

Excitation landscape of the CP43 photosynthetic antenna complex from multiscale simulations

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ELECTRONIC SUPPLEMENTARY INFORMATION

Additional Computational Details

Molecular Dynamics (MD) simulations

The initial structure of the Photosystem II (PSII) monomer used in this work is based on the high-resolution crystal structure of *T. vulcanus* (PDB ID: 3WU2).¹ The complete protein unit was embedded in a POPC lipid bilayer of dimension $176 \times 176 \text{ \AA}^2$ using Packmol-Memgen,² thoroughly solvated with a TIP3P water box (**Figure S1**) and neutralized with appropriate number of counterions in a 0.15M NaCl salt buffer. For the protein residues, waters and POPC bilayer we used the standard parameters from the AMBERff14SB,³ TIP3P⁴ and LIPID17⁵ force fields, respectively. The partial charges and force field parameters for the organic cofactors (plastoquinones, carotenoids, structural lipids) were obtained using GAFF2,⁶ bonded parameters for non-heme Fe and OEC were taken from earlier studies,⁷⁻⁹ while those of the remaining cofactors (Chl a, Pheo, heme) were obtained from literature.^{10, 11} The nonbonded parameters for the metal ions were based on their respective oxidation states using data sets available for the TIP3P water model.¹² For Na^+ and Cl^- ions, we used the Joung–Cheatham parameters compatible with the TIP3P water model.^{13, 14}

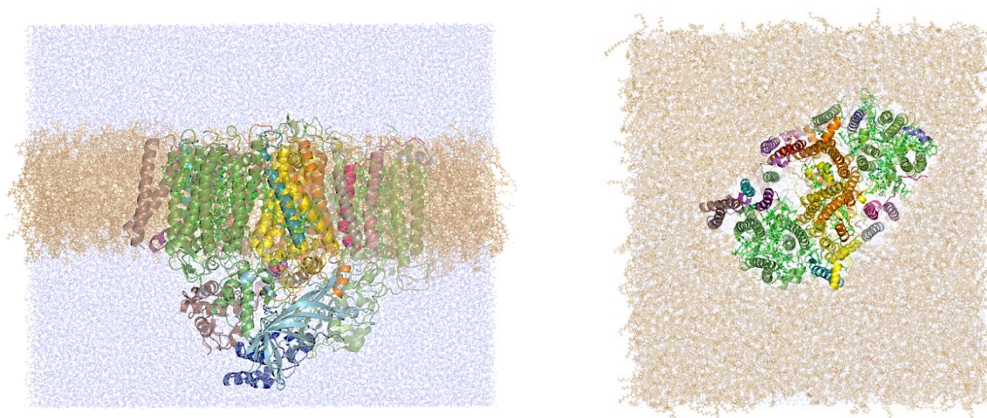


Figure S1. Side view and stromal (top) view of the molecular-mechanics (MM) model of the lipid bilayer bound PSII monomer used in this work (Na^+ and Cl^- counterions not shown for clarity).

A step-by-step minimization protocol was employed to remove energetically unfavorable geometric clashes in the system. In the heating phase, the system is first heated from 10 to 100 K in a succession of 5 ps in the NvT ensemble, followed by further heating from 100 to 303 K in the NpT ensemble for a total of 125 ps. The temperature during this step is maintained using the Langevin dynamics¹⁵ with a collision frequency of 5 ps^{-1} . During the equilibration phase, the C_α atoms of amino acids were restrained with a force constant of $20 \text{ kcal mol}^{-1} \text{ \AA}^{-2}$. Subsequently, the restraints on the C_α atoms were systematically reduced ($2 \text{ kcal mol}^{-1} \text{ \AA}^{-2}/500$

ps) and the system was further equilibrated for 65 ns to equilibrate the POPC bilayer. Thereafter, production run was initiated without any restraints and the temperature and pressure set at 303 K and 1 atm, respectively. During the entire procedure, the temperature was controlled using Langevin dynamics with a collision frequency of 1 ps^{-1} and the system pressure was controlled using the Berendsen barostat¹⁶ with anisotropic pressure scaling with a relaxation time of 2 ps. We employed the SHAKE algorithm¹⁷ to constrain the bonds involving hydrogens, therefore a time step of 2 fs could be used. The electrostatic interactions were treated using the Particle Mesh Ewald (PME) approach¹⁸ with a 10 \AA cut-off. The AMBER20 package¹⁹ was used to perform the energy minimizations and equilibration dynamics while the production MD simulations were performed in the GPU version of the pmemd module (*pmemd.cuda*).²⁰

Calculation of the absorption spectrum with the MD-PMM approach

For computing the absorption spectrum, after calculating the perturbed frequencies (ν) and transition dipoles ($\mu_{j,i}$) for each exciton state over the frames of the MD trajectory, we evaluate the excitation energy distribution using a suitable number of frequency bins. Subsequently, we utilize the excitation energy distribution and the corresponding transition dipoles to determine the molar extinction coefficient $\epsilon_{0,i}$ for the transitions from the ground to the i th excited state, thus providing the absorption spectrum according to:

$$\epsilon_{0,i} = \sum_{\nu_{\text{ref}}} \frac{\Gamma_A(\nu_{\text{ref}}) h \nu}{N} \frac{e^{-(\nu - \nu_{\text{ref}})^2 / 2\sigma^2}}{\sigma \sqrt{2\pi}} \quad (\text{S1})$$

$$\Gamma_A(\nu_{\text{ref}}) = \frac{|\mu_{0,j}|_{\nu_{\text{ref}}}^2}{6\epsilon_0 c \hbar^2} \quad (\text{S2})$$

Here, ν_{ref} , $n(\nu_{\text{ref}})$ and $|\mu_{0,j}|_{\nu_{\text{ref}}}^2$ are the frequency at the center of each bin, the corresponding number of MD frames and mean transition dipole square norm within the bin, respectively, $\hbar = h/2\pi$ with h the Planck constant, ϵ_0 is the vacuum dielectric constant, c is the speed of light and σ^2 is the variance associated to the semiclassical intra-QC vibrations neglected in the evaluation of the unperturbed properties. In the present case, the value of σ^2 ($\sigma = 10^{-4}$ Hartree) has been estimated on the basis of the full width at half maximum (FWHM) of the experimental spectrum of chlorophyll a in toluene,²¹ approximating the vacuum condition. The calculated spectral line shape in the Q_y region is reported in **Figure S2**. Note that the width of the

calculated bands (inhomogeneous broadening) is due to the explicit effect of the semiclassical fluctuations of the QCs and their environment along the MD trajectory and does not include any adjustable parameter.

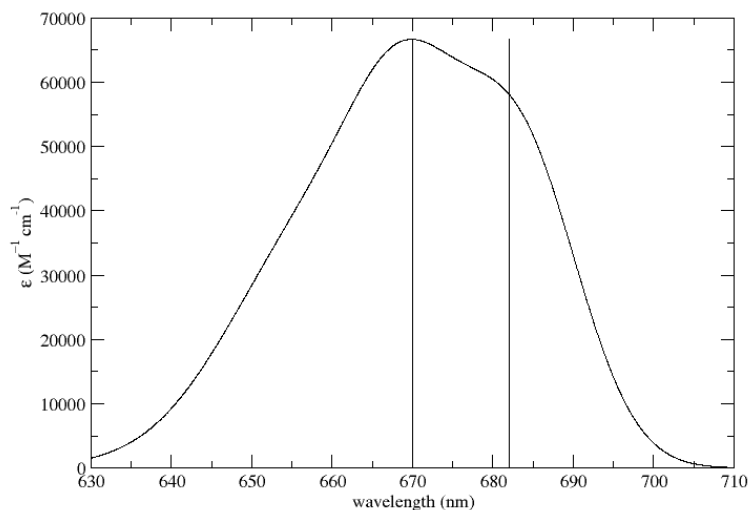


Figure S2. Room-temperature absorption spectrum of the CP43 complex calculated with the MD-PMM approach. The spectrum has been shifted by 0.000457 Hartree to lower energies in order to match the position of the main experimental peak measured at 293 K.

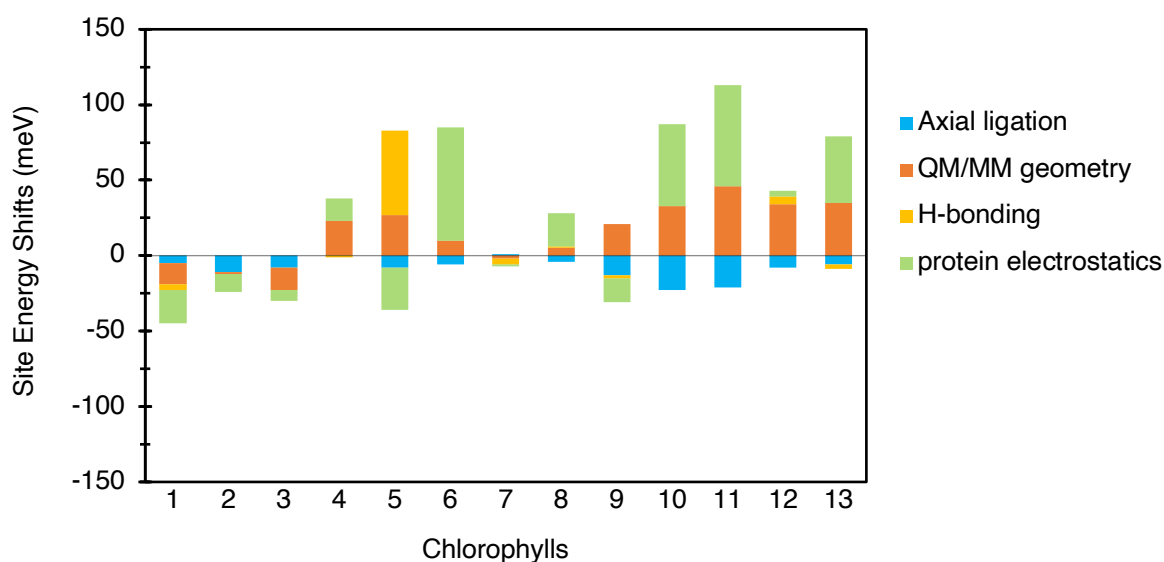


Figure S3. Decomposition of the electrostatic and non-electrostatic contributions (axial ligation, H-bonding, QM/MM geometry optimization) to the site energy shifts of the CP43 chlorophylls.

