Supporting Information

Marcus Inverted Region in Organic Long-Persistent Luminescence Host-Guest Systems Designed from Thermally Activated Delayed Fluorescence Molecule: A Mechanism Study

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1. Calculation Details

1.1 General Methods

All geometric structures are optimized with Gaussian16 Program (Revision C.01),[1] with Minnesota hybrid functional of M06-2X form[2] and def2-SVP basis sets developed by Ahlrich and co-workers used.[3] The Grimme's third dispersion correction (D3) is adopted for better consideration of intermolecular weak interactions.[4] Frequency calculations at the same level are performed for all structures on steady points to ensure no imaginary frequency exists. Excited states are calculated under the framework of time-independent density functional theory (TD-DFT) except for T_1 states are calculated by unrestricted Kohn-Sham method.

Wavefunction analysis (**Table S1** ~ **S4**) is carried out by Multiwfn Program (Development version 3.8)[5] and Visual Molecular Dynamics (VMD, version 1.9.3) is applied for better visualization of our results.[6] Spin-orbit coupling integrals (*H*) are calculated using Dalton2020 Program,[7-8] with both single- and double-electron spin-orbit integrals precisely calculated under CAM-B3LYP/def2-SVP level of theory (**Table S5**).[9] Phosphorescence oscillator strength is calculated with quadratic response theory[10-11] using Dalton2020 Program. Electronic coupling integrals (*V*) in non-adiabatic processes are calculated by fragment charge difference (FCD) method (**Table S6**).[12-13]

1.2 Realization of Fragment Charge Difference

Electronic coupling integrals (V) in non-adiabatic processes are calculated by fragment charge difference (FCD) method[12-13] according to **eq. S1**, where ΔE_{FC} stands for the vertical energy gap between the studied states. Elements of the donor-acceptor 2×2 charge difference matrix $\Delta\mathbf{q}$ are defined as **eq. S2**, where ρ_{mn} stands for the transition density matrix between state m and n. For diagonal elements Δq_{11} and Δq_{22}, ρ_{mn} refers to transition electronic density for excited states. For off-diagonal elements Δq_{12} and Δq_{21}, **eq. S3** is applied for symmetrizing. The integrals involved in FCD calculation can be calculated as summations on the introduced basis set according to Slater-Condon rule, which is performed by Multiwfn Program.[5]

$$V = \frac{\Delta E_{FC}\bar{\Delta}q_{12}}{\sqrt{\left(\Delta q_{11} - \Delta q_{22}\right)^2 + 4\bar{\Delta}q_{12}^2}} \#(eq.\ S1)$$

$$\Delta q_{mn} = q_{mn}^{D} - q_{mn}^{A} = \int_{r \in D} \rho_{mn}(r)dr - \int_{r \in A} \rho_{mn}(r)dr \#(eq.\ S2)$$

$$\bar{\Delta}q_{12} = \frac{1}{2}\left(\Delta q_{12} + \Delta q_{21}\right) \#(eq.\ S3)$$

Below we show an example for $S_1 \rightarrow S_3$ FCD calculation. Contents of input files and system commands are listed on the left, while explanations are on the right.

Gaussian16 input files: TD-DFT job.	
%NProcShared=16	
%OldChk=S1Opt.chk	*Use optimized S_1 state structure.*
%Chk=S1S3FCD.chk	*Save new checkpoint file for following steps.*
#P M062X/def2SVP EM=GD3	*Detailed output (#P) is necessary.*
TD(NStates=5,Root=1) IOp(9/40=4)	*S_1 state as target state. Output all configurations with coefficient > 10^{-4}.*
Guess=Read Geom=AllCheck	*Read optimized S_1 structure from %OldChk.*
Generate transition density matrix.	
formchk S1S3FCD.chk S1S3FCD.fchk	*Write formatted checkpoint files.*
Multiwfn S1S3FCD.fchk	*Read formatted checkpoint file into Multiwfn.*
18	*Electron excitation analysis.*
9	*Generate and export transition density matrix.*
S1S3FCD.log	*Read Gaussian16 output file.*
2	*Generate transition density matrix between two excited states.*
1,3	*Calculate transition density matrix between S_1 and S_3 states.*
Enter	*Use default threshold of product of two configuration coefficients.*
1	*Symmetrize as **eq. S3**.*
y	*Output TDM.fch file in current folder.*
Exit Multiwfn	
Integrate transition density in whole space.	
Multiwfn TDM.fch	*Reload transition density matrix into Multiwfn.*
100	*Other functions (Part 1).*
4	*Integrate a function in whole space.*
1	*Electron density. (Corresponds to transition density)*

Exit Multiwfn

Record final result (to calculate $q_{12}^{D}+q_{12}^{A}$, 559.9997404530) and accumulated value for atom centers 1-67 (303.9810126885, corresponding to PPT donor part, to calculate q_{12}^{D}) on screen. Total electron number of PPT part is 304 and that of CzPhAP is 256. Hence, we have:

$$\Delta q_{12}=q_{12}^{D}-q_{12}^{A}=2q_{12}^{D}-\left(q_{12}^{D}+q_{12}^{A}\right)$$
$$=2\times(303.9810126885-304)-(559.9997404530-304-256)=-0.0377150760\quad(eq.S4)$$

Since we have symmetrized transition density matrix elements before, here $\Delta q_{12}=\Delta q_{21}=\bar{\Delta}q_{12}$.

Calculate inter-fragment charge transfer.	
Multiwfn S1S3FCD.fch	*Read formatted checkpoint file into Multiwfn.*
18	*Electron excitation analysis.*
8	*Calculate inter-fragment charge transfer via IFCT method*
1	*Mulliken-like partition*
S1S3FCD.log	*Read Gaussian16 output file.*
1	*Perform the analysis for S_1 state.*
2	*Define two fragments.*
1-67	*Range of atom number for fragment 1. (PPT part)*
68-123	*Range of atom number for fragment 2. (CzPhAP part)*
0	*Exit this function.*
8	*Calculate inter-fragment charge transfer via IFCT method*
1	*Mulliken-like partition*
3	*Perform the analysis for S_3 state.*
2	*Define two fragments.*
1-67	*Range of atom number for fragment 1. (PPT part)*
68-123	*Range of atom number for fragment 2. (CzPhAP part)*
Exit Multiwfn	

Record two net charge transfer values as 0.71095 for S_1 state and 0.56279 for S_3 state. Hence, we have:

$$\Delta q_{11}=q_{11}^{D}-q_{11}^{A}=-\left(q_{11}^{A}-q_{11}^{D}\right)=-2\times0.71095=-1.42190\#(eq.\ S5)$$
$$\Delta q_{22}=q_{22}^{D}-q_{22}^{A}=-\left(q_{22}^{A}-q_{22}^{D}\right)=-2\times0.56279=-1.12558\#(eq.\ S6)$$

Substitute **eq. S4** ~ **S6** into **eq. S1** and ΔE_{FC} = 0.02353591 a.u. gives V = -0.00290303 a.u., or 636.7 cm^{-1}.

Notice that since we calculate transition density matrix as $S_1 \rightarrow S_3$ transition, the ΔE_{FC} value should hence be calculated as $E(S_3) - E(S_1)$, which is a positive value. Sometimes the final result of coupling integral is a negative value, however, this is not important due to square calculation in **eq. S1**. Positive or negative coupling integral is decided jointly by energy difference and extents of charge separation of two states. Detailed FCD results are listed in **Table S6**.

2. Supplemental Figures

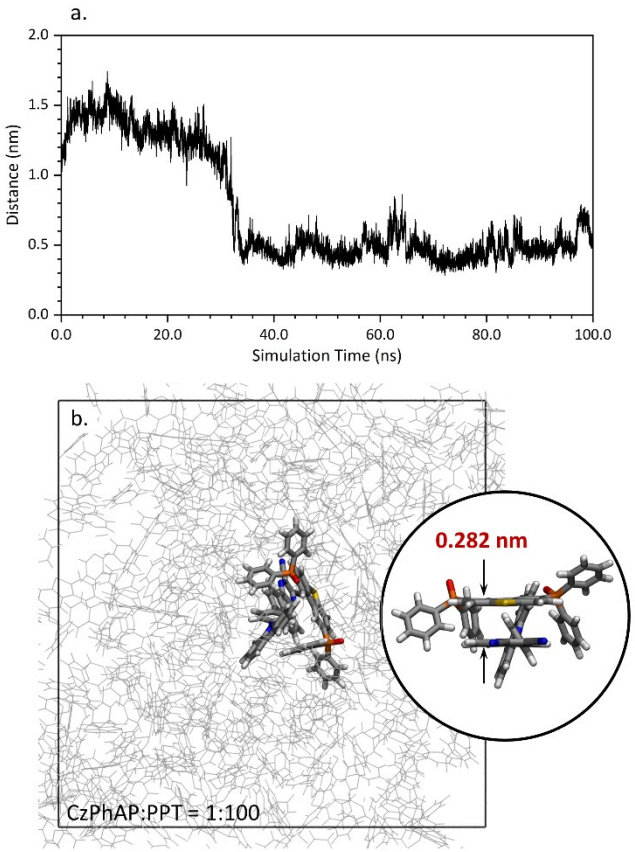

Figure S1. a). Distance between mass centres of AP moiety of CzPhAP and DBT moiety of PPT along the 100 ns MD simulataion after the annealing. This selected PPT molecule holds the longest binding conformation with dopant molecule CzPhAP among the 100 host molecules. **b).** The stacking conformation between CzPhAP and PPT with the minimum distance of 0.282 nm between mass centres in the MD simulation after annealing.

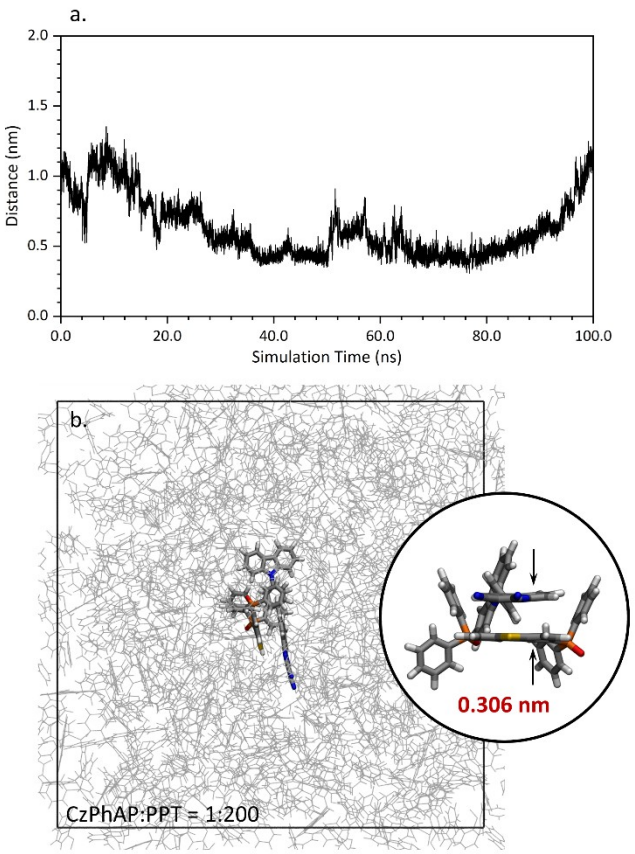

Figure S2. a). Distance between mass centres of AP moiety of CzPhAP and DBT moiety of PPT along the 100 ns MD simulataion after the annealing. This selected PPT molecule holds the longest binding conformation with dopant molecule CzPhAP among the 200 host molecules. **b).** The stacking conformation between CzPhAP and PPT with the minimum distance of 0.306 nm between mass centres in the MD simulation after annealing.

