	2.27525525121400	c
-7.41472286231141	-2.70432788901029	0.00000000000000	c
-7.81153166290388	-1.30153212824124	-2.27525525121400	c
-7.81153166290388	1.30153212824124	-2.27525525121400	c
-7.41472286231141	2.70432788901029	0.00000000000000	c
-7.88195650105249	2.27894229862786	4.08719272172692	h
-7.88195650105249	-2.27894229862786	4.08719272172692	h
-7.88195650105249	-2.27894229862786	-4.08719272172692	h
-7.88195650105249	2.27894229862786	-4.08719272172692	h
-6.04937808320135	-5.06917441627781	0.00000000000000	c
-5.03292571835047	-6.11421879842065	2.27525525121400	c
-5.03292571835047	-6.11421879842065	-2.27525525121400	c
-2.77860594455340	-7.41575092666187	2.27525525121400	c
-5.91460017489687	-5.68650341212144	4.08719272172692	h
-2.77860594455340	-7.41575092666187	-2.27525525121400	c
-5.91460017489687	-5.68650341212144	-4.08719272172692	h
-1.36534477911006	-7.77350230528809	0.00000000000000	c
-1.96735632615561	-7.96544571074929	4.08719272172692	h
-1.96735632615561	-7.96544571074929	-4.08719272172692	h
1.36534477911007	-7.77350230528809	0.00000000000000	c
2.77860594455340	-7.41575092666187	-2.27525525121400	c
2.77860594455340	-7.41575092666187	2.27525525121400	c

5.03292571835047	-6.11421879842064	-2.27525525121400	c
1.96735632615562	-7.96544571074929	-4.08719272172692	h
5.03292571835047	-6.11421879842064	2.27525525121400	c
1.96735632615562	-7.96544571074929	4.08719272172692	h
6.04937808320135	-5.06917441627780	0.00000000000000	c
5.91460017489687	-5.68650341212144	-4.08719272172692	h
5.91460017489687	-5.68650341212144	4.08719272172692	h
7.41472286231141	-2.70432788901028	0.00000000000000	c
7.81153166290387	-1.30153212824125	-2.27525525121400	c
7.81153166290387	-1.30153212824125	2.27525525121400	c
7.81153166290387	1.30153212824125	-2.27525525121400	c
7.88195650105249	-2.27894229862786	-4.08719272172692	h
7.81153166290387	1.30153212824125	2.27525525121400	c
7.88195650105249	-2.27894229862786	4.08719272172692	h
7.41472286231141	2.70432788901028	0.00000000000000	c
7.88195650105249	2.27894229862786	-4.08719272172692	h
7.88195650105249	2.27894229862786	4.08719272172692	h
-6.04937808320135	5.06917441627781	0.00000000000000	c
-5.03292571835047	6.11421879842065	2.27525525121400	c
-5.03292571835047	6.11421879842065	-2.27525525121400	c
-2.77860594455340	7.41575092666187	2.27525525121400	c
-5.91460017489687	5.68650341212144	4.08719272172692	h
-2.77860594455340	7.41575092666187	-2.27525525121400	c
-5.91460017489687	5.68650341212144	-4.08719272172692	h
-1.36534477911006	7.77350230528809	0.00000000000000	c
-1.96735632615561	7.96544571074929	4.08719272172692	h
-1.96735632615561	7.96544571074929	-4.08719272172692	h
6.04937808320135	5.06917441627780	0.00000000000000	c
5.03292571835047	6.11421879842064	-2.27525525121400	c
5.03292571835047	6.11421879842064	2.27525525121400	c
2.77860594455340	7.41575092666187	-2.27525525121400	c
5.91460017489687	5.68650341212144	-4.08719272172692	h

2.77860594455340	7.41575092666187	2.27525525121400	c
5.91460017489687	5.68650341212144	4.08719272172692	h
1.36534477911007	7.77350230528809	0.00000000000000	c
1.96735632615562	7.96544571074929	-4.08719272172692	h
1.96735632615562	7.96544571074929	4.08719272172692	h

\$end

C. [7]CP ground state

\$coord

9.20682682459690	1.86400946318501	3.48809597513607	c
9.78964715646856	1.89633336303083	0.92219865923740	c
9.18019122620897	-0.16729793580414	-0.65604654668834	c
8.46540093950357	-2.42247464416174	0.56772464434703	c
7.88093181223138	-2.45387840973225	3.13032936240868	c
7.98551518496730	-0.23310555934681	4.59701468669904	c
9.54602974406658	3.56208355410639	4.60928899620821	h
10.57026781074493	3.61925891675820	0.09945627393163	h
8.03857924649141	-4.09601946053386	-0.55696809854635	h
7.01751132008712	-4.15092301189166	3.91914020382704	h
-5.20062014042893	-0.32862072086594	-7.59100671480551	c
-5.86611255620982	-2.52665762172844	-6.23736282201678	c
-6.69048969739074	1.83393032457127	-7.10402955830714	c
-7.50197356330287	-2.43060096941991	-4.18571388947321	c
-4.86547701078541	-4.29220249161932	-6.58540716162301	h
-8.32465039403592	1.93476468114017	-5.04455586588479	c
-6.43879002331015	3.53629364050719	-8.23863307320133	h
-8.56546860682044	-0.12864616420043	-3.37134668840997	c
-7.70074852050807	-4.11332527129878	-3.01233419804611	h
-9.29570919304749	3.70748765237561	-4.63213284471234	h
-9.18019122620897	0.16729793580414	-0.65604654668834	c
-9.78964715646856	-1.89633336303083	0.92219865923740	c

-8.46540093950357	2.42247464416174	0.56772464434703	c
-9.20682682459690	-1.86400946318501	3.48809597513607	c
-10.57026781074493	-3.61925891675820	0.09945627393163	h
-7.88093181223138	2.45387840973225	3.13032936240868	c
-8.03857924649141	4.09601946053386	-0.55696809854635	h
-7.98551518496730	0.23310555934681	4.59701468669904	c
-9.54602974406658	-3.56208355410639	4.60928899620821	h
-7.01751132008712	4.15092301189166	3.91914020382704	h
6.25209546459963	-0.00122828073448	6.78538012556352	c
4.90687571497946	2.27680453551178	7.09362047860847	c
5.34398531614790	-2.10747424951198	8.14806033215055	c
2.53993358882331	2.31713288537983	8.23538254976672	c
5.56549354643373	3.98026692652931	6.13914356376474	h
2.97402284848593	-2.06630574629560	9.29271518105161	c
6.42783194926896	-3.86261589085341	8.16333528817194	h
1.39877558065501	0.08149608409107	9.12658921706413	c
1.43320500662569	4.05273464919709	8.13196595535034	h
2.26517790636822	-3.79023013571013	10.17589114777565	h
-6.25209546459963	0.00122828073448	6.78538012556352	c
-4.90687571497946	-2.27680453551178	7.09362047860847	c
-5.34398531614790	2.10747424951198	8.14806033215055	c
-2.53993358882331	-2.31713288537981	8.23538254976672	c
-5.56549354643373	-3.98026692652931	6.13914356376474	h
-2.97402284848593	2.06630574629560	9.29271518105161	c
-6.42783194926896	3.86261589085341	8.16333528817194	h
-1.39877558065501	-0.08149608409107	9.12658921706413	c
-1.43320500662569	-4.05273464919709	8.13196595535034	h
-2.26517790636822	3.79023013571013	10.17589114777565	h
8.56546860682044	0.12864616420042	-3.37134668840997	c
8.32465039403592	-1.93476468114017	-5.04455586588479	c
7.50197356330287	2.43060096941991	-4.18571388947321	c
6.69048969739074	-1.83393032457127	-7.10402955830714	c



