## Supporting Information: On the Role of the Special Pair in Photosystems as a Charge Transfer Rectifier

Huseyin Aksu,<sup>†</sup> Alexander Schubert,<sup>†,‡,§</sup> Srijana Bhandari,<sup>†</sup> Atsushi Yamada,<sup>¶</sup> Eitan Geva,<sup>‡</sup> and Barry D. Dunietz<sup>\*,†</sup>

Department of Chemistry and Biochemistry, Kent State University, Kent, OH 44242, USA, Department of Chemistry, University of Michigan, Ann Arbor, MI 48109, USA, and Center for Computational Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8577 Japan Received February 8, 2020; E-mail: bdunietz@kent.edu

S2-S5: SI Tables and Figures.

S4-S8: X-Ray atoms coord. (Å).

 $<sup>^\</sup>dagger \mathrm{Department}$  of Chemistry and Biochemistry, Kent State University, Kent, OH 44242, USA

 $<sup>^{\</sup>ddagger} \mathrm{Department}$  of Chemistry, University of Michigan, Ann Arbor, MI 48109, USA

 $<sup>\</sup>P$ Center for Computational Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8577 Japan

 $<sup>{}^{\</sup>S} \mbox{Present}$  address: The Institute of Physical Chemistry, Friedrich-Schiller-University, Jena, Germany

SI Table S1. Excited states of the special pair calculated with SRSH-PCM scheme at various dielectric constants. Structures are obtained in corresponding constant.

ε	state	main	excitation	oscillator	net charge						
		configuration	energy(eV)	strength							
	$S_1$	$H \rightarrow L(0.80)$ $H-1 \rightarrow L+1(0.37)$	1.8709	0.79	0.02						
CAS	$S_2$	$H \rightarrow L+1(0.67)$ $H \rightarrow L+1(0.71)$ $H-1 \rightarrow L(0.71)$	1.9225	0.02	0.02						
GAS	$\operatorname{CT}_1$	$\begin{array}{l} \mathrm{H\text{-}1} \rightarrow \mathrm{L}(\text{-}0.56) \\ \mathrm{H} \rightarrow \mathrm{L}(0.53) \end{array}$	2.3459	0.00	-0.46		$CT_1$	$H \rightarrow L(0.87)$	1.5645	0.23	-0.78
	$\mathrm{CT}_2$	$H \rightarrow L+1(0.58)$ $H-1 \rightarrow L(0.89)$ $H \rightarrow L(-0.22)$	2.4091	0.00	0.65		$\mathrm{CT}_2$	$H \rightarrow L+1(0.41)$ $H \rightarrow L(-0.41)$ $H \rightarrow L+1(0.80)$	1.6112	0.15	0.66
	$S_1$ $S_2$	$ \begin{array}{c} \mathrm{H} \rightarrow \mathrm{L}(0.22) \\ \mathrm{H} \rightarrow \mathrm{L}(0.92) \\ \mathrm{H} \rightarrow \mathrm{L}{+}1(0.92) \end{array} $	1.6690 1.7273	0.89 0.05	-0.14 0.01	2.3		$H^{-1} \rightarrow L(-0.36)$			
1.2	$\operatorname{CT}_1$	$H-1 \rightarrow L(0.88)$	1.9992	0.10	-0.69		S <sub>1</sub>	$\begin{array}{l} \text{H-1} \rightarrow \text{L+1}(0.94) \\ \text{H} \rightarrow \text{L}(0.26) \\ \end{array}$	1.7915	0.67	0.12
	$\mathrm{CT}_2$	$H-1 \rightarrow L+1(0.27)$ $H-1 \rightarrow L(-0.27)$ $H-1 \rightarrow L+1(0.94)$	2.0858	0.08	0.78		S <sub>2</sub>	$H \rightarrow L+1(0.40)$ $H-1 \rightarrow L(0.90)$ $H \rightarrow L(0.85)$	1.8069	0.03	-0.03
	$S_1$ $S_2$	$H \rightarrow L(0.94)$ $H \rightarrow L+1(0.95)$	1.6603 1.7193	0.81 0.07	-0.20 0.02		$CT_2$	$H \rightarrow L(0.42)$ $H \rightarrow L(-0.43)$	1.6037	0.14	0.70
1.3	$\operatorname{CT}_1$	$H-1 \rightarrow L(0.91)$	1.9606	0.13	-0.62			$\begin{array}{l} \mathrm{H} \rightarrow \mathrm{L+1(0.78)} \\ \mathrm{H-1} \rightarrow \mathrm{L(-0.38)} \end{array}$			
	$\mathrm{CT}_2$	$H-1 \rightarrow L+1(0.27)$ $H-1 \rightarrow L(-0.27)$ $H \rightarrow L+1(0.01)$	2.0395	0.10	0.75	2.4	$S_1$	$H-1 \rightarrow L+1(0.93)$ $H \rightarrow L(0.28)$	1.7891	0.68	0.11
	$S_1$ $S_2$	$H \rightarrow L(0.96)$ $H \rightarrow L+1(0.97)$	1.6496 1.7101	0.72 0.11	-0.27 0.09		$S_2$	$H \rightarrow L+1(0.41)$ $H-1 \rightarrow L(0.89)$	1.8070	0.04	-0.04
1.4	$\operatorname{CT}_1$	$\text{H-1} \rightarrow \text{L}(0.93)$	1.9327	0.15	-0.55		$CT_1$	$H \rightarrow L(0.82)$ $H \rightarrow L+1(0.46)$	1.5463	0.18	-0.84
	$\mathrm{CT}_2$	$H-1 \rightarrow L+1(0.27)$ $H-1 \rightarrow L(-0.27)$ $H_1 \rightarrow L+1(0.04)$	2.0025	0.13	0.72		$CT_2$	$H \rightarrow L(-0.45)$ $H \rightarrow L+1(0.74)$ $H \downarrow + L(0.20)$	1.5896	0.13	0.76
	$S_1$	$H-1 \rightarrow L+1(0.94)$ $H \rightarrow L(0.98)$	1.6384	0.64	-0.35	2.6		$H=1 \rightarrow L(-0.39)$			
1.5	$S_2$	$H \rightarrow L+1(0.98)$	1.7001	0.14	0.14		$S_1$	$\begin{array}{l} \text{H-1} \rightarrow \text{L+1(0.91)} \\ \text{H} \rightarrow \text{L(0.33)} \\ \end{array}$	1.7849	0.71	0.09
	CT <sub>1</sub>	$H-1 \rightarrow L(0.94)$ $H-1 \rightarrow L+1(0.27)$ $H_{-1} \rightarrow L(-0.27)$	1.9086	0.18	-0.48		S <sub>2</sub>	$H \rightarrow L+1(0.43)$ $H-1 \rightarrow L(0.87)$ $H \rightarrow L(0.80)$	1.8073	0.05	-0.03
	S12	$H^{-1} \rightarrow L^{+1}(0.94)$ $H \rightarrow L(0.98)$	1.6261	0.56	-0.42		CT <sub>2</sub>	$H \rightarrow L(0.30)$ $H \rightarrow L+1(0.48)$ $H \rightarrow L(-0.47)$	1.5776	0.14	0.81
1.6	$S_2$	$\mathrm{H} \rightarrow \mathrm{L+1}(0.98)$	1.6904	0.16	0.20			$H \rightarrow L+1(0.72)$ H-1 $\rightarrow L(-0.40)$			
	CT <sub>1</sub>	$H-1 \rightarrow L(0.94)$ $H-1 \rightarrow L+1(0.27)$ $H_1 \rightarrow L(0.27)$	1.8911	0.20	-0.42	2.8	5	$H-1 \to L+1(0.31)$	1 7000	0.72	0.00
	S1	$H-1 \rightarrow L(-0.27)$ $H-1 \rightarrow L+1(0.94)$ $H \rightarrow L(0.98)$	1.9458	0.20	-0.48		$S_1$	$H \rightarrow L+1(0.36)$ $H \rightarrow L+1(0.44)$	1.7822	0.75	-0.08
1.7	$S_2$	$H \rightarrow L+1(0.98)$	1.6840	0.18	0.27		$CT_1$	$H-1 \rightarrow L(0.86)$ $H \rightarrow L(0.78)$	1.5247	0.12	-0.89
	$CT_1$	$H-1 \rightarrow L(0.94)$ $H-1 \rightarrow L+1(0.28)$	1.8769	0.22	-0.37		$\mathrm{CT}_2$	$H \rightarrow L+1(0.50)$ $H \rightarrow L(-0.48)$	1.5653	0.11	0.84
	$\frac{CT_2}{S_1}$	$H-1 \rightarrow L(-0.28)$ $H \rightarrow L(0.50)$ $H \rightarrow L+1(0.77)$	1.9240	0.22	-0.54			$H \rightarrow L+1(0.69)$ $H-1 \rightarrow L(-0.41)$ $H-1 \rightarrow L+1(0.34)$			
	$S_2$	$H-1 \rightarrow L+1(0.32)$ $H \rightarrow L(0.83)$ $H \rightarrow L+1(-0.48)$	1.6737	0.15	0.38	3.0	$S_1$	$H \rightarrow L(0.39)$ H-1 $\rightarrow$ L+1(0.88)	1.7798	0.75	0.06
1.8	$CT_1$	$H \rightarrow L+1(-0.40)$	1.8531	0.24	-0.35		$S_2$	$H-1 \rightarrow L+1(0.85)$ $H \rightarrow L+1(0.46)$	1.8073	0.05	-0.02
		$\begin{array}{l} \mathrm{H-1} \rightarrow \mathrm{L+1(0.86)} \\ \mathrm{H} \rightarrow \mathrm{L+1(0.40)} \\ \end{array}$					$CT_1$	$H \rightarrow L(0.74)$ $H \rightarrow L+1(0.52)$	1.4873	0.06	-0.93
	CT <sub>2</sub>	$H-1 \rightarrow L(0.91)$ $H-1 \rightarrow L+1(-0.31)$ $H \rightarrow L(0.42)$	1.8716	0.25	0.42		$\mathrm{CT}_2$	$H-1 \rightarrow L(0.36)$ $H-1 \rightarrow L(-0.38)$ $H \rightarrow L+1(0.64)$	1.5300	0.08	0.91
	51	$H \rightarrow L(0.42)$ $H \rightarrow L+1(0.77)$ $H-1 \rightarrow L+1(0.36)$	1.3980	0.42	-0.58	4.0		$H \rightarrow L+1(0.04)$ $H \rightarrow L(0.48)$			
	$S_2$	$\begin{array}{l} \mathrm{H} \rightarrow \mathrm{L}(0.85) \\ \mathrm{H} \rightarrow \mathrm{L+1(-0.45)} \end{array}$	1.6611	0.14	0.45		$S_1$	$\begin{array}{l} H \rightarrow L(0.46) \\ H\text{-}1 \rightarrow L\text{+}1(0.84) \end{array}$	1.7755	0.80	0.03
1.9	$\mathrm{CT}_1$	$H \rightarrow L+1(-0.43)$	1.8308	0.29	-0.31		S <sub>2</sub>	$H-1 \rightarrow L(0.84)$ $H \rightarrow L+1(0.49)$ $H \rightarrow L(0.61)$	1.8062	0.03	-0.01
	$\mathrm{CT}_2$	$H-1 \rightarrow L+1(0.80)$ $H-1 \rightarrow L(0.94)$ $H-1 \rightarrow L+1(-0.23)$	1.8579	0.25	0.36		011	$H \rightarrow L(0.61)$ $H \rightarrow L+1(0.61)$ $H-1 \rightarrow L(0.42)$	1.4015	0.03	-0.94
	$S_1$	$H \rightarrow L(0.48)$ $H \rightarrow L+1(0.75)$	1.5911	0.39	-0.60		$\mathrm{CT}_2$	$\begin{array}{l} \text{H-1} \rightarrow \text{L}(0.40) \\ \text{H} \rightarrow \text{L+1}(0.52) \\ \end{array}$	1.4304	0.05	0.93
	$S_2$	$H-1 \rightarrow L+1(0.39)$ $H \rightarrow L(0.86)$ $H \rightarrow L+1(-0.44)$	1.6484	0.12	0.49	10.0	$S_1$	$H \rightarrow L(0.56)$ $H \rightarrow L(0.53)$	1.7662	0.74	0.01
2.0	$\operatorname{CT}_1$	$\rm H \rightarrow L{+}1({-}0.46)$	1.8278	0.34	-0.28		$S_2$	$\begin{array}{l} \mathrm{H\text{-}1} \rightarrow \mathrm{L\text{+}1}(0.75) \\ \mathrm{H\text{-}1} \rightarrow \mathrm{L}(0.59) \end{array}$	1.7896	0.12	-0.01
	$CT_2$	$H-1 \rightarrow L+1(0.86)$ $H-1 \rightarrow L(0.96)$ $H \rightarrow L(0.90)$	1.8489	0.24	0.31		$CT_1$	$H \rightarrow L+1(0.35)$ $H \rightarrow L+1(0.69)$ $H \rightarrow L(0.48)$	1.3500	0.02	-0.91
	CT <sub>1</sub>	$H \rightarrow L(0.90)$ $H \rightarrow L+1(0.37)$ $H \rightarrow L(-0.38)$	1.6267	0.30	-0.69		$CT_2$	$H \rightarrow L(0.48)$ $H-1 \rightarrow L(0.45)$ $H \rightarrow L(0.64)$	1.3697	0.05	0.90
9.1	012	$H \to L+1(0.84)$ $H-1 \to L(-0.33)$	1.0201	0.10	0.00			$H \rightarrow L+1(0.40)$ $H-1 \rightarrow L+1(0.51)$ $H \rightarrow L(0.42)$			
2.1	$S_1$ $S_2$	$H-1 \rightarrow L+1(0.97)$ $H \rightarrow L+1(0.36)$	$1.7789 \\ 1.8071$	0.62 0.02	0.13 -0.01	78	$S_1$	$H-1 \rightarrow L(0.42)$ $H-1 \rightarrow L+1(0.74)$	1.7637	0.74	0.09
	CT.	$H-1 \rightarrow L(0.92)$ $H \rightarrow L(0.88)$	1 5708	0.97	-0.73		S.	$H \rightarrow L(-0.56)$ $H_{-1} \rightarrow L(0.74)$	1 70/15	0.02	-0.07
	UI1	$H \rightarrow L+1(0.38)$	1.0100	0.27	-0.73		52	$H \rightarrow L+1(-0.55)$	1.1.040	5.04	0.01
	$\mathrm{CT}_2$	$\begin{array}{l} \mathrm{H} \rightarrow \mathrm{L}(\text{-}0.39) \\ \mathrm{H} \rightarrow \mathrm{L}{+}1(0.82) \\ \mathrm{H}{-}1 \rightarrow \mathrm{L}(\text{-}0.35) \end{array}$	1.6185	0.15	0.61						
2.2	$S_1$	$\text{H-1} \rightarrow \text{L+1}(0.95)$	1.7948	0.64	0.13						
	$S_2$	$\begin{array}{c} \mathrm{H} \rightarrow \mathrm{L}(0.23) \\ \mathrm{H} \rightarrow \mathrm{L}{+1}(0.38) \\ \mathrm{H}{-1} \rightarrow \mathrm{L}(0.91) \end{array}$	1.8069	0.03	-0.03						