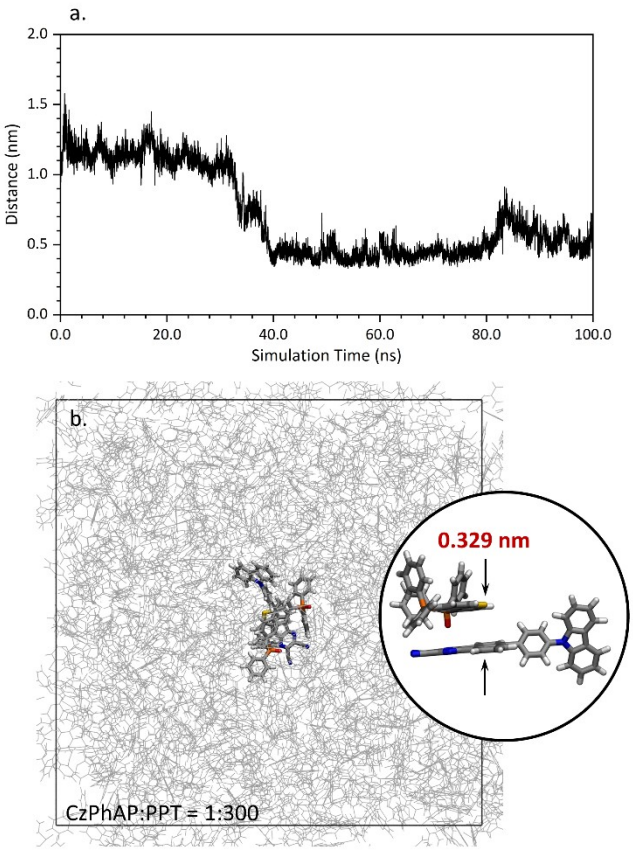

Figure S3. a). Distance between mass centres of AP moiety of CzPhAP and DBT moiety of PPT along the 100 ns MD simulataion after the annealing. This selected PPT molecule holds the longest binding conformation with dopant molecule CzPhAP among the 300 host molecules. **b).** The stacking conformation between CzPhAP and PPT with the minimum distance of 0.329 nm between mass centres in the MD simulation after annealing.

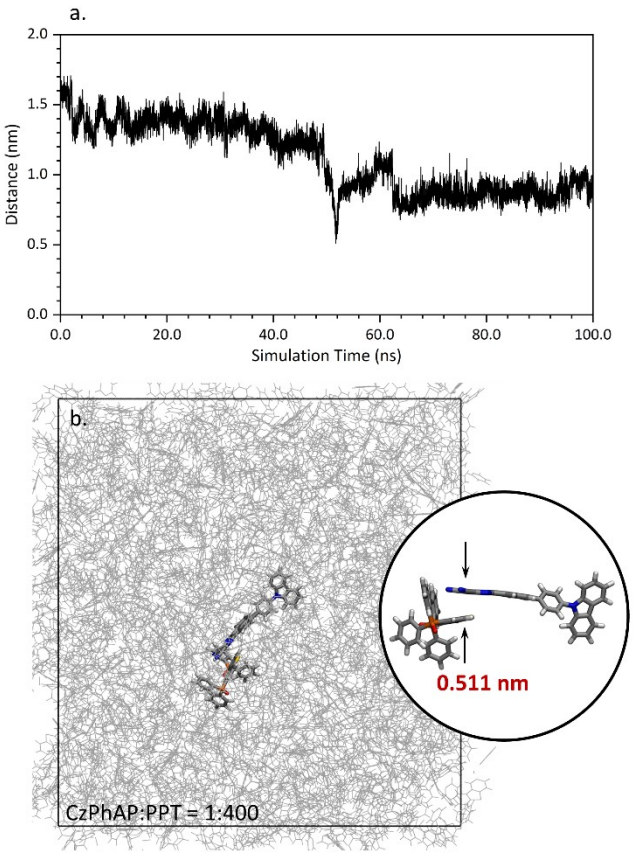

Figure S4. a). Distance between mass centres of AP moiety of CzPhAP and DBT moiety of PPT along the 100 ns MD simulataion after the annealing. This selected PPT molecule holds the longest binding conformation with dopant molecule CzPhAP among the 400 host molecules. **b).** The stacking conformation between CzPhAP and PPT with the minimum distance of 0.511 nm between mass centres in the MD simulation after annealing.

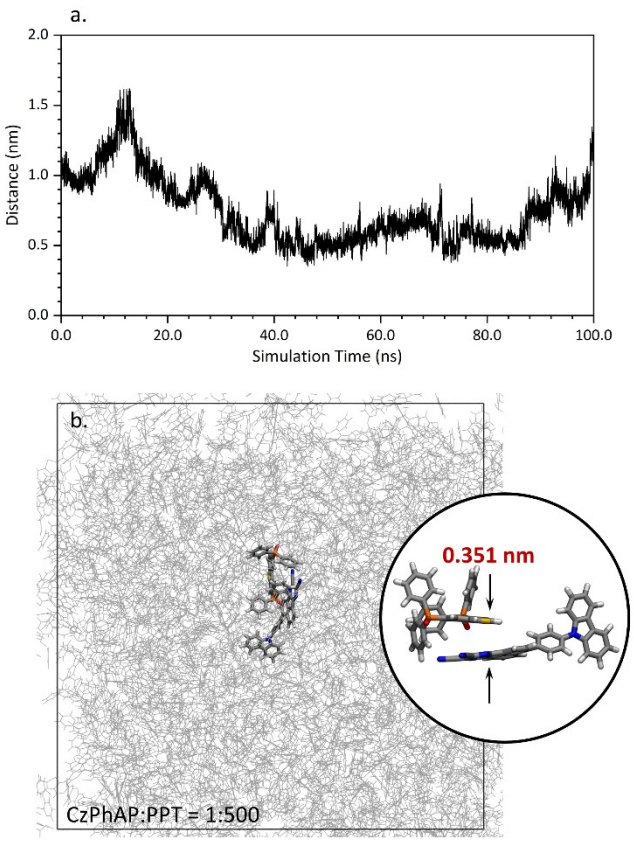

Figure S5. a). Distance between mass centres of AP moiety of CzPhAP and DBT moiety of PPT along the 100 ns MD simulataion after the annealing. This selected PPT molecule holds the longest binding conformation with dopant molecule CzPhAP among the 500 host molecules. **b).** The stacking conformation between CzPhAP and PPT with the minimum distance of 0.351 nm between mass centres in the MD simulation after annealing.

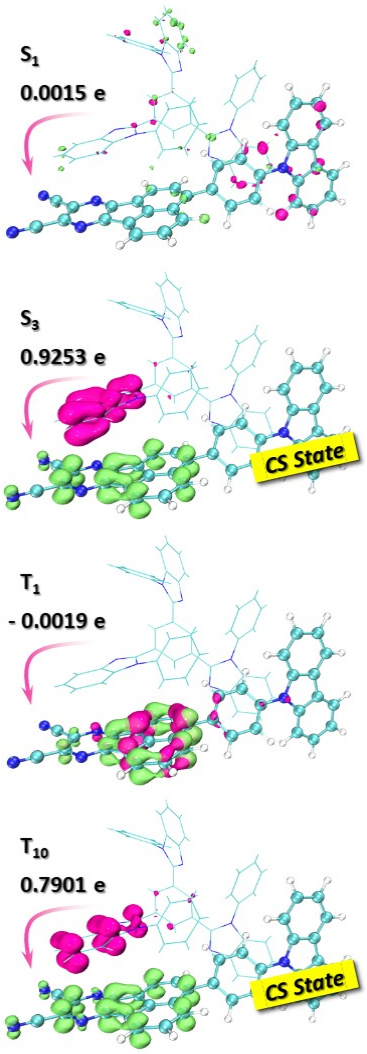

Figure S6. Isosurface (isovalue: 0.0030 a.u.) of electron-hole distribution and IFCT population change for different excited states of CzPhAP:TPBi host-guest system.

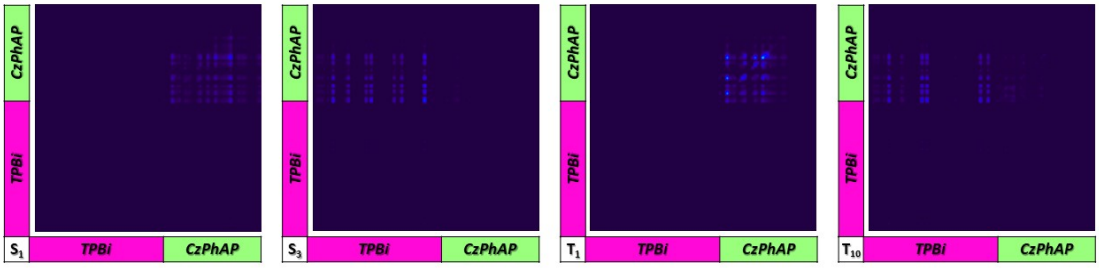

Figure S7. Atomic transition density matrices of key excited states in the form of heat maps for CzPhAP:TPBi host-guest system.

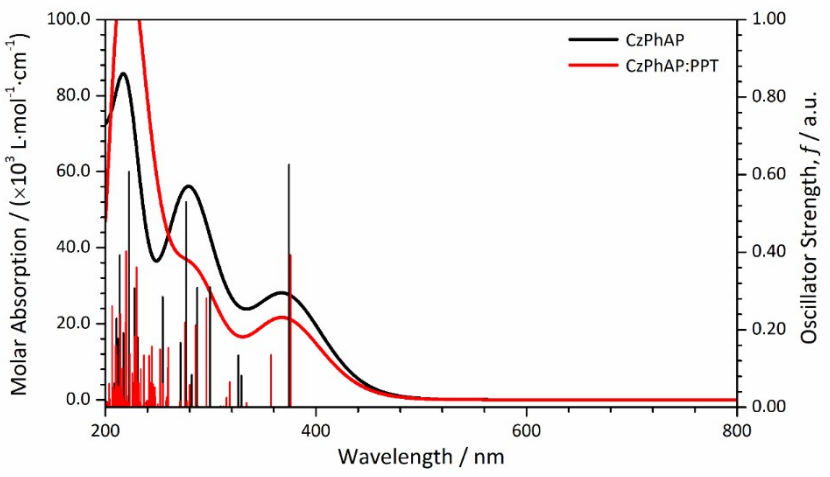

Figure S8. Predicted steady-state UV-Vis absorption spectra of CzPhAP molecule and CzPhAP:PPT host-guest system.