9.29570919304749	-3.70748765237561	-4.63213284471234	h
5.86611255620982	2.52665762172844	-6.23736282201678	c
7.70074852050807	4.11332527129878	-3.01233419804611	h
5.20062014042893	0.32862072086594	-7.59100671480551	c
6.43879002331015	-3.53629364050719	-8.23863307320133	h
4.86547701078541	4.29220249161932	-6.58540716162301	h
-2.69689139488000	-0.18330137199787	-8.84295896461014	c
-1.15943211567936	-2.34073767321000	-9.16125557119600	c
-1.46213852002746	2.16326831042873	-9.13581227690384	c
1.46213852002746	-2.16326831042873	-9.13581227690384	c
-2.00621579006121	-4.21923645847348	-9.19685703910250	h
1.15943211567936	2.34073767321000	-9.16125557119600	c
-2.55040225537088	3.91208648805905	-9.08352435464795	h
2.69689139488000	0.18330137199787	-8.84295896461014	c
2.55040225537088	-3.91208648805905	-9.08352435464795	h
2.00621579006121	4.21923645847348	-9.19685703910250	h

\$end

#### D. [7]CP excited state

\$coord

8.70197228470397	2.27095439195528	3.32624574747858	c
9.27959345085040	2.27147259792063	0.78522902182257	c
9.16257609318466	0.01479207357010	-0.68796940010307	c
9.07398615176265	-2.27147051418396	0.73757769423553	c
8.49491743767346	-2.27142031116243	3.27917199799577	c
7.95833881950327	0.01418826448790	4.60289532400941	c
8.65175953671777	4.07678226059535	4.31714766554304	h
9.65771888687066	4.07757650597040	-0.13002884871798	h
9.23108032820524	-4.08677036702468	-0.22206690861054	h
8.21676225192040	-4.08695596073292	4.21100406092268	h
-5.17850606369458	-0.07065746003302	-7.60606330904366	c

-6.25500887567621	-2.35047162908230	-6.65123932181987	c
-6.38560963282289	2.19272924509255	-6.77279101269685	c
-7.87655906808855	-2.34224299768625	-4.61106898180810	c
-5.62934765520493	-4.16921187265825	-7.38705643092674	h
-8.00645534674241	2.20087226273950	-4.73267816860786	c
-5.88559532983992	3.99867513650647	-7.62767872563736	h
-8.55494173484903	-0.05380924982226	-3.35851704832998	c
-8.45379296118343	-4.15485143567035	-3.82175030192256	h
-8.72751407526083	4.01158005980429	-4.06600124156845	h
-9.16257609318466	-0.01479207357010	-0.68796940010307	c
-9.27959345085040	-2.27147259792063	0.78522902182257	c
-9.07398615176265	2.27147051418396	0.73757769423553	c
-8.70197228470397	-2.27095439195528	3.32624574747858	c
-9.65771888687066	-4.07757650597040	-0.13002884871798	h
-8.49491743767346	2.27142031116243	3.27917199799577	c
-9.23108032820524	4.08677036702468	-0.22206690861054	h
-7.95833881950327	-0.01418826448790	4.60289532400941	c
-8.65175953671777	-4.07678226059535	4.31714766554304	h
-8.21676225192040	4.08695596073292	4.21100406092268	h
6.25420021119580	0.05042155925413	6.74625461193145	c
5.06813311338956	2.33226910067686	7.55339843340128	c
5.19422335579229	-2.20793982598626	7.77222447588202	c
2.72120102649512	2.32148838222907	8.68760480324785	c
5.89901910901037	4.15112228594798	7.06070631171970	h
2.84843587572624	-2.21858631175280	8.90653819427675	c
6.16146650265169	-4.00809178733916	7.51161644729230	h
1.36910105978325	0.02805964526595	9.10737365731685	c
1.80505775410520	4.13232047873189	9.03820145449814	h
2.05643506076438	-4.02594834546801	9.49764293496675	h
-6.25420021119580	-0.05042155925413	6.74625461193145	c
-5.06813311338956	-2.33226910067686	7.55339843340128	c
-5.19422335579229	2.20793982598626	7.77222447588202	c

-2.72120102649512	-2.32148838222907	8.68760480324785	c
-5.89901910901037	-4.15112228594798	7.06070631171970	h
-2.84843587572624	2.21858631175280	8.90653819427675	c
-6.16146650265169	4.00809178733916	7.51161644729230	h
-1.36910105978325	-0.02805964526595	9.10737365731685	c
-1.80505775410520	-4.13232047873189	9.03820145449814	h
-2.05643506076438	4.02594834546801	9.49764293496675	h
8.55494173484903	0.05380924982226	-3.35851704832998	c
8.00645534674241	-2.20087226273950	-4.73267816860786	c
7.87655906808855	2.34224299768625	-4.61106898180810	c
6.38560963282289	-2.19272924509255	-6.77279101269685	c
8.72751407526083	-4.01158005980429	-4.06600124156845	h
6.25500887567621	2.35047162908230	-6.65123932181987	c
8.45379296118343	4.15485143567035	-3.82175030192256	h
5.17850606369458	0.07065746003302	-7.60606330904366	c
5.88559532983992	-3.99867513650647	-7.62767872563736	h
5.62934765520493	4.16921187265825	-7.38705643092674	h
-2.71284727633441	-0.03941644569436	-8.79850449049866	c
-1.26958260592342	-2.29191409426928	-9.13842137113165	c
-1.33615848592767	2.25403486124001	-9.13870936763152	c
1.33615848592767	-2.25403486124001	-9.13870936763152	c
-2.21642480678664	-4.12010508288279	-9.20060466460297	h
1.26958260592342	2.29191409426928	-9.13842137113165	c
-2.33506574213584	4.05452944476415	-9.18967783876252	h
2.71284727633441	0.03941644569436	-8.79850449049866	c
2.33506574213584	-4.05452944476415	-9.18967783876252	h
2.21642480678664	4.12010508288279	-9.20060466460297	h

\$end

### E. [8]CP ground state

\$coord

-9.66426319750793	5.42724461628590	2.01995446924215	c
-10.67130751346339	2.99602457079550	2.01995446924215	c
-10.41558586638854	1.39642390926991	-0.09824310318391	c
-9.52220896715663	2.52174455835546	-2.33983804111907	c
-8.51636121018523	4.95007585491837	-2.33983804111907	c
-8.35235221180988	6.37751058049834	-0.09824310318391	c
-9.77084852869434	6.55246774355065	3.74509463860763	h
-11.54232762755714	2.27573887761560	3.74509463860763	h
-9.33437513452720	1.37812642137858	-4.04429980636908	h
-7.57488249365243	5.62591741787412	-4.04429980636908	h
-10.41558586638854	-1.39642390926991	0.09824310318391	c
-9.52220896715663	-2.52174455835546	2.33983804111907	c
-10.67130751346339	-2.99602457079550	-2.01995446924215	c
-8.51636121018523	-4.95007585491837	2.33983804111907	c
-9.33437513452720	-1.37812642137858	4.04429980636908	h
-9.66426319750793	-5.42724461628590	-2.01995446924215	c
-11.54232762755714	-2.27573887761560	-3.74509463860763	h
-8.35235221180988	-6.37751058049834	0.09824310318391	c
-7.57488249365243	-5.62591741787412	4.04429980636908	h
-9.77084852869434	-6.55246774355065	-3.74509463860763	h
-6.37751058049833	-8.35235221180988	-0.09824310318391	c
-4.95007585491837	-8.51636121018524	-2.33983804111907	c
-5.42724461628590	-9.66426319750793	2.01995446924215	c
-2.52174455835546	-9.52220896715663	-2.33983804111907	c
-5.62591741787412	-7.57488249365243	-4.04429980636908	h
-2.99602457079550	-10.67130751346339	2.01995446924215	c
-6.55246774355065	-9.77084852869434	3.74509463860763	h
-1.39642390926991	-10.41558586638854	-0.09824310318391	c
-1.37812642137858	-9.33437513452720	-4.04429980636908	h
-2.27573887761559	-11.54232762755714	3.74509463860763	h
-6.37751058049833	8.35235221180988	0.09824310318391	c
-4.95007585491837	8.51636121018524	2.33983804111907	c