**SI Table S2.** Excited states energies at  $\epsilon$ =2.0 for the dimers of Figure 5(B) and 5(C) where the distinctly oriented PFGs are removed. Figure 5(B) dimer exhibits same orientation as in Figure 5(A). In Figure 5(C), the monomers are shifted towards each other to obtain a stacked dimer geometry.

	state	excitation	oscillator	net charge
		energy(eV)	strength	(e)
	$S_1$	1.9371	0.91	0.00
	$S_2$	2.0131	0.00	0.00
5(b)				
	$CT_1$	2.2277	0.00	0.61
	$CT_2$	2.2597	0.05	-0.62
	$CT_1$	2.0530	0.02	-0.80
	$CT_2$	2.0675	0.02	0.76
5(c)				
	$S_1$	2.1392	0.00	0.05
	$S_2$	2.2905	0.53	0.02

SI Table S3. Diabatic states-based energy parameters and rates. Excited state ( $S_{D1}$ ), Electronic coupling ( $V_{el}$ ), CT state energy, and CT-optimized energies (CT\*), driving force ( $\Delta E$ ), reorganization energy ( $E_r^{tot}$ ), activation energy ( $E_A$ ), Marcus CT rate ( $k_M$ ) and Fermi golden rule CT rate ( $k_{FGR}$ ). For the CT states, CT<sub>AB</sub> and CT<sub>BA</sub> are provided at the first and second row, respectively, for each dielectric value.

ε	$S_{D1}$	CT	$CT^*$	$V_{\rm el}$	$ \Delta E $	$E_r^{\rm tot}$	$E_{\mathbf{a}}$	$k_{ m M}$	$k_{\rm FGR}$
	[eV]	[eV]	[eV]	[eV]	[eV]	[eV]	[eV]	$[s^{-1}]$	$[s^{-1}]$
1.2	1.7493	1.9136	1.6126	0.099	0.136	0.301	0.023	$1.25 \times 10^{14}$	$1.66 \times 10^{14}$
		2.0274	1.7264	0.102	0.022		0.064	$2.60 \mathrm{x10}^{13}$	$1.42 \mathrm{x} 10^{14}$
1.3	1.7506	1.8626	1.5536	0.097	0.188	0.309	0.012	$1.79 \mathrm{x} 10^{14}$	$1.81 \mathrm{x} 10^{14}$
		1.9739	1.6649	0.107	0.077		0.044	$6.40 \mathrm{x} 10^{13}$	$1.52 \mathrm{x} 10^{14}$
1.4	1.7515	1.8185	1.5085	0.099	0.243	0.310	0.0036	$2.56 \mathrm{x} 10^{14}$	$1.80 \mathrm{x} 10^{14}$
		1.9289	1.6189	0.105	0.134		0.0250	$1.26 \mathrm{x} 10^{14}$	$1.59 \mathrm{x} 10^{14}$
1.5	1.7531	1.7819	1.4709	0.098	0.282	0.311	0.0007	$2.81 \mathrm{x10}^{14}$	$1.82 \mathrm{x10}^{14}$
		1.8892	1.5782	0.102	0.175		0.0147	$1.78 \mathrm{x} 10^{14}$	$1.49 \mathrm{x} 10^{14}$
1.6	1.7323	1.7257	1.4127	0.110	0.320	0.313	0.0001	$3.62 \mathrm{x} 10^{14}$	$1.84 \mathrm{x} 10^{14}$
		1.8215	1.5085	0.060	0.224		0.0063	$2.24 \mathrm{x} 10^{14}$	$7.29 \mathrm{x} 10^{13}$
1.7	1.7370	1.7042	1.3912	0.104	0.341	0.313	0.0006	$3.16 \mathrm{x} 10^{14}$	$1.65 \mathrm{x10}^{14}$
		1.7899	1.4769	0.063	0.260		0.0022	$1.19 \mathrm{x} 10^{14}$	$6.62 \mathrm{x} 10^{13}$
1.8	1.7325	1.6902	1.3752	0.098	0.357	0.315	0.0014	$2.71 \mathrm{x} 10^{14}$	$1.45 \mathrm{x} 10^{14}$
		1.7624	1.4474	0.064	0.285		0.0007	$1.09 \mathrm{x} 10^{14}$	$6.32 \mathrm{x} 10^{13}$
1.9	1.7454	1.6750	1.3600	0.095	0.385	0.315	0.0039	$2.31 \mathrm{x} 10^{14}$	$1.32 \mathrm{x} 10^{14}$
		1.7375	1.4225	0.064	0.323		0.00001	$1.22 \mathrm{x} 10^{14}$	$6.27 \mathrm{x} 10^{13}$
2.0	1.7474	1.6614	1.3454	0.092	0.402	0.316	0.0059	$2.01 \mathrm{x} 10^{14}$	$1.20 \mathrm{x} 10^{14}$
		1.7160	1.4000	0.066	0.347		0.0183	$1.26 \mathrm{x} 10^{14}$	$6.68 \mathrm{x} 10^{13}$
2.1	1.7326	1.6193	1.3023	0.058	0.430	0.317	0.0101	$6.78 \mathrm{x} 10^{13}$	$4.31 \mathrm{x} 10^{13}$
		1.6773	1.3603	0.074	0.373		0.0025	$1.48 \mathrm{x} 10^{14}$	$8.14 \mathrm{x} 10^{13}$
2.2	1.7356	1.6086	1.2896	0.058	0.449	0.319	0.0132	$5.98 \mathrm{x} 10^{13}$	$3.91 \mathrm{x} 10^{13}$
		1.6637	1.3447	0.072	0.391		0.0041	$1.31 \mathrm{x} 10^{14}$	$7.55 \mathrm{x} 10^{13}$
2.3	1.7386	1.5986	1.2786	0.056	0.460	0.320	0.0153	$5.13 \mathrm{x} 10^{13}$	$3.45 \mathrm{x} 10^{13}$
		1.6523	1.3323	0.070	0.406		0.0058	$1.16 \mathrm{x} 10^{14}$	$6.92 \mathrm{x} 10^{13}$
2.4	1.7403	1.5897	1.2687	0.055	0.472	0.321	0.0196	$4.18 \mathrm{x} 10^{13}$	$3.18 \mathrm{x} 10^{13}$
		1.6414	1.3204	0.069	0.420		0.0076	$1.05 \mathrm{x} 10^{14}$	$6.42 \mathrm{x} 10^{13}$
2.5	1.7422	1.5819	1.2619	0.053	0.480	0.320	0.0200	$3.84 \mathrm{x} 10^{13}$	$2.85 \mathrm{x} 10^{13}$
		1.6312	1.3112	0.068	0.431		0.0002	$9.43 \text{x} 10^{13}$	$5.92 \mathrm{x} 10^{13}$
2.6	1.7438	1.5733	1.2523	0.052	0.492	0.321	0.0227	$3.31 \mathrm{x} 10^{13}$	$2.65 \mathrm{x10}^{13}$
		1.6222	1.3012	0.067	0.443		0.0116	$8.47 \mathrm{x} 10^{13}$	$5.41 \mathrm{x} 10^{13}$
2.8	1.7465	1.5600	1.2350	0.050	0.512	0.325	0.0269	$2.59 \mathrm{x} 10^{13}$	$2.34 \mathrm{x} 10^{13}$
		1.6062	1.2812	0.065	0.465		0.0151	$6.93 \mathrm{x} 10^{13}$	$4.61 \mathrm{x} 10^{13}$
3.0	1.7480	1.5462	1.2202	0.048	0.528	0.326	0.0312	$2.01 \mathrm{x} 10^{13}$	$2.07 \mathrm{x} 10^{13}$
		1.5911	1.2651	0.064	0.483		0.0003	$5.78 \mathrm{x} 10^{13}$	$4.19 \mathrm{x} 10^{13}$
3.5	1.7527	1.5207	1.1937	0.044	0.559	0.327	0.0411	$1.15 \mathrm{x} 10^{13}$	$1.57 \mathrm{x} 10^{13}$
		1.5654	1.2384	0.059	0.514		0.0015	$3.62 \mathrm{x} 10^{13}$	$3.28 \mathrm{x} 10^{13}$
4.0	1.7560	1.5022	1.1702	0.042	0.586	0.332	0.0486	$1.09 \mathrm{x} 10^{13}$	$1.45 \times 10^{13}$
		1.5477	1.2157	0.058	0.540		0.0067	$1.86 \mathrm{x} 10^{13}$	$2.87 \mathrm{x} 10^{13}$
5.0	1.7600	1.4757	1.1437	0.039	0.616	0.332	0.0607	$4.22 \mathrm{x} 10^{12}$	$9.26 \times 10^{12}$
		1.5226	1.1906	0.050	0.569		0.0423	$1.42 \mathrm{x} 10^{13}$	$1.90 \times 10^{13}$
10.0	1.7573	1.4115	1.0685	0.033	0.689	0.343	0.0872	$1.07 \mathrm{x} 10^{12}$	$5.12 \times 10^{12}$
		1.4409	1.0979	0.050	0.659		0.0223	$4.28 \times 10^{12}$	$1.36 \mathrm{x} 10^{13}$
78.0	1.7534	1.3584	1.0094	0.027	0.744	0.349	0.1118	$2.74 \mathrm{x} 10^{11}$	$2.77 \mathrm{x} 10^{12}$
		1.3773	1.0283	0.048	0.725		0.1013	$1.30 \mathrm{x} 10^{12}$	$9.63 \times 10^{12}$



**SI Figure S1.** FGR CT rates for the full range of dielectric constants up to 78. Black and red curves correspond to  $CT_{AB}$  and  $CT_{BA}$  processes, respectively.



**SI Figure S2.** Marcus CT rates for the full range of dielectric constants up to 78. Black and red curves correspond to  $CT_{AB}$  and  $CT_{BA}$  processes, respectively



**SI Figure S3.** HRF distributions due to electron transfer  $(P_A^+ P_B^-)$  in the special pair for dielectric constants 1.6 (upper panel) and 78 (lower panel) due to acceptor and donor monomer contributions.



**SI Figure S4.** HRF distributions due to electron transfer  $(P_A^- P_B^+)$  in the special pair for dielectric constants 1.6 (upper panel) and 78 (lower panel) due to acceptor and donor monomer contributions.



**SI Figure S5.** The time-dependent integrand of the FGR-expression (solid lines), without the  $F_r^{ex}(t)$  window function, decays at  $\epsilon = 1.6$  (highest rate) on a sub-100 fs timescale. The semi-classical contribution of an external reorganization energy  $E^{ex}$  of 0.01 eV leads to a window function  $F_r^{ex}(t)$  (red dashed line) with only negligible effect on the FGR rate.

SI Table S4. The atomic coordinates of the X-Ray structure of special pair (Å).