3. Computational Results

3.1 Transition Dipole Moments

(**Table S1** and **S2** are on the next page.)

Table S1. Transition dipole moments and oscillator strengths between excited states (CzPhAP:PPT)

S State *i*	S State *j*	*x*	*y*	*z*	Δ*E* (eV)	f_{ij}	T State *i*	T State *j*	*x*	*y*	*z*	Δ*E* (eV)	f_{ij}
0	0	-2.42286	0.85590	-1.23118	0.00000	0.00000	(S) 0	(S) 0	-2.42286	0.85590	-1.23118	0.00000	0.00000
0	1	-2.20589	0.14617	-0.05315	3.29970	0.39532	(S) 0	1	-4.13955	-0.14320	0.59115	2.53550	1.08744
0	2	1.18261	-0.12178	-0.48062	3.47090	0.13983	(S) 0	2	-0.15009	2.29071	0.08617	2.90190	0.37519
0	3	-0.20527	0.16915	-0.29015	3.71150	0.01409	(S) 0	3	0.67502	1.96311	-0.83505	3.34510	0.41032
0	4	-0.02144	0.12190	-0.17970	3.79290	0.00442	(S) 0	4	0.30714	0.10791	0.32265	3.42540	0.01763
0	5	-0.77597	-0.17876	0.28048	3.89630	0.06804	(S) 0	5	0.31699	0.62805	-0.16580	3.45860	0.04427
0	6	0.51060	0.07011	-0.01179	3.93590	0.02563	(S) 0	6	-1.21401	0.82854	0.25219	3.51640	0.19159
0	7	0.06315	-0.02464	0.16860	3.97440	0.00322	(S) 0	7	2.95266	0.60910	-0.53234	3.56380	0.81833
0	8	-0.02783	-0.00115	0.02834	4.11060	0.00016	(S) 0	8	0.00178	1.96755	0.31245	3.61660	0.35166
0	9	0.00348	-0.00225	-0.00576	4.15810	0.00001	(S) 0	9	0.21970	0.11495	-0.33735	3.71780	0.01597
0	10	1.62520	0.16182	-0.38280	4.19010	0.28887	(S) 0	10	-2.32335	-0.09831	0.56660	3.75070	0.52641
1	1	-4.90672	1.24571	2.37188	0.00000	0.00000	1	1	-3.66761	0.98795	-0.74746	0.00000	0.00000
1	2	5.64865	-0.39011	1.27348	0.17120	0.14127	1	2	-0.42548	0.42341	-0.01837	0.36640	0.00324
1	3	0.85160	-0.24423	-0.19252	0.41180	0.00829	1	3	0.81004	-0.07365	0.80972	0.80960	0.02613
1	4	3.28833	0.22508	0.23147	0.49320	0.13192	1	4	0.01579	0.01005	-0.01800	0.88990	0.00001
1	5	1.35288	0.12610	-1.62692	0.59660	0.06567	1	5	1.68215	-0.12101	-0.52181	0.92310	0.07048
1	6	0.10334	0.82128	0.38430	0.63620	0.01298	1	6	-0.88012	-0.23906	-0.06883	0.98090	0.02010
1	7	-0.03783	-0.06092	-0.01085	0.67470	0.00009	1	7	-0.36168	0.05691	-0.11048	1.02830	0.00368
1	8	-0.01256	-0.07216	-0.04181	0.81090	0.00014	1	8	-0.19826	-0.36663	-0.43177	1.08110	0.00954
1	9	0.02388	0.02077	0.09352	0.85840	0.00020	1	9	-0.59306	0.46855	0.42388	1.18230	0.02175
1	10	-0.67356	0.50440	0.27317	0.89040	0.01707	1	10	-0.24165	0.07250	0.07344	1.21520	0.00206
2	2	-7.83511	1.19058	2.25881	0.00000	0.00000	2	2	-2.35287	0.73831	-1.07775	0.00000	0.00000
2	3	-2.21171	0.07741	-0.40399	0.24060	0.02983	2	3	0.06928	-0.04035	-0.49976	0.44320	0.00278
2	4	-3.44473	0.11428	1.38153	0.32200	0.10877	2	4	0.04087	0.01776	0.00431	0.52350	0.00003
2	5	-4.15432	-0.12779	0.07860	0.42540	0.18010	2	5	1.72186	0.04364	-0.11785	0.55670	0.04065
2	6	-0.50517	0.12014	0.63071	0.46500	0.00760	2	6	-0.32991	-0.07253	0.54649	0.61450	0.00621
2	7	0.14033	-0.02979	-0.06830	0.50350	0.00031	2	7	-0.00643	0.20801	0.25125	0.66190	0.00173
2	8	-0.17618	-0.10604	0.07187	0.63970	0.00074	2	8	0.05381	-0.03340	0.33929	0.71470	0.00209
2	9	-0.04269	-0.03298	-0.14935	0.68720	0.00042	2	9	0.10356	-0.05897	-0.00176	0.81590	0.00028
2	10	0.90759	-0.55754	-0.19506	0.71920	0.02066	2	10	-0.11238	-0.00834	0.02037	0.84880	0.00027
3	3	-0.19109	-0.08660	3.85592	0.00000	0.00000	3	3	-1.48367	0.70852	2.23112	0.00000	0.00000
3	4	-0.49002	-0.08668	0.59270	0.08140	0.00119	3	4	-0.03651	-0.01668	0.02114	0.08030	0.00000
3	5	-1.92507	0.19075	-0.47853	0.18480	0.01798	3	5	-1.39579	0.09503	-0.25762	0.11350	0.00563
3	6	-0.34859	0.10484	0.13862	0.22440	0.00083	3	6	-0.32475	-0.24964	-1.01255	0.17130	0.00501
3	7	0.05122	0.00987	-0.05412	0.26290	0.00004	3	7	-0.22684	-0.15586	-0.63029	0.21870	0.00253
3	8	-0.06794	0.06672	-0.00356	0.39910	0.00009	3	8	-1.09608	-0.17033	-1.50858	0.27150	0.02332
3	9	-0.01117	-0.00664	-0.04711	0.44660	0.00003	3	9	0.95932	0.07819	0.78150	0.37270	0.01404
3	10	-0.30818	0.23623	-0.18634	0.47860	0.00218	3	10	0.16938	-0.00236	0.02897	0.40560	0.00029
4	4	-5.17372	0.87602	0.23456	0.00000	0.00000	4	4	-2.15142	0.93419	-1.29299	0.00000	0.00000
4	5	-3.11832	0.63503	0.16815	0.10340	0.02573	4	5	-0.14732	0.00417	0.04770	0.03320	0.00002
4	6	0.67589	-0.06976	-1.24362	0.14300	0.00704	4	6	0.07639	-0.00731	0.01401	0.09100	0.00001
4	7	-0.00711	0.00449	0.14591	0.18150	0.00009	4	7	-0.05773	-0.01349	0.09531	0.13840	0.00004
4	8	-0.19030	0.01224	-0.02061	0.31770	0.00029	4	8	0.00551	-0.02903	-0.00196	0.19120	0.00000
4	9	-0.02846	-0.02165	-0.11771	0.36520	0.00014	4	9	0.00834	0.04769	0.02220	0.29240	0.00002
4	10	2.44137	-0.07895	0.03030	0.39720	0.05807	4	10	0.01086	0.00642	-0.00081	0.32530	0.00000
5	5	-6.93764	0.36662	0.47879	0.00000	0.00000	5	5	-9.78862	0.93035	1.03285	0.00000	0.00000
5	6	-0.66257	0.60962	0.43945	0.03960	0.00097	5	6	3.52424	-0.15620	0.19155	0.05780	0.01767
5	7	0.10691	-0.03617	-0.04744	0.07810	0.00003	5	7	0.41796	-0.09469	0.24010	0.10520	0.00062
5	8	-0.23530	0.04855	0.04374	0.21430	0.00031	5	8	0.07022	0.00875	0.44109	0.15800	0.00077
5	9	-0.02296	-0.02429	-0.13629	0.26180	0.00013	5	9	2.53314	-0.21201	-0.11066	0.25920	0.04111
5	10	-0.29662	0.45773	-0.00933	0.29380	0.00214	5	10	0.91530	-0.04141	-0.17200	0.29210	0.00622
6	6	-2.74077	0.67816	2.91818	0.00000	0.00000	6	6	-2.97147	0.61514	0.70100	0.00000	0.00000
6	7	0.10109	0.09083	-0.50723	0.03850	0.00026	6	7	0.12684	-0.04270	0.58931	0.04740	0.00042
6	8	-0.00333	0.01380	-0.10037	0.17470	0.00004	6	8	0.20235	-0.13348	0.83475	0.10020	0.00185
6	9	-0.00558	-0.00067	-0.01475	0.22220	0.00000	6	9	-0.87666	-0.12460	0.90357	0.20140	0.00790
6	10	-1.79139	0.03759	-1.20574	0.25420	0.02905	6	10	-0.39271	-0.00578	0.14163	0.23430	0.00100
7	7	-2.14912	0.92335	-1.23837	0.00000	0.00000	7	7	-2.98083	0.87886	-0.64618	0.00000	0.00000
7	8	0.06688	-0.19601	-0.01743	0.13620	0.00014	7	8	0.43076	-0.16965	0.45826	0.05280	0.00055
7	9	0.00264	-0.00195	0.00372	0.18370	0.00000	7	9	-0.91929	0.37787	0.07291	0.15400	0.00375
7	10	0.06453	-0.05063	0.27719	0.21570	0.00044	7	10	-0.16856	0.06199	0.01112	0.18690	0.00015
8	8	-1.52173	0.92762	-1.41949	0.00000	0.00000	8	8	-2.40445	0.88032	-0.19195	0.00000	0.00000
8	9	0.27624	-0.00722	-0.06899	0.04750	0.00009	8	9	0.27872	-0.09545	-0.59397	0.10120	0.00109
8	10	-0.01931	0.02059	0.06072	0.07950	0.00001	8	10	0.04857	-0.02251	-0.06918	0.13410	0.00003
9	9	-	1.38302	3.04503	0.00000	0.00000	9	9	-4.81738	0.57707	1.16156	0.00000	0.00000
9	10	0.04356	0.00500	0.02491	0.03200	0.00000	9	10	-0.65719	-0.01843	0.34730	0.03290	0.00045
10	10	-7.14272	0.88374	1.66403	0.00000	0.00000	10	10	-1.56243	0.91571	-1.41616	0.00000	0.00000

Table S2. Transition dipole moments and oscillator strengths between excited states (CzPhAP:TPBi)