-5.42724461628590	9.66426319750793	-2.01995446924215	c
-2.52174455835546	9.52220896715663	2.33983804111907	c
-5.62591741787412	7.57488249365243	4.04429980636908	h
-2.99602457079550	10.67130751346339	-2.01995446924215	c
-6.55246774355065	9.77084852869434	-3.74509463860763	h
-1.39642390926991	10.41558586638854	0.09824310318391	c
-1.37812642137858	9.33437513452720	4.04429980636908	h
-2.27573887761559	11.54232762755714	-3.74509463860763	h
6.37751058049834	8.35235221180988	-0.09824310318391	c
4.95007585491837	8.51636121018524	-2.33983804111907	c
5.42724461628590	9.66426319750793	2.01995446924215	c
2.52174455835546	9.52220896715663	-2.33983804111907	c
5.62591741787412	7.57488249365243	-4.04429980636908	h
2.99602457079550	10.67130751346339	2.01995446924215	c
6.55246774355065	9.77084852869433	3.74509463860763	h
1.39642390926991	10.41558586638854	-0.09824310318391	c
1.37812642137859	9.33437513452720	-4.04429980636908	h
2.27573887761560	11.54232762755714	3.74509463860763	h
8.35235221180988	6.37751058049834	0.09824310318391	c
9.66426319750793	5.42724461628590	-2.01995446924215	c
8.51636121018524	4.95007585491837	2.33983804111907	c
10.67130751346339	2.99602457079550	-2.01995446924215	c
9.77084852869434	6.55246774355065	-3.74509463860763	h
9.52220896715663	2.52174455835546	2.33983804111907	c
7.57488249365243	5.62591741787412	4.04429980636908	h
10.41558586638854	1.39642390926991	0.09824310318391	c
11.54232762755714	2.27573887761560	-3.74509463860763	h
9.33437513452720	1.37812642137858	4.04429980636908	h
1.39642390926991	-10.41558586638854	0.09824310318391	c
2.99602457079550	-10.67130751346339	-2.01995446924215	c
2.52174455835546	-9.52220896715663	2.33983804111907	c
5.42724461628590	-9.66426319750793	-2.01995446924215	c

2.27573887761560	-11.54232762755714	-3.74509463860763	h
4.95007585491837	-8.51636121018524	2.33983804111907	c
1.37812642137859	-9.33437513452720	4.04429980636908	h
6.37751058049834	-8.35235221180988	0.09824310318391	c
6.55246774355065	-9.77084852869433	-3.74509463860763	h
5.62591741787412	-7.57488249365243	4.04429980636908	h
8.35235221180988	-6.37751058049834	-0.09824310318391	c
8.51636121018524	-4.95007585491837	-2.33983804111907	c
9.66426319750793	-5.42724461628590	2.01995446924215	c
9.52220896715663	-2.52174455835546	-2.33983804111907	c
7.57488249365243	-5.62591741787412	-4.04429980636908	h
10.67130751346339	-2.99602457079550	2.01995446924215	c
9.77084852869434	-6.55246774355065	3.74509463860763	h
10.41558586638854	-1.39642390926991	-0.09824310318391	c
9.33437513452720	-1.37812642137858	-4.04429980636908	h
11.54232762755714	-2.27573887761560	3.74509463860763	h

\$end

#### F. [8]CP excited state

\$coord

-9.37689515598826	5.29571104195904	2.18520944500475	c
-10.37509934024828	2.88583296230088	2.18520944500475	c
-10.40793556718229	1.37247170434156	-0.04198509126882	c
-9.88673752725537	2.68268829629610	-2.33201542828291	c
-8.88792623545454	5.09403206321304	-2.33201542828291	c
-8.33000586683381	6.38903776858070	-0.04198509126882	c
-9.28589631444338	6.32178206346360	3.96983214121699	h
-11.03629521959665	2.09594528707949	3.96983214121699	h
-10.02881439088962	1.69166891374644	-4.13195731691172	h
-8.28763322349189	5.89525210262670	-4.13195731691172	h
-10.40793556718229	-1.37247170434156	0.04198509126882	c

-9.88673752725537	-2.68268829629610	2.33201542828291	c
-10.37509934024828	-2.88583296230088	-2.18520944500475	c
-8.88792623545454	-5.09403206321304	2.33201542828291	c
-10.02881439088962	-1.69166891374644	4.13195731691172	h
-9.37689515598826	-5.29571104195904	-2.18520944500475	c
-11.03629521959665	-2.09594528707949	-3.96983214121699	h
-8.33000586683381	-6.38903776858070	0.04198509126882	c
-8.28763322349189	-5.89525210262670	4.13195731691172	h
-9.28589631444338	-6.32178206346360	-3.96983214121699	h
-6.38903776858070	-8.33000586683381	-0.04198509126882	c
-5.09403206321304	-8.88792623545456	-2.33201542828291	c
-5.29571104195904	-9.37689515598826	2.18520944500475	c
-2.68268829629611	-9.88673752725537	-2.33201542828291	c
-5.89525210262670	-8.28763322349189	-4.13195731691172	h
-2.88583296230087	-10.37509934024828	2.18520944500475	c
-6.32178206346360	-9.28589631444338	3.96983214121699	h
-1.37247170434156	-10.40793556718229	-0.04198509126882	c
-1.69166891374645	-10.02881439088962	-4.13195731691172	h
-2.09594528707948	-11.03629521959665	3.96983214121699	h
-6.38903776858070	8.33000586683381	0.04198509126882	c
-5.09403206321304	8.88792623545456	2.33201542828291	c
-5.29571104195904	9.37689515598826	-2.18520944500475	c
-2.68268829629611	9.88673752725537	2.33201542828291	c
-5.89525210262670	8.28763322349189	4.13195731691172	h
-2.88583296230087	10.37509934024828	-2.18520944500475	c
-6.32178206346360	9.28589631444338	-3.96983214121699	h
-1.37247170434156	10.40793556718229	0.04198509126882	c
-1.69166891374645	10.02881439088962	4.13195731691172	h
-2.09594528707948	11.03629521959665	-3.96983214121699	h
6.38903776858070	8.33000586683381	-0.04198509126882	c
5.09403206321304	8.88792623545454	-2.33201542828291	c
5.29571104195904	9.37689515598826	2.18520944500475	c

2.68268829629611	9.88673752725535	-2.33201542828291	c
5.89525210262670	8.28763322349189	-4.13195731691172	h
2.88583296230087	10.37509934024828	2.18520944500475	c
6.32178206346360	9.28589631444338	3.96983214121699	h
1.37247170434157	10.40793556718229	-0.04198509126882	c
1.69166891374645	10.02881439088962	-4.13195731691172	h
2.09594528707948	11.03629521959665	3.96983214121699	h
8.33000586683381	6.38903776858070	0.04198509126882	c
9.37689515598826	5.29571104195904	-2.18520944500475	c
8.88792623545454	5.09403206321304	2.33201542828291	c
10.37509934024828	2.88583296230087	-2.18520944500475	c
9.28589631444338	6.32178206346360	-3.96983214121699	h
9.88673752725537	2.68268829629611	2.33201542828291	c
8.28763322349189	5.89525210262670	4.13195731691172	h
10.40793556718229	1.37247170434157	0.04198509126882	c
11.03629521959665	2.09594528707948	-3.96983214121699	h
10.02881439088962	1.69166891374645	4.13195731691172	h
1.37247170434157	-10.40793556718229	0.04198509126882	c
2.88583296230087	-10.37509934024828	-2.18520944500475	c
2.68268829629611	-9.88673752725535	2.33201542828291	c
5.29571104195904	-9.37689515598826	-2.18520944500475	c
2.09594528707948	-11.03629521959665	-3.96983214121699	h
5.09403206321304	-8.88792623545454	2.33201542828291	c
1.69166891374645	-10.02881439088962	4.13195731691172	h
6.38903776858070	-8.33000586683381	0.04198509126882	c
6.32178206346360	-9.28589631444338	-3.96983214121699	h
5.89525210262670	-8.28763322349189	4.13195731691172	h
8.33000586683381	-6.38903776858070	-0.04198509126882	c
8.88792623545454	-5.09403206321304	-2.33201542828291	c
9.37689515598826	-5.29571104195904	2.18520944500475	c
9.88673752725537	-2.68268829629611	-2.33201542828291	c
8.28763322349189	-5.89525210262670	-4.13195731691172	h



10.37509934024828	-2.88583296230087	2.18520944500475	c
9.28589631444338	-6.32178206346360	3.96983214121699	h
10.40793556718229	-1.37247170434157	-0.04198509126882	c
10.02881439088962	-1.69166891374645	-4.13195731691172	h
11.03629521959665	-2.09594528707948	3.96983214121699	h