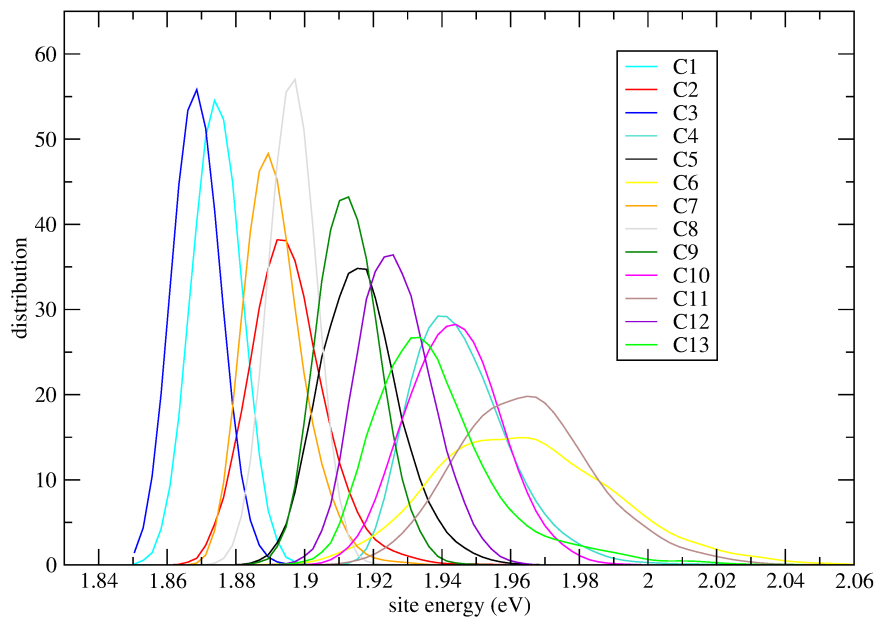


Figure S4. Distributions of the site energy for all Chl-a molecules (which include their respective axial ligands) in the CP43 complex performing the MD-PMM calculations over the last 30 ns of the MD trajectory (3000 frames in total).

Table S1. TD-DFT (ω B97X-D3(BJ)/def2-TZVP) excitation energies E (in eV) of the S_2/Q_x states and corresponding oscillator strengths for the CP43 chlorophylls computed *in vacuo*, with QM/MM on an isolated CP43 protein, and with QM/MM in the complete PSII monomer. The geometries in all cases are derived from QM/MM optimizations within the PSII monomer. Shifts are reported in meV with respect to the gas-phase values.

Site	TD-DFT Gas-phase		TD-DFT QM/MM Isolated CP43			TD-DFT QM/MM Full PSII monomer		
	E	f_{osc}	E	f_{osc}	Shift	E	f_{osc}	Shift
C1	2.354	0.04	2.296	0.03	-58	2.260	0.02	-94
C2	2.372	0.04	2.307	0.03	-65	2.280	0.02	-92
C3	2.370	0.02	2.303	0.02	-67	2.283	0.01	-87
C4	2.427	0.03	2.359	0.01	-68	2.375	0.02	-52
C5	2.475	0.16	2.417	0.12	-58	2.440	0.15	-35
C6	2.383	0.06	2.457	0.09	74	2.464	0.11	81
C7	2.421	0.05	2.392	0.04	-29	2.382	0.05	-39
C8	2.394	0.05	2.412	0.03	18	2.452	0.07	58
C9	2.404	0.06	2.354	0.06	-50	2.342	0.06	-62
C10	2.362	0.07	2.424	0.11	62	2.450	0.12	88
C11	2.371	0.07	2.473	0.18	102	2.468	0.17	97
C12	2.418	0.08	2.433	0.09	15	2.409	0.09	-9
C13	2.423	0.07	2.413	0.08	-10	2.449	0.12	26

Table S2. TD-DFT Transition Dipole moments of the CP43 chlorophylls *in vacuo*.

Chl	S ₀ -S ₁					S ₀ -S ₂				
	T (debye)	T ² (au ²)	T _x (au)	T _y (au)	T _z (au)	T (debye)	T ² (au ²)	T _x (au)	T _y (au)	T _z (au)
C1	5.4223	4.5507	1.6598	0.9657	0.9292	1.7877	0.4947	-0.0116	-0.3280	-0.6220
C2	5.5418	4.7535	0.7559	1.9560	-0.5969	1.9422	0.5839	0.0872	-0.4145	0.6360
C3	5.6286	4.9036	1.6110	-1.4899	-0.2976	1.6609	0.4270	-0.2455	0.2258	0.5619
C4	5.5886	4.8341	-1.4121	-1.5491	-0.6636	1.8808	0.5475	0.1257	0.3485	0.6405
C5	5.5772	4.8146	1.3595	-1.2380	-1.1974	2.8896	1.2924	-0.1356	0.1439	1.1195
C6	5.4903	4.6656	0.5175	2.0624	0.3799	2.5398	0.9984	-0.4580	-0.5103	-0.7268
C7	5.6640	4.9655	2.0657	0.4489	-0.7050	2.0711	0.6639	-0.6712	-0.3362	-0.3168
C8	5.5771	4.8142	-1.5829	1.2619	-0.8464	2.3161	0.8303	0.2265	-0.3135	0.8250
C9	5.5291	4.7318	0.7763	2.0238	-0.1832	2.1829	0.7375	0.0540	0.5222	-0.6796
C10	5.4721	4.6347	0.7634	1.8828	-0.7121	2.8377	1.2464	0.2472	-0.5897	0.9152
C11	5.4245	4.5545	-0.8384	0.8208	-1.7827	2.7056	1.1331	0.1478	-0.0549	-1.0527
C12	5.4414	4.5830	1.0225	-1.8759	0.1356	2.6893	1.1194	-0.2525	0.7593	0.6922
C13	5.5280	4.7298	-1.7554	-0.9651	0.8468	2.8140	1.2257	0.5441	-0.0466	-0.9631

Table S3. Comparison of CP43 chlorophyll site energies from the literature. All values are in eV.

Site	Muh et al. ^{22 a}	Muh et al. ^{22 b}	Shibata et al. ^{23 c}	Shibata et al. ^{23 d}	Sarnagadharan et al. ²⁴	Saito et al. ²⁵	QM/MM (this work)	PMM (this work)
C1	1.839	1.843	1.853	1.842	1.818	2.127	1.846	1.873
C2	1.851	1.857	1.860	1.863	1.831	2.154	1.867	1.894
C3	1.843	1.840	1.853	1.862	1.817	2.114	1.861	1.867
C4	1.845	1.843	1.831	1.829	1.866	2.142	1.928	1.945
C5	1.846	1.847	1.853	1.834	1.842	2.152	1.938	1.915
C6	1.861	1.859	1.853	1.855	1.851	2.129	1.970	1.963
C7	1.839	1.838	1.833	1.841	1.842	2.122	1.885	1.890
C8	1.834	1.832	1.846	1.856	1.841	2.122	1.915	1.895
C9	1.828	1.834	1.825	1.818	1.848	2.096	1.881	1.912
C10	1.836	1.835	1.884	1.902	1.845	2.115	1.955	1.942
C11	1.823	1.823	1.862	1.830	1.831	2.136	1.986	1.964
C12	1.833	1.839	1.849	1.842	1.839	2.110	1.926	1.925
C13	1.861	1.858	1.873	1.870	1.865	2.142	1.961	1.937

^a Based on 3ARC¹^b Based on 4IL6²⁶^c Fit of linear optical spectra^d Fit of absorption and LD spectra

Table S4. Excitonic coupling constants (upper panel) and corresponding standard deviations (lower panel) between CP43 chlorophylls computed using the MD-PMM approach. All values are reported in cm^{-1} .

Chl	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13
C1		10.89	21.90	3.09	-3.07	-12.22	21.05	7.15	10.89	2.70	-2.52	0.63	-0.11
C2	6.05		8.14	154.07	-8.67	-16.15	-1.01	16.94	23.26	73.09	5.05	12.33	-10.27
C3	5.31	7.89		-36.43	4.48	-0.45	7.88	-4.39	-11.26	23.04	8.19	25.02	5.71
C4	1.07	8.80	3.02		-3.40	4.57	-2.08	-1.53	-0.97	-34.68	-4.46	-4.72	5.09
C5	0.86	1.08	0.36	0.48		25.46	-98.32	-5.90	-31.38	-1.18	-0.81	-1.55	5.03
C6	1.38	0.72	0.64	0.20	1.88		-77.69	-1.14	-32.26	-12.14	-4.85	-4.15	10.23
C7	1.53	1.89	0.98	0.42	5.26	15.33		17.84	-112.59	-4.61	-9.06	-34.46	26.34
C8	0.25	0.87	0.47	0.81	3.34	0.54	2.23		130.37	66.94	1.78	2.11	-5.16
C9	0.71	1.85	1.11	0.86	1.45	1.32	10.64	10.68		16.20	-117.64	36.43	-6.15
C10	1.12	7.47	2.36	3.33	1.13	0.46	1.95	4.51	12.58		-97.23	19.40	-11.76
C11	0.34	0.73	0.72	0.67	0.42	0.26	0.64	4.72	5.37	5.87		25.24	-13.91
C12	0.79	1.40	2.18	0.46	0.66	1.56	5.37	0.90	6.66	1.77	1.07		-48.50
C13	0.57	0.38	1.15	0.18	0.26	0.45	0.87	0.41	1.72	0.74	1.11	9.71	

Table S5. Relative center-to-center distances (in Å) of the 13 CP43 Chls, Chl_{ZD1} and D1-RC pigments based on the 3WU2 crystal structure.¹ Distances less than 12 Å are shown in red, 12–15 Å are shown in pink. In CP43, C5 is closest the D1 pigments (Chl_{ZD1}, Phe_{D1} and Chl_{D1}) while C4 is closer to P_{D1} (distances in green).

	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	Chl _{ZD1}	
C2		13.1													
C3		12.7	12.1												
C4		22.0	11.2	16.3											
C5		23.9	20.9	29.3	30.5										
C6		16.9	24.1	25.3	35.1	16.9									
C7		18.8	18.9	22.1	29.4	12.1	8.7								
C8		26.5	17.5	24.9	23.6	14.6	24.1	15.5							
C9		22.5	16.4	19.1	23.6	17.9	19.9	11.7	9.1						
C10		20.8	10.2	15.1	14.3	21.6	25.8	18.3	11.4	9.6					
C11		31.2	21.9	24.5	24.4	25.9	30.5	22.2	11.9	10.7	11.8				
C12		20.0	20.7	16.4	28.6	24.7	16.7	13.3	20.8	12.0	17.5	20.0			
C13		28.0	26.0	19.9	30.6	32.8	26.8	22.5	24.7	16.1	19.9	18.3	10.4		
Chl _{ZD1}		33.7	34.3	43.7	42.4	21.9	31.2	31.4	34.9	38.9	39.8	46.6	43.8	53.0	
Chl _{D1}		41.0	33.3	45.4	35.4	28.5	44.0	39.2	31.9	39.6	36.3	41.8	49.1	55.1	24.7
Phe _{D1}		39.0	30.8	42.6	34.7	21.5	38.3	32.7	24.4	32.7	31.4	34.7	43.0	48.7	24.3
P _{D1}		38.9	29.1	40.8	28.1	30.6	45.1	39.3	29.7	37.0	31.6	37.4	46.8	51.3	32.0

Table S6. QM/MM and TD-DFT (ω B97X-D3(BJ)/def2-TZVP) computed excitation energies (in eV) and corresponding oscillator strengths and NTO analysis for selected chlorophyll pairs in CP43. The geometries in all cases are derived from QM/MM optimizations of the pigments embedded inside the complete PSII monomer for snapshot 1. (LE: local excitations, CT: Charge Transfer states).