S State *i*	S State *j*	*x*	*y*	*z*	Δ*E* (eV)	f_{ij}	T State *i*	T State *j*	*x*	*y*	*z*	Δ*E* (eV)	f_{ij}
0	0	-4.34162	0.12650	3.25154	0.00000	0.00000	(S) 0	(S) 0	-4.34162	0.12650	3.25154	0.00000	0.00000
0	1	-2.18662	-0.02521	0.24109	3.31060	0.39257	(S) 0	1	-4.10541	0.40412	0.64255	2.52860	1.07982
0	2	-0.18251	0.49386	0.11946	3.55210	0.02537	(S) 0	2	-0.06415	-1.65607	-1.65790	2.87370	0.38690
0	3	0.02121	-0.02518	-0.03899	3.64460	0.00023	(S) 0	3	-0.69296	0.24250	0.46649	3.40580	0.06313
0	4	0.16930	0.09583	-0.11682	3.86690	0.00488	(S) 0	4	0.06678	0.30003	-0.27043	3.43060	0.01409
0	5	-0.57786	0.08997	0.24068	3.89610	0.03818	(S) 0	5	0.99317	0.67068	0.98521	3.44860	0.20335
0	6	-0.09129	-0.17135	0.14459	3.98220	0.00572	(S) 0	6	-0.49071	1.89494	1.77595	3.57110	0.61117
0	7	-0.05727	-0.01691	0.01018	4.01630	0.00036	(S) 0	7	3.14493	0.20887	0.23962	3.58090	0.87657
0	8	0.08553	0.02188	0.00041	4.05360	0.00077	(S) 0	8	0.18459	-1.31167	-0.99626	3.63240	0.24447
0	9	-1.65225	0.11883	0.41137	4.17320	0.29786	(S) 0	9	0.07262	0.58973	-1.69393	3.63750	0.28718
0	10	-0.24792	-0.00068	0.09145	4.24000	0.00725	(S) 0	10	0.24959	0.30862	0.42044	3.64720	0.02987
1	1	-	-0.38341	3.79736	0.00000	0.00000	1	1	-6.02273	0.03870	3.27645	0.00000	0.00000
1	2	-1.33386	0.27254	0.16077	0.24150	0.01112	1	2	-0.29167	-0.24043	-0.21658	0.34510	0.00160
1	3	-0.54079	0.27386	-0.01251	0.33400	0.00301	1	3	-2.30593	-0.08700	0.22115	0.87720	0.11549
1	4	3.56034	-0.06250	-0.64522	0.55630	0.17849	1	4	-0.04043	0.00042	0.02106	0.90200	0.00005
1	5	4.31619	-0.04981	-0.65646	0.58550	0.27345	1	5	-0.04732	0.00106	0.00806	0.92000	0.00005
1	6	0.11485	-0.00901	-0.03602	0.67160	0.00024	1	6	0.33153	-0.01249	-0.15514	1.04250	0.00343
1	7	1.36587	0.19198	-0.33560	0.70570	0.03484	1	7	-0.04158	-0.22067	-0.29261	1.05230	0.00351
1	8	-0.51332	-0.04310	0.10225	0.74300	0.00502	1	8	0.25855	0.21764	0.04268	1.10380	0.00314
1	9	1.75236	0.47387	0.25263	0.86260	0.07099	1	9	0.25890	0.10511	-0.00601	1.10890	0.00212
1	10	0.11550	0.32639	0.22750	0.92940	0.00391	1	10	-0.46279	0.08067	0.00851	1.11860	0.00605
2	2	-4.00420	-5.38219	4.85871	0.00000	0.00000	2	2	-3.92017	-0.16754	3.48244	0.00000	0.00000
2	3	0.08216	-0.07386	0.21105	0.09250	0.00013	2	3	-1.18638	0.46489	0.12999	0.53210	0.02139
2	4	0.25586	-2.23116	0.57230	0.31480	0.04142	2	4	-0.04403	0.03130	-0.01470	0.55690	0.00004
2	5	0.93390	1.15147	-0.06209	0.34400	0.01856	2	5	-0.01792	-0.02237	0.00890	0.57490	0.00001
2	6	-0.01214	0.04724	-0.03206	0.43010	0.00004	2	6	0.09329	0.52738	-0.06433	0.69740	0.00497
2	7	0.13008	-0.04897	0.11983	0.46420	0.00038	2	7	0.10539	0.22615	-0.28894	0.70720	0.00253
2	8	0.04804	0.26518	-0.14282	0.50150	0.00114	2	8	-0.03927	0.71475	-0.24326	0.75870	0.01062
2	9	0.36740	0.11173	-0.33234	0.62110	0.00392	2	9	0.05630	0.25052	-0.11712	0.76380	0.00149
2	10	1.03349	0.63633	0.11933	0.68790	0.02506	2	10	-0.10595	-1.14229	0.23966	0.77350	0.02603
3	3	-4.06724	-7.08197	4.40179	0.00000	0.00000	3	3	-	-0.37492	4.17845	0.00000	0.00000
3	4	0.56593	0.52826	0.05319	0.22230	0.00328	3	4	-0.13362	-0.03893	0.03108	0.02480	0.00001
3	5	0.78809	-0.68406	0.00329	0.25150	0.00671	3	5	-0.11751	0.01599	0.01350	0.04280	0.00001
3	6	-0.05484	-0.08500	-0.03189	0.33760	0.00009	3	6	0.80184	-0.48603	0.02533	0.16530	0.00356
3	7	-0.48320	-0.03565	-0.24079	0.37170	0.00267	3	7	0.63211	-0.47558	0.01332	0.17510	0.00269
3	8	-0.08597	0.45531	-0.19207	0.40900	0.00252	3	8	0.65402	-0.77874	0.25572	0.22660	0.00610
3	9	-0.03221	-0.18301	-0.05160	0.52860	0.00048	3	9	0.72358	-0.28786	0.03966	0.23170	0.00345
3	10	-0.51680	-0.18288	-0.16977	0.59540	0.00480	3	10	-1.20527	0.72679	-0.13825	0.24140	0.01183
4	4	-6.82894	-0.94662	3.61973	0.00000	0.00000	4	4	-4.08076	-0.01548	3.11930	0.00000	0.00000
4	5	-3.22739	-0.16555	-0.35569	0.02920	0.00756	4	5	0.00879	0.00670	0.00140	0.01800	0.00000
4	6	-0.11382	-0.02204	-0.05451	0.11530	0.00005	4	6	0.02109	-0.07134	0.04076	0.14050	0.00002
4	7	1.08283	0.34209	0.50862	0.14940	0.00567	4	7	0.07750	-0.04871	0.01044	0.15030	0.00003
4	8	0.54227	0.10746	-0.01857	0.18670	0.00140	4	8	0.05669	-0.14216	0.05345	0.20180	0.00013
4	9	-1.73875	0.32993	0.06989	0.30630	0.02354	4	9	0.03853	-0.06450	0.02238	0.20690	0.00003
4	10	-0.70280	0.12471	0.23602	0.37310	0.00517	4	10	0.03957	0.02880	-0.01706	0.21660	0.00001
5	5	-	-0.26375	3.90262	0.00000	0.00000	5	5	-4.68643	-0.24314	3.00785	0.00000	0.00000
5	6	-0.30593	-0.01401	-0.00994	0.08610	0.00020	5	6	0.00688	-0.00691	-0.01280	0.12250	0.00000
5	7	1.36254	1.16986	0.95564	0.12020	0.01219	5	7	-0.00293	0.02540	-0.01554	0.13230	0.00000
5	8	0.74152	0.03893	-0.00943	0.15750	0.00213	5	8	-0.01363	-0.05005	-0.01249	0.18380	0.00001
5	9	-0.21867	0.30641	0.35105	0.27710	0.00180	5	9	-0.01061	0.08839	-0.01667	0.18890	0.00004
5	10	0.59634	-0.32806	0.26969	0.34390	0.00452	5	10	-0.00198	-0.22149	0.03749	0.19860	0.00025
6	6	-4.10724	-0.10607	3.10003	0.00000	0.00000	6	6	-5.16355	-1.14781	3.84049	0.00000	0.00000
6	7	0.21008	0.14906	0.06765	0.03410	0.00006	6	7	-0.00849	-0.17350	0.17396	0.00980	0.00001
6	8	-0.03068	-0.11679	-0.13568	0.07140	0.00006	6	8	0.36258	-2.35267	0.42219	0.06130	0.00878
6	9	0.11946	-0.15580	0.07566	0.19100	0.00021	6	9	0.11825	-1.06911	0.19183	0.06640	0.00194
6	10	0.06782	0.08238	-0.06009	0.25780	0.00009	6	10	0.41611	-0.47636	-0.04553	0.07610	0.00075
7	7	-	-5.36582	0.51388	0.00000	0.00000	7	7	-5.16667	-0.71070	3.45764	0.00000	0.00000
7	8	-0.56581	-0.27664	-0.15667	0.03730	0.00038	7	8	0.37701	-0.87179	0.35831	0.05150	0.00130
7	9	-0.83772	-0.06777	-0.15429	0.15690	0.00281	7	9	0.10209	-0.35880	0.15967	0.05660	0.00023
7	10	-0.18880	0.49533	0.39090	0.22370	0.00238	7	10	-0.26797	0.95044	-0.32739	0.06630	0.00176
8	8	-3.39661	-0.15844	2.93468	0.00000	0.00000	8	8	-4.47738	-3.48988	4.24967	0.00000	0.00000
8	9	0.17446	-0.06748	-0.03454	0.11960	0.00011	8	9	-0.01254	-1.66545	0.44814	0.00510	0.00037
8	10	-0.24706	-0.09158	-0.09459	0.18640	0.00036	8	10	0.35271	-0.67975	-0.14259	0.01480	0.00022
9	9	-8.46135	-2.35108	4.42614	0.00000	0.00000	9	9	-4.47245	-0.65325	3.47081	0.00000	0.00000
9	10	-2.87220	1.45573	-0.63051	0.06680	0.01762	9	10	0.24553	-0.62208	-0.00488	0.00970	0.00011
10	10	-	-3.74380	2.77647	0.00000	0.00000	10	10	-4.91147	-6.09968	4.32766	0.00000	0.00000

3.2 Inter-Fragment Charge Transfer Analysis

Table S3. Inter-fragment charge transfer and electron-hole distribution (CzPhAP:PPT).