\$end

**G. [9]CP ground state**

\$coord

3.02356238649206	-1.96355625300778	-12.04443987674381	c
5.49665192814150	-1.91495145080967	-11.14676438560122	c
6.46082920295828	0.21713683743011	-9.86932225388120	c
4.96257108592507	2.41679919206647	-9.91204012745927	c
2.49326822429013	2.36992616649763	-10.81206136753447	c
1.39406901617311	0.11952235915203	-11.71373524085353	c
2.30515049458660	-3.69299521840279	-12.90924879887227	h
6.66061618301584	-3.60750098707134	-11.33246405711716	h
5.64042581873181	4.12326049457569	-8.97589024783538	h
1.31426609435114	4.04099912961360	-10.55445465939775	h
8.60542581452998	0.06534622144563	-8.07788528734187	c
8.99153395804789	-2.18748287691716	-6.71368483982999	c
9.95468486803651	2.21139594525307	-7.25288951944537	c
10.31288478269362	-2.19880362611775	-4.44224008854009	c
8.01370286604782	-3.90568923451660	-7.29606559414503	h
11.27651242288428	2.20007975930760	-4.97727925289032	c
9.86884056026677	3.95602429594458	-8.34981974203139	h
11.31580618991464	0.04207256595968	-3.41321955241661	c
10.32694828507725	-3.92632815873819	-3.31801140226409	h
12.19413006337946	3.93595461655561	-4.34524991496586	h
11.80745991653414	0.16712372979239	-0.66074636099830	c
11.10859338908087	2.35533516069022	0.68443503102954	c

12.42622150581895	-1.98367682078761	0.78747919863736	c
10.65396409276078	2.28056705821643	3.27286250435605	c
10.64532467475089	4.07676823615550	-0.35062278961888	h
11.96526758536728	-2.06159434477107	3.37626699642530	c
13.16200621276588	-3.66782476740686	-0.14867714107350	h
10.87040122982677	0.01048843387787	4.64551218775617	c
9.84978944866107	3.94436592492592	4.18704081094333	h
12.34599167266308	-3.80520810360034	4.41111159156439	h
-1.39406901617311	-0.11952235915203	-11.71373524085353	c
-2.49326822429013	-2.36992616649763	-10.81206136753447	c
-3.02356238649206	1.96355625300778	-12.04443987674381	c
-4.96257108592507	-2.41679919206647	-9.91204012745927	c
-1.31426609435114	-4.04099912961360	-10.55445465939775	h
-5.49665192814150	1.91495145080968	-11.14676438560122	c
-2.30515049458658	3.69299521840279	-12.90924879887227	h
-6.46082920295828	-0.21713683743011	-9.86932225388120	c
-5.64042581873181	-4.12326049457569	-8.97589024783538	h
-6.66061618301584	3.60750098707134	-11.33246405711716	h
-11.31580618991464	-0.04207256595968	-3.41321955241661	c
-10.31288478269362	2.19880362611775	-4.44224008854009	c
-11.27651242288428	-2.20007975930760	-4.97727925289032	c
-8.99153395804789	2.18748287691716	-6.71368483982999	c
-10.32694828507725	3.92632815873819	-3.31801140226409	h
-9.95468486803651	-2.21139594525307	-7.25288951944537	c
-12.19413006337946	-3.93595461655561	-4.34524991496586	h
-8.60542581452998	-0.06534622144563	-8.07788528734187	c
-8.01370286604782	3.90568923451660	-7.29606559414503	h
-9.86884056026677	-3.95602429594458	-8.34981974203139	h
-11.80745991653414	-0.16712372979239	-0.66074636099830	c
-12.42622150581895	1.98367682078761	0.78747919863736	c
-11.10859338908087	-2.35533516069022	0.68443503102954	c
-11.96526758536728	2.06159434477107	3.37626699642530	c

-13.16200621276588	3.66782476740686	-0.14867714107350	h
-10.65396409276078	-2.28056705821643	3.27286250435605	c
-10.64532467475089	-4.07676823615550	-0.35062278961888	h
-10.87040122982677	-0.01048843387787	4.64551218775617	c
-12.34599167266308	3.80520810360034	4.41111159156439	h
-9.84978944866107	-3.94436592492592	4.18704081094333	h
9.46094991784954	-0.26290892049771	7.04606662300838	c
8.97213888781869	1.77122150156262	8.69579320503575	c
8.07196480172174	-2.49460529973929	7.45983531317104	c
6.95764928580645	1.70229440474054	10.38799191138694	c
10.11634196212496	3.48340136497388	8.57235417681083	h
6.04967393335812	-2.55354939370318	9.13363098261177	c
8.40693714827496	-4.13235837808228	6.25393348795199	h
5.30809237453961	-0.39146122480717	10.50218584191533	c
6.58954219212898	3.36418403351845	11.55068119270278	h
4.87637158299786	-4.24551388493799	9.17491371769549	h
-5.30809237453961	0.39146122480717	10.50218584191533	c
-6.04967393335812	2.55354939370318	9.13363098261177	c
-6.95764928580645	-1.70229440474054	10.38799191138694	c
-8.07196480172174	2.49460529973929	7.45983531317104	c
-4.87637158299786	4.24551388493799	9.17491371769549	h
-8.97213888781869	-1.77122150156262	8.69579320503575	c
-6.58954219212898	-3.36418403351845	11.55068119270278	h
-9.46094991784954	0.26290892049771	7.04606662300838	c
-8.40693714827496	4.13235837808228	6.25393348795199	h
-10.11634196212496	-3.48340136497388	8.57235417681083	h
2.69738898780504	-0.21283354335586	11.50027346910558	c
1.13352085129012	-2.35687296628168	11.75013856414223	c
1.48617515028857	2.15068731711995	11.72659182268008	c
-1.48617515028857	-2.15068731711995	11.72659182268008	c
1.96644006310658	-4.24169520700438	11.78738529114758	h
-1.13352085129012	2.35687296628168	11.75013856414223	c

2.60063198019075	3.88303451844175	11.66781213008362	h
-2.69738898780504	0.21283354335586	11.50027346910558	c
-2.60063198019075	-3.88303451844175	11.66781213008362	h
-1.96644006310658	4.24169520700438	11.78738529114758	h

\$end

## H. [9]CP excited state

\$coord

2.90812575358870	-2.15483807613368	-11.77709161451906	c
5.36212266670777	-2.14013131477236	-10.88574542602548	c
6.47924434854526	0.08353858763481	-9.86623200500402	c
5.11419129059515	2.35960329012435	-10.27513153169020	c
2.65989972492856	2.34536805455329	-11.16942151660049	c
1.37487920231691	0.05366904701898	-11.72391052935529	c
2.11236305691398	-3.93530012673903	-12.44251243411343	h
6.41719368787173	-3.91037491952717	-10.88003736487234	h
5.90939512033473	4.15255278732574	-9.64744951728478	h
1.62859766364748	4.12806839054461	-11.20624880362955	h
8.58758736955771	0.00181825529476	-8.09957303798344	c
9.26468524596695	-2.28642077108648	-6.86843475530129	c
9.75165875482511	2.22634804643072	-7.13623536123570	c
10.57197032144613	-2.29250833766172	-4.60721004370909	c
8.53892176249246	-4.07926035905311	-7.57615483544331	h
11.05792687831241	2.22020950199606	-4.87606133089665	c
9.53364163189525	4.01229013071754	-8.14061744361442	h
11.30500082842788	-0.01093594006684	-3.39574166310145	c
10.81802584005616	-4.09012290234692	-3.63254446181629	h
11.82494615852517	4.00065235887056	-4.17755598052986	h
11.78109767799548	0.05752410547548	-0.68604862466395	c
11.45442849255408	2.32711663977687	0.71179019573829	c
12.10318793700382	-2.17341312134352	0.78034053648705	c