Mg	-4.2856000000000000	4.14067000000000001	-3.9274900000000001	Mg	-9.7476000000000000	-0.16733000000000000	0.0385100000000000
C	-0.978600000000000000	3 57866999999999998	-4 83349000000000003	C	-12.5626000000000000	-2.0153300000000001	-0.95549000000000000
č	-5.05460000000000000	0.999669999999999999	-5 16448999999999998	С	-7.8276000000000000	-2.13832999999999998	-2.04748999999999998
č	-7 34960000000000000	4 25867000000000004	-2 365489999999999999	С	-7.1856000000000000	2.150669999999999999	0.1625100000000000
č	-3 10760000000000000	6 6666600000000000	-1 794/89999999999999	$\mathbf{C}$	-11.905600000000000	2.18567000000000000	1.4395100000000001
N	-3.18360000000000000	2 59066999999999998	-4 9374900000000004	Ν	-10.1106000000000000	-1.91733000000000000	-1.16849000000000000
C	-1.85160000000000000	2.676660000000000000	-5 303/90000000000	$\mathbf{C}$	-11.355600000000001	-2.52833000000000000	-1.397489999999999999
ĉ	1 56160000000000000	1 56267000000000000	6 3024800000000000	С	-11.160600000000001	-3.6923300000000001	-2.308489999999999999
C	2 76760000000000000	0.67067000000000000	6 254480000000007	С	-9.669600000000001	-3.9023300000000001	-2.28349000000000000000000000000000000000000
c	-3 75460000000000000	1 40867000000000000	-5 389/90000000003	$\mathbf{C}$	-9.1196000000000000	-2.5673300000000001	-1.87049000000000000
c	-0.32560000000000000	0.7356700000000000	-6.010/8000000000000	С	-11.621600000000001	-3.3353299999999999999	-3.7214900000000002
c	-0.15960000000000000	-0.4323300000000000	-6 951/899999999999	$\mathbf{C}$	-11.654600000000000000000000000000000000000	-4.44132999999999998	-4.720489999999999999
ĉ	0.831/000000000000000	1 420330000000000000	6 4334800000000000	С	-12.84859999999999999	-5.3313300000000003	-4.53648999999999997
0	0.8314000000000000	2 61332000000000000	6 578490000000000	0	-13.4596000000000000	-5.3023300000000004	-3.45848999999999998
ő	1.9694000000000000	-1 0/23300000000000	-5 7294900000000000	0	-13.2986000000000000	-6.2343299999999999999	-5.57948999999999998
N	5.0336000000000000	2 008660000000000000	3 8534800000000000	Ν	-7.8336000000000000	-0.06433000000000000	-0.72649000000000000000000000000000000000000
C	6.04360000000000000	1.674670000000000000	4 4654900000000000	С	-7.24060000000000000	-0.9973300000000000	-1.5244899999999999999999999999999999999999
C	7 38660000000000000	1.17667000000000001	4 281480000000000	С	-5.8736000000000000	-0.61533000000000000	-1.7184900000000001
C	-7.58000000000000000000000000000000000000	2.0616600000000000	2 480400000000001	Ċ	-5.74360000000000000	0.71067000000000000	-1.37049000000000000
C	7 1126000000000000	2.0010099999999999999	2 1774000000000000	Ċ	-6.9566000000000000	0.9866700000000000	-0.59149000000000000
C	-7.1130000000000000	1.0616700000000000	-3.1774900000000000	Ċ	-4.71360000000000000	1.585669999999999999	-0.8254899999999999999
õ	10.0046000000000000	0.06267000000000000	-2.8414899999999999999	Ō	-4.0006000000000000	1.319669999999999999	0.08751000000000000
C	10.01850000000000000	2.2616700000000000	2.04940999999999999999	Ċ	-3.91460000000000000	1.8966700000000001	-2.06348999999999998
N	=10.0185999999999999999	5.2010700000000000	2.455400000000000	N	-9.53459999999999999	1.7696700000000001	0.9025100000000000
C	-5.1180000000000000	5.2806600000000002	-2.400400000000002	C	-8.3506000000000000	2.5286700000000000	0.8515100000000000
C	-0.400000000000000000	5.2600099999999999999 6 5676600000000007	-2.04949000000000000	č	-8.5266000000000000	3.7686700000000002	1.7095100000000000
Ĉ	-0.18900000000000000	6.05767000000000000000000000000000000000	-1.33049000000000000	č	-10.0296000000000000	3.9256700000000002	1.79550999999999999
Ĉ	-3.4030000000000000	6.9570700000000002 6.2646700000000002	1 725 40000000000000	č	-10.5656000000000000	2.541669999999999999	1.4665100000000000
N	-4.4070000000000000	4.02567000000000000	-1.7204900000000000	Ň	-11.7256000000000000	0.03667000000000000	0.32751000000000000
C	-2.304000000000000	4.9330700000000000	-5.5094699999999999999	C	-12.4675999999999999999999999999999999999999	1.02767000000000001	0.9105100000000000
Č	-2.1080000000000000	6.28767000000000000	-2.3004899999999999999	č	-13.8896000000000000	0.67967000000000000	0.8805100000000000
C	-0.75900000000000000	5.49767000000000000	2 5684000000000000000000000000000000000000	Ċ	-13.9806000000000001	-0.43133000000000000	0.1125100000000000
Č	-0.2320000000000000	5.4270700000000000 4.5446700000000000	-3.3084900000000002	č	-12.645600000000000000000000000000000000000	-0.85533000000000000	-0.18249000000000000
C	-1.3240000000000000	4.34407000000000000	-3.9414699999999999999	Ċ	-14.8736000000000000	-1.34233000000000000	-0.56549000000000000
õ	2.0644000000000000	5.0400700000000004 5.4646600000000000	-4.34849000000000000	õ	-16.10259999999999999	-1.43433000000000001	-0.53349000000000000
C	2.0044000000000000	2.0516700000000000	-4.550489999999999997 5.2264800000000007	Č	-14.0146000000000000	-2.33232999999999998	-1.3804900000000000000000000000000000000000
C	0.4194000000000000	4 58767000000000000	-5.5204899999999999997 6.666480000000000	Ċ	-14.39059999999999999	-3.74332999999999998	-0.971490000000000000
õ	0.2394000000000000	4.0656600000000000	-0.0004899999999999990	õ	-13.642600000000000000000000000000000000000	-4.3553300000000004	-0.1924900000000000000000000000000000000000
0	0.8374000000000000	4.0050099999999999999	-7.0194899999999999999	Õ	-15.5855999999999999999999999999999999999	-4.28932999999999996	-1.390490000000000000000000000000000000000
C	-0.57000000000000000	6.2616600000000000	-0.8344899999999999997 8.0714000000000007	Ċ	-16.049600000000002	-5.41533000000000000	-0.86349000000000000
Ĉ	-0.7390000000000000	0.2010099999999999999	-8.0714900000000007	č	-14.6796000000000001	-6.6613300000000004	-5.51248999999999997
п	2.02740000000000000000	-2.09652999999999999	-4.9634699999999999998	Ĥ	-7.2249400000000000	-2.733369999999999999999999999999999999999	-2.63720000000000000
п u	-3.320010000000000	4.220480000000000000	-5.56290000000000000	Н	-6.396250000000000	2.813229999999999999	0.2171600000000000
п u	-8.292370000000000	4.52946000000000002	-1.9317400000000000	Н	-12.56387999999999999	2.85910999999999998	1.8616200000000001
11 11	-2.110330000000000	2.01062000000000002	7.254600000000000	н	-11.71360999999999999999999999999999999999999	-4.55978999999999996	-2.0142300000000000
п	-1.307810000000000	2.0100299999999999999	7.2265000000000000	Н	-9.404170000000001	-4.658489999999999996	-1.57450000000000000
п u	-3.1030300000000000	0.3202900000000000	-7.23030000000000004 5.8684500000000000	Н	-9.2849799999999999	-4.2315800000000001	-3.226129999999999999
11 11	-2.551180000000000	1 26662000000000000	-5.808450000000002	Н	-12.6120199999999999	-2.9372500000000001	-3.6473300000000002
п u	0.3343700000000000	1.300030000000000000	-0.095079999999999999	Н	-10.887210000000000	-2.6495199999999999999999999999999999999999	-4.0892400000000002
и П	1 105020000000000	0.03740000000000000	7.02020209999999999999	Н	-11.687410000000000	-4.01837000000000000	-5.70279999999999999999
п u	-1.103020000000000	-0.91905000000000000	7.876000000000002	Н	-10.7756300000000000000000000000000000000000	-5.0359400000000001	-4.5835600000000003
11 U	7 7722400000000000	-0.03807000000000000	4 682720000000000	Н	-5.11680000000000000	-1.2281599999999999999999999999999999999999	-2.0601200000000000
11 11	-7.7733400000000000	4.044880000000000000	-4.0827300000000000	н	-4.580020000000000	2.132029999999999999	-2.8676800000000000
п u	-9.29005999999999999	4.044660000000000000 2.10070000000000000	-2.323019999999999999	Н	-3.321760000000000	1.0462199999999999999	-2.3283700000000001
п	10.702020000000000	3.19970000000000000	-1.31494000000000000	Н	-3.2743000000000000	2.73275999999999999	-1.87406000000000001
п	7 518820000000000	5.47080000000000000	-5.2040100000000002	Н	-8.0784699999999999	4.6222200000000004	1.24523999999999999
п	7.010020000000000	0.4074499999999999999	-0.3040300000000000000000000000000000000	Н	-8.060150000000000	3.68251999999999998	2.66862999999999998
л U	-7.2133200000000000 5.264580000000000	00100000000000000000000000000000000000	-1.9004900000000000000 0.60274000000000000	Н	-10.3248300000000000000000000000000000000000	4.223349999999999999	2.77994999999999999
п	-0.3040800000000000000	6.021829999999999999 6.60841000000000	-0.093/4000000000000	Н	-10.4026700000000000000000000000000000000000	4.6789500000000004	1.133459999999999999
н u	-0.320700000000000	0.0084100000000000	0.200000000000000000	н	-14.66266000000000000000000000000000000000	1.1783399999999999999999999999999999999999	1.348200000000000000
п	-0.213910000000000	0.99549000000000002	-2.100139999999999999	н	-14 1476400000000000	-2 24947000000000000	-2 4389500000000000
H	1.096340000000000	3.1250200000000000	-0.383849999999999998	н	-16 98273000000000	-5 6662200000000000	-1 323070000000002
H	-1.446890000000000	1.075029999999999999	-7.9667000000000003	н	-16 194120000000000	-5 2837399000000000	0.188510000000000
H	-1.151360000000000	5.5513100000000000	-8.76919999999999997	Н	-15 3460900000000002	-6 2039499999999999999	-1 030969999999999999
H	0.1789900000000000	0.03152999999999999	-8.42808999999999992	н	-14 889419999999999	-7 319609999999999999	-6 32951999999999999
H	3.485210000000000	-1.7001900000000000	-4.482929999999999996	н	-15 320449000000000	-5 8063700000000000	-5 5696500000000000
H	2.934010000000000	-2.872209999999999999	-5.55580000000000002	н	-14 850080000000000	-7 17372999999999999	-4 58875999999999999
п	1.9483100000000000	-2.30144000000000000	-4.20192999999999996				

SI Table S5. The atomic coordinates of the X-Ray structure of BChl monomer ( $P_A$ ) molecule (Å).

Mg	-9.7476000000000000	-0.1673300000000000	0.038510000000000
С	-12.5626000000000000	-2.0153300000000001	-0.9554900000000000
С	-7.8276000000000000	-2.13832999999999998	-2.04748999999999998
С	-7.1856000000000000	2.1506699999999999999999999999999999999999	0.16251000000000000
Ċ	-11 905600000000000	2 1856700000000000	1 4395100000000001
Ň	-10 110600000000000000	-1 9173300000000000	-1 1684900000000000
C	11 255600000000000	2 52822000000000000	1 307/8000000000000
č	-11.355000000000000	2.60222000000000000	-1.3974099999999999999
č	-11.1000000000000000	-5.0925500000000000	-2.308489999999999999
C	-9.669600000000000	-3.9023300000000001	-2.2834900000000000
C	-9.119600000000000	-2.5673300000000001	-1.8704900000000000
С	-11.621600000000001	-3.33532999999999999	-3.7214900000000002
С	-11.65460000000000000	-4.44132999999999998	-4.720489999999999999
$\mathbf{C}$	-12.84859999999999999	-5.3313300000000003	-4.5364899999999997
0	-13.4596000000000000	-5.3023300000000004	-3.4584899999999998
0	-13.2986000000000000	-6.234329999999999999	-5.5794899999999998
Ν	-7.8336000000000000	-0.06433000000000000	-0.72649000000000000
С	-7.240600000000000000000000000000000000000	-0.99733000000000000	-1.524489999999999999
$\mathbf{C}$	-5.8736000000000000	-0.61533000000000000	-1.7184900000000001
č	-5 7436000000000000	0.71067000000000000	-1.3704900000000000
č	-6.956600000000000000	0.98667000000000000	-0.591/9000000000000
č	4 71260000000000000	1 5856600000000000	0.82548000000000000
õ	-4.7130000000000000	1.3100000000000000000000000000000000000	-0.823483333333333333
g	-4.0006000000000000	1.319009999999999999	0.0875100000000000
C	-3.9146000000000000	1.8966700000000000	-2.06348999999999998
N	-9.5345999999999999	1.7696700000000001	0.9025100000000000
C	-8.3506000000000000	2.52867000000000000	0.8515100000000000
С	-8.5266000000000000	3.7686700000000002	1.7095100000000001
$\mathbf{C}$	-10.0296000000000000	3.92567000000000002	1.79550999999999999
$\mathbf{C}$	-10.5656000000000000	2.541669999999999999	1.46651000000000000
Ν	-11.7256000000000000	0.03667000000000000	0.3275100000000000
$\mathbf{C}$	-12.46759999999999999	1.0276700000000001	0.9105100000000000
С	-13.8896000000000000	0.67967000000000000	0.8805100000000000
С	-13.980600000000001	-0.43133000000000000	0.11251000000000000
Ċ	-12.6456000000000000	-0.85533000000000000	-0.1824900000000000
č	-14 873600000000000000	-1 34233000000000000	-0.5654900000000000
õ	16 1025000000000000	1.42422000000000000000000000000000000000	0.5224000000000000
č	-10.102333333333333333	2 2222200000000000	1 280/000000000000
ä	-14.0140000000000000	-2.3323299999999999999	-1.38049000000000000
õ	-14.590599999999999999	-3.143329999999999999	-0.9714900000000000
0	-13.042000000000000	-4.3553300000000004	-0.1924900000000000
0	-15.58559999999999999	-4.2893299999999999	-1.3904900000000000
C	-16.049600000000002	-5.4153300000000000	-0.8634900000000000
С	-14.679600000000001	-6.661330000000004	-5.51248999999999997
Н	-7.2249400000000000	-2.733369999999999999	-2.63720000000000000
Н	-6.396250000000000	2.813229999999999999	0.21716000000000000
н	-12.5638799999999999	2.8591099999999998	1.861620000000001
Н	-11.71360999999999999	-4.5597899999999996	-2.0142300000000000
Н	-9.404170000000001	-4.65848999999999996	-1.57450000000000000
Н	-9.28497999999999999	-4.2315800000000001	-3.226129999999999999999999999999999999999
Н	-12.612019999999999	-2.9372500000000001	-3.6473300000000002
н	-10.887210000000000	-2 649519999999999999	-4 0892400000000002
н	-11 68741000000000	-4 01837000000000000	-5 702799999999999999
ц	10.775620000000000	5.0250400000000000	4 5825600000000000
п	-10.775050000000000	1 2281500000000000	-4.5855000000000000
п	-5.110800000000000	-1.228159999999999999	-2.0601200000000000
H	-4.580020000000000	2.13202999999999999	-2.8676800000000000
H	-3.321760000000000	1.04621999999999999	-2.3283700000000001
Н	-3.2743000000000000000000000000000000000000	2.732759999999999999	-1.8740600000000001
Н	-8.0784699999999999	4.6222200000000004	1.245239999999999999
Н	-8.060150000000000	3.6825199999999998	2.6686299999999998
Η	-10.324830000000000	4.223349999999999999	2.77994999999999999
Η	-10.402670000000001	4.6789500000000004	1.133459999999999999
Η	-14.662660000000001	1.17833999999999999	1.3482000000000001
Н	-14.147640000000001	-2.2494700000000001	-2.4389500000000002
н	-16.982730000000000	-5.6662200000000000	-1.3230700000000000
H	-16 194120000000000	-5 2837399999999999	0.188510000000000
п	15.246000000000000	6 20204000000000000	1.0200600000000000
ш	14 8804100000000000	7 2106000000000000	-1.000000000000000000000000000000000000
п	-14.88941999999999999	-1.5190099999999999999	-0.978918888888888
H	-10.32044999999999999	-5.80637000000000003	-5.5696500000000002
Н	-14.850080000000000	-7.173729999999999999	-4.5887599999999997