State	Hole^{D}	Electron^{D}	Hole^{D}	Electron^{D}	Redis^{D}	Redis^{A}	D→A	A→D	Net IFCT
S_1	0.4917	0.0342	0.5083	0.9658	0.0168	0.4909	0.4749	0.0174	0.4575
S_2	0.3673	0.0315	0.6327	0.9685	0.0116	0.6128	0.3557	0.0199	0.3358
S_3	*0.8756*	*0.0338*	*0.1244*	*0.9662*	*0.0296*	*0.1202*	*0.8460*	*0.0042*	*0.8418*
S_4	0.1667	0.0350	0.8333	0.9650	0.0058	0.8041	0.1609	0.0292	0.1317
S_5	0.1442	0.0381	0.8558	0.9619	0.0055	0.8232	0.1387	0.0326	0.1061
S_6	0.6745	0.0441	0.3255	0.9559	0.0297	0.3112	0.6448	0.0143	0.6305
S_7	0.0286	0.0318	0.9714	0.9682	0.0009	0.9405	0.0276	0.0309	-0.0033
S_8	0.0204	0.0324	0.9796	0.9676	0.0007	0.9479	0.0197	0.0317	-0.0120
S_9	0.0000	0.0278	1.0000	0.9722	0.0000	0.9722	0.0000	0.0278	-0.0278
S_{10}	0.3272	0.0393	0.6728	0.9607	0.0129	0.6463	0.3144	0.0264	0.2880
T_1	0.0725	0.0345	0.9275	0.9655	0.0025	0.8955	0.0700	0.0320	0.0380
T_2	0.0636	0.0382	0.9364	0.9618	0.0024	0.9006	0.0611	0.0358	0.0253
T_3	*0.6083*	*0.0450*	*0.3917*	*0.9550*	*0.0274*	*0.3740*	*0.5810*	*0.0176*	*0.5634*
T_4	0.0212	0.0353	0.9788	0.9647	0.0007	0.9443	0.0204	0.0345	-0.0141
T_5	0.1349	0.0565	0.8651	0.9435	0.0076	0.8162	0.1273	0.0489	0.0784
T_6	0.6119	0.3352	0.3881	0.6648	0.2051	0.2580	0.4068	0.1301	0.2767
T_7	0.1275	0.0522	0.8725	0.9478	0.0067	0.8269	0.1208	0.0456	0.0752
T_8	0.6664	0.5033	0.3336	0.4967	0.3354	0.1657	0.3310	0.1679	0.1631
T_9	0.4244	0.1240	0.5756	0.8760	0.0526	0.5042	0.3717	0.0714	0.3003
T_{10}	0.0087	0.0045	0.9913	0.9955	0.0000	0.9868	0.0087	0.0045	0.0042

Table S4. Inter-fragment charge transfer and electron-hole distribution (CzPhAP:TPBi).

State	Hole^D	Electron^D	Hole^D	Electron^D	Redis^D	Redis^A	D→A	A→D	Net IFCT
S_1	0.0234	0.0246	0.8671	0.9712	0.0006	0.8422	0.0228	0.0213	0.0015
S_2	0.7574	0.0201	0.2386	0.9788	0.0152	0.2335	0.7414	0.0048	0.7366
S_3	*0.9450*	*0.0189*	*0.0534*	*0.9802*	*0.0178*	*0.0523*	*0.9263*	*0.0010*	*0.9253*
S_4	0.1715	0.0228	0.7887	0.9758	0.0039	0.7697	0.1674	0.0180	0.1494
S_5	0.1138	0.0254	0.7927	0.9718	0.0029	0.7704	0.1106	0.0201	0.0905
S_6	0.0276	0.0249	0.9701	0.9739	0.0007	0.9448	0.0268	0.0241	0.0027
S_7	0.8448	0.0236	0.1355	0.9745	0.0199	0.1321	0.8232	0.0032	0.8200
S_8	0.0231	0.0214	0.9742	0.9778	0.0005	0.9525	0.0226	0.0209	0.0017
S_9	0.3864	0.0289	0.5737	0.9648	0.0112	0.5535	0.3728	0.0166	0.3562
S_{10}	0.6562	0.0238	0.3133	0.9712	0.0156	0.3043	0.6372	0.0075	0.6297
T_1	0.0279	0.0300	0.9611	0.9676	0.0008	0.9300	0.0270	0.0289	-0.0019
T_2	0.0827	0.0260	0.9132	0.9723	0.0022	0.8879	0.0804	0.0238	0.0566
T_3	0.0841	0.0367	0.7779	0.9421	0.0031	0.7328	0.0793	0.0285	0.0508
T_4	0.0232	0.0283	0.9733	0.9701	0.0007	0.9442	0.0225	0.0275	-0.0050
T_5	0.9691	0.9583	0.0279	0.0371	0.9287	0.0010	0.0360	0.0268	0.0092
T_6	0.2353	0.0275	0.7605	0.9708	0.0065	0.7383	0.2284	0.0209	0.2075
T_7	0.1394	0.0260	0.8546	0.9713	0.0036	0.8300	0.1354	0.0222	0.1132
T_8	0.5506	0.0552	0.3639	0.8564	0.0304	0.3116	0.4715	0.0201	0.4514
T_9	0.1531	0.0475	0.4286	0.5173	0.0073	0.2217	0.0792	0.0204	0.0588
T_{10}	*0.8263*	*0.0343*	*0.1667*	*0.9632*	*0.0283*	*0.1605*	*0.7959*	*0.0057*	*0.7902*

3.3 Coupling Integrals

Table S5. Spin-orbit coupling matrices elements

Initial State	Final State	*x* / a.u.	*y* / a.u.	*z* / a.u.	SOC, *H* / cm^{-1}
S_1	T_1	0.00000013	0.00000095	-0.00001019	2.2448
S_1	T_3	0.00000128	0.00000502	-0.00000118	1.1653
S_3	T_1	0.00000221	0.00000030	-0.00000198	0.6541
S_3	T_3	-0.00000174	0.00000004	-0.00000790	1.7742
T_1	S_1	0.00001297	0.00001431	-0.0000005	4.2372
T_1	S_3	-0.00001134	0.00000359	0.00001484	4.1712
T_3	S_1	-0.00000223	0.00000025	-0.00000434	1.0716
T_3	S_3	-0.00000011	-0.00000426	0.00000273	1.1010

Table S6. Results of electronic coupling integrals calculated by FCD method.

Initial State	Final State	Net Initial	IFCT,	Net Final	IFCT,	Δq_{11}	Δq_{22}	Δq_{12}	ΔE_{FC} / eV	V_{12} / cm^{-1}
S_1	S_3		0.71095		0.56279	1.42190	1.12558	-0.03772	0.64045	636.7
S_3	S_1		0.69440		0.73935	1.38880	1.47870	-0.12455	-0.43678	1655.7
T_1	T_3		0.02899		0.14947	0.05798	0.29894	-0.00587	0.80972	145.5
T_3	T_1		0.66466		0.04622	1.32932	0.09244	-0.07424	-0.30284	158.7

4. Geometric Structures

CzPhAP:PPT S_0 state

1	C	5.183090	1.348208	0.839672
2	C	4.779829	2.698035	0.841958
3	C	3.439643	3.045162	0.970471
4	C	2.496351	2.021655	1.111961
5	C	2.879874	0.667103	1.082548
6	C	4.233972	0.335207	0.949429
7	H	5.526573	3.493474	0.782840
8	H	3.136741	4.092698	0.985475
9	H	4.574064	-0.703764	0.977724
10	C	0.535012	0.486304	1.407130
11	C	-0.679933	-0.190654	1.574915
12	C	-0.674299	-1.577492	1.541578
13	C	0.522153	-2.302898	1.350339
14	C	1.726654	-1.618290	1.224121
15	C	1.739615	-0.219948	1.239086
16	H	-1.611201	0.361130	1.714331
17	H	-1.618711	-2.115091	1.654551
18	H	2.670162	-2.154731	1.115511
19	S	0.772090	2.222309	1.368799
20	P	6.923589	0.780545	0.882373
21	O	6.998917	-0.641374	1.350297
22	C	7.639596	1.023829	-0.761400
23	C	7.752091	1.935876	2.019700
24	C	7.377760	2.140851	-1.559542
25	C	8.445301	-0.011749	-1.242883
26	C	8.270755	3.177626	1.638866
27	C	7.853895	1.512807	3.349473
28	C	7.924239	2.225530	-2.837738
29	H	6.718481	2.938522	-1.212239
30	C	8.999184	0.081982	-2.517683
31	H	8.604568	-0.890660	-0.615094
32	C	8.865198	4.003481	2.592395
33	H	8.232276	3.496069	0.594705
34	C	8.450994	2.340542	4.298058
35	H	7.473816	0.524793	3.618384
36	C	8.737697	1.196765	-3.313606
37	H	7.692260	3.089008	-3.462750
38	H	9.622827	-0.727721	-2.899322
39	C	8.951490	3.586970	3.920792
40	H	9.271953	4.970807	2.294107
41	H	8.532359	2.009269	5.334394
42	H	9.160140	1.259083	-4.317843
43	H	9.420923	4.233536	4.663951
44	P	0.477346	-4.126343	1.456833
45	O	0.195638	-4.629458	2.836850
46	C	2.053935	-4.701364	0.764334
47	C	-0.829833	-4.681284	0.302185
48	C	2.633113	-4.191242	-0.407190
49	C	2.701406	-5.712046	1.479797
50	C	-0.611324	-5.035768	-1.033773
51	C	-2.108181	-4.832438	0.855089
52	C	3.850686	-4.694969	-0.857370
53	H	2.158285	-3.373270	-0.956915
54	C	3.918408	-6.217570	1.021401
55	H	2.241224	-6.079118	2.399866
56	C	-1.667501	-5.501568	-1.817387
57	H	0.390558	-4.976312	-1.463692
58	C	-3.165366	-5.285243	0.066762
59	H	-2.251025	-4.623304	1.918029
60	C	4.491037	-5.710190	-0.143246
61	H	4.308690	-4.281983	-1.757153
62	H	4.425954	-7.002907	1.583141
63	C	-2.946239	-5.618115	-1.270778
64	H	-1.488012	-5.784784	-2.855544
65	H	-4.158707	-5.399851	0.503308
66	H	5.449166	-6.097106	-0.493246
67	H	-3.770189	-5.985587	-1.884498
68	N	4.911364	3.733093	-2.747430
69	N	5.544414	-0.343179	-2.802859
70	C	4.062762	2.976377	-2.551060
71	C	4.508179	0.113721	-2.581399
72	C	2.974038	2.051259	-2.324587
73	C	3.190128	0.657932	-2.341816
74	N	1.763141	2.588736	-2.126124
75	N	2.192608	-0.221545	-2.172717
76	C	0.785602	1.726583	-1.954030
77	C	1.001642	0.305278	-1.985013
78	C	-0.640358	1.967701	-1.711164
79	C	-0.290227	-0.358145	-1.780066
80	C	-1.232443	0.687137	-1.597069
81	C	-1.430079	3.086212	-1.570293
82	C	-0.713581	-1.664858	-1.735482
83	C	-2.591347	0.471652	-1.332075
84	C	-2.805127	2.899785	-1.287371
85	H	-1.010982	4.090152	-1.648114
86	C	-2.093180	-1.914231	-1.499502
87	H	-0.021455	-2.495691	-1.877838
88	C	-3.396194	1.645902	-1.148959
89	C	-3.005224	-0.893908	-1.302577
90	H	-3.431274	3.780817	-1.135428
91	H	-2.439867	-2.948334	-1.471975
92	C	-4.835940	1.547515	-0.803510