Pair	Mg-Mg (Å)	State	Es (eV)	f_{osc}	NTO character	weight	
C12-C13	10.1	1	1.920	0.21	LE (C12)	0.84	
					LE (C12)	0.19	
		2	1.967	0.24	LE (C13)	0.83	
					LE (C13)	0.19	
		3	2.410	0.06	LE (C12)	0.77	
LE (C12)	0.24						
4	2.46	0.15	LE (C13)	0.81			
			LE (C13)	0.19			
5	3.222	0.12	delocalized exciton + CT		0.88		
C2-C10	10.4	1	1.843	0.13	LE(C2)	0.84	
					LE(C2)	0.20	
		2	1.943	0.26	LE (C10) + CT (C2 \rightarrow C10)		0.86
					LE (C10)	0.10	
		3	2.001	0.07	LE (C10) + CT (C2 \rightarrow C10)		0.89
LE (C10)	0.10						
4	2.255	0.03	LE(C2)	0.69			
			LE(C2)	0.34			
5	2.465	0.17	LE (C10)	0.83			
			LE (C10)	0.19			
C6-C7	9.0	1	1.885	0.13	LE(C7)	0.84	
					LE(C7)	0.20	
		2	1.963	0.26	LE (C6)	0.84	
					LE (C6)	0.19	
		3	2.384	0.07	LE(C7)	0.74	
LE(C7)	0.28						
4	2.453	0.03	LE (C6)	0.79			
			LE (C6)	0.21			
5	3.218	0.17	delocalized exciton + CT		0.80		
C8-C9	9.5	1	1.882	0.23	LE(C9)	0.82	
					LE(C9)	0.20	
		2	1.913	0.24	LE (C8)	0.83	
					LE (C8)	0.18	
		3	2.352	0.04	LE(C9)	0.77	
LE(C9)	0.25						
4	2.441	0.06	LE (C8)	0.75			
			LE (C8)	0.26			
5	3.251	0.33	LE(C9)	0.67			
			LE(C9)	0.27			
C9-C10	9.3	1	1.888	0.17	LE(C9)	0.83	
					LE(C9)	0.20	
		2	1.942	0.25	LE(C10)	0.84	
					LE(C10)	0.18	
		3	2.365	0.04	LE(C9)	0.76	
LE(C9)	0.26						
4	2.433	0.11	LE(C10)	0.81			
			LE(C10)	0.21			
5	3.094	0.00	CT (C10 \rightarrow C9)		1.00		
C7-C9	11.4	1	1.868	0.39	LE (C9)	0.44	
					LE (C7)	0.41	

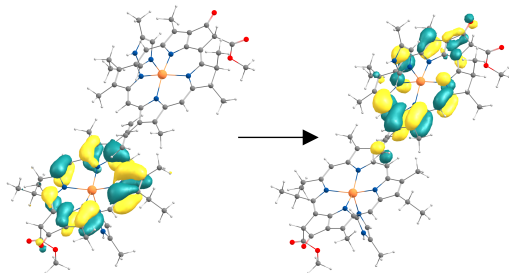
		2	1.891	0.09	LE (C7)	0.43
					LE (C9)	0.40
		3	2.350	0.07	LE (C9)	0.73
					LE (C9)	0.24
		4	2.37	0.04	LE (C7)	0.69
					LE (C7)	0.28
		5	3.278	0.30	LE (C9)	0.44
					LE (C7)	0.28
C9-C11	11.0	1	1.864	0.30	LE (C9)	0.83
					LE (C9)	0.20
		2	1.981	0.20	LE (C11)	0.83
					LE (C11)	0.18
		3	2.329	0.07	LE (C9)	0.76
					LE (C9)	0.27
		4	2.466	0.14	LE (C11)	0.83
					LE (C11)	0.19
		5	3.071	0.00	CT (C9 → C11)	1.00
C2-C4	11.8	1	1.868	0.32	LE(C2)	0.75
					LE(C2)	0.20
		2	1.899	0.098	LE(C4)	0.73
					LE(C4)	0.22
		3	2.291	0.02	LE(C2)	0.69
					LE(C2)	0.34
		4	2.320	0.00	LE(C4)	0.63
					LE(C4)	0.40
		5	3.166	0.64	LE(C4)	0.61
					LE(C4)	0.42
C8-C10	11.2	1	1.899	0.23	LE(C8)	0.80
					LE(C8)	0.17
		2	1.950	0.24	LE(C10)	0.80
					LE(C10)	0.17
		3	2.439	0.16	LE(C8)	0.62
					LE(C8)	0.22
		4	2.445	0.04	LE(C10)	0.67
					LE(C10)	0.18
		5	3.127	0.00	CT (C10 → C8)	1.00
C10-C11	11.9	1	1.958	0.34	LE(C10)	0.80
					LE(C10)	0.17
		2	1.994	0.18	LE(C11)	0.79
					LE(C11)	0.17
		3	2.451	0.26	LE(C10)	0.75
					LE(C10)	0.17
		4	2.484	0.11	LE(C11)	0.76
					LE(C11)	0.16
		5	2.546	0.00	CT (C10 → C11)	1.00
C5-C7	12.1	1	1.882	0.35	LE(C7)	0.78
					LE(C7)	0.18
		2	1.933	0.17	LE(C5)	0.79
					LE(C5)	0.16
		3	2.392	0.05	LE(C7)	0.72
					LE(C7)	0.30
		4	2.440	0.13	LE(C5)	0.83
					LE(C5)	0.19
		5	3.331	0.50	LE(C7)	0.64
					LE(C7)	0.34

Table S7. QM/MM and TD-DFT (ω B97X-D3(BJ)/def2-TZVP) computed excitation energies (in eV) and corresponding oscillator strengths and NTO analysis for the C2-C10 pair in CP43. The geometries in all cases are derived from QM/MM optimizations of the pigments embedded inside the complete PSII monomer in snapshots 2-10 (LE: local excitations, CT: Charge Transfer states).

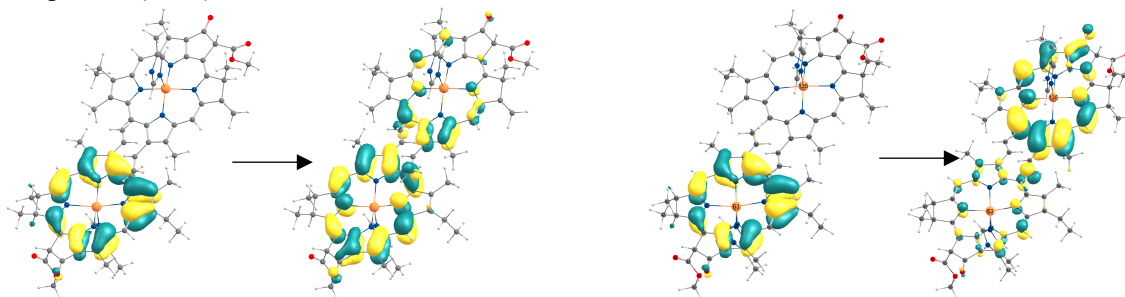
Snapshot	Mg-Mg (Å)	State	Es (eV)	f_{osc}	NTO character	weights
2	10.6	1	1.875	0.20	LE(C2)	0.83
					LE(C2)	0.22
		2	1.967	0.26	LE (C10)	0.85
					LE (C10)	0.18
		3	2.230	0.00	CT (C2 → C10)	0.98
		4	2.320	0.04	LE(C2)	0.69
					LE(C2)	0.34
		5	2.478	0.15	LE (C10)	0.80
					LE (C10)	0.21
3	10.3	1	1.838	0.12	LE (C2) + CT (C2 → C10)	0.87
					LE(C2)	0.17
		2	1.901	0.10	LE (C2) + CT (C2 → C10)	0.94
					LE(C2)	0.06
		3	1.998	0.23	LE (C10)	0.85
					LE (C10)	0.18
		4	2.273	0.02	LE(C2)	0.68
					LE(C2)	0.35
		5	2.447	0.01	CT (C2 → C10)	0.98
4	10.3	1	1.868	0.18	LE(C2)	0.83
					LE(C2)	0.22
		2	1.979	0.27	LE (C10)	0.85
					LE (C10)	0.17
		3	2.099	0.00	CT (C2 → C10)	0.99
		4	2.298	0.04	LE(C2)	0.69
					LE(C2)	0.34
		5	2.491	0.18	LE (C10)	0.81
					LE (C10)	0.20
5	10.1	1	1.869	0.18	LE(C2)	0.83
					LE(C2)	0.22
		2	1.953	0.28	LE (C10)	0.85
					LE (C10)	0.18
		3	2.237	0.00	CT (C2 → C10)	0.98
		4	2.279	0.04	LE(C2)	0.69
					LE(C2)	0.34
		5	2.461	0.14	LE (C10)	0.80
					LE (C10)	0.22
6	10.1	1	1.855	0.19	LE(C2)	0.83
					LE(C2)	0.22
		2	1.981	0.29	LE (C10)	0.85
					LE (C10)	0.17
		3	2.237	0.00	CT (C2 → C10)	0.90
		4	2.288	0.03	LE(C2)	0.58
					LE(C2)	0.44

		5	2.509	0.17	LE (C10)	0.81
					LE (C10)	0.21
7	10.2	1	1.842	0.18	LE(C2)	0.84
					LE(C2)	0.21
		2	1.966	0.15	LE (C10) + CT (C2 → C10)	0.92
					LE (C10)	0.10
		3	2.018	0.14	LE (C10) + CT (C2 → C10)	0.88
					LE (C10)	0.12
		4	2.271	0.04	LE(C2)	0.69
					LE(C2)	0.34
		5	2.509	0.14	LE (C10)	0.87
					LE (C10)	0.14
8	10.4	1	1.859	0.17	LE(C2)	0.83
					LE(C2)	0.21
		2	1.939	0.31	LE (C10)	0.85
					LE (C10)	0.17
		3	2.102	0.00	CT (C2 → C10)	0.99
		4	2.282	0.04	LE(C2)	0.70
					LE(C2)	0.33
		5	2.461	0.15	LE (C10)	0.81
					LE (C10)	0.20
9	9.9	1	1.803	0.11	LE (C2) + CT (C2 → C10)	0.88
					LE(C2)	0.15
		2	1.895	0.13	LE (C2) + CT (C2 → C10)	0.91
					LE(C2)	0.10
		3	1.955	0.23	LE (C10)	0.86
					LE (C10)	0.17
		4	2.240	0.03	LE(C2)	0.69
					LE(C2)	0.34
		5	2.440	0.05	LE (C10) + CT (C2 → C10)	0.94
10	10.5	1	1.856	0.18	LE(C2)	0.83
					LE(C2)	0.23
		2	1.923	0.29	LE (C10)	0.85
					LE (C10)	0.18
		3	2.257	0.00	LE (C2) + CT (C2 → C10)	0.59
					LE (C10)	0.42
		4	2.309	0.04	LE (C2) + CT (C2 → C10)	0.76
					LE(C2)	0.24
		5	2.436	0.13	LE (C10)	0.80
					LE (C10)	0.22