SI Table S6. The atomic coordinates of the X-Ray structure of BChl monomer  $(P_B)$  molecule (Å).

Mg	-4.2856000000000000	4.1406700000000001	-3.9274900000000001
С	-0.9786000000000000	3.57866999999999998	-4.8334900000000003
С	-5.0546000000000000	0.999669999999999999	-5.16448999999999998
С	-7.3496000000000000	4.2586700000000004	-2.365489999999999999
С	-3.1076000000000000	6.666669999999999999	-1.79448999999999999
Ν	-3.1836000000000000	2.5906699999999998	-4.937490000000004
С	-1.8516000000000000	2.6466699999999999999	-5.30349000000000000
С	-1.5616000000000000	1.56267000000000000	-6.3024899999999997
С	-2.76760000000000000000000000000000000000	0.67067000000000000	-6.2544899999999997
С	-3.7546000000000000000000000000000000000000	1.4086700000000001	-5.389490000000003
С	-0.3256000000000000	0.73567000000000000	-6.010489999999999999
С	-0.1596000000000000	-0.43233000000000000	-6.9514899999999997
С	0.8314000000000000	-1.4203300000000001	-6.433489999999999999
0	0.607400000000000	-2.613329999999999999	-6.5784900000000004
0	1.9694000000000000	-1.04233000000000000	-5.7294900000000002
Ν	-5.9336000000000000	2.908669999999999999	-3.853489999999999999
С	-6.0436000000000000	1.6746700000000001	-4.46549000000000000
С	-7.3866000000000000	1.1766700000000001	-4.28148999999999998
С	-8.054600000000001	2.061669999999999999	-3.4804900000000001
С	-7.113600000000000000000000000000000000000	3.1486700000000001	-3.1774900000000001
С	-9.365600000000001	1.96167000000000000	-2.84148999999999998
0	-10.09460000000000000000000000000000000000	0.96267000000000000	-2.849489999999999999
С	-10.01859999999999999	3.2616700000000001	-2.4964900000000001
Ν	-5.118600000000000000000000000000000000000	5.3536700000000002	-2.455490000000002
С	-6.4606000000000000	5.28066999999999998	-2.04949000000000000000000000000000000000
С	-6.7896000000000000	6.5676699999999997	-1.3304900000000000
С	-5.4636000000000000	6.9576700000000002	-0.74549000000000000
С	-4.46760000000000000000000000000000000000	6.3646700000000003	-1.725490000000000000
Ν	-2.5046000000000000	4.93567000000000000	-3.36948999999999999
С	-2.168600000000000000000000000000000000000	5.9976700000000003	-2.566489999999999999
С	-0.7396000000000000	6.2876700000000003	-2.64249000000000000
С	-0.2526000000000000	5.42767000000000000	-3.5684900000000002
С	-1.3246000000000000000000000000000000000000	4.5446700000000000000000000000000000000000	-3.941489999999999999
С	0.890400000000000	5.0406700000000004	-4.34849000000000000
0	2.0644000000000000	5.464669999999999999	-4.35048999999999997
С	0.4194000000000000	3.95167000000000000	-5.32648999999999997
С	0.2394000000000000	4.5876700000000001	-6.66648999999999996
0	0.8374000000000000	4.065669999999999999	-7.619489999999999999
0	-0.5766000000000000	5.64567000000000000	-6.83448999999999997
С	-0.7596000000000000	6.26166999999999996	-8.0714900000000007
С	2.6274000000000000000000000000000000000000	-2.0983299999999998	-4.98348999999999998
Н	-5.320610000000000	0.08560000000000000	-5.562900000000000000
Н	-8.292370000000000	4.3294800000000002	-1.95174000000000000
Η	-2.770530000000000	7.4561700000000002	-1.2216800000000001
Н	-1.367810000000000	2.01062999999999999	-7.2546900000000001
Н	-3.165030000000000	0.5202900000000000	-7.2365000000000004
н	-2.537780000000000	-0.3004400000000000	-5.868450000000002
Н	0.534370000000000	1.3666300000000000	-6.0956799999999998
н	-0.433770000000000	0.33746000000000000	-5.02325999999999996
Н	-1.105020000000000	-0.9190300000000000	-7.0705900000000002
Н	0.199290000000000	-0.0586700000000000	-7.88769999999999997
н	-7.773340000000000	0.30808000000000000	-4.6827300000000003
н	-9.2900399999999999	4.04488000000000000	-2.5230199999999998
Н	-10.44004999999999999	3.19970000000000000	-1.51494000000000000
н	-10.793020000000000	3.47080000000000001	-3.2046100000000002
Н	-7.518820000000000	6.407449999999999999	-0.5640300000000000
н	-7.213320000000000	7.31658000000000001	-1.9664900000000001
н	-5.364580000000000	8.021829999999999996	-0.6937400000000000
н	-5.326750000000000	6.60841000000000001	0.25660000000000000
Н	-0.2139100000000000	6.99549000000000002	-2.1061399999999999999999999999999999999999
Н	1.0963400000000000	3.12502000000000000	-5.38384999999999998
н	-1.4468900000000000000000000000000000000000	7.07502999999999999	-7.9667000000000003
Н	-1.1513600000000000000000000000000000000000	5.55131000000000000	-8.769199999999999997
Н	0.1789900000000000	6.63152999999999999	-8.42808999999999999
Н	3.4852100000000000	-1.70019000000000001	-4.4829299999999999996
н	2.934010000000000	-2.87220999999999999	-5.6558000000000002
н	1.948310000000000	-2.5014400000000001	-4.26152999999999996

SI Table S7. The atomic coordinates of structure demonstrated in Figure 5(b) (Å).

				Ma	0.082660000000000	1 102780000000000	6 086180000000000
Mg	5.065200000000000	-6.520420000000000	-8.902910000000000	C	2 40550000000000000	-1.193780000000000	-0.9801800000000000 6 4076700000000000
С	5.2075900000000000	-9.8855299999999999	-8.058790000000000	C	-2.4055000000000000	4.274470000000000	-0.4070700000000000
С	1.6782200000000000000000000000000000000000	-6.634730000000000	-8.341070000000000	Ĉ	4.2720400000000000	-4.374470000000000	-5.001050000000000
С	4.727610000000000	-3.437980000000000	-10.323510000000001	Ĉ	4.372940000000000	-1.3299800000000000	7.226400000000000
$\mathbf{C}$	8.259480000000000	-6.752640000000000	-10.315910000000001	U N	1.147400000000000	2.280720000000000	-7.330490000000000
Ν	3.655650000000000	-8.057570000000000	-8.2281499999999999	N	-0.56497000000000	-2.514400000000000	-6.19471000000000
$\mathbf{C}$	3.9697900000000000	-9.364260000000000	-7.851000000000000	C	-1.93137000000000	-2.235950000000000	-6.168350000000000
$\mathbf{C}$	2.736710000000000	-10.090890000000000	-7.342350000000000	C	-2.72804000000000	-3.487950000000000	-5.851660000000000
$\mathbf{C}$	1.652870000000000	-9.002380000000000	-7.409060000000000	C	-1.629420000000000	-4.428180000000000	-5.320050000000000
$\mathbf{C}$	2.363270000000000	-7.830260000000000	-8.040310000000000	C	-0.351080000000000	-3.741410000000000	-5.744560000000000
Ν	3.464380000000000	-5.311080000000000	-9.395210000000001	N	2.407700000000000	-2.551080000000000	-6.359230000000000
$\mathbf{C}$	2.194580000000000	-5.496010000000000	-8.9283199999999999	C	2.1365000000000000000000000000000000000000	-3.838220000000000	-5.992580000000000
$\mathbf{C}$	1.448270000000000	-4.260220000000000	-9.06272000000001	С	3.345360000000000	-4.632380000000000	-6.105680000000000
С	2.287410000000000	-3.339120000000000	-9.600790000000000	С	4.326810000000000	-3.8123800000000000	-6.5586400000000000
С	3.575430000000000	-4.0193600000000000	-9.827240000000000	$\mathbf{C}$	3.730180000000000	-2.4707300000000000	-6.697730000000000
Ν	6.303330000000000	-5.289270000000000	-10.180040000000000	Ν	2.547090000000000	0.281440000000000	-7.147970000000000
С	5.985720000000000	-4.053410000000000	-10.52225999999999999	$\mathbf{C}$	3.822640000000000	-0.0318900000000000	-7.283470000000000
С	7.137660000000000	-3.311510000000000	-11.170500000000001	$\mathbf{C}$	4.686140000000000	1.165810000000000	-7.6256000000000000
С	8.253460000000000	-4.366310000000000	-11.2060000000000000000000000000000000000	$\mathbf{C}$	3.6756900000000000	2.324450000000000	-7.655770000000000
С	7.619770000000000	-5.5718900000000000	-10.530510000000000	$\mathbf{C}$	2.348550000000000	1.6432000000000000000000000000000000000000	-7.363540000000000
Ν	6.4566000000000000	-7.973750000000000	-9.1693599999999999	Ν	-0.301390000000000	0.365050000000000	-6.816280000000000
С	7.735760000000000	-7.9352600000000000	-9.693310000000000	$\mathbf{C}$	-0.148710000000000	1.711350000000000	-7.090360000000000
C	8.3809299999999999	-9.17418999999999999	-9.527490000000000	$\mathbf{C}$	-1.3976900000000000	2.360350000000000	-7.10652000000000
С	7.443670000000000	-9.996990000000000	-8.873880000000000	$\mathbf{C}$	-2.3475000000000000	1.354050000000000	-6.840090000000000
C	6.298930000000000	-9.209840000000000	-8.685510000000001	$\mathbf{C}$	-1.615040000000000	0.170410000000000	-6.675300000000000
č	7.200330000000000	-11.313420000000001	-8.334050000000000	$\mathbf{C}$	-3.7524600000000000	1.049100000000000	-6.68201000000000
Ō	7.916750000000000	-12.29768999999999999	-8.2809899999999999	Ο	-4.739480000000000	1.765510000000000	-6.728420000000000
č	5 7246900000000000	-11 2835500000000000	-7 750960000000000	$\mathbf{C}$	-3.849050000000000	-0.500690000000000	-6.418270000000000
й	0.6353300000000000	-6 5957500000000000	-8 0416399999999999	Н	0.901960000000000	-5.413540000000000	-5.347240000000000
н	4 6811700000000000	-2.3977100000000000	-10.620260000000000	Н	5.426050000000000	-1.406050000000000	-7.384520000000000
н	9 286470000000000	-6.813630000000000	-10 668410000000000	Н	1.163410000000000	3.349740000000000	-7.536570000000000
н	2 509160000000000	-10 8786200000000000	-8.06822000000000	Н	-3.4844500000000000	-3.288930000000000	-5.085880000000000
н	1 290630000000000	-8 71064000000000	-6.41452000000000	Н	-1.683100000000000	-5.4445600000000000	-5.721860000000000
н	7 4001900000000000	-2 /31770000000000	-10 572/6000000000	Н	5.186070000000000	1.010620000000000	-8.587750000000000
ц	8 558270000000000	4 610160000000000	12 22854000000001	Н	3.901330000000000	3.084550000000000	-6.902020000000000
н	5 8204600000000000	11 4687000000000000	6 67527000000000	Н	-4.435730000000000	-0.950740000000000	-7.225010000000000
п п	0.7767200000000000	0.2007200000000000	7.002220000000000	Н	3.420640000000000	-5.690480000000000	-5.887360000000000
11	0.110130000000000	4 11802000000000	-7.992220000000000	Н	-1.559170000000000	3.415730000000000	-7.286120000000000
и П	6.8485500000000000	-4.118930000000000	12 162580000000000	Н	-1.650730000000000	-4.5083700000000000	-4.227130000000000
и п	0.0400000000000000000000000000000000000	-2.330410000000000000000000000000000000000	10.671270000000000	н	5.468910000000000	1.299430000000000	-6.872470000000000
п	9.100070000000000	-4.0403400000000000	-10.0713700000000000	Н	3.652470000000000	2.823080000000000	-8.62886999999999999
п	9.90193999999999999	-9.4197900000000000 10 59710000000000	-9.009299999999999999	Н	-3.2726400000000000	-3.8827800000000000	-6.6837800000000000
п	2.0000000000000000000000000000000000000	10.027100000000001	-0.3098000000000000	н	-4 3327400000000000	-0.7594400000000000	-5 4995800000000000
H	0.00239000000000000	-12.008620000000000	-8.159829999999999999	н	5 302680000000000	-4 076510000000000	-6 76590000000000000
н	2.0664700000000000	-2.3531600000000000	-9.810790000000001		5.5520000000000000000000000000000000000	1.070010000000000	0.1000000000000000000000000000000000000

SI Table S8. The atomic coordinates of structure demonstrated in Figure 5(c) (Å).