93	H	-4.055177	-1.140911	-1.140619
94	C	-5.268394	0.743314	0.261421
95	C	-5.792558	2.287347	-1.511792
96	C	-6.615067	0.667066	0.599205
97	H	-4.536189	0.174704	0.838254
98	C	-7.139516	2.228420	-1.170010
99	H	-5.473722	2.915246	-2.345786
100	C	-7.559947	1.411982	-0.115025
101	H	-6.946874	0.026881	1.417781
102	H	-7.877203	2.819396	-1.714616
103	N	-8.926394	1.340950	0.227776
104	C	-9.971509	1.062359	-0.650874
105	C	-9.455946	1.533133	1.502492
106	C	-9.928815	0.761354	-2.016135
107	C	-11.190437	1.074623	0.065739
108	C	-8.805317	1.871888	2.693404
109	C	-10.860104	1.377224	1.445494
110	C	-11.134813	0.496141	-2.655384
111	H	-8.985064	0.726589	-2.560652
112	C	-12.389897	0.804496	-0.601313
113	C	-9.587047	2.027717	3.832636
114	H	-7.725651	2.018216	2.728904
115	C	-11.623662	1.539625	2.606278
116	C	-12.355877	0.521456	-1.961203
117	H	-11.129068	0.259710	-3.720437
118	H	-13.336289	0.812436	-0.057991
119	C	-10.981316	1.859112	3.796130
120	H	-9.103904	2.290844	4.774732
121	H	-12.707977	1.420742	2.573645
122	H	-13.282485	0.310125	-2.495600
123	H	-11.562246	1.987510	4.709834

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1	C	4.867008	1.618936	0.695525
2	C	4.390915	2.910269	0.418744
3	C	3.024741	3.175147	0.408318
4	C	2.147515	2.116192	0.682191
5	C	2.609994	0.801557	0.900295
6	C	3.977777	0.554847	0.905950
7	H	5.094818	3.718415	0.209958
8	H	2.649045	4.176190	0.195962
9	H	4.394291	-0.439044	1.093951
10	C	0.254648	0.519182	1.089326
11	C	-0.945429	-0.183825	1.253858
12	C	-0.873906	-1.566111	1.408473
13	C	0.362281	-2.231816	1.427292
14	C	1.556137	-1.500286	1.316404
15	C	1.505813	-0.129173	1.118849
16	H	-1.905601	0.333198	1.229110
17	H	-1.800712	-2.137133	1.486913
18	H	2.523284	-2.003779	1.354887
19	S	0.415392	2.220855	0.780879
20	P	6.644825	1.177769	0.888639
21	O	6.746910	-0.288147	1.167679
22	C	7.493177	1.696047	-0.618311
23	C	7.231622	2.282461	2.212684
24	C	7.842622	3.022455	-0.899208
25	C	7.756605	0.681962	-1.543760
26	C	8.597852	2.583176	2.288968
27	C	6.370843	2.731185	3.220984
28	C	8.448875	3.330933	-2.112941
29	H	7.654637	3.812702	-0.167692
30	C	8.351912	1.001458	-2.762525
31	H	7.481884	-0.347427	-1.306358
32	C	9.091278	3.336714	3.351441
33	H	9.277442	2.227892	1.510863
34	C	6.866809	3.485421	4.283183
35	H	5.306361	2.489473	3.182309
36	C	8.696728	2.321795	-3.044655
37	H	8.721302	4.362785	-2.338047
38	H	8.538095	0.212277	-3.492102
39	C	8.225673	3.790529	4.346972
40	H	10.155754	3.569182	3.403155
41	H	6.189827	3.833422	5.064510
42	H	9.160264	2.570386	-4.000663
43	H	8.612996	4.382023	5.177959
44	P	0.464574	-4.043994	1.745072
45	O	0.371993	-4.353411	3.204679
46	C	2.022917	-4.531694	0.962585
47	C	-0.887610	-4.813682	0.799467
48	C	2.442963	-4.035851	-0.280895
49	C	2.841108	-5.402733	1.686215
50	C	-0.708451	-5.430161	-0.443313
51	C	-2.141844	-4.859245	1.422246
52	C	3.681180	-4.412180	-0.794378
53	H	1.837315	-3.317185	-0.841269
54	C	4.075570	-5.786441	1.160461
55	H	2.505376	-5.752953	2.664845
56	C	-1.784789	-6.052473	-1.075078
57	H	0.276864	-5.442844	-0.913539
58	C	-3.219608	-5.466342	0.780560
59	H	-2.255444	-4.441693	2.425744
60	C	4.494300	-5.290452	-0.073186
61	H	4.018456	-3.998698	-1.746049
62	H	4.719634	-6.461608	1.725445
63	C	-3.041580	-6.060922	-0.469514

64	H	-1.638936	-6.537481	-2.041261
65	H	-4.196043	-5.495183	1.266248
66	H	5.469119	-5.574319	-0.472231
67	H	-3.882483	-6.547192	-0.966486
68	N	5.332182	2.538241	-2.906917
69	N	5.658270	-1.559063	-2.646018
70	C	4.413153	1.856621	-2.745421
71	C	4.631628	-1.032233	-2.566183
72	C	3.242073	1.037423	-2.546890
73	C	3.348489	-0.388631	-2.469886
74	N	2.080315	1.674784	-2.440890
75	N	2.274846	-1.174171	-2.307051
76	C	1.012379	0.905129	-2.276231
77	C	1.115679	-0.555325	-2.221592
78	C	-0.360096	1.263501	-2.072560
79	C	-0.214256	-1.088722	-2.013963
80	C	-1.066178	0.041510	-1.897676
81	C	-1.071015	2.477823	-1.958141
82	C	-0.763538	-2.368933	-1.908111
83	C	-2.443168	-0.043522	-1.599302
84	C	-2.431139	2.415848	-1.646355
85	H	-0.572018	3.436512	-2.103317
86	C	-2.139885	-2.474204	-1.663535
87	H	-0.150498	-3.262160	-2.028813
88	C	-3.137149	1.215113	-1.434328
89	C	-2.969951	-1.356964	-1.509479
90	H	-2.975779	3.353061	-1.515223
91	H	-2.584618	-3.468508	-1.585017
92	C	-4.555009	1.278540	-1.038315
93	H	-4.035824	-1.512541	-1.346199
94	C	-5.078078	0.451856	-0.025275
95	C	-5.426512	2.212399	-1.629538
96	C	-6.405804	0.544241	0.371376
97	H	-4.425604	-0.270348	0.468170
98	C	-6.753006	2.317567	-1.232801
99	H	-5.053380	2.857904	-2.426272
100	C	-7.256277	1.479188	-0.230841
101	H	-6.798855	-0.112675	1.148728
102	H	-7.412339	3.054684	-1.693538
103	N	-8.605870	1.574595	0.166885
104	C	-9.708320	1.540826	-0.684458
105	C	-9.060095	1.713943	1.476240
106	C	-9.753678	1.370369	-2.072155
107	C	-10.888892	1.660510	0.084931
108	C	-8.328297	1.835543	2.662256
109	C	-10.473277	1.772036	1.470519
110	C	-11.005219	1.348644	-2.677521
111	H	-8.843029	1.248787	-2.658765
112	C	-12.135372	1.635366	-0.548475
113	C	-9.040928	1.990478	3.846200
114	H	-7.238398	1.819408	2.659577
115	C	-11.166073	1.928990	2.674984
116	C	-12.186346	1.485114	-1.929193
117	H	-11.068373	1.217979	-3.758779
118	H	-13.052572	1.727418	0.035668
119	C	-10.445035	2.031709	3.858783
120	H	-8.494049	2.086285	4.785346
121	H	-12.256404	1.974679	2.681749
122	H	-13.150408	1.464845	-2.438173
123	H	-10.970818	2.152941	4.806283

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1	C	5.293089	1.666712	0.795835
2	C	4.884072	2.998723	0.536104
3	C	3.546080	3.329864	0.467969
4	C	2.602136	2.301859	0.650622
5	C	2.998788	0.957054	0.886633
6	C	4.361433	0.650431	0.966618
7	H	5.638149	3.772802	0.378870
8	H	3.226583	4.351501	0.262920
9	H	4.721305	-0.364537	1.157507
10	C	0.634019	0.777999	0.881854
11	C	-0.596758	0.131821	0.943751
12	C	-0.599401	-1.264880	1.151813
13	C	0.588597	-1.973253	1.311058
14	C	1.822504	-1.292232	1.244652
15	C	1.849821	0.080495	1.016766
16	H	-1.532842	0.681654	0.830020
17	H	-1.558330	-1.788453	1.165239
18	H	2.760129	-1.839421	1.369130
19	S	0.889239	2.482302	0.594945
20	P	7.048640	1.126758	0.875883
21	O	7.102278	-0.306557	1.297982
22	C	7.684431	1.422459	-0.790329
23	C	7.862100	2.324843	1.975095
24	C	8.075651	2.678067	-1.269259
25	C	7.671472	0.312221	-1.640027
26	C	9.234191	2.565524	1.828660
27	C	7.167721	2.915753	3.037226
28	C	8.452807	2.818275	-2.601441
29	H	8.091655	3.545581	-0.604567
30	C	8.036330	0.463595	-2.976165
31	H	7.359219	-0.659434	-1.252512
32	C	9.897777	3.401094	2.724082
33	H	9.784125	2.098428	1.008314
34	C	7.833560	3.752516	3.931203