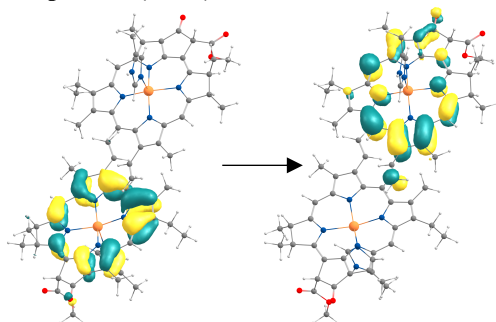
Snapshot 2 (5 ns), S3



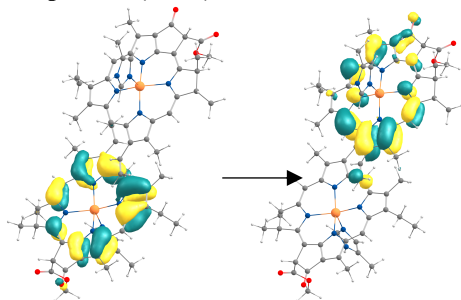
Snapshot 3 (10 ns), S1 and S2



Snapshot 4 (15 ns), S3



Snapshot 5 (20 ns), S3



Snapshot 6 (25 ns), S3

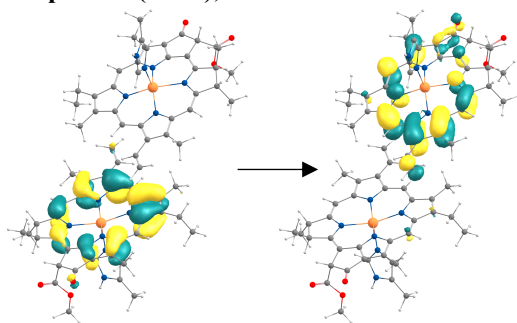
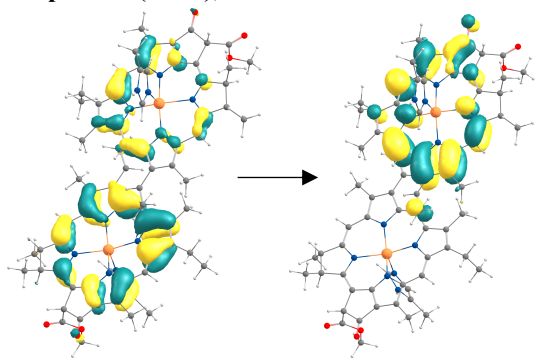
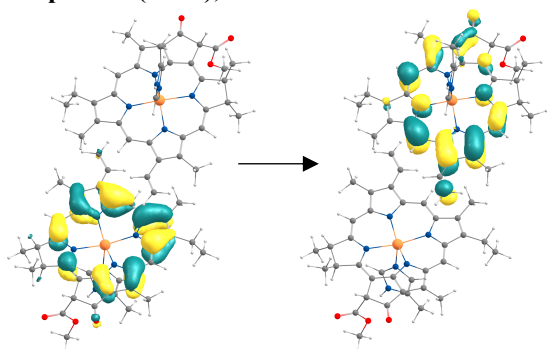


Figure S5. Natural Transition Orbitals (NTOs) for the lowest excited state with significant CT character for the C2-C10 dimer in snapshots 2-10.

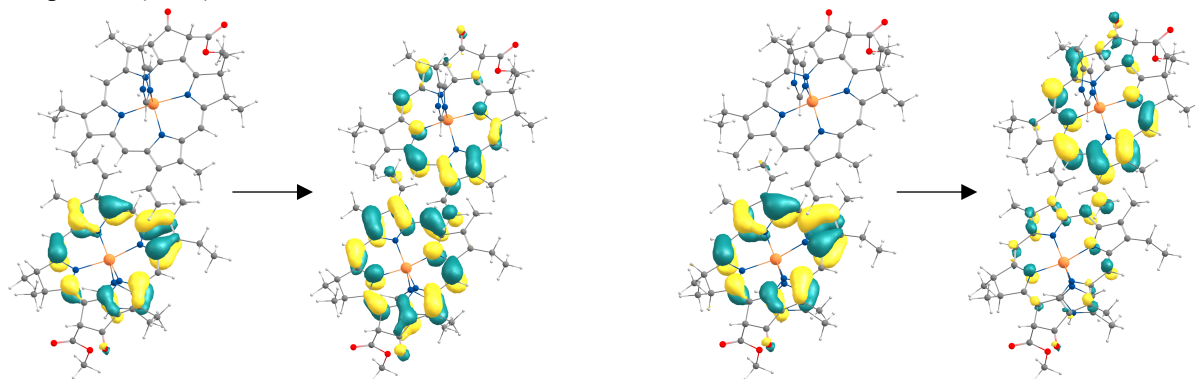
Snapshot 7 (30 ns), S2



Snapshot 8 (35 ns), S3



Snapshot 9 (40 ns), S1 and S2



Snapshot 10 (45ns), S3

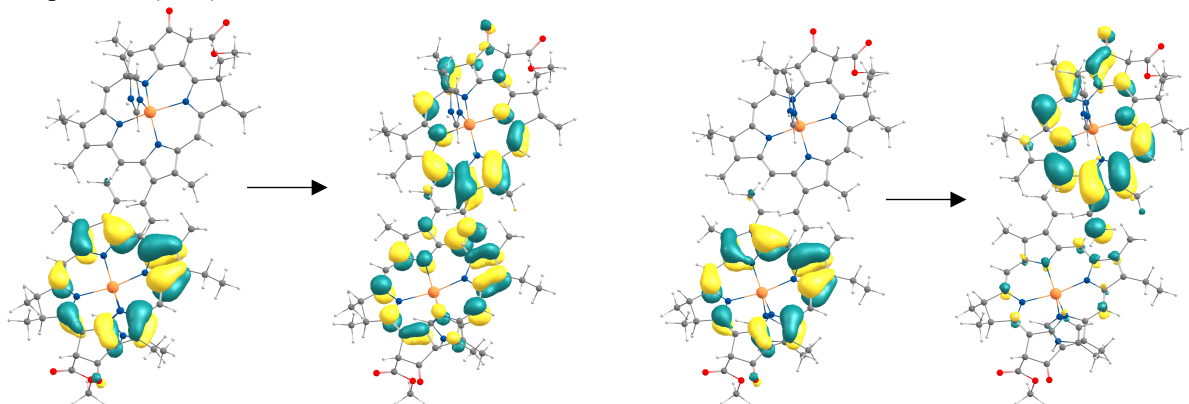


Figure S5 (continued). Natural Transition Orbitals (NTOs) for the lowest excited state with significant CT character for the C2-C10 dimer in snapshots 2-10.

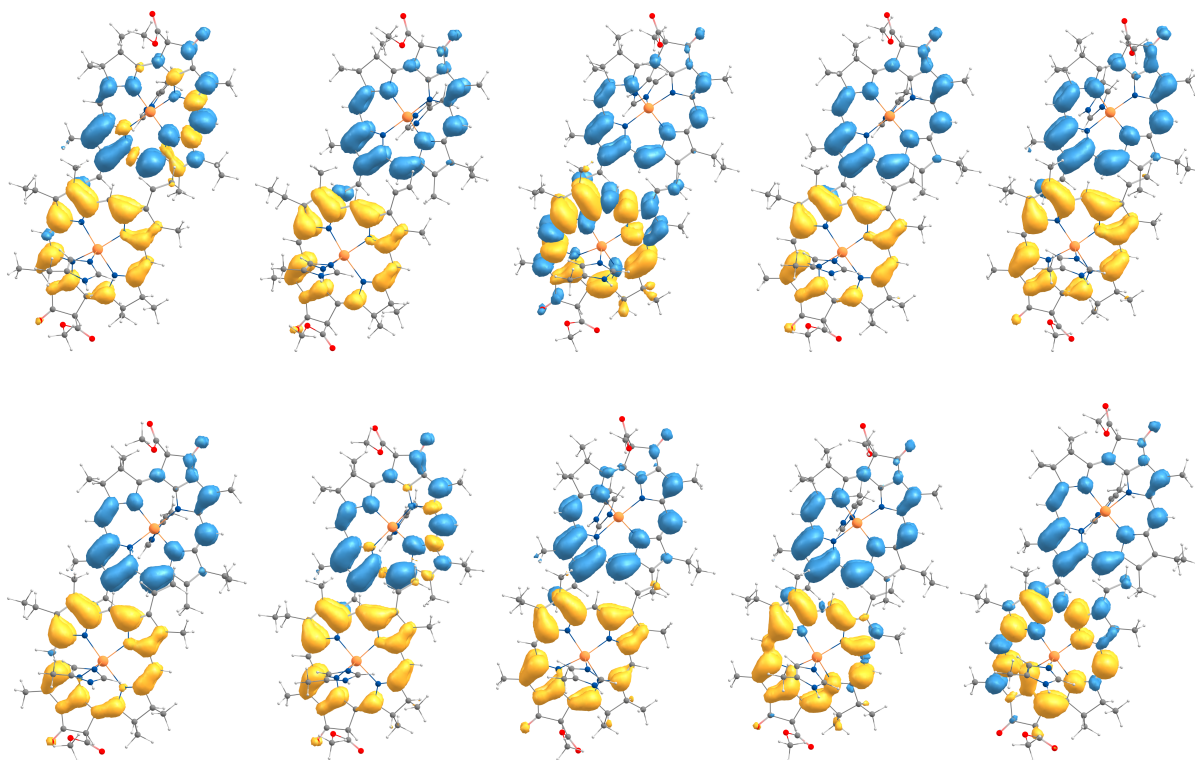


Figure S6. TD-DFT difference densities for the lowest excited states with CT character for the C2-C10 dimer in the ‘crystal-like’ (snapshot 1) and snapshots 2-10.