Mg         Losh (n/1123802)         -0.23317182(1233)         -0.81231006512213         -0.81231006512213         -0.6337319246063         -9.29241330011571         -0.5292017824277263           C         1.25170278812245         -6.434107807015410         -8.4866200006177777         C         6.63373192460373         -9.62241330011571         -4.653413714450707           C         4.2280605571212         -5.581795012681004         -9.82646070457380         C         10.0139068739007         -5.4453737164582         -1.36224751314523         -7.31225682923383           C         3.231776017412119         -9.0459781172056         -7.788211724839771         C         3.8178670002284         -9.2124510180647           C         2.107075152119         -9.045978117706731822         -0.3615074677106218452         -1.227151575803934         -0.1622181614429667           C         1.19754068413736         -5.2272420739353         -0.5059979798281         -9.31416673135851         -0.5029817106428           C         1.062687787153023         -1.31056970351833         -9.0424635239856415         -9.025187200304         -5.01480527141429           C         1.062687787153023         -1.31056970351833         -0.0146993893839         -9.07410065930825415         -9.025418720700442         -5.0950591287164         -5.02528187207700542         -5.0805957784776442830		4 4014 - 0110004000	a 0.001 (50001 50054	0.040010005100510	Ma	6 602557400992416	-6 887881603952142	-6 446523257236870
$ \begin{array}{c} C & 1.3072000789121 \\ C & 1.25170007891221 \\ C & 1.42808005527121 \\ C & 4.3470687015421 \\ C & 4.34706870154220 \\ C & 4.3470687015420 \\ C & 4.347068701541620 \\ C & 4.347068701620 \\ C & 4.3411653016000051852 \\ C & 4.100690570820218 \\ C & 4.3480692019847 \\ C & 4.3690872167167 \\ C & 7.09024205521710 \\ C & 5.38658003906782 \\ C & 4.3470687811720 \\ C & 4.3470682781400 \\ C & 4.347068278140 \\ C & 4.347068278140 \\ C & 4.34706827814 \\ C & 4.3470687814 \\ C & 4.34706878177904744 \\ C & 10.34287042804 \\ C & 5.3865800390678 \\ C & 4.347068781420 \\ C & 5.3865800390678 \\ C & 5.38658$	Mg	4.681670112386202	-6.263147802153376	-8.642919665162513	C	3 2070738/17750372	-6.459162631615193	-5.202017824277263
$ \begin{array}{c} C & 1.251 (02788124) 5 & -0.437 (098 (014) 210 & -8.4860 2000.0147 (6) \\ -4.2808005571212 & -3.387776611714616 & -10.40108915520498 \\ C & 10.01319008796097 & -6.844337717144453 & -6.488844222703053 \\ C & 8.006338115153320 & -6.58175012681004 & -9.826668070487380 \\ C & 3.34774425029743 & -9.162113216216895 & -7.788211724339771 \\ C & 3.48774425029743 & -9.162113216216895 & -7.788211724339771 \\ C & 2.210707571755119 & -9.045078175718 & -9.09405871070531822 \\ C & 1.152365013162021 & -8.794755508314400 & -7.51904903597088 \\ C & 4.2007055990224 & -9.83141567313551 & -4.05294816429667 \\ 1.152365013162021 & -5.227426042980416 & -9.54844350374188 \\ N & 0.097623023425 & -8.0045175083932 & -4.07297473770642 \\ N & 3.09672494573976 & -5.227426042980416 & -9.54844350374188 \\ N & 0.097623023425 & -8.0045175083932 & -4.0779473770642 \\ C & 1.9662339556415 & -9.023187 & -9.0231872907023 & -5.0089901288732 \\ C & 1.106508778155023 & -1.010555183 & -9.48024685425386 \\ C & 0.1761007494363239 & -9.073187216 & -5.24349873533372 \\ C & 3.243817759477623 & -3.94668515522 & -10.0533823390462 \\ C & 9.1438094790218 & -9.143869290219847 & -5.46399472083304 \\ C & 3.243817759477623 & -3.9461865115522 & -10.0533823390426 \\ C & 9.007630846259858 & -9.974010869661378 & -4.9739777317692 \\ C & 5.1671441131382 & -3.04718207555822366 \\ C & 0.9076544543314 & -3.24118908801459 & -10.073875452746 \\ C & 1.018428770325166 & -4.513204757616 & -5.43484973553327 \\ C & 6.003277809642 & -3.397180215055582236 \\ C & 7.37400479661273828 & -10.993877547404447 \\ C & 10.18428770325166 & -4.5132047592146 & -5.874597146458437 \\ N & 6.633904255955 \\ C & 7.3741001579457968 & -5.43848973553327 \\ C & 0.033747806429 & -8.398179049449 \\ -5.3785029614430 & -5.338162505148 & -5.74989473413465 \\ C & 5.39738122653741 & -6.8798977831168 \\ C & 5.39738122653748 & -8.9929419665449 \\ N & 5.39738122653748 & -8.9929419665449 \\ N & 7.34922864573987 & -2.275545266449 \\ D & -5.39731226657378 & -8.86509980840928 \\ N & 5.27758296614304 & -5.3381665508 \\ N & 5.27758296614304 & -5.33$	C	4.730720566929421	-9.684315730269967	-7.837267430732884	Č	6 683373192465033	-9 802441350011572	-4 635419174807075
$ \begin{array}{c} C & 4.280800055211212 & -3.387(76310/4106 + 0.5826407047380 \\ S. 4.28080055211212 & -7.387663043266 \\ S. 4.3875424552481 & -5.3126563043266 \\ S. 4.387541245502743 & -0.16211321621685 & -7.78821172483971 \\ C & 3.38774425502743 & -0.16211321621685 & -7.78821172483971 \\ C & 3.317886700002219 & -3.648530625803 & -4.29376711656964283 \\ C & 2.210705781757119 & -9.04507811779063 & -7.46651705753182 \\ C & 1.15236591362021 & -5.271266259036 \\ C & 1.15236591362021 & -5.27126029065 \\ C & 1.15759503322 & -4.67079173770644 \\ C & 5.1910935897088 \\ C & 2.2070659900234 & -9.39141567313585 & -4.67079173770644 \\ C & 1.07864555484192 & -5.350623610055 & -9.14227754484380037148 \\ C & 1.966253023413258 & -0.954164 & -9.561443830037148 \\ C & 1.9662530585415 & -9.26138720270023 & -5.00895912837220 \\ C & 1.96625305787155033 & -1.4105570735183 & -9.4892465542588 \\ C & 9.17610074463538 & -0.949246554258410 \\ C & 1.9662653057415 & -9.26138720270023 & -5.008995912837220 \\ C & 1.966263057815 & -9.02494655425840 \\ C & 1.9662530587115 & -9.07427623411085 \\ C & 1.966253057415 & -9.07428524110944552741545 \\ C & 1.9662530527105 & -5.8434532797350 \\ C & 9.3145507352075215716 & -5.8434532797350 \\ C & 5.31671441311312 & -3.96168611105522 \\ C & 9.207654517729 \\ C & 1.24326457373769 & -9.9131168544534 \\ C & 8.00931067476861 & -5.38665800396782 & -6.8799177313769 \\ C & 5.30757552726 & -5.4375582973515 & -1.01439775022 & -7.547502642489431 \\ C & 5.00237678517729 & -4.32839257322386 & -0.939494841065337 \\ C & 5.00373786040961 & -5.33865190306782 & -6.87993777313769 \\ C & 7.005595965473 & -0.87750479977315 & -0.1783975102 & -7.547502627315 \\ C & 7.71555926751176 & -7.7125552526135 & -0.1093743165347 \\ C & 1.01828770355816 & -4.541320237964 & -0.6738934758970 \\ C & 7.00559347575929 & -4.32839257322386 & -0.939821438570 \\ C & 5.003737866429 & -8.99847244594 & -5.3758529664960 \\ C & 7.33953475575929 & -4.373928716344 \\ C & 7.03735891054914 & -5.3758529474 \\ C & 1.01832877855898 & -3.338116984393 \\ C & 7.178459732328 & -0.117839743 & -0.0178378 & -0$	C	1.251702788122455	-6.434709870454210	-8.486620030547767	C	10 013108088706007	-6 844357371644583	-6.488864222703053
$ \begin{array}{c} c \\ s. 0.003361 1753292 \\ s. 0.003361 1753292 \\ c. 1.5236051312320 \\ c. 1.52360513120 \\ c. 1.523605131620 \\ c. 1.52360513162 \\ c. 1.52360513162 \\ c. 1.52360513160 \\ c. 1.52360513162 \\ c. 1.536052305141 \\ c. 1.52360513162 \\ c. 1.536052305141 \\ c. 1.536052305541 \\ c. 1.5160522 \\ c. 1.51637055522325 \\ c. 1.53605203305765 \\ c. 2.5176517292 \\ c. 2.51765171292 \\ c. 2.51765171579497623 \\ c. 2.3965182010 \\ c. 2.34281775497623 \\ c. 2.396582011652 \\ c. 1.51320457055822316 \\ c. 2.39714380493162371 \\ c. 2.39714380493162371 \\ c. 2.39714890090191847 \\ c. 2.43695427348562 \\ c. 2.37101675942623 \\ c. 2.397148912400 \\ c. 2.3970582104 \\ c. 2.39705829252 \\ c. 2.517652027115 \\ c. 2.517552027115 \\ c. 2.51755202$	C	4.428080055271212	-3.38///0310/41010	-10.460169815820498	č	6 653732661643051	-3 463247751945231	-7 312256882933360
N         3.221421911323294         -1.839/9513052905         -1.839/9513052905         -1.839/9513052905         -1.835305103023         -1.835305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -1.825305103023         -5.0148052711159           C         1.97540644137360         -5.22742604289339         -0.4010266903184         -9.831165570385145         -9.63318570270023         -5.0148052711159           C         1.984646822083173         -3.94468661810552         -0.106533660699218         -9.143869290219847         -5.63098472087033         -5.0148052711576         -5.4639847208304           C         3.94488348839         -10.010260351835         C         10.106539660699218         -9.143869290219847         -5.6309857203711676         -5.84384973553227         -5.63098472083304           C         3.94488348839         -10.0102690351835         C         10.10653966069218         -9.143869290219847         -5.7639977313769         -5.4739771316792         -5.433849773137692         -5.873580477035562731         -6.530955503039756         -5.473937773137692         <	C	8.006358115153320	-6.581795012681004	-9.826468070487380	N	5 138697700825863	-7 998603847064761	-5 212485159186647
$ \begin{array}{c} c \\ c \\ 2.107678175219 \\ c \\ 1.152365913162021 \\$	N	3.221421571753294	-7.837626330432863	-8.139795415629605	C	3 8178867600022000	-7.648536625580023	-4 923767116659348
$ \begin{array}{c} C & 2.2107658173(22119 & -9.901597811779963 & -7.466517057531822 & C & 3.107016599306234 & -9.83141565135852 & -1.05294814492677 \\ C & 1.917549684113736 & -7.615615074657518 & -8.089181944373992 & C & 5.11800806789281 & -9.17251575890332 & -4.670794737706442 \\ C & 1.97894555484192 & -5.2274504298016 & -9.54443850374188 & N & 8.09762830334532 & -8.00561575890342 & -4.57019473770644 \\ C & 1.97894555484192 & -5.32662361010955 & -9.14225744842801 & C & 7.89662390534532 & -8.005611578990449 & -4.957047263211150 \\ C & 1.946496822083173 & -3.28441533469833 & -9.480294685425386 & C & 9.17610079463633 & -9.974910866963178 & -4.95704726321190 \\ C & 1.946496822083173 & -3.28441533469833 & -0.0010269031835 & C & 0.10653905402374 & -5.680590396782 & -5.84384973553272 \\ C & 6.32170760741695 & -5.14345529739534 & -9.9133111685445344 & N & 8.096310667469661 & -5.38665800396782 & -6.87939773137692 \\ C & 6.92076545439314 & -3.24118680801045 & -10.0934794547047 & C & 0.1084287704258166 & -4.5412047957602 & -7.5845750424498431 \\ C & 8.002376785177292 & -4.2363925732286 & -10.993479441762 & 0.1084287704258166 & -4.54120437957602 & -7.884570424498431 \\ C & 7.37101579457968 & -5.43785692732386 & -10.9934794417 & C & 10.184287704258166 & -4.54120437957602 & -7.88457042449813 \\ C & 7.30450915177679 & -7.72555262743815 & -0.171190307945331 & C & 5.3975584054904 & -3.99782148273901 & -6.87106458492473 \\ C & 7.39428615793072 & -1.27184505222822 & -8.6650990849238 \\ C & 5.8873247896429 & -3.471850674669 & -4.230705529024 & -6.652913106579830 \\ C & 7.34945091517767 & -7.72555262743848 & -9.171190307945331 \\ C & 5.9873247826512 & -7.71184505228242 & -8.6650990849238 \\ N & 5.2778586014304 & -5.32970129158042 & -6.87106458492473 \\ C & 7.0985591389745 & -9.8170647566755 & C & 4.918290996301 & -3.3015761570672625 \\ C & 4.9048985587875 & -9.8192423874949 & -7.61729408317367 \\ C & 7.39236615793072 & -2.1867704676665697 \\ C & 4.92187885498 & -5.472649673716 & -5.549297278186 & -5.549294778578 & -5.54929475788322 \\ C & 5.66628414465 & -10.18$	C	3.487744295029743	-9.162113216216895	-7.788211724839771	C	3 13/801810617380	8 728701585662803	4 114670062188452