11.00078876238963	2.30077477421467	3.28408131775247	c
11.31148877739433	4.12589459005785	-0.28173652516371	h
11.64869305171222	-2.20011966748256	3.35096722845920	c
12.62361201691262	-3.93900222927576	-0.14583940228124	h
10.83637324957730	0.00243578222264	4.66306128451318	c
10.51856789123887	4.07873016655261	4.20458841950643	h
11.82866582147819	-3.98611892017416	4.36397103714331	h
-1.37487796754287	-0.05367090983837	-11.72391019140733	c
-2.65989848490116	-2.34536963472216	-11.16941995507813	c
-2.90812433626348	2.15483633826584	-11.77709160606636	c
-5.11418987353494	-2.35960442473979	-10.27512933726933	c
-1.62859664998079	-4.12807008632267	-11.20624712317783	h
-5.36212111111018	2.14013008403528	-10.88574497611220	c
-2.11236152563805	3.93529819286497	-12.44251281243779	h
-6.47924284249662	-0.08353943898329	-9.86623058192279	c
-5.90939345177457	-4.15255356437534	-9.64744584837669	h
-6.41719215811648	3.91037374671566	-10.88003761298538	h
-11.30499991755322	0.01093725350554	-3.39574048344924	c
-10.57196821564552	2.29250931196045	-4.60720875707634	c
-11.05792689146916	-2.22020826042855	-4.87606009076935	c
-9.26468277960904	2.28642114589635	-6.86843327419260	c
-10.81802331254834	4.09012397240448	-3.63254339211867	h
-9.75165836635724	-2.22634751929470	-7.13623388961263	c
-11.82494715028650	-4.00065069196992	-4.17755485104670	h
-8.58758588566555	-0.00181827710042	-8.09957149564679	c
-8.53891805134170	4.07926038544464	-7.57615310500011	h
-9.53364191941468	-4.01228972700856	-8.14061591488249	h
-11.78109748036149	-0.05752246014388	-0.68604760110669	c
-12.10318723950087	2.17341486517201	0.78034137052038	c
-11.45442985946829	-2.32711510408346	0.71179129141957	c
-11.64869314008890	2.20012131471551	3.35096825827625	c
-12.62361020727607	3.93900417796706	-0.14583872775097	h

-11.00079100261447	-2.30077351309828	3.28408261191542	c
-11.31149083311055	-4.12589312678695	-0.28173533722915	h
-10.83637483992517	-0.00243452850448	4.66306273353604	c
-11.82866515993140	3.98612080829789	4.36397196178335	h
-10.51857128290359	-4.07872920489636	4.20458991587560	h
9.46324591647697	-0.11762706293207	7.04416135858727	c
8.73200900012611	2.08178987080156	8.40683690014483	c
8.35332057244092	-2.41646116941688	7.87696643137219	c
6.73544146299027	2.05179007193725	10.08860226265072	c
9.69153238001936	3.87077380788744	8.05207141052612	h
6.35286576247910	-2.44505620428587	9.55448262807566	c
8.91936661730101	-4.19604602074927	7.00836657484739	h
5.29986244453720	-0.17787627727448	10.54046485800374	c
6.19188732485419	3.82194507049109	10.99096329406364	h
5.44420135767413	-4.25140519592733	9.94161408772177	h
-5.29986354656123	0.17787554682398	10.54046591596471	c
-6.35286694044267	2.44505581895987	9.55448490719861	c
-6.73544271423614	-2.05179041864845	10.08860305849748	c
-8.35332212812867	2.41646159020640	7.87696914325373	c
-5.44420251002283	4.25140455779020	9.94161693394030	h
-8.73201039928945	-2.08178975644527	8.40683783551044	c
-6.19188892800323	-3.82194552011817	10.99096391022155	h
-9.46324763494641	0.11762771842320	7.04416316752599	c
-8.91936847919545	4.19604688920087	7.00837025443170	h
-9.69153340729900	-3.87077380972053	8.05207133758574	h
2.71861959857817	-0.09867655873517	11.49357554042645	c
1.22157726990348	-2.31664928430872	11.75607412180656	c
1.38719496629906	2.22190037525503	11.75575863334442	c
-1.38719603650129	-2.22190204613603	11.75575668098417	c
2.12626117595444	-4.16607375120942	11.81515520974304	h
-1.22157832884334	2.31664751583992	11.75607667439082	c
2.42174684714871	4.00261811679150	11.77109724449140	h

-2.71862060127678	0.09867513199086	11.49357587666660	c
-2.42174789837123	-4.00261975821870	11.77109387366196	h
-2.12626219244633	4.16607180363034	11.81515998359343	h

\$end

### I. [10]CP ground state

\$coord

-2.57605611595498	13.54569099397748	1.31656202294016	c
-2.57605611595498	13.54569099397748	-1.31656202294016	c
-0.44312491592716	12.74358219206801	-2.69556486857915	c
1.78734256427802	12.29945174499846	-1.31357076655723	c
1.78734256427802	12.29945174499846	1.31357076655723	c
-0.44312491592716	12.74358219206801	2.69556486857915	c
-4.29793011203162	14.07909953783424	2.31922402408512	h
-4.29793011203162	14.07909953783424	-2.31922402408512	h
3.49010358788574	11.69407653210880	-2.30544961683238	h
3.49010358788574	11.69407653210880	2.30544961683238	h
-0.60479780754823	11.87937599237010	-5.35132384286776	c
-2.81977553878351	10.66149554160521	-6.18344821540654	c
1.50958817691284	11.76620113288085	-6.96787515349079	c
-2.81535640351749	9.12630838043336	-8.31561651668844	c
-4.50856046502844	10.71309533848576	-5.00272977246068	h
1.51179781706314	10.23354356670480	-9.10699885391279	c
3.21625516438524	12.82123953061750	-6.48910111196910	h
-0.59786931561068	8.73051486245481	-9.73365308214669	c
-4.50169830205026	8.02016527868086	-8.74015019813184	h
3.22093867511818	10.12420014975237	-10.25636527845635	h
-0.42454706435748	6.49034111110500	-11.40158810540732	c
1.84558012523901	5.10496109514501	-11.50856194374531	c
-2.57051132315660	5.36984484062326	-12.51724638929916	c
1.88690521601660	2.61055215878657	-12.34032353347257	c

3.56065300886143	5.90326402976773	-10.69036277438971	h
-2.53450286048847	2.86964897789891	-13.33479746052796	c
-4.32967466865365	6.43850880590818	-12.64576644117644	h
-0.34431616215279	1.37192310846293	-13.09476674858236	c
3.63055950819245	1.52670201988005	-12.15218139439271	h
-4.26564319850670	2.02856581720198	-14.07643080482035	h
-0.60479780754823	11.87937599237010	5.35132384286776	c
-2.81977553878351	10.66149554160521	6.18344821540654	c
1.50958817691284	11.76620113288085	6.96787515349079	c
-2.81535640351749	9.12630838043336	8.31561651668844	c
-4.50856046502844	10.71309533848576	5.00272977246068	h
1.51179781706314	10.23354356670480	9.10699885391279	c
3.21625516438524	12.82123953061750	6.48910111196910	h
-0.59786931561068	8.73051486245481	9.73365308214669	c
-4.50169830205026	8.02016527868086	8.74015019813184	h
3.22093867511818	10.12420014975237	10.25636527845635	h
-0.34431616215279	1.37192310846293	13.09476674858236	c
1.88690521601660	2.61055215878657	12.34032353347257	c
-2.53450286048847	2.86964897789891	13.33479746052796	c
1.84558012523901	5.10496109514501	11.50856194374531	c
3.63055950819245	1.52670201988005	12.15218139439271	h
-2.57051132315660	5.36984484062326	12.51724638929916	c
-4.26564319850670	2.02856581720198	14.07643080482035	h
-0.42454706435748	6.49034111110500	11.40158810540732	c
3.56065300886143	5.90326402976773	10.69036277438971	h
-4.32967466865365	6.43850880590818	12.64576644117644	h
-0.39973006725299	-1.42338763863518	13.07208402328324	c
1.70431891644126	-2.94594241461783	13.66269971154989	c
-2.47884765368416	-2.63652437155847	11.93842993534643	c
1.84981980143884	-5.44593645169436	12.85221413226239	c
3.29574066066753	-2.12970210919650	14.69072822792366	h
-2.32129892364056	-5.12321152141070	11.10764234474286	c