35	H	6.101415	2.719667	3.171972
36	C	8.426971	1.713475	-3.453841
37	H	8.757987	3.794554	-2.980162
38	H	8.003797	-0.399854	-3.641898
39	C	9.197128	3.997145	3.772945
40	H	10.965963	3.586175	2.603757
41	H	7.286526	4.211777	4.755625
42	H	8.709816	1.831483	-4.501104
43	H	9.717695	4.652672	4.472737
44	P	0.604163	-3.739001	1.828963
45	O	0.565600	-3.859292	3.318621
46	C	2.104119	-4.404320	1.067194
47	C	-0.829372	-4.540021	1.046322
48	C	2.510455	-4.079549	-0.235152
49	C	2.891227	-5.236430	1.868043
50	C	-0.745524	-5.308662	-0.119179
51	C	-2.046020	-4.451596	1.735320
52	C	3.706031	-4.594807	-0.731489
53	H	1.926578	-3.394949	-0.859159
54	C	4.082004	-5.756156	1.360402
55	H	2.566373	-5.448933	2.888958
56	C	-1.878179	-5.959932	-0.606940
57	H	0.209442	-5.417544	-0.637702
58	C	-3.180080	-5.088618	1.235244
59	H	-2.085367	-3.906333	2.681501
60	C	4.487531	-5.434243	0.065972
61	H	4.039573	-4.319381	-1.732771
62	H	4.702505	-6.401205	1.983917
63	C	-3.095509	-5.844118	0.065004
64	H	-1.807002	-6.567195	-1.510473
65	H	-4.126740	-5.015301	1.772403
66	H	5.428693	-5.825761	-0.322759
67	H	-3.979683	-6.356430	-0.317829
68	N	5.105466	2.269521	-2.633296
69	N	5.302515	-1.780983	-2.382356
70	C	4.139602	1.639055	-2.551854
71	C	4.280417	-1.239416	-2.374558
72	C	2.931267	0.862237	-2.439514
73	C	3.003909	-0.574153	-2.361114
74	N	1.779499	1.523879	-2.397692
75	N	1.914516	-1.333889	-2.265905
76	C	0.686429	0.781798	-2.287089
77	C	0.759043	-0.689980	-2.232258
78	C	-0.677906	1.170240	-2.089947
79	C	-0.565439	-1.195187	-2.037714
80	C	-1.400797	-0.040035	-1.908175
81	C	-1.360851	2.385280	-1.937057
82	C	-1.133257	-2.468403	-1.907698
83	C	-2.777046	-0.106768	-1.574331
84	C	-2.720691	2.339307	-1.593836
85	H	-0.852964	3.340308	-2.071956
86	C	-2.502311	-2.546427	-1.635940
87	H	-0.532119	-3.369729	-2.024761
88	C	-3.445823	1.154319	-1.391281
89	C	-3.313149	-1.411825	-1.464741
90	H	-3.249512	3.283633	-1.445088
91	H	-2.962591	-3.531688	-1.540790
92	C	-4.868576	1.230229	-0.988039
93	H	-4.375294	-1.549244	-1.261923
94	C	-5.370164	0.467581	0.079939
95	C	-5.752227	2.103653	-1.641219
96	C	-6.702353	0.557427	0.468019
97	H	-4.699796	-0.203585	0.620324
98	C	-7.080988	2.215953	-1.245618
99	H	-5.387647	2.699580	-2.479827
100	C	-7.567279	1.435441	-0.192930
101	H	-7.085057	-0.052112	1.288170
102	H	-7.755028	2.908847	-1.751768
103	N	-8.922406	1.530831	0.198769
104	C	-10.021537	1.371260	-0.639575
105	C	-9.379910	1.791053	1.486539
106	C	-10.059614	1.063245	-2.003685
107	C	-11.206253	1.531418	0.116542
108	C	-8.650918	2.052583	2.651564
109	C	-10.794608	1.800969	1.480868
110	C	-11.308795	0.939515	-2.600955
111	H	-9.143446	0.918512	-2.576603
112	C	-12.450765	1.401881	-0.509497
113	C	-9.366836	2.303905	3.816516
114	H	-7.560804	2.066433	2.644746
115	C	-11.490532	2.056780	2.667291
116	C	-12.495116	1.110810	-1.867302
117	H	-11.366644	0.700665	-3.663963
118	H	-13.371344	1.524340	0.063776
119	C	-10.772036	2.302493	3.830837
120	H	-8.822515	2.510238	4.739330
121	H	-12.581845	2.066117	2.674791
122	H	-13.457320	1.007982	-2.369877
123	H	-11.300177	2.502168	4.763672

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1	C	-4.822946	-1.529031	0.741019
2	C	-4.331079	-2.847379	0.681887
3	C	-2.970009	-3.105683	0.780927
4	C	-2.096490	-2.024020	0.942839
5	C	-2.568623	-0.698399	0.963026

6	C	-3.945128	-0.455525	0.860816	54	C	-4.080058	6.060326	0.953340
7	H	-5.023043	-3.682102	0.551659	55	H	-2.389483	6.051255	2.322166
8	H	-2.592796	-4.127604	0.733046	56	C	1.549211	5.909663	-1.834560
9	H	-4.357630	0.557788	0.886230	57	H	-0.483688	5.288987	-1.479665
10	C	-0.230315	-0.367164	1.195999	58	C	3.090289	5.618463	0.003891
11	C	0.945278	0.384040	1.316261	59	H	2.236599	4.804747	1.821555
12	C	0.848227	1.767837	1.314314	60	C	-4.618425	5.509985	-0.208275
13	C	-0.401508	2.416517	1.210425	61	H	-4.335064	4.102227	-1.825911
14	C	-1.563778	1.657006	1.127593	62	H	-4.646664	6.798781	1.522238
15	C	-1.484401	0.260040	1.101562	63	C	2.834164	6.031750	-1.304340
16	H	1.916751	-0.107934	1.391807	64	H	1.339460	6.257178	-2.847257
17	H	1.761430	2.363390	1.382986	65	H	4.087262	5.739373	0.430446
18	H	-2.544059	2.133218	1.076198	66	H	-5.609516	5.814346	-0.547755
19	S	-0.353619	-2.114341	1.114956	67	H	3.633256	6.467841	-1.905997
20	P	-6.597677	-1.090890	0.780348	68	N	-5.239642	-3.027109	-2.726832
21	O	-6.768337	0.392324	0.677681	69	N	-5.684144	1.033360	-2.619911
22	C	-7.439649	-1.998954	-0.542274	70	C	-4.333575	-2.329322	-2.570868
23	C	-7.208008	-1.846436	2.326207	71	C	-4.647628	0.539167	-2.499021
24	C	-7.679807	-3.377500	-0.498259	72	C	-3.182149	-1.470154	-2.401271
25	C	-7.842251	-1.248312	-1.650280	73	C	-3.338981	-0.054887	-2.378943
26	C	-8.587352	-2.045820	2.471808	74	N	-1.997091	-2.059044	-2.290089
27	C	-6.355114	-2.130844	3.397896	75	N	-2.297760	0.781519	-2.266525
28	C	-8.297055	-4.006409	-1.575717	76	C	-0.962446	-1.234448	-2.160794
29	H	-7.403544	-3.958540	0.385743	77	C	-1.120719	0.205467	-2.163472
30	C	-8.459070	-1.885097	-2.726377	78	C	0.425198	-1.528224	-1.992331
31	H	-7.659760	-0.171829	-1.656046	79	C	0.204428	0.809200	-2.025691
32	C	-9.103509	-2.533656	3.669476	80	C	1.098075	-0.261067	-1.889552
33	H	-9.258621	-1.820628	1.639376	81	C	1.208202	-2.738389	-1.937197
34	C	-6.874111	-2.619946	4.596733	82	C	0.690715	2.124165	-2.013344
35	H	-5.279348	-1.970236	3.299679	83	C	2.481122	-0.107883	-1.683306
36	C	-8.680505	-3.260391	-2.690988	84	C	2.547514	-2.616159	-1.732767
37	H	-8.481171	-5.081206	-1.546061	85	H	0.729383	-3.711576	-2.036847
38	H	-8.765899	-1.301815	-3.595735	86	C	2.060739	2.301358	-1.857892
39	C	-8.246185	-2.823088	4.732136	87	H	0.022707	2.977083	-2.127648
40	H	-10.178247	-2.688406	3.774858	88	C	3.238754	-1.344518	-1.515630
41	H	-6.202747	-2.841366	5.427605	89	C	2.951547	1.215114	-1.701837
42	H	-9.159450	-3.756861	-3.536516	90	H	3.142574	-3.525787	-1.644831
43	H	-8.650741	-3.207235	5.669919	91	H	2.465692	3.315557	-1.849520
44	P	-0.487593	4.236944	1.365450	92	C	4.614283	-1.370758	-1.063452
45	O	-0.254427	4.718653	2.762291	93	H	4.017660	1.425071	-1.623580
46	C	-2.100615	4.702494	0.676642	94	C	5.120087	-0.402849	-0.160828
47	C	0.782017	4.916371	0.236913	95	C	5.500120	-2.399791	-1.467324
48	C	-2.642840	4.151296	-0.494356	96	C	6.427200	-0.449537	0.293539
49	C	-2.822794	5.654032	1.401562	97	H	4.458417	0.378598	0.212471
50	C	0.524899	5.355811	-1.066054	98	C	6.809591	-2.445131	-1.021135
51	C	2.064491	5.077444	0.777471	99	H	5.157743	-3.162673	-2.167123
52	C	-3.902396	4.553413	-0.931886	100	C	7.291761	-1.467927	-0.136154
53	H	-2.110452	3.374228	-1.051285	101	H	6.797399	0.310108	0.982942

102	H	7.473550	-3.248986	-1.341188
103	N	8.618843	-1.513904	0.318651
104	C	9.750532	-1.678340	-0.483622
105	C	9.030332	-1.400334	1.648890
106	C	9.848365	-1.780871	-1.874853
107	C	10.900382	-1.669281	0.337881
108	C	8.262446	-1.276805	2.811120
109	C	10.439409	-1.492754	1.702558
110	C	11.119975	-1.906788	-2.424118
111	H	8.964937	-1.751276	-2.512401
112	C	12.167746	-1.796739	-0.238443
113	C	8.936940	-1.214188	4.025912
114	H	7.173767	-1.243321	2.774955
115	C	11.094194	-1.427916	2.936203
116	C	12.270142	-1.922105	-1.618714
117	H	11.222900	-1.990111	-3.506941
118	H	13.061108	-1.791279	0.388157
119	C	10.337911	-1.281333	4.092835
120	H	8.360456	-1.115800	4.946784
121	H	12.181971	-1.497774	2.987092
122	H	13.250923	-2.023867	-2.083967
123	H	10.832984	-1.227331	5.062740

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1	C	5.040066	1.639978	0.721073
2	C	4.673221	2.967263	0.451452
3	C	3.330818	3.340499	0.374402
4	C	2.363818	2.353145	0.574612
5	C	2.714990	1.006415	0.786757
6	C	4.057441	0.652551	0.871916
7	H	5.442320	3.734778	0.341630
8	H	3.051017	4.377252	0.186799
9	H	4.366307	-0.368154	1.113679
10	C	0.335182	0.914098	0.914144
11	C	-0.919285	0.287687	1.092429
12	C	-0.948795	-1.084899	1.308927
13	C	0.235540	-1.844248	1.321377
14	C	1.482560	-1.197477	1.169155
15	C	1.536937	0.166367	0.962619
16	H	-1.840519	0.871483	1.061936
17	H	-1.912240	-1.580596	1.438138
18	H	2.411742	-1.765597	1.223685
19	S	0.628431	2.592292	0.655084
20	P	6.745058	1.072440	1.128293
21	O	6.664004	-0.101027	2.056090
22	C	7.590505	0.706519	-0.421611
23	C	7.528362	2.525155	1.890769
24	C	7.492514	1.521779	-1.552071
25	C	8.332742	-0.477521	-0.462799
26	C	8.166500	3.541590	1.172052
27	C	7.465087	2.586594	3.287440
28	C	8.144607	1.156399	-2.726904
29	H	6.880360	2.425290	-1.544164
30	C	8.993819	-0.830549	-1.636523
31	H	8.363287	-1.114341	0.423424
32	C	8.715435	4.629407	1.850265
33	H	8.255396	3.479168	0.085462
34	C	8.017955	3.674516	3.959899
35	H	6.994870	1.764120	3.830984
36	C	8.899045	-0.016184	-2.764763
37	H	8.037991	1.781894	-3.614093
38	H	9.568859	-1.756520	-1.677815
39	C	8.637523	4.697444	3.241384
40	H	9.215656	5.420667	1.290220
41	H	7.972279	3.720785	5.048935
42	H	9.402879	-0.307134	-3.687846
43	H	9.072478	5.547702	3.769100
44	P	0.234880	-3.611250	1.845911
45	O	0.061351	-3.703253	3.328404
46	C	1.805479	-4.271080	1.228460
47	C	-1.098040	-4.475926	0.961439
48	C	2.334479	-3.969743	-0.035796
49	C	2.514750	-5.091770	2.109604
50	C	-0.876300	-5.304373	-0.143869
51	C	-2.383421	-4.376522	1.509192
52	C	3.569502	-4.491874	-0.411762
53	H	1.821128	-3.287426	-0.719605
54	C	3.745247	-5.622968	1.721460
55	H	2.098099	-5.288233	3.099980
56	C	-1.941123	-5.994912	-0.721612
57	H	0.130945	-5.424625	-0.547966
58	C	-3.448751	-5.053216	0.918023
59	H	-2.533987	-3.791450	2.419662
60	C	4.270643	-5.322462	0.465935
61	H	3.992089	-4.228924	-1.382487
62	H	4.302278	-6.260158	2.409561
63	C	-3.228074	-5.860336	-0.199044
64	H	-1.763820	-6.644457	-1.579815
65	H	-4.450118	-4.968440	1.342482
66	H	5.241654	-5.723389	0.171663
67	H	-4.060001	-6.399629	-0.654492
68	N	5.183631	2.711037	-3.216095
69	N	5.699120	-1.352551	-2.414621
70	C	4.312999	1.994678	-2.962812
71	C	4.653867	-0.859866	-2.449344
72	C	3.184488	1.142761	-2.674364