$ \begin{array}{c} C & 1.5236591310221 & -8.794785596314640 & -7.5190.9935897088 & C & -2.57047265718 & -8.00545175890333 & -1.670794737706442 \\ \hline 1.0798478455488192 & -5.3506233610055 & -9.14275744842801 & C & 7.89662539586615 & -9.2618872027002 & -5.008959512837230 \\ \hline 1.062687787153023 & -4.131055970351833 & -9.480294685425386 & D & 9.7610079436383 & -9.97401086993178 & -4.957047263241190 \\ \hline 1.062687787153023 & -4.131055970351833 & -9.480294685425386 & D & 9.17610079436389 & -9.974010869930178 & -4.957047263241190 \\ \hline 1.04649823035643173 & -3.284415334698339 & -10.011026090351835 & C & 9.415929752157167 & -7.909226265327166 & -5.843849735533272 \\ \hline 5.16341759497623 & -3.96486810552 & -10.0933723804862 & C & 9.415929752157167 & -7.909226265327166 & -5.843849735533272 \\ \hline 5.716714413113182 & -3.067182204909 & -10.3057058523362 & C & 9.390403693452374 & -5.658065093977602 & -7.854750424489431 \\ C & 6.290765454393149 & -3.241180688010459 & -10.99347540740447 & C & 10.18427703258166 & -4.541320437957602 & -7.84750424489431 \\ \hline C & 8.002376785177292 & -4.32639259732386 & -10.99349481106537 & C & 7.85053475796295 & -4.078393904255023 & -7.4775761271595 \\ \hline C & 7.1001579457668 & -5.43756622743915 & -10.17324478224653 & C & 7.85053475796295 & -4.078393904255023 & -7.4938971638134 \\ \hline C & 7.00857591387742 & -8.9629041966149 & -8.4718360740066 & -3.99782143827390 & -6.871066468402473 \\ \hline C & 7.0085751387425 & -9.819242387449 & -8.47183507410026 & C & 3.3021502245478 & -4.23307055829241 & -6.69739300 + 6.871066468402473 \\ C & 7.0085578138725 & -9.8119242387449 & -8.471835074100626 & C & 3.93735890540904 & -3.99782143827390 & -5.573018493120300 \\ \hline 7.3422846573937 & -9.81924239864573937 & -1.117345302996561 & -1.01134724242457 & -8.33051254594448 & -5.67761942984024 \\ C & 5.068448745845742 & -5.887159713933 & -4.3471496849485425 & -5.88715971393348 & -5.071639429427613340 \\ C & 7.0698567814465 & -2.379535512020332 & -0.85913415263001 H & 10.078713127872 & -3.851149683667784 & -5.442485761 \\ D & 9.8246573037 & -4.34712465784998 & -$	C	2.210705781752119	-9.904597811779963	-7.466517057531822	C	4 200706500306234	0.831/15673135851	4.052048164420667
$ \begin{array}{c} 191734968413736 & -7.615013074657318 & -5.08918194373392 & C & 5.17050307331325 & -5.015451750890444 & -5.501480527714584 \\ C & 1.789645554841912 & -5.350623361010955 & -9.142275744812891 & C & 7.89662339556161 & -9.263188720270023 & -5.008995912837230 \\ C & 1.946496822083173 & -3.284415334698339 & -10.041026690351835 & C & 10.16539660699218 & -9.143869290219847 & -4.55014805277147582341190 \\ C & 1.946496822083173 & -3.284415334698339 & -10.041026690351835 & C & 10.06539660699218 & -9.143869290219847 & -5.453998472083304 \\ C & 3.243817759497623 & -3.9646866181065522 & -10.05038233804862 & C & 9.41592752157167 & -7.909226265327106 & -5.843849735533272 \\ C & 6.037170760741695 & -5.14344532973550 & -0.913311685445334 & N & 8.096310667469661 & -5.386658003936782 & -6.873939773137692 \\ C & 5.90754545393149 & -3.24118688010459 & -10.993877540740447 & C & 10.184287703251166 & -4.5113204375764724489431 \\ C & 8.002376785177292 & -4.326392507322386 & -10.993494441065337 & C & 9.169369346259858 & -3.395160963168493 & -7.6477376912719595 \\ C & 7.371101579457968 & -5.437556829743915 & -10.173244782024653 & C & 7.889534757959295 & -4.07893904255023 & -7.298389716381434 \\ C & 5.3277129525271767 & -7.72545522822 & -8.665099808409238 & N & 5.27585269614430 & -5.3297101291580429 & -6.8571066468102473 \\ C & 7.008955913897452 & -9.815924238473490 & -9.07770647967253 & C & 4.191892009963001 & -3.3011576137610424 & -6.9339054985857 \\ C & 7.008955913897452 & -9.815924238473494 & -8.27887706566697 & C & 4.10182859358466 & -5.422336123581426 & -5.66785394498516 \\ C & 5.16848985528879 & -11.117345302949561 & -7.61723706671767 & C & 1.92176693548726 & -5.422336123581426 & -5.66785394798712 \\ C & 5.068551389742 & -9.815921241434 & -8.27887706566697 & C & 4.1018389358786 & -5.42233612381426 & -5.6672834274267518933 & -4.43419568142054 & -5.573018493120300 \\ C & 7.34923645799972 & -12.67751479677 & -9.28286770656697 & C & 4.10163859358786 & -5.42233612381426 & -5.6672894479671892 \\ C & 5.06825841 & -8.279711972313292 & -5.2469668977$	C	1.152365913162021	-8.794785596314640	-7.519049935897088	C	4.200700333500234 5.418008067080281	-9.172515758903932	-4.670794737706442
N         3.096/24945793976         -5.27426042980416         -9.34843850374188         A         -5.005302502502202         -5.006305110955         -5.30062531010955         -5.30062531010955         -5.30062531010955         -5.008995712372023         -5.008995712372324           C         1.062687787153023         -4.13105507051833         -9.480294685425386         C         9.17010079436389         -9.974910866963178         -4.957047263241190           C         3.24313775497623         -3.964686618105522         -10.041026690351835         C         9.0701067460661         -5.38665800303672         -5.843849735533272           C         6.033170760741695         -5.143446329793540         -9.91311685445334         N         8.006310667460661         -5.38665800303672         -5.843849735533272           C         6.5920765454339149         -3.241180688010459         -0.09344841065337         C         10.1933646259858         -3.339516093164893         -6.8773791271592           C         7.371001579457068         -5.43756829743915         -10.173244782024653         C         7.859534757952952         -4.078393904255023         -7.29853871683710679303           C         7.391015794779         -7.7184505252882         -8.65099808409238         N         5.27585266144344         -5.327701271584444394         -6.871066468402473         -6.87106646840247	C	1.917549684413736	-7.615615074657518	-8.089181944373992	N	8.007628302334325	8.005451750800444	5 501/805271/15/0
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N	3.096724945793976	-5.227426042980416	-9.548443850374188	C	7 806625305856415	0.263188720270023	5 008005012837230
$ \begin{array}{c} C & 1.062687787153023 & -1.31005970351833 & -9.480294683425386 & C & 0.101005390300 & -0.14386920219847 & -5.46399472083304 \\ C & 3.243817759407623 & -3.28441532468830 & -9.913311685445334 & N & 8.06631667469661 & -5.843849735538272 \\ N & 6.033170760741695 & -5.143445320739540 & -9.913311685445334 & N & 8.06631667469661 & -5.843849735538272 \\ C & 5.716714413113182 & -3.967185204280490 & -10.430570585823396 & C & 9.300493693452374 & -5.658005279823011 & -6.96292734858023 \\ C & 6.920765454393149 & -3.24118968810459 & -10.939877540740477 & C & 10.18428770328166 & -4.541320437957602 & -7.584750424489431 \\ R & 8.002376785177292 & -4.326392597322386 & -10.993408471065337 & C & 9.109306846259585 & -3.391510066168493 & 7.647737612171595 \\ C & 7.371001579457968 & -5.437856829732386 & -10.173244782024653 & C & 7.58953475795295 & -4.078393904255023 & -7.288389716381434 \\ N & 6.132175253227115 & -7.711845052528480 & -9.017110307945331 & C & 5.39755940549040 & -3.997821438273901 & -6.871064668402473 \\ C & 7.03954591517767 & -7.725542564849 & -9.017706479676253 & C & 4.101892009063010 & -3.310157613670424 & -6.60339054985847 \\ C & 7.008559387452 & -8.9912901066549 & -9.037706479676253 & C & 4.010638593585860 & -5.42233612358142 & -5.06678534469 \\ C & 5.89735122653732 & -8.91924238374949 & -8.2868790656597 & C & 4.010638593585860 & -5.42233612358142 & -5.066785344693 \\ C & 5.1684898552879 & -11.117345302949561 & -7.610273906371367 & C & 1.921766035486729 & -5.887158713053486 & -5.01761524884024 \\ C & 7.239236455793797 & -12.167751410911430 & -7.992112398654382 & O & 1.00878131270872 & -3.6714969856374 & -5.504294027613346 \\ C & 5.16848985528479 & -11.117345302949561 & -7.610273906371367 & C & 1.92176633486729 & -5.887158713053486 & -5.01761524884024 \\ C & 7.3492384579372 & -2.811982019065439 & -0.652841053132816 \\ H & 0.0286479179837 & -2.4307575272 & -3.651494294767 & -2.91763934255954284 \\ H & 0.1822417538937 & -6.43972521241135 & -8.25264796665897 & H & 2.291760374386774 & -5.52089818277316 \\ H & 0.026609711206 & -$	C	1.798945554848192	-5.350623361010955	-9.142275744842891	C	0 176100704363830	9.203100720270023	4 057047263241100
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C	1.062687787153023	-4.131055970351833	-9.480294685425386	C	10 106520660600218	-3.374310800303178	5 46200847208221130
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	1.946496822083173	-3.284415334698339	-10.041026690351835	C	0.415020752157167	7 000226265227106	5 942940725522272
N         6.03170760741605         5.143445329739540         -9.913311685445334         N         6.30501700149001         -0.3000300395162         -0.538037131032           C         5.717413131342         -3.96118204280409         -10.43877540740447         C         9.1094369345234         -5.5800300527882301         -6.338027234585023           C         8.00237678517720         -4.326392597322386         -10.9934748202465337         C         9.169369846259858         -3.3951603616493         -7.647737691271595           C         7.371010579457966         -5.43756829743915         -7.71184505252822         -8.665099808409238         N         5.2758526614430         -5.329701291580429         -6.87106468402473           C         7.439450915177679         -7.72554526544840         -9.171190307945331         C         5.397358940549040         -3.997821438273001         -6.87106648402473           C         7.008955913897452         -9.811924238374949         -8.47183070400260         C         4.011638593585860         -5.42236123581426         -5.67685394798322           C         5.897332126537328         -8.99620011665449         -8.28687706656597         C         1.05736192643933         -4.34195681420544         -5.570318493120300           O         7.34923864573972         -12.16751410911430         -7.992112398654382	С	3.243817759497623	-3.964686618105522	-10.050338233804862	N	9.413929732137107	= 1.909220203327100	-0.04004970000272
$ \begin{array}{c} {\rm C} & 5.71671441311312 \\ {\rm C} & 5.907654543931 \\ {\rm C} & 6.9027654543931 \\ {\rm C} & 8.002376785177292 \\ {\rm C} & 4.32639259732238 \\ {\rm C} & -10.993494841065337 \\ {\rm C} & 7.3710017525322718 \\ {\rm C} & -5.437856829713915 \\ {\rm C} & -7.71184505522822 \\ {\rm C} & 8.60639080840238 \\ {\rm C} & 7.43945091517767 \\ {\rm C} & -7.725545262541840 \\ {\rm C} & -9.171190307945331 \\ {\rm C} & 5.275852696144304 \\ {\rm C} & -3.39712191580429 \\ {\rm C} & -6.87106448492473 \\ {\rm C} & 8.009327378966429 \\ {\rm P} & 8.99540232673724 \\ {\rm P} & -7.725545262541840 \\ {\rm P} & -9.171190307945331 \\ {\rm C} & 5.2973852406144304 \\ {\rm C} & -3.397821438273901 \\ {\rm C} & -6.87106468402473 \\ {\rm C} & 8.009327378966429 \\ {\rm P} & 8.99540232673764 \\ {\rm P} & 9.03770676253 \\ {\rm C} & 4.19189200963001 \\ {\rm C} & -3.301157613670424 \\ {\rm C} & 6.9393545287 \\ {\rm C} & -4.1835070400260 \\ {\rm C} & 3.302150224254378 \\ {\rm C} & -4.233070558290241 \\ {\rm C} & -6.07202803318210 \\ {\rm C} & 5.897331226537328 \\ {\rm P} & 8.996290419665449 \\ {\rm P} & 8.286877906566597 \\ {\rm C} & 4.010638593585860 \\ {\rm C} & -5.422336125581426 \\ {\rm C} & 5.16484985852887 \\ {\rm P} & 1.117345302949561 \\ {\rm C} & 7.610279306371367 \\ {\rm C} & 1.92176693548729 \\ {\rm C} & 1.9273619264393 \\ {\rm C} & 4.3149568142044 \\ {\rm C} & 5.1731305346 \\ {\rm C} & 5.16484985852887 \\ {\rm P} & 1.117345302949561 \\ {\rm C} & -7.610279306371367 \\ {\rm C} & 1.92176693548729 \\ {\rm C} & 1.00878131270872 \\ {\rm C} & 3.35712204376 \\ {\rm P} & 3.273268710278 \\ {\rm C} & 8.355122004376 \\ {\rm C} & -2.3753521202032 \\ {\rm C} & -0.665284105312816 \\ {\rm P} & 0.4702868472924415 \\ {\rm C} & -0.088472524541 \\ {\rm C} & -2.37535351202032 \\ {\rm C} & -2.409541432876201 \\ {\rm C} & -2.3753251200323 \\ {\rm C} & -2.409541432876201 \\ {\rm C} & -0.372785333 \\ {\rm H} & 9.29913340956838 \\ {\rm C} & -0.1709367910618 \\ {\rm C} & -4.67599489976301078 \\ {\rm C} & -3.5871871087288 \\ {\rm C} & -0.17093673146728 \\ {\rm C} & -2.409541432876201 \\ {\rm C} & -2.409541432876201 \\ {\rm C} & -2.375673284918 \\ {\rm H} & 1.052245544445 \\ {\rm C} & -2.40854143204555 \\ {\rm C} & -2.409573418941205 \\ {\rm C} & -2.409573418941205 \\ {\rm C$	Ν	6.033170760741695	-5.143445329793540	-9.913311685445334	C	0.090310007409001	-0.00000000000000000000000000000000000	-0.019391113131092 6.02602792405002