-4.15713645019730	-1.53591683940972	11.46746544723790	h
-0.08511256782081	-6.54422148076977	11.38112183593706	c
3.55278895225311	-6.52710008011557	13.27908797381634	h
-3.88751688656383	-5.88537135642556	10.00881506388230	h
-0.39973006725299	-1.42338763863518	-13.07208402328324	c
1.70431891644126	-2.94594241461783	-13.66269971154989	c
-2.47884765368416	-2.63652437155847	-11.93842993534643	c
1.84981980143884	-5.44593645169436	-12.85221413226239	c
3.29574066066753	-2.12970210919650	-14.69072822792366	h
-2.32129892364056	-5.12321152141070	-11.10764234474286	c
-4.15713645019730	-1.53591683940972	-11.46746544723790	h
-0.08511256782081	-6.54422148076977	-11.38112183593706	c
3.55278895225311	-6.52710008011557	-13.27908797381634	h
-3.88751688656383	-5.88537135642556	-10.00881506388230	h
1.46909322196273	-12.58063999574096	-2.70700770740416	c
3.45763833687292	-11.48398437062629	-1.31722164914960	c
-0.33936056392048	-13.95836465092712	-1.31580874690159	c
3.45763833687292	-11.48398437062629	1.31722164914960	c
4.90693706522348	-10.39807106744789	-2.29915639405433	h
-0.33936056392048	-13.95836465092712	1.31580874690159	c
-1.83400327840511	-14.97632682793655	-2.30739237876182	h
1.46909322196273	-12.58063999574096	2.70700770740416	c
4.90693706522348	-10.39807106744789	2.29915639405433	h
-1.83400327840511	-14.97632682793655	2.30739237876182	h
0.30049898350751	-8.79584778457863	-9.76762579181710	c
-1.70890352395388	-10.05568570302962	-8.55240096793880	c
2.75860691271456	-9.45429506893420	-8.97715351888272	c
-1.30700263059936	-11.52176395444100	-6.40667335209942	c
-3.64531499836209	-9.75730399539737	-9.19209743009199	h
3.16318980397786	-10.95282052239185	-6.85705138883141	c
4.39208416909732	-8.61635444263894	-9.91348925463588	h
1.13083978391766	-11.84420225737664	-5.38385284416829	c

-2.94354955358690	-12.25587366058964	-5.39007105834340	h
5.10086089972819	-11.30350417386189	-6.24693273964684	h
1.13083978391766	-11.84420225737664	5.38385284416829	c
3.16318980397786	-10.95282052239185	6.85705138883141	c
-1.30700263059936	-11.52176395444100	6.40667335209942	c
2.75860691271456	-9.45429506893420	8.97715351888272	c
5.10086089972819	-11.30350417386189	6.24693273964684	h
-1.70890352395388	-10.05568570302962	8.55240096793880	c
-2.94354955358690	-12.25587366058964	5.39007105834340	h
0.30049898350751	-8.79584778457863	9.76762579181710	c
4.39208416909732	-8.61635444263894	9.91348925463588	h
-3.64531499836209	-9.75730399539737	9.19209743009199	h

\$end

#### J. [10]CP excited state

\$coord

-2.92146140328528	13.28464254671639	1.30642384278540	c
-2.92147507772240	13.28464252756546	-1.30641063354700	c
-0.68513650607759	12.80831280860590	-2.71576682714554	c
1.59678231699081	12.77356020881507	-1.30701302155576	c
1.59679551104191	12.77355555804140	1.30697977076441	c
-0.68510916004990	12.80830774249111	2.71575655448978	c
-4.70702156381158	13.57967466849846	2.29278690229629	h
-4.70704647778050	13.57966944838524	-2.29275486317308	h
3.39137649178492	12.50194305593750	-2.28108744229477	h
3.39139888865250	12.50193083232899	2.28103525860115	h
-0.73836342778425	11.95016470857376	-5.33553454988560	c
-2.97240369585999	10.90683377832251	-6.39055864515902	c
1.48755680356804	11.68370026325899	-6.81433489195639	c
-2.90512762767876	9.36846149532925	-8.50251259194851	c
-4.76336620881880	11.11646090690607	-5.39500092989734	h

1.55436482922347	10.14759102140549	-8.92691566230411	c
3.21714797951964	12.64486072011863	-6.23794135677224	h
-0.59868916227465	8.75463918856156	-9.72588351262017	c
-4.64541197263311	8.43077987795527	-9.08052800941681	h
3.33526197780044	9.94866179131436	-9.94477621772445	h
-0.40906616941418	6.53096794133241	-11.34466770928538	c
1.93147739474085	5.26046310980442	-11.66286332234762	c
-2.56983899602815	5.26150065766414	-12.31089091963563	c
2.04782278393239	2.77786009759460	-12.47325605805795	c
3.67333837031437	6.16319550292474	-11.03619671629078	h
-2.45475302077219	2.77884683086124	-13.11667582504431	c
-4.39006913154771	6.22770175229399	-12.35047576614289	h
-0.16867710312541	1.37214227230231	-13.02425788432556	c
3.87559990080128	1.82774347013983	-12.45091890550522	h
-4.18696019721240	1.86869766184141	-13.76392592502693	h
-0.73831155623063	11.95015521931322	5.33552324391503	c
-2.97235075396186	10.90684890704529	6.39057366058401	c
1.48762416527108	11.68366391928060	6.81429558276580	c
-2.90506718701761	9.36847774771963	8.50252790295154	c
-4.76332231889546	11.11649435435860	5.39503612180946	h
1.55444042533360	10.14755302905480	8.92687529096228	c
3.21721957819085	12.64480380599700	6.23788038440342	h
-0.59862142985869	8.75462955942172	9.72587193935523	c
-4.64535549657107	8.43081691524986	9.08056500711453	h
3.33534918754004	9.94859837795632	9.94471067742367	h
-0.16866379010936	1.37213516215681	13.02425874857753	c
2.04784768107894	2.77782883226074	12.47324120600525	c
-2.45472446883876	2.77886380229945	13.11668662762869	c
1.93152358077162	5.26043059185798	11.66284136633509	c
3.87561483132179	1.82769328268866	12.45089680242774	h
-2.56978806769113	5.26151866940454	12.31090244491247	c
-4.18693871288120	1.86873234647257	13.76394259292190	h

-0.40900871050499	6.53096014543827	11.34465987120199	c
3.67338965633437	6.16314192343580	11.03615827430754	h
-4.39000585451218	6.22774227170074	12.35050540914902	h
-0.12333278114397	-1.38321829340086	13.02520746381461	c
2.15219197154872	-2.79674206926478	13.20843016914854	c
-2.31765897638944	-2.78566902630266	12.38584423299966	c
2.29223649330865	-5.28078909231110	12.41004119163075	c
3.86197790992594	-1.89074584511559	13.91830351766656	h
-2.17454580318275	-5.26578891164382	11.57705058096752	c
-4.14385535292645	-1.83599397066367	12.30214618425613	h
0.17300114193524	-6.54744269141300	11.34850170964203	c
4.11353498857435	-6.23852496637401	12.51512268644746	h
-3.90169478049516	-6.16256880481719	10.90623600260124	h
-0.12331689355085	-1.38321065762535	-13.02520271191232	c
2.15222411717049	-2.79671075007203	-13.20840723272152	c
-2.31763333359072	-2.78568373401762	-12.38585508659082	c
2.29228949303494	-5.28075482353933	-12.41001210910243	c
3.86200508872813	-1.89069803927088	-13.91827159596971	h
-2.17450087526680	-5.26580276545789	-11.57706273267708	c
-4.14383964002992	-1.83602673695357	-12.30216794245631	h
0.17305760191195	-6.54743157620079	-11.34849286330065	c
4.11360113480330	-6.23846849505545	-12.51506996076850	h
-3.90164662022595	-6.16260220491531	-10.90626593516318	h
1.16059635620092	-12.75300438822092	-2.72072172418073	c
3.39453892724758	-12.29560851260083	-1.30586897447056	c
-0.94907313162364	-13.62943156393153	-1.30651257986557	c
3.39452760090838	-12.29561271501070	1.30589884874300	c
5.11654395667704	-11.71250073893300	-2.27285295434276	h
-0.94908595991685	-13.62943144011941	1.30650102584867	c
-2.65679814628609	-14.23777617101348	-2.28632301610988	h
1.16057186360936	-12.75300896671654	2.72073088772692	c
5.11652547401641	-11.71251164946081	2.27289962279782	h