73	C	3.341377	-0.264879	-2.473385
74	N	1.999872	1.744286	-2.618830
75	N	2.297616	-1.074973	-2.269723
76	C	0.961982	0.951965	-2.400015
77	C	1.110235	-0.495452	-2.251528
78	C	-0.418831	1.284645	-2.216329
79	C	-0.198858	-1.052998	-2.007290
80	C	-1.082324	0.054159	-1.955629
81	C	-1.148026	2.473848	-2.147403
82	C	-0.718633	-2.341291	-1.798557
83	C	-2.462916	-0.045981	-1.627604
84	C	-2.510582	2.391053	-1.802487
85	H	-0.681376	3.439243	-2.344068
86	C	-2.099748	-2.466157	-1.536700
87	H	-0.091791	-3.230042	-1.876408
88	C	-3.186338	1.184361	-1.527186
89	C	-2.954312	-1.374030	-1.439625
90	H	-3.081002	3.318892	-1.715596
91	H	-2.516940	-3.465234	-1.401824
92	C	-4.606815	1.229725	-1.110548
93	H	-4.013889	-1.541706	-1.248372
94	C	-5.066450	0.504476	0.001573
95	C	-5.529795	2.040281	-1.789959
96	C	-6.394404	0.569429	0.408320
97	H	-4.367648	-0.121844	0.560020
98	C	-6.854967	2.128384	-1.377134
99	H	-5.200228	2.606578	-2.663040
100	C	-7.298636	1.385732	-0.278722
101	H	-6.743103	-0.012279	1.263027
102	H	-7.559358	2.773661	-1.904380
103	N	-8.648388	1.457874	0.132988
104	C	-9.757077	1.231787	-0.677792
105	C	-9.091205	1.759840	1.417354
106	C	-9.810120	0.864514	-2.026539
107	C	-10.932390	1.390178	0.093026
108	C	-8.350653	2.092652	2.556543
109	C	-10.505288	1.729180	1.437064
110	C	-11.065541	0.680089	-2.594521
111	H	-8.900609	0.720714	-2.610171
112	C	-12.183381	1.198747	-0.503300
113	C	-9.053756	2.373436	3.722641
114	H	-7.261744	2.138240	2.529788
115	C	-11.188287	2.015904	2.623838
116	C	-12.243140	0.848962	-1.846608
117	H	-11.135065	0.394384	-3.645177
118	H	-13.096876	1.319268	0.081550
119	C	-10.457719	2.332152	3.762607
120	H	-8.500139	2.635226	4.625623
121	H	-12.279099	1.994531	2.650641
122	H	-13.210628	0.697691	-2.326221
123	H	-10.975656	2.556817	4.695451

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1	C	-0.767988	-1.487976	-1.460700
2	C	-0.055329	-3.783064	-1.147017
3	C	1.519521	-1.975109	-0.824959
4	C	0.518514	-1.055312	-1.137804
5	C	-1.055006	-2.855702	-1.456828
6	C	-1.783063	-0.476797	-1.812971
7	C	1.242075	-3.341560	-0.854436
8	C	-0.417317	-5.213324	-1.153981
9	C	2.849900	-1.484891	-0.405813
10	H	0.740305	0.011230	-1.121652
11	H	-2.051408	-3.225969	-1.704044
12	N	-1.551469	0.546596	-2.588714
13	N	-3.097216	-0.538622	-1.371999
14	H	2.043125	-4.047308	-0.631387
15	N	0.132027	-6.138068	-0.276648
16	N	-1.279084	-5.741323	-1.977977
17	N	2.978754	-0.560237	0.627727
18	N	3.984277	-1.811499	-0.949883
19	C	-2.753980	1.213176	-2.695459
20	C	-3.745075	0.550945	-1.941756
21	C	-3.621755	-1.345633	-0.326912
22	C	-0.442800	-7.358018	-0.595378
23	C	0.947655	-5.888015	0.859726
24	C	-1.321416	-7.081768	-1.664765
25	C	4.336161	-0.280573	0.718012
26	C	1.972729	-0.133675	1.533237
27	C	4.941879	-1.080478	-0.276483
28	C	-3.064344	2.399567	-3.374221
29	C	-5.046506	1.048300	-1.810048
30	C	-4.858436	-1.972015	-0.489329
31	C	-2.913383	-1.483628	0.872610
32	C	-0.306251	-8.634777	-0.043154
33	C	0.513182	-4.997706	1.845515
34	C	2.179814	-6.531962	0.981283
35	C	-2.078353	-8.117683	-2.230636
36	C	5.085328	0.536221	1.573301
37	C	1.915421	1.206881	1.917179
38	C	1.051454	-1.048244	2.058201
39	C	6.333792	-1.066700	-0.441330
40	C	-4.359338	2.884382	-3.271331
41	H	-2.297896	2.913688	-3.954585
42	C	-5.334997	2.219039	-2.499666
43	H	-5.795463	0.557518	-1.186277

44	C	-5.388472	-2.734477	0.550133	91	C	2.619923	2.198510	-1.737579
45	H	-5.391131	-1.867008	-1.435338	92	C	4.381382	4.332605	0.616496
46	C	-3.442458	-2.265324	1.895921	93	C	9.070927	3.222014	-0.235053
47	H	-1.950532	-0.981750	0.995888	94	N	8.871832	0.771292	-2.833702
48	C	-1.068272	-9.643836	-0.617437	95	C	1.923092	4.075808	0.326097
49	H	0.362968	-8.828089	0.795961	96	C	1.271543	2.469863	-1.392614
50	C	1.330509	-4.735365	2.942552	97	H	2.857747	1.468221	-2.513816
51	H	-0.458825	-4.512543	1.733516	98	C	4.204168	5.193672	1.675487
52	C	2.984766	-6.274497	2.090078	99	N	10.200607	3.286749	-0.010039
53	H	2.504998	-7.215524	0.195263	100	C	0.902424	3.351739	-0.378201
54	C	-1.938732	-9.390539	-1.698088	101	C	1.768066	4.960766	1.432520
55	H	-2.753017	-7.908538	-3.060815	102	H	0.475144	1.952138	-1.936353
56	C	6.464976	0.530553	1.395857	103	C	2.873859	5.499550	2.068713
57	H	4.621408	1.137488	2.355568	104	H	5.056175	5.614248	2.211149
58	C	0.932659	1.638404	2.806535	105	C	-0.526900	3.402526	0.010644
59	H	2.635344	1.910173	1.501172	106	H	0.768832	5.202010	1.798101
60	C	0.065900	-0.605006	2.937075	107	H	2.719187	6.170505	2.914602
61	H	1.115018	-2.100891	1.780708	108	C	-1.253822	4.589549	0.166247
62	C	7.082168	-0.262823	0.406709	109	C	-1.197204	2.187078	0.209082
63	H	6.798923	-1.678932	-1.214092	110	C	-2.614014	4.561767	0.468693
64	H	-4.635830	3.806224	-3.785059	111	H	-0.757687	5.551691	0.024184
65	H	-6.336275	2.648702	-2.425714	112	C	-2.556709	2.151105	0.473049
66	C	-4.680485	-2.889801	1.740388	113	H	-0.637657	1.250602	0.145844
67	H	-6.355707	-3.221075	0.420318	114	C	-3.288985	3.339208	0.580125
68	H	-2.888829	-2.377870	2.829846	115	H	-3.159345	5.493951	0.610654
69	H	-0.991744	-10.657929	-0.222896	116	H	-3.062952	1.194107	0.570937
70	C	2.566768	-5.371225	3.066342	117	N	-4.685850	3.288364	0.767897
71	H	0.999326	-4.033470	3.709853	118	C	-5.371275	2.284949	1.458921
72	H	3.950961	-6.771804	2.182055	119	C	-5.621117	4.046337	0.055367
73	H	-2.514342	-10.216333	-2.118038	120	C	-4.889006	1.293362	2.323781
74	H	7.085123	1.151593	2.045243	121	C	-6.754887	2.405460	1.198296
75	C	-0.002400	0.737936	3.312563	122	C	-5.429807	5.092996	-0.854534
76	H	0.893529	2.692315	3.087899	123	C	-6.914617	3.533969	0.304872
77	H	-0.647559	-1.323479	3.345265	124	C	-5.807054	0.406558	2.874828
78	H	8.168938	-0.236499	0.303683	125	H	-3.831022	1.211846	2.569572
79	H	-5.093206	-3.496236	2.547463	126	C	-7.661079	1.504736	1.767850
80	H	3.204221	-5.162120	3.925981	127	C	-6.551168	5.626435	-1.480003
81	H	-0.776475	1.078497	4.001387	128	H	-4.437231	5.460438	-1.106250
82	C	5.073952	2.814500	-1.042621	129	C	-8.029409	4.089174	-0.331740
83	C	7.187422	2.243634	-1.508852	130	C	-7.180304	0.498862	2.595961
84	N	6.827070	3.866601	0.235370	131	H	-5.446069	-0.377908	3.541616
85	C	3.609600	2.863021	-1.049331	132	H	-8.728958	1.594921	1.561768
86	C	5.548371	3.711767	-0.026379	133	C	-7.843012	5.139817	-1.220986
87	N	5.886789	2.092273	-1.782193	134	H	-6.418637	6.439746	-2.195167
88	C	7.654777	3.121996	-0.510118	135	H	-9.027287	3.691071	-0.139846
89	C	8.121773	1.431347	-2.257115	136	H	-7.871115	-0.216605	3.043067
90	C	3.246820	3.796574	-0.046050	137	H	-8.699705	5.585163	-1.727508

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