$ \begin{array}{c} {\rm C} & 6.920765454393149 \\ {\rm c} & .3.241189668010459 \\ {\rm c} & .0.993877540740447 \\ {\rm c} & .0.93367754517929 \\ {\rm c} & .3.241189668010459 \\ {\rm c} & .0.993877540740447 \\ {\rm c} & .0.93367754517292 \\ {\rm c} & .3.27001579457968 \\ {\rm c} & .4.37856829743915 \\ {\rm c} & .1.0.434294841065337 \\ {\rm c} & .5.437856829743915 \\ {\rm c} & .1.0173244782024653 \\ {\rm c} & .5.373589064904 \\ {\rm c} & .3.997821438273901 \\ {\rm c} & .5.27585269144304 \\ {\rm c} & .3.997821438273901 \\ {\rm c} & .5.27585269144304 \\ {\rm c} & .3.997821438273901 \\ {\rm c} & .5.27585269144304 \\ {\rm c} & .3.997821438273901 \\ {\rm c} & .5.27585269144304 \\ {\rm c} & .3.997821438273901 \\ {\rm c} & .6.871066468402473 \\ {\rm c} & .6.9390549858547 \\ {\rm c} & .7.008955913897452 \\ {\rm c} & .9.811924238374949 \\ {\rm s} & .8.471835070400260 \\ {\rm c} & .5.89733122653738 \\ {\rm s} & .8.99609419665449 \\ {\rm c} & .8.2867790656597 \\ {\rm c} & 4.10163859358860 \\ {\rm c} & .4.233070558290241 \\ {\rm c} & .666785394798322 \\ {\rm c} & .666785794798322 \\ {\rm c} & .666785794798322 \\ {\rm c} & .666785794798322 \\ {\rm c} & .666785794798327 \\ {\rm c} & .1.117345302949651 \\ {\rm c} & .1.163634287212243 \\ {\rm s} & .8.040336224799427 \\ {\rm c} & 1.9573612926543933 \\ {\rm c} & .1.6871312708722 \\ {\rm c} & .1.67751410911430 \\ {\rm c} & .7.092112398654382 \\ {\rm c} & .1.08781312708722 \\ {\rm c} & .1.0871353468 \\ {\rm c} & .5.164898582884 \\ {\rm c} & .5.16489858287 \\ {\rm c} & .1.117345302949561 \\ {\rm c} & .6.67944883844566 \\ {\rm c} & .0.133417248193405 \\ {\rm d} & .6.324507178937 \\ {\rm c} & .6.6769488384566 \\ {\rm c} & .0.133417248193405 \\ {\rm d} & .6.5246946156883947 \\ {\rm d} & .3.276673102780 \\ {\rm c} & .3.5551224034753 \\ {\rm c} & .5.1749408947009 \\ {\rm d} & .3.2767873102780 \\ {\rm c} & .5.58743184707410062 \\ {\rm d} & .0.382450718937 \\ {\rm c} & .6.6769488384566 \\ {\rm d} & .0.33417248193405 \\ {\rm d} & .6.5246941412870 \\ {\rm d} & .3.276873102780 \\ {\rm d} & .3.277187332206855914 \\ {\rm d} & .5.294825761092 \\ {\rm d} & .3.2776873102780 \\ {\rm d} & .3.27726873102780 \\ {\rm d} & .3.27726873102780 \\ {\rm d} & .3.55512240347053 \\ {\rm d} & .5.550798036375 \\ {\rm d} & .0.4447378494345$	С	5.716714413113182	-3.967182304280490	-10.430570585823396	C	9.090490090402074	-0.0000000279620011	-0.990927294090029
$ \begin{array}{c} \mathbb{C} & 8.002376785177292 & 4.326302597322386 & -10.99349481065337 & \mathbb{C} & 5.0303640239539 & -3.9910090510094255023 & -7.298389116381434 \\ \mathbb{N} & 6.132175253227115 & -7.71184505252822 & -8.665099808409238 & \mathbb{N} & 5.275852696144304 & -5.329701291580429 & -6.45291310579930 \\ \mathbb{C} & 7.439450915177679 & -7.72545262548480 & -9.171190307945331 & \mathbb{C} & 5.397358940549040 & -3.99781438273901 & -6.871066468402473 \\ \mathbb{C} & 8.009327378966429 & -8.995402366739764 & -9.037706479676253 & \mathbb{C} & 4.19189200963001 & -3.30157613670424 & -6.603390548958547 \\ \mathbb{C} & 7.008955913897452 & -9.811924238374949 & -8.471835070400260 & \mathbb{C} & 3.302150224254378 & -4.233070558290241 & -6.107202803318210 \\ \mathbb{C} & 5.897331226537328 & -8.996200419665449 & -8.286877905666597 & \mathbb{C} & 4.010638593585860 & -5.422330123581426 & -5.966785394798322 \\ \mathbb{C} & 6.662184774836515 & -11.163634287212243 & -8.40336224799427 & \mathbb{C} & 1.957361926543933 & -4.434195681420544 & -5.573018493120300 \\ \mathbb{C} & 7.349238645739372 & -12.167751410911430 & -7.992112398654382 & \mathbb{O} & 1.008781312708722 & -3.67146983636784 & -5.540294027613346 \\ \mathbb{C} & 5.168489858528879 & -11.117345302949561 & -7.610279306371367 & \mathbb{C} & 1.921766935486729 & -5.887158713053486 & -5.017615242844024 \\ \mathbb{H} & 0.188241783884702 & -6.390725212441453 & -8.271494080497009 & \mathbb{H} & 6.70134724424525 & -10.81022458594944 & -4.231877861598499 \\ \mathbb{H} & 4.37086567841465 & -2.3775551220032 & -10.8513415263611 & \mathbb{H} & 11.082374267518993 & -6.917899354892501 & -6.665284105312816 \\ \mathbb{H} & 0.70233206885941 & 8.529711972313292 & -6.524694656808907 & \mathbb{H} & 3.3924651686731669 & -10.710394707010618 & -4.64759966356705 \\ \mathbb{H} & 0.7033220688591 & -8.529711972313292 & -6.524694566808907 \\ \mathbb{H} & 1.050414514441269 & -4.87384139043625 & -8.8609854849998 \\ \mathbb{H} & 0.702389654761 & -2.09541332876201 & -10.32267933837481 & \mathbb{H} & 10.50414514441269 \\ -0.633440870741061 & -12.009367728563334 & \mathbb{H} & 9.39979330956838 & -2.271463974131486 & -5.92398189277316 \\ \mathbb{H} & 0.09376344650411 & -3.975047230976777 & -9.285536$	С	6.920765454393149	-3.241189688010459	-10.993877540740447	C	0 160260046250050	-4.041020407907002 2.205160062168402	-7.304730424409431 7.647727601271505
$ \begin{array}{c} C & 7.311001579457968 & -5.437856829743915 & -10.173244782024653 \\ C & 7.439450915177679 & -7.72554526254848 & -9.171190307945331 \\ C & 7.439450915177679 & -7.72554526254848 & -9.171190307945331 \\ C & 8.009327378966429 & -8.995402326739764 & -9.037706479676253 \\ C & 4.09327378966429 & -8.995402326739764 & -9.037706479676253 \\ C & 7.008955913897452 & -9.81192423837494 & -8.471835070400260 \\ C & 3.030215024254378 & -4.23307058290241 & -6.07020020318210 \\ C & 5.89731226537328 & -8.996290419665449 & -8.286877906566597 \\ C & 4.010638593585860 & -5.422336123581426 & -5.966785394798322 \\ C & 6.662184774836515 & -11.163634287212243 & -8.040336224799427 \\ C & 1.927766192654393 & -4.43119508142054 & -5.573018493120300 \\ C & 5.168489858528879 & -11.117345302949561 & -7.610279306371367 \\ C & 1.921766935486729 & -3.87158713053486 & -5.01761524284024 \\ H & 0.18824178388470 & -6.39072521241435 & -8.271494080497009 \\ H & 4.370865678414465 & -2.37953551202032 & -10.859134152636011 \\ H & 0.1862477888470 & -6.4907252245415 & -8.271494080497009 \\ H & 2.019509099711206 & -10.68048725245415 & -8.215948257610922 \\ H & 8.207112332618482 & -4.682944807048016 & -12.009367728563934 \\ H & 0.1954142387610 & -0.455254041762 & -8.13752800647029 \\ H & 9.209703440365045 & -10.710398679010618 & -4.647509963596705 \\ H & 0.00937634465041 & -3.975047230976777 & -9.285536727689802 \\ H & 0.209771128216 & -9.0452544041762 & -8.13752880647029 \\ H & 9.2997033090568483 & -2.01875088282586 & -6.906942557501343 \\ H & 0.00937634465041 & -3.975047230976777 & -9.285536727689802 \\ H & 4.020374069818506 & -2.271463974131486 & -6.942612962985045 \\ H & 0.00937634465041 & -3.975047230976777 & -9.285536727689802 \\ H & 4.020374069818506 & -2.271463974131486 & -6.942612962985045 \\ H & 0.202969868489$	С	8.002376785177292	-4.326392597322386	-10.993494841065337	C	9.109309840239838	-3.393100903108493	-7.04//3/0912/1090
N       6.132175253227115       -7.711845052522822       -8.665099808409238       N       5.273552090144304       -3.0270121806429       -6.322115105429       -6.312351426       -6.107202803318210       -6.017202803318210       -5.3973512255327212       -8.40336224799427       C       1.937361925543933       -4.43419568142054       -5.573018493120300         O       7.349238645793972       -12.167751410911430       -7.992112398654382       O       1.008781312708722       -3.671496983636784       -5.540294027613346         C       5.16848985528879       -11.117345302949561       -7.610279306371367       C       1.921766935486729       -5.887158713053486       -5.10761524284024       -5.510294027613346       -4.317861598499       -4.32177861598499       -4.3177861598499       -4.3177861598499       -4.3177861598499       -4.665284105312816       -10.13247545149474424525       -10.81024585	С	7.371001579457968	-5.437856829743915	-10.173244782024653	N	1.009004101909290 5.075050c0c144904	-4.076595904255025	-1.290309110301434 C 452012100570020
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Ν	6.132175253227115	-7.711845052522822	-8.665099808409238	IN C	0.270802090144304	-0.329701291080429	-0.452915100579950
$ \begin{array}{c} C & 8.009327378966429 & -8.995402326739764 & -9.037706479676253 \\ C & 7.008955913897452 & -9.811924238374949 & -8.471835070400260 \\ C & 3.3021502245245478 & -4.23070558290241 & -6.10720280318210 \\ C & 5.897331226537328 & -8.996290419665449 & -8.286877906566597 \\ C & 4.010638593585860 & -5.422336123581426 & -5.966785394798322 \\ C & 6.662184774836515 & -11.163634287212243 & -8.040336224799427 \\ C & 1.997361926543933 & -4.434195681420544 & -5.573018493120300 \\ O & 7.349238645793972 & -12.167751410911430 & -7.992112398654382 \\ O & 1.008781312708722 & -3.671496983636784 & -5.540294027613346 \\ C & 1.982417833884702 & -6.390725212441435 & -8.271494080497009 \\ H & 0.188241783884702 & -6.390725512441435 & -8.271494080497009 \\ H & 4.370865678414465 & -2.379535512020332 & -10.859134152636011 \\ H & 9.045026630017778 & -6.676946883844566 & -10.133417248193405 \\ H & 0.072332206885941 & -8.529711972313292 & -6.524694656808907 \\ H & 2.01950909711206 & -10.68084872544515 & -8.215948257610922 \\ H & 8.207112332618482 & -4.682944807048016 & -12.0093677285673102780 & -8.35512240347053 & -3.117934255954284 \\ H & 0.772332206885941 & -8.529711972313292 & -6.524694656808907 \\ H & 8.207112332618482 & -4.682944807048016 & -12.009367728563934 \\ H & 5.094843685161185 & -11.442762293723376 & -6.566258423598884 \\ H & 1.01594135164871669 & -10.7193967910618 & -4.647509963596705 \\ H & 7.170589952964700 & -2.409541432876201 & -10.322679328334781 \\ H & 0.0993763445054516185 & -11.442762293723376 & -6.566258423598884 \\ H & 1.115923977308537 & -6.434713276838148 & -5.520389182727316 \\ H & 0.286097711282160 & -9.045525440411762 & -8.13752880647029 \\ H & 0.099376344650441 & -3.975047230976777 & -9.285536727689802 \\ H & 0.009376344650441 & -3.975047230976777 & -9.285536727689802 \\ H & 4.02037068918506 & -2.271463974131486 & -6.942612962985045 \\ H & 0.02866673784517465 & -10.40070188758446 & -6.49291786725455 \\ H & 9.00409056407393 & -9.2766936952784 & -9.356779863665558 \\ H & 9.132207402787555 & -2.910039945331830 & -8.626288576424587 \\ H & 2$	С	7.439450915177679	-7.725545262548480	-9.171190307945331	C	0.397308940049040	-3.997821438273901	-0.8/10004084024/3
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\mathbf{C}$	8.009327378966429	-8.995402326739764	-9.037706479676253	C	4.191892009903001	-3.310137013070424	-0.093390349838347