-2.65682272374845	-14.23777014189796	2.28629469141094	h
0.43460779584861	-8.77361522537465	-9.74157138735577	c
-1.68217858964353	-9.96431406890651	-8.59470717617846	c
2.83589945496828	-9.60664369842366	-8.87457227315891	c
-1.43231735150572	-11.48170622774333	-6.48264456577477	c
-3.58102618643871	-9.58077951319778	-9.29371787822593	h
3.08635176122684	-11.12424046275652	-6.76329594414999	c
4.55080834074319	-8.90825386017967	-9.77608258160162	h
0.95604497153637	-11.93519526330647	-5.34425469281143	c
-3.14609432110864	-12.17900708518368	-5.57720939581712	h
4.98548568827179	-11.59972537405128	-6.12274045352755	h
0.95599864050168	-11.93520435958995	5.34426375056199	c
3.08629767473795	-11.12427267347356	6.76332984769683	c
-1.43237180064467	-11.48169487523124	6.48262896465996	c
2.83583689964581	-9.60667882299082	8.87460699569971	c
4.98543409627264	-11.59977304214076	6.12279324928945	h
-1.68224150946342	-9.96430212776119	8.59469044878761	c
-3.14614561140990	-12.17897989957692	5.57717543510625	h
0.43454432582183	-8.77362710869575	9.74158042190232	c
4.55074267051273	-8.90831008101220	9.77613933701420	h
-3.58109315636032	-9.58074779708706	9.29367920518715	h

\$end

### K. [11]CP ground state

\$coord

-4.99105488909000	14.33468522197785	1.31544195973726	c
-7.40124223815483	13.27941179483616	1.39456534899558	c
-8.27741970176179	11.69049019667176	-0.55415106690661	c
-6.73404452394109	11.46469928155410	-2.70954171790644	c
-4.31866940337403	12.49512209089655	-2.77342756666738	c
-3.31710574685771	13.83007819850923	-0.69789429364867	c

-4.36878533387088	15.50002812350611	2.89810200374820	h
-8.59926103331856	13.63164015136124	3.03665051868250	h
-7.34498641779170	10.25936665029908	-4.26628556166891	h
-3.11358742086612	12.05944785378977	-4.38584100500925	h
-10.43363232055842	9.93623463200563	-0.24764439244180	c
-10.78846280114480	8.70141605294718	2.08179238947485	c
-11.88392121614282	9.07261732018871	-2.30798236260909	c
-12.23911315198990	6.51546611611173	2.25743467105657	c
-9.71382147943076	9.32215926410423	3.72816319231328	h
-13.35062406306211	6.89615416885675	-2.12516159076182	c
-11.78970563857287	10.07451079870837	-4.10871037099353	h
-13.42283148240981	5.46081536035075	0.11919108379829	c
-12.25661005581816	5.48288441429039	4.04094825505869	h
-14.38351373126658	6.24550391493873	-3.78729399116399	h
-14.24378275004954	2.78560094098991	0.16663929129859	c
-13.94514033047856	1.27759072090441	-2.00649423871800	c
-14.89836810994167	1.52619814320162	2.42213532704916	c
-13.96726998978769	-1.34730108806534	-1.86597575656282	c
-13.45258901795319	2.16612361745813	-3.79951157926548	h
-14.90285765268907	-1.10077962242504	2.56854878604279	c
-15.31808425341627	2.62132733691920	4.11839998259368	h
-14.27407628230608	-2.60148066114683	0.46008404188768	c
-13.49412292037812	-2.44003595656056	-3.54917881593605	h
-15.31588512214701	-2.00707900641480	4.37505923164577	h
7.28855387292493	12.26761563766543	0.28573024702214	c
7.82870511021114	10.83998610823302	2.46734421351523	c
9.05376079029126	12.11910423628468	-1.70616711352684	c
9.83439627022153	9.14830737029491	2.54025039429301	c
6.52699446413781	10.88321485318860	4.06327569553262	h
11.05376085131507	10.40823116694065	-1.64265424057653	c
8.81346628008842	13.30351035294967	-3.37704513919114	h
11.40737870344374	8.77185968902750	0.42802065005452	c

10.04232223026298	7.92454586158334	4.18590183036432	h
12.32189007623541	10.28740630332922	-3.26548223857559	h
14.50254971136686	1.29082558793445	0.33438262155202	c
13.82346077017549	2.51891414765139	-1.92658498605804	c
14.73964881067507	2.80763024036770	2.51163519202242	c
13.07594348524520	5.04177631968826	-1.93631907371583	c
13.63752597539229	1.41764467653244	-3.65987968871323	h
13.99372286677413	5.32917422898934	2.50135670887716	c
15.42637546259728	1.96824893788945	4.26587951414662	h
12.97266476448519	6.45713493056033	0.31430837976078	c
12.32364098293593	5.85194089928512	-3.67664829608771	h
14.11216602939315	6.42014980814384	4.24782550416662	h
14.44527705910491	-1.50251555024587	0.46292752703418	c
15.04708607354729	-3.07659375774861	-1.59886022745846	c
13.31132353601415	-2.66334302242298	2.57135928087439	c
14.27741098129754	-5.59332473500513	-1.66528540716004	c
16.06501967012238	-2.29536009333952	-3.21408641063613	h
12.52502977823899	-5.16746625555355	2.49492736895303	c
12.81958427613806	-1.51733333158387	4.21271569185667	h
12.84303680090129	-6.66027650961020	0.31287468779006	c
14.72240063740424	-6.72358587796527	-3.33160294182530	h
11.43651147272470	-5.90050647439587	4.08282659871800	h
-13.46543375743084	-5.26830233332862	0.69130641601318	c
-13.68547569790311	-7.02961433479332	-1.29387128000940	c
-11.99694990628294	-5.99375076111044	2.78778776657808	c
-12.26499711641392	-9.24507421171393	-1.31648668514242	c
-14.92778233508185	-6.61555718909428	-2.88779147544334	h
-10.56103498606194	-8.19366330793976	2.75209171312920	c
-11.78549680105965	-4.69239609595214	4.37239604029131	h
-10.52863459157059	-9.80027575051374	0.62919437728076	c
-12.44045870563971	-10.51935917367931	-2.92767665359002	h
-9.26574140368139	-8.54481814507550	4.31474900034709	h

-0.78971268332763	-14.11976547599565	-0.71983569298070	c
0.40895041087102	-12.86548088229511	-2.73870485389697	c
0.79594934234453	-15.25241836030916	1.09724881135742	c
3.00847756020178	-12.51707322477092	-2.78797275792176	c
-0.73479449621162	-11.94769305254620	-4.18555460680980	h
3.40669238560777	-14.90632266319204	1.04498024910266	c
-0.03183494056703	-16.36807621280900	2.62236269701147	h
4.57063839029359	-13.40465793060430	-0.82377467797894	c
3.81278031702024	-11.33563874705383	-4.27186820872664	h
4.55412625186203	-15.76048796872051	2.53076145247436	h
-8.44533741150629	-11.64347333580780	0.31722087840190	c
-7.00500814084967	-12.51978056185655	2.37966579044742	c
-7.52531137385934	-12.23310721356267	-2.11225368846976	c
-4.61466376890895	-13.56170999274565	2.03485526247879	c
-7.69959293622938	-12.25397732756874	4.30211255172196	h
-5.15168370568109	-13.30475835390137	-2.45793789325336	c
-8.60419706655508	-11.66992815896340	-3.77527611336637	h
-3.55023230229030	-13.81575290388646	-0.39267018806944	c
-3.47651374278424	-14.00673590132766	3.69573964246712	h
-4.47298125030758	-13.62016661427670	-4.37871356389283	h
7.16465862943400	-12.38521443065993	-0.59182808817727	c
8.48028044091660	-11.41950393667589	-2.69664899460358	c
8.23502438072253	-11.91381811611363	1.80044444449450	c
10.49415663314998	-9.75672261852766	-2.40482302628140	c
7.82802214966386	-11.86293733296939	-4.60116339184246	h
10.27331978141412	-10.27757290647976	2.08990948570022	c
7.33723435412131	-12.68638163736403	3.48811883973416	h
11.32920140511459	-8.99482123373190	0.00710835517943	c
11.30676541626338	-8.88757801164131	-4.08773263182344	h
10.95964537153483	-9.88182233251137	3.99302613209093	h
-0.55475699865191	14.24420023973882	-0.51054600359875	c
1.04310418614302	14.09459595838741	-2.63700450299558	c