Table S8. Comparison of different range-separated functionals to compute the Chl a ionization potential (IP) and electron affinity (EA), the energy of the Highest Occupied Molecular Orbital (HOMO) for Chl and Chl⁻.²⁷ All energy values are in eV. HFX is the range of exact (Hartree–Fock) exchange included in each functional, and ω (in Bohr⁻¹) is the parameter controlling the range separation.

DFT Method	HFX	ω	HOMO (Chl)	IP (Chl ⁺ /Chl)	HOMO (Chl ⁻)	EA (Chl/Chl ⁻)	CT state energy
CAM-B3LYP ²⁸	19–65%	0.33	-6.1184	6.2733	-1.7153	1.9350	1.302
LC-BLYP ²⁹	0–100%	0.33	-6.8345	6.2740	-2.5112	2.0611	1.930
ω B97 ³⁰	0–100%	0.40	-6.8535	6.0935	-2.5049	2.0602	2.104
ω B97X-V ³¹	16.7–100%	0.30	-6.7753	6.2733	-2.6160	1.9738	1.943
ω B2PLYP ³²	53–100%	0.30	-6.5902	6.5702	-2.4626	1.7388	--
LC-PBE ³³	0–100%	0.47	-7.1880	6.3005	-3.0015	2.3925	1.958

Example ORCA input file for the QM/MM TD-DFT calculations conducted in the present work

```
! QMMM NoTrah
! wB97X-D3BJ RIJCOSX verytightSCF

%tddft
  TDA false
  nroots 8
  maxdim 20
  donto true
  NT0Thresh 1e-4
end

%pal nprocs 8 end
%maxcore 16000

%basis
  Basis "Def2-TZVP"
  AuxJ "Def2/J"
  AuxC "Def2-TZVP/C"
  AuxJK "Def2/JK"
end

%qmmm
  ORCAFFfilename "ps2-A1-final.ORCAFF.prms"
  Embedding Electrostatic
  ChargeAlteration CS
  QMAatoms end
end

*pdbfile 0 1 chl-opt.pdb
```

Note: complete ORCA output files of all TD-DFT calculations are provided in a separate supporting data set hosted by the Open Research Data Repository of the Max Planck Society at: <https://doi.org/10.17617/3.S2DPUE>

Cartesian coordinates (in Å) of QM regions from the QM/MM geometry optimizations of the 13 CP43 chlorophylls and of Chl_{ZD1}

Note: These coordinates are also provided as a separate plain-text file.

Note: PDB files that contain the optimized QM structures within the complete MM setup of the PSII monomer, as well as complete force field parameter files to enable reproduction of the complete simulations, are provided in a separate supporting data set, hosted by the Open Research Data Repository of the Max Planck Society at: <https://doi.org/10.17617/3.S2DPUE>

To facilitate use of these PDB files, the list below indicates the correspondence between the Chl labels used in this work and the residue numbers in the PDB files.

Site	Chl in PDB	Ligand in PDB
C1	1146	H563
C2	1147	H756
C3	1148	H444
C4	2736	
C5	1149	H767
C6	1150	H577
C7	2737	
C8	1151	H770
C9	1152	H379
C10	1153	H382
C11	2738	N365
C12	1154	H490
C13	1155	H458
Chl _{ZD1}	1145	H118

C1
88

C	109.942118107884	63.430277071805	84.822841610029
H	110.322679352993	63.116007714856	85.804607033856
H	110.804500421759	63.627637971882	84.172264450002
C	109.101613289299	64.661100257664	84.890923304930
N	108.250592035459	64.958301115770	85.939133238347
H	108.073006836008	64.357949026038	86.748335579086
C	107.634384261784	66.136312757261	85.677126360575
H	106.931717627102	66.619112486604	86.348183605036
N	108.034263990189	66.611440268213	84.507586647159
C	108.950608015071	65.708943093134	84.009156337919
H	109.444867511205	65.882903568564	83.058714690414
C	105.347785579216	72.189962612159	86.868265664590
C	103.733718163019	65.817335356744	80.216258965993
C	111.308839955818	68.698235780702	79.332540123928
C	110.292131579939	71.451380096640	86.889078934188
N	106.295464378594	69.379503129451	85.136102569923
C	104.022687090885	65.866345641133	78.900884518309
C	111.161269572482	70.143228894689	78.837531947464
C	108.793026019970	71.267102581316	87.390381634199

N	105.706267861219	67.858564116940	82.627807203343
O	111.143644262299	72.102576682389	87.474145483635
C	108.823929640112	70.451266203735	88.679818728651
N	109.096204941100	69.520082792793	84.166025411821
C	109.417716838471	70.557997018899	90.980244798628
C	108.100838096093	70.515960790211	86.263749417908
C	104.189542310911	68.301180287148	84.515857558075
C	106.678729088412	67.103593682265	80.511397939647
C	110.691168098837	69.186622580913	82.361439645729
C	104.233148246463	68.614106395636	87.675746856187
C	102.249491435827	66.442519363344	82.870353190403
C	108.755627213884	67.118098628373	78.178270684389
C	112.640148222905	70.808821812397	84.345432392646
C	106.755967133968	70.197114253492	86.135174169240
C	104.512321207117	67.710584638169	83.276667946663
C	107.991821541485	67.598299202693	80.635000914229
C	110.378174396038	69.642536292142	83.648780380073
O	108.589101563829	69.256449223241	88.740097714047
C	105.622682083308	70.680145375268	87.020193814580
C	103.623470833292	66.885403132014	82.483441415897
C	108.972497173789	67.621066498467	79.566926360526
C	111.228936986821	70.382946508984	84.575249122971
O	109.184116643763	71.225515011409	89.718145159365
C	104.473607205384	69.714274589920	86.632879262690
C	104.296713168305	66.595474333931	81.300604630375
C	110.094903706703	68.245133229688	80.076813041149
C	110.390228775243	70.704076847663	85.643635247253
C	104.978793047490	69.108243365295	85.331797676717
C	105.622429403659	67.203704363600	81.422980661596
C	109.801563585587	68.565181255403	81.463841962917
C	109.102472896176	70.168664653417	85.335030246205
N	108.516371449011	68.171196840295	81.762227207103
Mg	107.466715523073	68.436950725918	83.559843386837
H	106.260662094161	72.747491247714	87.108062612362
H	104.578196292601	72.519744502759	87.578772241207
H	102.946738707870	65.116177668923	80.522659929958
H	111.507875051838	68.025399001892	78.485351820530
H	112.184189746108	68.661572789765	79.998810123747
H	104.748033736692	66.568615655774	78.491573642369
H	103.521598687603	65.200573830688	78.198380705427
H	111.030952694655	70.803549999722	79.704034144403
H	110.276675501309	70.258355576228	78.195969657190
H	112.049275960258	70.475335951168	78.277439327391
H	108.391217816758	72.266859080293	87.614080280230
H	110.500757393525	70.439410784982	91.114847825893
H	108.922752406407	69.580713959110	90.996802042183
H	109.026285192080	71.216569146599	91.760984056157
H	103.172289580094	68.132585810947	84.874480697068
H	106.461486715780	66.587066169244	79.577899600782
H	111.705888982572	69.370901063886	82.003092684536
H	103.829625273773	69.036087606376	88.605164886372
H	105.169734257727	68.086261118070	87.911397131907
H	103.505379951294	67.879765389362	87.304702915456
H	102.119153677149	66.438742807903	83.960631582615
H	102.042085779085	65.422085212626	82.514631177958
H	101.462208172697	67.084382072425	82.441962881486
H	109.717791462217	66.976632735348	77.669716044930
H	108.147717799763	67.816390610855	77.577921295814

H	108.230733860005	66.150238842843	78.172502672158
H	113.224957273718	70.045279921901	83.811755630332
H	113.137628781757	71.039550307505	85.296196034917
H	112.664685047832	71.727808709819	83.735998244179
H	105.904374075608	70.522890104011	88.073427243833
H	103.524518732935	70.249027269323	86.483927779333
O	111.134884149960	74.175737939602	89.542747143064
H	111.984206170065	74.654646201668	89.485901327557
H	111.132019455426	73.549341469669	88.791083786571
H	109.353647105734	62.592315497268	84.397766716665
H	105.044292548816	72.563432777818	85.862592706228

C2

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C	104.198845310509	76.223534278193	92.770829455742
H	103.270897577928	75.822743362857	93.199356512176
H	104.283925482458	77.278827620695	93.066655190295
C	104.151677147447	76.078199913746	91.271178653396
C	104.929129848303	76.874623952010	90.419196528843
H	105.591191431235	77.627526796479	90.847812018336
C	104.855069531952	76.748894270171	89.031468556578
H	105.464931258332	77.386383496160	88.386825199218
C	103.993284464617	75.800506255114	88.459631339715
O	103.860714871392	75.635114991498	87.106372490455
H	104.714359019004	75.869118207760	86.676293991394
C	103.206319006636	74.999914609977	89.294765880370
H	102.562340260859	74.251539309387	88.833515142770
C	103.285072653223	75.147615443075	90.678635555311
H	102.654920054835	74.528055329416	91.320701434815
C	99.764159298549	81.172105365391	82.673045782781
H	99.413426276764	81.146353993573	83.711017774299
H	99.469191939096	80.238572613223	82.177436575913
C	101.238873336170	81.377196727407	82.524221462910
N	102.000302787158	82.156296468401	83.373639671780
H	101.631750308683	82.598684309964	84.219584889718
C	103.224125955700	82.336531718586	82.817704329114
H	104.020121383308	82.908878609322	83.282126038355
N	103.298605190111	81.702813255117	81.651830553106
C	102.068918899790	81.100254725628	81.462304988033
H	101.862904408535	80.503735176036	80.579076675816
C	108.681254409124	78.892345577814	83.690329038377
C	106.127560398117	85.803599439210	77.518501102113
C	101.414815465675	79.555155110525	75.981659465428
C	104.430961683970	76.633606936166	83.039843650114
N	106.410348054554	80.874281061551	81.864416377175
C	106.813518837207	86.955945133920	77.380878730208
C	99.981326929289	80.043322535884	76.248424647387
C	105.357520331519	77.687957620127	83.760286406594
N	105.916806560523	82.759364885909	79.600619905367
O	104.131504124868	75.543894491726	83.500261079783
C	104.720359164240	78.336546985177	84.986984118757
N	104.364677193919	79.160693250034	80.538401874323
C	102.666001583012	78.940781487036	85.990616814419
C	105.567008026770	78.797107312115	82.731695119055
C	107.480106545979	83.034881747291	81.488198600002
C	104.682076913594	83.086772291976	77.503934022036
C	102.916295764225	78.692522517102	78.637593503640