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\mathbf{C}$	7.008955913897452	-9.811924238374949	-8.471835070400260	č	3.302130224234378	-4.233070338290241	-0.107202803318210
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\mathbf{C}$	5.897331226537328	-8.996290419665449	-8.286877906566597	č	4.010038393383800	-0.422330123081420	-0.900/80394/98322
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$\mathbf{C}$	6.662184774836515	-11.163634287212243	-8.040336224799427	Č	1.997301920943933	-4.434195081420544	-0.073018493120300
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0	7.349238645793972	-12.167751410911430	-7.992112398654382	O C	1.008781312708722	-3.071496983636784	-5.540294027613346
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\mathbf{C}$	5.168489858528879	-11.117345302949561	-7.610279306371367	C	1.921766935486729	-5.887158713053486	-5.017615242884024
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Η	0.188241783884702	-6.390725212441435	-8.271494080497009	H	6.701347244244525	-10.810224585949445	-4.231877861598499
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	Η	4.370865678414465	-2.379535512020332	-10.859134152636011	H	11.082374267518993	-6.917899354892501	-6.665284105312816
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	Н	9.045026630017778	-6.676946883844566	-10.133417248193405	H	6.633245071798373	-2.430601909393331	-7.651847407410062
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	Η	2.019509099711206	-10.680848725245415	-8.215948257610922	H	2.873726873102780	-8.355512240347053	-3.117934255954284
H7.170589952964700-2.409541432876201-10.322679328334781H10.504145144112609-4.873384139043625-8.580699854849998H8.207112332618482-4.682944807048016-12.009367728563934H9.399793309056838-2.621875088282586-6.906942557501343H5.094843685161185-11.442762293723376-6.566258423598884H1.115923977308537-6.434713276838148-5.520389182727316H0.286097711282160-9.045525440411762-8.137528800647029H9.299103440365045-10.9838837848520-4.58560268003750H0.009376344650441-3.975047230976777-9.285536727689802H4.020374069818506-2.271463974131486-6.942612962985045H6.720296968408930-2.816767859044978-11.981264036725435H4.408008607858338-10.183226743305575-3.038312690206619H8.952903298656379-3.988489997637410-10.57503759483466H11.087822891459020-4.300028684239243-7.017884347235350H9.004099056407393-9.276690369522784-9.356779863665558H9.132207402787055-2.910039945331830-8.626285876424587H2.260163784517465-10.400701887585464-6.492917867256669H2.202845100081345-9.061198700262814-4.581197197652243H4.594362468306144-11.832026860594315-8.212049097382748H1.672636390897452-5.861540342898767-3.949736381909533H1.777486084130031-2.281118550798253-10.410820084441989H11.166932470908383-9.3	Η	0.772332206885941	-8.529711972313292	-6.524694656808907	H	3.924651686731669	-10.710939679010618	-4.647509963596705
H8.207112332618482-4.682944807048016-12.009367728563934H9.399793309056838-2.621875088282586-6.906942557501343H5.094843685161185-11.442762293723376-6.566258423598884H1.115923977308537-6.434713276838148-5.520389182727316H0.286097711282160-9.045525440411762-8.137528800647029H9.299103440365045-10.983883878848520-4.585500268003750H0.009376344650441-3.975047230976777-9.285536727689802H4.020374069818506-2.271463974131486-6.942612962985045H6.720296968408930-2.816767859044978-11.981264036725435H4.408008607858338-10.183226743305575-3.03831269026619H8.952903298656379-3.988489997637410-10.572503759483466H11.087822891459020-4.300028684239243-7.017884347235350H9.004099056407393-9.276690369522784-9.356779863665558H9.132207402787055-2.910039945331830-8.626285876424587H2.260163784517465-10.400701887585464-6.492917867256669H2.202845100081345-9.061198700262814-4.581197197652243H4.594362468306144-11.832026860594315-8.212049097382748H1.672636390897452-5.861540342898767-3.949736381909533H1.777486084130031-2.281118550798253-10.410820084441989H11.166932470908383-9.320999202371636-5.593296299762109	Η	7.170589952964700	-2.409541432876201	-10.322679328334781	H	10.504145144412609	-4.873384139043625	-8.580699854849998
H       5.094843685161185       -11.442762293723376       -6.566258423598884       H       1.115923977308537       -6.434713276838148       -5.520389182727316         H       0.286097711282160       -9.045525440411762       -8.137528800647029       H       9.299103440365045       -10.983883878848520       -4.585560268003750         H       0.009376344650441       -3.975047230976777       -9.285536727689802       H       4.020374069818506       -2.271463974131486       -6.942612962985045         H       6.720296968408930       -2.816767859044978       -11.981264036725435       H       4.408008607858338       -10.183226743305575       -3.038312696026619         H       8.952903298656379       -3.988489997637410       -10.572503759483466       H       11.087822891459020       -4.300028684239243       -7.017884347235350         H       9.004099056407393       -9.276690369522784       -9.356779863665558       H       9.132207402787055       -2.910039945331830       -8.626285876424587         H       2.200163784517465       -10.400701887585464       -6.492917867256669       H       2.202845100081345       -9.061198700262814       -4.581197197652243         H       1.577486084130031       -2.281118550798253       -10.410820084441989       H       11.166932470908383       -9.320999202371636       -5.93296299762109 </td <td>Η</td> <td>8.207112332618482</td> <td>-4.682944807048016</td> <td>-12.009367728563934</td> <td>H</td> <td>9.399793309056838</td> <td>-2.621875088282586</td> <td>-6.906942557501343</td>	Η	8.207112332618482	-4.682944807048016	-12.009367728563934	H	9.399793309056838	-2.621875088282586	-6.906942557501343
H       0.286097711282160       -9.045525440411762       -8.137528800647029       H       9.299103440365045       -10.983883878848520       -4.5856026809750         H       0.009376344650441       -3.975047230976777       -9.285536727689802       H       4.020374069818506       -2.271463974131486       -6.942612962985045         H       6.720296968408930       -2.816767859044978       -11.981264036725435       H       4.408008607858338       -10.183226743305575       -3.038312696026619         H       8.952903298656379       -3.988489997637410       -10.572503759483466       H       11.087822891459020       -4.30002864239243       -7.01788434723550       -8.626285876424587         H       9.004099056407393       -9.27669036952784       -9.356779863665558       H       9.132207402787055       -2.910039945331830       -8.626285876424587         H       2.200163784517465       -10.400701887585464       -6.492917867256669       H       2.202845100081345       -9.061198700262814       -4.581197197652243         H       1.577486084130031       -2.281118550798253       -10.410820084441989       H       1.166932470908383       -9.320999202371636       -5.593296299762109	Η	5.094843685161185	-11.442762293723376	-6.566258423598884	Н	1.115923977308537	-6.434713276838148	-5.520389182727316
H       0.009376344650441       -3.975047230976777       -9.285536727689802       H       4.020374069818506       -2.271463974131486       -6.942612962985045         H       6.720296968408930       -2.816767859044978       -11.981264036725435       H       4.408008607858338       -10.183226743305575       -3.03831269026619         H       8.952903298656379       -3.988489997637410       -10.572503759483466       H       11.087822891459020       -4.300028684239243       -7.017884347235350         H       9.004099056407393       -9.27669036952784       -9.356779863665558       H       9.132207402787055       -2.91003994531830       -8.626285876424587         H       2.260163784517465       -10.400701887585464       -6.492917867256669       H       2.202845100081345       -9.061198700262814       -4.581197197652243         H       4.594362468306144       -11.832026860594315       -8.212049097382748       H       1.672636390897452       -5.861540342898767       -3.949736381909533         H       1.777486084130031       -2.281118550798253       -10.410820084441989       H       11.166932470908383       -9.320999202371636       -5.593296299762109	Н	0.286097711282160	-9.045525440411762	-8.137528800647029	Н	9.299103440365045	-10.983883878848520	-4.585560268003750
H6.720296968408930-2.816767859044978-11.981264036725435H4.408008607858338-10.183226743305575-3.038312696026619H8.952903298656379-3.988489997637410-10.572503759483466H11.087822891459020-4.300028684239243-7.017884347235350H9.004099056407393-9.276690369522784-9.356779863665558H9.132207402787055-2.910039945331830-8.626285876424587H2.260163784517465-10.400701887585464-6.492917867256669H2.202845100081345-9.061198700262814-4.581197197652243H4.594362468306144-11.832026860594315-8.212049097382748H1.672636390897452-5.861540342898767-3.949736381909533H1.777486084130031-2.281118550798253-10.410820084441989H11.166932470908383-9.320999202371636-5.593296299762109	Н	0.009376344650441	-3.975047230976777	-9.285536727689802	Н	4.020374069818506	-2.271463974131486	-6.942612962985045
H8.952903298656379-3.988489997637410-10.572503759483466H11.087822891459020-4.300028684239243-7.017884347235350H9.004099056407393-9.276690369522784-9.356779863665558H9.132207402787055-2.910039945331830-8.626285876424587H2.260163784517465-10.400701887585464-6.492917867256669H2.202845100081345-9.061198700262814-4.581197197652243H4.594362468306144-11.832026860594315-8.212049097382748H1.672636390897452-5.861540342898767-3.949736381909533H1.777486084130031-2.281118550798253-10.410820084441989H11.166932470908383-9.320999202371636-5.593296299762109	Η	6.720296968408930	-2.816767859044978	-11.981264036725435	Н	4.408008607858338	-10.183226743305575	-3.038312696026619
H9.004099056407393-9.276690369522784-9.356779863665558H9.132207402787055-2.910039945331830-8.626285876424587H2.260163784517465-10.400701887585464-6.492917867256669H2.202845100081345-9.061198700262814-4.581197197652243H4.594362468306144-11.832026860594315-8.212049097382748H1.672636390897452-5.861540342898767-3.949736381909533H1.777486084130031-2.281118550798253-10.410820084441989H11.166932470908383-9.320999202371636-5.593296299762109	Η	8.952903298656379	-3.988489997637410	-10.572503759483466	Н	11.087822891459020	-4.300028684239243	-7.017884347235350
H       2.260163784517465       -10.400701887585464       -6.492917867256669       H       2.202845100081345       -9.061198700262814       -4.581197197652243         H       4.594362468306144       -11.832026860594315       -8.212049097382748       H       1.672636390897452       -5.861540342898767       -3.949736381909533         H       1.777486084130031       -2.281118550798253       -10.410820084441989       H       11.166932470908383       -9.320999202371636       -5.593296299762109	Η	9.004099056407393	-9.276690369522784	-9.356779863665558	Н	9.132207402787055	-2.910039945331830	-8.626285876424587
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Η	2.260163784517465	-10.400701887585464	-6.492917867256669	Н	2.202845100081345	-9.061198700262814	-4.581197197652243
H 1.777486084130031 -2.281118550798253 -10.410820084441989 H 11.166932470908383 -9.320999202371636 -5.593296299762109	Η	4.594362468306144	-11.832026860594315	-8.212049097382748	Н	1.672636390897452	-5.861540342898767	-3.949736381909533
	Η	1.777486084130031	-2.281118550798253	-10.410820084441989	H	11.166932470908383	-9.320999202371636	-5.593296299762109