0.64604295014627	14.36726084010361	1.86422010228051	c
3.62871831356636	13.69387223386704	-2.38402770818148	c
0.23664811462783	14.15290445053278	-4.53249646000624	h
3.23723312236375	14.00989002561580	2.11539647407461	c
-0.48661963534312	14.56775901136938	3.57424033949525	h
4.77407289593739	13.46378592568255	0.00941441997658	c
4.74577354256506	13.37000826295647	-4.08568619089464	h
4.05669069321683	14.02210001438239	4.00700597969610	h

\$end

#### L. [11]CP excited state

\$coord

-4.86819356702687	14.10398522167339	1.78991665635486	c
-7.25231256973855	13.03100359474916	1.83627531846664	c
-8.27612896228167	11.78164244354074	-0.30538657790002	c
-6.88486129258070	12.02873603465436	-2.58160400535410	c
-4.49637877340787	13.09058899480883	-2.62385704768822	c
-3.31158742806799	13.99820476774133	-0.39537657856817	c
-4.15407215208560	14.97481199879666	3.51476100391154	h
-8.33227067100412	13.09797492129676	3.59069798248852	h
-7.60305224414994	11.16705940142526	-4.30942477538031	h
-3.44340824025992	13.02773548606742	-4.39177094082731	h
-10.37619045166494	10.00010408338625	-0.13031548062543	c
-10.96972474653541	8.81013053109892	2.19559018652062	c
-11.64914421570353	9.05338456836603	-2.29407640556664	c
-12.39937122638429	6.62210887295825	2.29201424584464	c
-10.09903765412269	9.48892104294993	3.93494659696221	h
-13.08505671639383	6.87092870534812	-2.19539661538500	c
-11.44794802217309	10.02431708794151	-4.10117880436344	h
-13.35061961469406	5.46037054287114	0.07218244126457	c
-12.59786577497102	5.66814955542681	4.10663515839818	h

-13.97048866836276	6.19418072475855	-3.92892586377907	h
-14.14924644264430	2.81639626856420	0.08816868512834	c
-14.05977720165213	1.33986486092604	-2.14659599985666	c
-14.65026175556852	1.47680673563551	2.35916274388417	c
-14.07790078229159	-1.27454925032072	-2.06992194609652	c
-13.74496405893340	2.25865034003071	-3.96299283058273	h
-14.65896000483897	-1.13647825824023	2.43788952893714	c
-14.96846694809857	2.51641862860063	4.10996740038167	h
-14.17868458976272	-2.61200698488008	0.24933803511238	c
-13.77502452176376	-2.30755220542379	-3.82677285392326	h
-14.98179665849961	-2.07157813550515	4.24647322969866	h
7.28407181361018	12.39663614467370	0.18334151317762	c
8.12963887319057	11.26732072345358	2.46362090863518	c
8.81394348107154	11.94967603672891	-1.97700402072073	c
10.09699877036254	9.54712245501179	2.50285291584839	c
7.08757525081945	11.58539005897041	4.21061428946106	h
10.77626504619557	10.22192672882312	-1.94031719142123	c
8.40143287657663	12.92744032625857	-3.74301764759713	h
11.37168158142538	8.81295391681697	0.26349723988811	c
10.51361187726963	8.58021025451879	4.27331859946656	h
11.84130607446866	9.89947247030855	-3.67552818217026	h
14.35987663958056	1.27294174492408	0.20742558139592	c
13.85002156531786	2.58336793468110	-2.07376783193794	c
14.47013617064758	2.77397574651149	2.42871411102202	c
13.12602469409524	5.09759927003967	-2.07988114841301	c
13.79558468917875	1.54446187168864	-3.85239972783391	h
13.74851971787091	5.28640448353105	2.42207963585761	c
15.07497949784794	1.92177820213908	4.20507123533040	h
12.85879937513476	6.48914299426674	0.19446309124862	c
12.53072255600082	5.94069110729622	-3.86271016235812	h
13.80855560917603	6.33755076537921	4.19415128505056	h
14.33530166567517	-1.48569697736416	0.28645542535016	c

14.60840827047877	-3.00427343864514	-1.90784583324448	c
13.61679177189891	-2.77585597749450	2.52196806941285	c
13.86364755321626	-5.51080576974483	-1.94388912839577	c
15.36195240954451	-2.17146343905848	-3.63613619423515	h
12.86084268282381	-5.27786312559929	2.48215573716803	c
13.43332630818625	-1.72770793742489	4.28612528130417	h
12.77160285201241	-6.69216029008764	0.20566503971584	c
14.05656920991229	-6.56373429948969	-3.70466728697493	h
12.12326769587679	-6.09289985146827	4.22272179541430	h
-13.40543436202905	-5.25807104416685	0.38276101078719	c
-13.30486922020041	-6.84886497403358	-1.77449190795679	c
-12.31351679152320	-6.24703857014107	2.62025027625605	c
-11.90636754024914	-9.05808672234818	-1.78666830716240	c
-14.29758713451747	-6.29649537350594	-3.49452167200157	h
-10.90431933006598	-8.44907640758790	2.60377896010182	c
-12.38396008483351	-5.14427707206139	4.35899167373392	h
-10.48455278777449	-9.84220006692641	0.35153622122538	c
-11.84605633255999	-10.16861768690530	-3.52103268935388	h
-9.93153704014534	-8.98860064285364	4.33614662846910	h
-0.77858018492393	-14.33537025256987	-0.46050628011295	c
0.53746761882238	-13.66507151429624	-2.69784857944823	c
0.75396207717682	-14.99801106672046	1.64077068203590	c
3.12692782840315	-13.31770755422663	-2.72172743908980	c
-0.51916435045026	-13.19723976746770	-4.40227433836830	h
3.34592609330797	-14.65124028606919	1.61655397842039	c
-0.12344610453251	-15.73396414195331	3.35410813216835	h
4.61314704927316	-13.61236338047177	-0.50976397137559	c
3.99111562880892	-12.59333034935202	-4.44466708787952	h
4.41552723690578	-15.12697553626912	3.31265553496049	h
-8.42297699613354	-11.67120140783337	0.17180022164956	c
-7.05830732901622	-12.50715970244193	2.32518214052559	c
-7.40606958389288	-12.39691717248996	-2.20200058768579	c

-4.69315587668719	-13.60223114628787	2.11693436671029	c
-7.81970132654242	-12.18422405918882	4.21170320360853	h
-5.04208525845839	-13.49174156015584	-2.41059506124727	c
-8.42087644820593	-11.93658567182351	-3.93409872895722	h
-3.50392753277671	-13.94959078821990	-0.26160537844989	c
-3.66232330683079	-14.03500189396180	3.84765266485632	h
-4.31776527954794	-13.90764293387158	-4.29333108763707	h
7.14285174308426	-12.51975693582561	-0.35399656408124	c
8.45714132951661	-11.64343633421224	-2.52225229368940	c
8.25038547898340	-11.89672753214352	2.00763918923088	c
10.44493964856984	-9.95649714750556	-2.33830687617509	c
7.83228520441348	-12.21659900229309	-4.39976542293227	h
10.23975845480586	-10.21034307855879	2.19104409279945	c
7.41444395967444	-12.61289052251441	3.74875374494833	h
11.28017476082769	-9.00993014085936	0.02850927498451	c
11.26249298021318	-9.22323369341972	-4.08067442884316	h
10.92946154835847	-9.71923498885688	4.06874052161685	h
-0.57942499723626	14.38884392325639	-0.28914189277008	c
0.96548864909019	14.28463175235061	-2.48070101534026	c
0.73366311082341	14.48904898464631	2.04840131949096	c
3.54566224391123	13.89273438717412	-2.33163828293905	c
0.10512869985105	14.39515200337002	-4.34851314940295	h
3.31420068978457	14.10147080740461	2.19751064557383	c
-0.31620964626483	14.71318794098916	3.80629660043384	h
4.79353400086066	13.57758325966612	0.02147124383230	c
4.59482812662068	13.65107834963979	-4.08746250334074	h
4.19304005950736	14.09590400500217	4.06089333091910	h

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