C	108.028511754229	82.432158265103	84.531514047537
C	107.867191476582	85.878569246850	80.266471284547
C	102.604673805306	82.417773738813	75.248290183522
C	102.607880683244	75.867429110933	80.094838491846
C	106.468800680362	79.853557680100	82.773782661709
C	106.820774155478	83.490978364674	80.326849097306
C	103.919754999681	81.904823321746	77.456815550760
C	103.515127008070	78.312770036689	79.846117827234
O	105.344745152210	78.900225081064	85.865575396400
C	107.629541798353	80.021719984797	83.739498561057
C	107.037608354204	84.779437753028	79.698039721286
C	102.970117338918	81.563044447012	76.414865415704
C	103.333543539074	77.071589714638	80.583309072126
O	103.374776679622	78.283945639759	84.920999615299
C	108.165757811464	81.433531223651	83.379345203484
C	106.275886126961	84.783092153637	78.531951981572
C	102.460934599649	80.320341937840	76.734823823753
C	104.046607328913	77.245958858873	81.767257909726
C	107.336170588496	81.820992841787	82.160727010299
C	105.573989772696	83.501406638319	78.496909218958
C	103.108908671542	79.916923048541	77.973541050933
C	104.673407068801	78.525508536622	81.674531414136
N	103.966625132523	80.910606648571	78.395609838926
Mg	104.890960376983	81.118604886675	80.305283518789
H	108.288456021201	77.982597538835	84.160353644029
H	109.572055365405	79.182956054588	84.260662945155
H	105.360963182963	85.597978132860	76.764015390105
H	101.480397677508	78.484350485721	76.229168821684
H	101.615538277399	79.637261671159	74.898748821990
H	107.605565532275	87.250466990561	78.063611414791
H	106.596773249544	87.627262601133	76.553616720324
H	99.243078440428	79.407403322319	75.738408762542
H	99.845572588866	81.072343249274	75.888156738916
H	99.758176615427	80.026060497410	77.324800535688
H	106.280997208749	77.208762674154	84.101407416370
H	101.689404054729	78.453540315241	86.051054091385
H	102.552491893080	80.006727054142	85.742258048302
H	103.214433710061	78.831644506711	86.933238842498
H	108.210655991824	83.724792184780	81.912668647218
H	104.540185680698	83.770157423893	76.664977305028
H	102.228365711174	77.982413064320	78.174417101426
H	106.972900039782	82.537494244899	84.817758033458
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H	107.414763846899	86.856919028357	80.057827526768
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H	103.492064485845	82.795113858600	74.721555574797
H	102.030478890700	83.304590444275	75.554560749578
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H	109.003699772400	78.623900779050	82.657104603431

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N	118.025397228004	78.657980601955	80.697041416870
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N	116.397214497171	76.490699700570	82.256125139549
C	120.963038205554	72.119669512245	78.104447979392
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C	113.583848590985	78.771672915336	83.586539565508
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C	113.293147587956	79.330633966893	81.244589642633
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O	109.622026674785	89.162081946888	85.796719297116
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H	93.514011913525	69.326720519731	72.152791939662
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H	92.587750315367	73.924537953554	60.452643657779
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H	90.672038446879	71.478205819829	73.265423413381
H	92.102197253313	72.529414596246	73.232532609775
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H	91.744587932533	68.793309095972	60.994539062445
H	93.924641603743	78.137043396562	67.932986809437
H	90.439381521685	74.778351969544	56.887093136813
H	87.372890734290	71.218220336778	63.301388860486

C6
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C	107.143995063652	60.720112847273	64.958542399277
H	107.745781255096	60.863921916631	65.862975172716
H	107.308325167790	61.583058826800	64.303823259606

C	105.701274850629	60.588193219663	65.294442355566
N	104.740654688500	60.326493117567	64.328026033183
H	104.911245497922	60.060825829122	63.349524123210
C	103.536767123945	60.232252514454	64.936447464451
H	102.611988306310	59.997600123119	64.418769249022
N	103.660572438269	60.451605855827	66.237943895588
C	105.002749624446	60.675931466224	66.475881298176
H	105.384678278917	60.870453849887	67.472681098861
C	97.539667998666	61.092761914117	64.740941401694
C	103.5610555074686	65.396234549929	70.026833470045
C	104.178281827148	57.616628808090	71.901224925327
C	99.583698595029	56.486191617809	65.221253026195
N	100.633099737692	61.152499931873	65.934438204330
C	103.965721099741	66.672630049993	69.889327826376
C	103.063561690472	57.249879195490	72.895165852427
C	99.353353851735	57.837416618761	64.402922564872
N	102.249984079938	62.587313702329	68.005401797398
O	99.129457397233	55.409515538908	64.837410695437
C	100.084087698535	57.669927053899	63.076449501801
N	101.287553784762	58.683412068110	67.409938758698
C	102.204542832028	56.989685555622	62.166773120357
C	99.944173740312	58.930292528971	65.287741740225
C	101.102693083583	63.559639922613	66.062031066515
C	103.544763472000	62.285755352640	70.066919724386
C	102.407506705715	57.613030688479	69.302857467558
C	100.590025162971	62.689738675670	62.985713319395
C	102.156125865336	66.253022024155	67.275907825816
C	105.094457698128	60.684052963690	72.282574076210
C	101.179405257841	54.956728470657	67.985739899639
C	99.900265120666	60.306223333640	65.141522524193
C	101.881192066119	63.652138068504	67.237291624823
C	103.503356903389	60.880951115351	70.204186278032
C	101.612808450162	57.542375359710	68.142526444467
O	99.576377362625	57.788903089825	61.968322797351
C	98.993956096055	61.102332850059	64.216612267050
C	102.363656372660	64.890076468482	67.827221471595
C	104.173000673976	60.118340174880	71.251235337839
C	101.052229276749	56.365205014688	67.513799429242
O	101.366182733605	57.323189549769	63.297804014760
C	99.687693409827	62.486872382476	64.210960065106
C	103.004790392959	64.537053487465	69.004075048089
C	103.821536471379	58.798753876498	71.055310708940
C	100.392087647803	56.845126130222	66.367074203499
C	100.517815764961	62.432549356838	65.493964729519
C	102.944552476357	63.076113169580	69.085598770007
C	102.962917990759	58.765984791847	69.874403515267
C	100.578658425910	58.261397030368	66.361954721939
N	102.799963777378	60.045840489132	69.386280792008
Mg	102.001905312525	60.605271232055	67.546155267534
H	97.157906175168	60.063586631361	64.759944931744
H	96.882668394026	61.667000759352	64.072911844202
H	103.641197104300	64.947368193724	71.022259831565
H	105.106107137946	57.821877211364	72.456954164609
H	104.393612018153	56.747007355794	71.258101588397
H	103.955789623262	67.206375091556	68.941528323199
H	104.342930288852	67.211680922389	70.753118713142
H	102.857670883239	58.089029172012	73.574099590340
H	103.347101512823	56.378561107979	73.503090489319

H	102.127038756697	57.013128047490	72.370603182131
H	98.286400516979	57.957613399272	64.168001901856
H	102.633830944542	57.908084051586	61.744427916515
H	101.638544576703	56.444432316676	61.403810913858
H	103.005657876609	56.365780181647	62.573078735212
H	100.902524689924	64.502575882586	65.549779113814
H	104.118887298771	62.816805695351	70.827617930714
H	102.628683597333	56.668277086755	69.802948712285
H	99.993741449417	62.717740899717	62.059744248524
H	101.321022607869	61.870884395145	62.901854487129
H	101.149137374396	63.632148466922	63.062928392280
H	101.856060985902	66.953280012776	68.069779519474
H	101.382545588486	66.259912338417	66.501049431441
H	103.078756771725	66.649354579781	66.821536460738
H	105.490260963587	59.898712466390	72.936966265862
H	104.609803309184	61.436030449193	72.919911820174
H	105.954690620179	61.187002577095	71.812846863046
H	102.208590385892	54.586709290762	67.853530423349
H	100.512338904901	54.296499118781	67.417860176612
H	100.935764412245	54.864409646029	69.054967042778
H	98.970875935791	60.668036288856	63.203094236740
H	98.958481553036	63.311369184712	64.252337097204
H	107.486993266825	59.795057427159	64.450582389277
H	97.402577143414	61.503222004996	65.773127296058

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C	101.812000000000	74.147000000000	67.884000000000
H	101.678000000000	74.825000000000	67.025000000000
H	102.382000000000	74.635000000000	68.685000000000
O	102.459000000000	72.928000000000	67.508000000000
H	103.401000000000	73.118000000000	67.316000000000
C	104.465000000000	72.010000000000	70.146000000000
C	96.892000000000	66.752000000000	66.698000000000
C	102.306000000000	66.972000000000	60.799000000000
C	107.093000000000	70.352000000000	66.415000000000
N	102.607000000000	69.741000000000	68.062000000000
C	95.974000000000	66.214000000000	67.527000000000
C	103.085000000000	65.650000000000	60.887000000000
C	106.363000000000	70.648000000000	67.781000000000
N	100.103000000000	68.580000000000	66.782000000000
O	108.288000000000	70.553000000000	66.225000000000
C	107.059000000000	69.967000000000	68.951000000000
N	103.884000000000	69.205000000000	65.465000000000
C	107.942000000000	67.920000000000	69.723000000000
C	104.917000000000	70.184000000000	67.564000000000
C	100.389000000000	69.448000000000	69.065000000000
C	99.267000000000	67.380000000000	64.815000000000
C	103.723000000000	68.445000000000	63.150000000000
C	102.129000000000	69.687000000000	71.612000000000
C	97.480000000000	68.365000000000	69.445000000000
C	99.330000000000	66.348000000000	61.840000000000
C	106.803000000000	69.323000000000	63.066000000000
C	103.846000000000	70.194000000000	68.449000000000
C	99.647000000000	68.819000000000	68.049000000000
C	100.362000000000	67.541000000000	63.939000000000
C	104.456000000000	68.988000000000	64.214000000000

O	107.343000000000	70.497000000000	70.006000000000
C	103.855000000000	70.621000000000	69.913000000000
C	98.326000000000	68.242000000000	68.223000000000
C	100.429000000000	67.045000000000	62.573000000000
C	105.853000000000	69.381000000000	64.216000000000
O	107.312000000000	68.670000000000	68.665000000000
C	102.365000000000	70.466000000000	70.317000000000
C	98.027000000000	67.583000000000	67.038000000000
C	101.694000000000	67.348000000000	62.109000000000
C	106.088000000000	69.831000000000	65.516000000000
C	101.727000000000	69.843000000000	69.087000000000
C	99.152000000000	67.833000000000	66.132000000000
C	102.384000000000	68.028000000000	63.189000000000
C	104.855000000000	69.718000000000	66.229000000000
N	101.541000000000	68.154000000000	64.274000000000
Mg	101.920000000000	69.221000000000	66.047000000000
H	103.956000000000	72.750000000000	69.515000000000
H	105.531000000000	72.022000000000	69.895000000000
H	96.798000000000	66.526000000000	65.632000000000
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H	96.004000000000	66.349000000000	68.606000000000
H	95.186000000000	65.566000000000	67.143000000000
H	103.912000000000	65.731000000000	61.607000000000
H	103.505000000000	65.352000000000	59.914000000000
H	102.428000000000	64.839000000000	61.235000000000
H	106.430000000000	71.731000000000	67.963000000000
H	107.197000000000	67.643000000000	70.481000000000
H	108.729000000000	68.517000000000	70.200000000000
H	108.354000000000	67.029000000000	69.242000000000
H	99.858000000000	69.575000000000	70.007000000000
H	98.417000000000	66.827000000000	64.412000000000
H	104.255000000000	68.305000000000	62.207000000000
H	102.503000000000	70.244000000000	72.478000000000
H	102.638000000000	68.716000000000	71.586000000000
H	101.061000000000	69.491000000000	71.773000000000
H	96.419000000000	68.479000000000	69.172000000000
H	97.766000000000	69.237000000000	70.048000000000
H	97.549000000000	67.477000000000	70.092000000000
H	99.308000000000	65.267000000000	62.054000000000
H	99.441000000000	66.455000000000	60.751000000000
H	98.340000000000	66.735000000000	62.121000000000
H	106.979000000000	68.293000000000	62.723000000000
H	107.770000000000	69.756000000000	63.346000000000
H	106.411000000000	69.875000000000	62.198000000000
H	104.454000000000	69.872000000000	70.457000000000
H	101.925000000000	71.473000000000	70.428000000000
O	101.535000000000	71.215000000000	65.753000000000
H	101.875000000000	71.854000000000	66.449000000000
H	101.197000000000	71.796000000000	65.048000000000
H	100.819857000000	73.894143000000	68.292571000000
H	104.396429000000	72.428571000000	71.176000000000

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C	96.212002418105	79.573444006904	62.726824265818
H	96.113178490932	79.171658970183	63.743477333323

H	96.766303091423	78.849494049062	62.110145787337
C	96.923622617470	80.880380448324	62.780137489744
N	97.290614739638	81.588693347005	61.647702541293
H	97.065456049817	81.382873268754	60.658365867204
C	97.945567841841	82.702960902311	62.041793076729
H	98.324659252607	83.447222343743	61.350921990609
N	98.026124902752	82.762254499137	63.368086677330
C	97.383898801690	81.634243241325	63.838002395982
H	97.271210443107	81.439656121796	64.897820679919
C	101.457741777628	87.001491646284	60.252839364510
C	102.481829676886	81.821146373134	67.911233482247
C	95.409052594277	85.641358384256	68.572898139744
C	96.599665339080	87.551910979383	60.771037925856
N	100.189131778642	84.835239581554	62.521470963150
C	103.416114662022	80.860629813172	68.051847495454
C	95.412639487147	87.070256740687	69.128121627133
C	97.848950374349	86.812720270355	60.149636872009
N	100.692404832293	83.611787846044	65.200616602749
O	95.830012543002	88.208013142264	60.078970844546
C	97.366373793643	85.751640470934	59.178522064463
N	97.709433828616	85.906378845323	63.698622504049
C	98.042210651224	84.184333704278	57.538216839408
C	98.537441251113	86.130388696877	61.331071361243
C	102.138010615343	83.520286189886	63.213641863934
C	99.843533759284	83.441915662462	67.496023259050
C	96.276009274619	86.189416300476	65.649060211453
C	101.771929325474	83.195070012937	60.067890959849
C	104.010455439980	81.886093717058	65.095200863862
C	97.972266600116	84.095925411925	69.906078921449
C	94.699804161751	88.181897223101	63.698597970493
C	99.769933424383	85.502377587687	61.400593033385
C	101.820812307146	83.202805736057	64.551125854634
C	98.651588529355	84.187988477859	67.383586141046
C	96.603090241331	86.483103241206	64.317251574698
O	96.252952141698	85.244467076146	59.157786481217
C	100.879783350124	85.574705510895	60.367653869902
C	102.670513608496	82.435287951707	65.440986309178
C	97.735790761474	84.473675979985	68.482140448089
C	95.888083006154	87.337244275466	63.390438892802
O	98.344135658434	85.365491966515	58.321513077966
C	101.867697884314	84.499330629660	60.871904662512
C	102.030759263795	82.418326131139	66.672241283969
C	96.685575608536	85.184271915774	67.936135550068
C	96.580943772152	87.208523444678	62.177666067488
C	101.408472137819	84.275792431574	62.307160157270
C	100.786135956169	83.172696645970	66.501279624555
C	97.011481687356	85.384861078583	66.530345119806
C	97.677379769324	86.328955150925	62.435756013581
N	98.189134918244	84.738346315387	66.222162419868
Mg	99.007819041257	84.434084875537	64.326663216291
H	100.781614209792	87.624998767520	59.657823824739
H	102.429245933813	86.973239430838	59.743207090113
H	101.976491557680	82.171686483598	68.817377289024
H	95.145300351088	84.952556251882	69.382403617216
H	94.606526950065	85.550753358355	67.823134597204
H	103.941138668704	80.410678259883	67.211806009940
H	103.647369076652	80.447582968084	69.031655158743
H	95.742226406897	87.794754933054	68.369600284953

H	96.081843167036	87.152600721024	69.993209628167
H	94.405374395866	87.357407869398	69.462529120534
H	98.482496355699	87.546358211484	59.629438435790
H	98.943727578396	83.984958017158	56.950542937644
H	97.185810385790	84.373120486768	56.877572044758
H	97.795348417691	83.335542741532	58.187466448511
H	103.084759373803	83.124524492809	62.841696280288
H	100.060107234242	83.048292351553	68.490596453039
H	95.368432944971	86.647426199911	66.046086992700
H	102.081397546475	83.349734877806	59.023181749080
H	100.736513176952	82.821522219572	60.062375151643
H	102.402019608802	82.409215796096	60.506349506459
H	104.727011765952	82.053474778908	65.913109815616
H	104.416334208157	82.350607486416	64.189044790393
H	103.986168030329	80.801081462781	64.910985616167
H	98.877577691644	84.586204651094	70.297488950333
H	98.132226764660	83.014836885961	70.035926576725
H	97.134321192773	84.396348761021	70.542568724118
H	93.915418144755	87.607812635370	64.212541539343
H	94.269134518186	88.590777532283	62.778737897808
H	94.971482050503	89.023379031524	64.356954513510
H	100.490421039635	85.298870616866	59.379877256775
H	102.906996527486	84.865535108672	60.846843030177
O	98.801903198594	89.723680458424	61.338288438225
H	98.838886868992	89.379982738160	62.245688036978
H	99.404622637301	90.497010655249	61.335295438262
H	95.191117856033	79.697669909424	62.308198212604
H	101.598620984311	87.518738624495	61.229843402774

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C	112.231601448480	79.264739847073	64.394074052524
H	112.998091165317	79.124943672995	63.618893753726
H	112.408587807293	78.524307888592	65.190048746320
C	110.846874582298	79.126000870546	63.851681136882
N	110.494257402590	78.390640522974	62.731256027769
H	111.111207268865	77.951245264970	62.038809195305
C	109.138658117228	78.403513875809	62.627255125895
H	108.594841417204	77.914032142007	61.826052637772
N	108.598829921982	79.100337501000	63.618869199187
C	109.651331769031	79.552164155086	64.383382416413
H	109.480113587685	80.149756683517	65.273921559346
C	101.737283822947	74.257645906570	67.813923610687
H	101.511632305577	75.041848014882	67.071179085803
H	102.388316818007	74.676979904787	68.595757792804
O	102.343825338913	73.116914119191	67.218749626018
H	103.287457544627	73.336817798885	67.055446678858
C	108.369448199811	77.964339331199	69.043654870921
C	108.033150601967	84.796551539228	62.394207375087
C	103.992476843215	78.732766176255	59.189442994528
C	105.202436290460	75.190134242653	66.493152876580
N	106.931073420848	79.687604616075	66.369614049484
C	108.679861123884	85.971123892270	62.528504983203
C	102.503688160903	79.115609014666	59.148991109762
C	105.704155383536	76.233180320606	67.580140568793
N	107.040726337526	81.759220924879	64.221116777643
O	104.932707953376	74.019545492861	66.755393406048

C	104.527971157878	76.439222349236	68.533912502526
N	105.604514673066	77.971158625926	64.345165611849
C	102.459274623723	77.605287977364	68.766141237097
C	106.097009183363	77.464122972263	66.776270755269
C	107.855965380460	81.954399050223	66.527780076374
C	106.400721834216	82.241558466158	61.899634639240
C	104.784742167117	77.646136820914	62.068486364568
C	106.933948883159	81.305805763645	69.467866982417
C	108.913972930841	84.729349736201	65.521560328763
C	105.128380381130	81.679811619242	59.055328675379
C	104.215595832075	74.668480692938	63.156902943291
C	106.723465535053	78.622319213141	67.211379389623
C	107.677582172963	82.443699191458	65.219135092223
C	105.759307142588	81.039866395034	61.531517833552
C	105.043046964728	77.161445089999	63.360722253067
O	104.339891129355	75.794138609783	69.538314639289
C	107.235496024175	78.905254300270	68.614448409079
C	108.131810121651	83.732973798320	64.732464746417
C	105.177159332786	80.756540418137	60.230346317233
C	104.756311131358	75.842476165967	63.897855063187
O	103.678298773397	77.378587802944	68.033455113514
C	107.690667028655	80.381916589961	68.520187413359
C	107.737797628665	83.805480410421	63.400257290329
C	104.728155098268	79.450946185885	60.276899304862
C	105.135713624532	75.915686741876	65.243072820050
C	107.484893094310	80.718223116028	67.056198686168
C	107.024153135208	82.562140743926	63.109625030267
C	105.045206950861	78.947298757657	61.602952908355
C	105.648766598862	77.231360215439	65.455865407331
N	105.665438326910	79.937744107204	62.335190885141
Mg	106.614478585648	79.738369081811	64.195151986497
H	109.263897096333	78.163039928658	68.437426495030
H	108.094519477422	76.908660820541	68.928085872831
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H	104.459769315797	78.968925560375	58.217940476420
H	109.018989209782	86.350191834923	63.488841409431
H	108.910378634755	86.579413634176	61.656408739166
H	101.996057136217	78.756073886322	60.054033353039
H	101.999988997483	78.690374613711	58.269011541515
H	102.379087797426	80.206825950831	59.109806610842
H	106.502757080476	75.770123734251	68.173330821101
H	101.652397113216	77.656093222481	68.026920646564
H	102.543595859585	78.564481544570	69.294010540016
H	102.281823713996	76.797929875915	69.486061049804
H	108.335330709960	82.630203730652	67.237732213157
H	106.430174695979	83.010320200399	61.126438164718
H	104.306545064049	76.960368557857	61.366025579306
H	107.199581036716	82.359681054657	69.319211562234
H	107.139903678574	81.039090411653	70.513903858036
H	105.854776002079	81.211064278766	69.314788057929
H	109.946732196230	84.820467933898	65.146287088284
H	108.974309713535	84.444891977532	66.579408170652
H	108.473992790514	85.736500382439	65.472336001677
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H	104.107896338866	81.780850013641	58.655425361860
H	103.564221395673	74.066090751075	63.805643265896

H	105.033972402959	74.004978976502	62.830657654182
H	103.656770062075	74.974102808786	62.261821251141
H	106.388851306823	78.809981470388	69.313526571042
H	108.768165185229	80.463389362412	68.735808775228
H	112.380159215574	80.277277827089	64.825761495171
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O	107.831847229185	90.953776043531	68.004925163651
C	105.330496593975	89.263901741858	67.530233280090
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C	108.472442737168	85.019874931608	74.482228292146
C	108.902441196822	88.308518693788	71.663690349427
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C	105.024629744073	84.620824306231	69.821217501735

C	106.763237853211	83.358373512065	73.669946773731
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Mg	107.409602335674	85.552079254966	71.632939578429
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H	111.018714684249	89.078231037358	77.226450781338
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H	102.704995586577	89.085532909422	67.850411653266
H	103.187852203458	90.801188426205	67.770511035641
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C	110.200040596092	88.931077857412	66.070296308015
C	105.338077991612	94.006308652806	62.299788106227
C	108.620551318019	90.881914946497	55.486768830767
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C	110.531966682556	88.004718564601	66.989814952860
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N	109.935999072977	89.290682381082	62.390816277866
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C	109.609993063962	88.556108324238	55.035508667165
N	108.282987624334	90.801751589057	59.002265544191
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C	109.784678437088	89.680816742584	57.309878492639
C	111.709409638837	87.931377884878	61.382888010637
C	108.501022915276	90.471123697303	63.999364479759
C	106.704093026303	92.437053907297	59.917292247096
C	113.091225760921	86.394549807741	59.034356298979
C	112.272632055756	87.153693121010	64.406238175812
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C	106.318321865173	93.144402352701	56.792489244671
C	110.696137631268	89.018926903488	58.111371294619
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C	107.732186977239	91.266835551756	63.121279311356
C	107.332301294314	91.808911609623	58.821966208520
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N	107.820638681149	91.228057868791	61.757113080475
Mg	108.921691713209	89.794289232058	60.669894830713
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H	113.883485403046	88.520589138908	56.711387913400
H	109.787532811894	89.877204985992	66.430013950530
H	104.559528857025	93.892992306801	63.068597571169
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H	113.788188785977	86.193526894826	58.207145271137
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H	105.840856773628	91.707663590809	65.414469997206
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H	105.844262330299	93.797457374333	57.532810583875
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H	108.812954711720	95.330338270332	53.837644256609
H	109.137668295588	94.232907729936	52.801741362452
H	105.548358452107	87.098273617295	59.399615265200
H	113.093600037826	90.084645046364	57.043624327252

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H	110.012951792232	70.291065489010	66.370297781700
C	111.958880475450	70.723119409333	65.672760121747
H	111.740795585147	71.473620718584	64.920065786883
N	113.164258347922	70.264244208239	65.986331788871
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H	113.822693058932	68.828236547543	67.441872950393
C	115.025814455289	72.871781918308	70.532273444832
C	118.131951499006	66.496456532865	63.973880770229
C	114.273716603513	72.059587684490	59.705258521065
C	113.695651362981	75.955150000336	66.790377708368
N	115.720243394032	71.621228333173	67.324391961116
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C	114.676504034063	73.787776061456	67.425067565081
C	116.954973103950	69.549734529143	67.746789138451
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N	115.084663659401	70.938743740069	63.200486333188
Mg	115.027697230826	71.027068326729	65.312947135765
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H	119.745577274640	65.807813453679	65.202310284652
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H	116.855525473439	69.211003638991	59.776361928642
H	115.277355149706	69.455994915868	58.999087751554
H	115.508454601381	68.155268092878	60.177903034303
H	112.674062685752	75.590103621725	62.373375679845
H	113.580115999246	76.839335071631	63.258683714382
H	111.961113637788	76.397468856193	63.788812404835
H	116.713227530196	73.672273150852	69.444357013974
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C	124.056189892033	83.140776609506	59.724518477926
C	124.927743149147	83.650070318217	58.750067371571
H	125.357250855329	84.645840353859	58.890202401584
C	125.244164300259	82.922736320553	57.601904734320
H	125.907650759211	83.334014361312	56.838461678858
C	124.704731740178	81.642175972526	57.414282301720

O	124.993648253728	80.978560868099	56.255202503599
H	124.539905715427	80.102575721665	56.281564260944
C	123.892078628689	81.088039492858	58.412494475652
H	123.512825640215	80.071648415821	58.298545244613
C	123.575740804892	81.835352755153	59.544956528254
H	122.920319619897	81.393403149915	60.299650951505
C	119.014569482519	81.534698093669	59.833898275720
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H	118.050608324771	81.282040358820	59.366869115083
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N	120.201167370213	79.645118854376	58.675726660466
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C	120.571324714289	79.684546058850	60.835526153093
H	120.601049092224	79.916011589365	61.894611788942
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C	118.423214229173	75.474901200445	65.015747275754
C	124.952124591120	80.024462137468	65.731438662514
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N	122.465307703204	75.736791789824	59.815685863060
C	117.519033482869	74.565693614815	65.424406881697
C	126.115523100338	79.142446566525	66.212910930015
C	125.340689515881	76.843310479153	57.487510225702
N	120.903438696495	76.102155765566	62.343032328998
O	127.402947515074	78.263419387756	57.397523249087
C	124.671362876286	77.538256130044	56.330111556233
N	124.291909199985	77.796745641164	60.871804485300
C	124.574781313514	77.886619216090	54.006537812257
C	124.391047812741	76.606313953312	58.651210090375
C	120.432701706491	74.545870900041	60.505514482655
C	120.930164022473	77.199277887249	64.536019786341
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C	120.463039131115	74.742773094470	57.310969346152
C	118.101486175168	73.612705551942	62.376927251872
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C	123.331758300678	75.719242869613	58.750992965688
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C	125.139792979276	78.760428389667	61.411595933593
O	123.805561315681	78.403145545705	56.445499658900
C	122.984375242825	74.596121498124	57.790478012394
C	119.100361571381	74.681454268307	62.664926233317
C	122.752192554292	78.676645147550	65.530816133675
C	126.190421617600	79.088845828851	60.480689616768
O	125.173123913629	77.182296448738	55.131229864509
C	121.556424504628	74.205334752053	58.240229629057
C	119.210166030696	75.471530080337	63.800419130921
C	123.892268430401	79.253295120178	65.009604432388
C	125.949040816220	78.275235094613	59.358853722486
C	121.464034925240	74.842014244412	59.618675525809
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C	124.777293683747	77.516151354295	59.662179739151
N	122.842971807808	78.101434497322	63.285868581319
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H	118.613074299862	76.317801735338	65.687105637463
H	124.511149453052	80.538954562648	66.594273954241
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H	126.884295054897	79.748435752088	66.714292271044
H	126.585327394149	78.614428736619	65.370525497249
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H	125.883463277266	75.956306882665	57.132569648985
H	125.058193074102	77.489313513302	53.114253547491
H	124.751636843290	78.964122939374	54.091610261402
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H	120.435880276018	77.231038783223	65.507455054341
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H	127.005570169873	81.008583058462	60.040581450452
H	128.231740280063	79.755071601844	60.363337561589
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H	121.444083669951	73.114212204858	58.311906512437
H	122.764130245710	84.724519649378	60.515645065281
H	119.464784702153	82.394796200562	59.293341891174
H	124.146738270111	72.958577772272	58.816146234436

Chlz-D1

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C	74.262563985213	71.123412331221	80.117565905605
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C	74.267613373371	68.051122322530	82.072028949681
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C	78.530702283773	63.997715282684	83.267952862898
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C	69.072378397676	63.466921866207	79.628329005121
C	74.136383715966	65.007163678305	85.843619663373
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C	75.566425203347	65.235457824859	83.848415272745
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C	78.508840004928	67.746761079346	82.131294292813
C	78.294764638389	65.737011148012	76.479290614429
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C	72.456875258925	64.431133062245	78.359419429843
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O	75.501259095278	67.823957192466	84.989943810698
C	78.089832385185	65.472698994723	83.180172525315
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C	75.768838978915	65.166569507628	76.499109412164
C	70.469675107899	63.913152183320	79.332046954175
C	73.373387095561	64.758923759988	84.633742750516
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C	74.783520338753	65.004051459232	77.563012748887
C	71.480475596459	64.244573147007	80.327035069430
C	74.231601597352	64.929845967609	83.507586401159
N	72.662123975633	64.570846100616	79.702123653288
Mg	74.398075308809	65.381932494002	80.584829363763
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H	78.099344961254	63.559463665919	84.175996547512
H	74.481659229878	64.556889258656	74.891596990943
H	68.412666414429	63.721557931165	78.783621761563
H	68.674967460098	64.023265837510	80.492292713886
H	77.200574423621	65.773380600454	74.135033527194
H	75.827556880915	65.163513943208	73.031714308286
H	69.614955586010	61.682014235543	80.765669745253
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H	67.947979397865	61.656204171961	80.135350490374
H	76.333293270414	64.798092059634	85.881170519182
H	75.471882399834	68.848488306235	87.500109029877
H	77.073223454263	69.007058270201	86.729593778516
H	76.949748108558	68.338612794682	88.399520299366
H	78.616930010492	66.190687693350	79.200156961548
H	73.136633717054	64.439660541745	76.355246295932
H	70.292788346103	63.953817049091	82.072773203721
H	79.228226274248	68.045136842923	82.907563393426
H	77.506267891932	68.061682710944	82.458449321710
H	78.753113873194	68.287876616527	81.206641825600
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H	79.103835145693	65.761679041390	77.220300261128
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H	69.395202025092	63.680856478685	76.812014064459
H	70.873382445384	62.862433644399	76.281155295019

H	70.315071681284	63.289352547383	84.408877010274
H	70.173489935444	64.984990433343	84.882180359927
H	71.089585874695	63.871466727396	85.911884344828
H	78.357156858166	66.013662744120	84.098746856976
H	79.551459072961	65.925325060334	81.573082536503
H	75.289165037607	71.507529442906	79.946925804049
H	79.616943226798	63.779397450177	83.304050133430

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