Supporting Information: The Negligible Effect of the Single Vacancy Defect on the Ultrafast Excitation Energy Transfer from Porphyrin to Single-Walled Carbon Nanotubes

Xiao-Ying Xie[a], Ya-Qi Xu[a], Xi Zhao[b], Wen-Kai Chen[b]*

[a]The Laboratory of Theoretical and Computational Chemistry, School of Chemistry and Chemical Engineering, Yantai University, Yantai 264005, China;

[b]College of Chemistry and Materials Science, Hebei Key Laboratory of Inorganic Nano-Materials, Hebei Normal University, Shijiazhuang 050024, China

E-mail: wenkaichen@hebtu.edu.cn

Content

1. Theoretical Methods

1.1 sTDA-xTB Framework

Simulating the nonadiabatic dynamics of large defect-hybridized systems such as single vacancy (SV) defective single-walled carbon nanotube (SWCNT) and tetraphenyl porphyrin (H2TPP) nanohybrid, i.e., H2TPP@SV-CNT(6,5), comprising over 400 atoms and 85 excited states, demands computationally efficient quantum mechanical methods. Ab initio nonadiabatic dynamics (NAMD) approaches are computationally unaffordable. In this work, to balance the efficiency and precision, we perform the NAMD simulations at a semi-empirical extended tight-binding based simplified Tamm-Dancoff approximation (sTDA-xTB) level.[1-3]

1.1.1 Ground-State Optimization and Molecular Dynamics: GFN1-xTB Method

All ground-state calculations, including geometry optimization and molecular dynamics (MD), utilize the GFN1-xTB method.[4] GFN1-xTB is a semi-empirical approximation to density functional theory (DFT) within the extended tight-binding (xTB) framework. It provides an efficient description of structures, vibrational frequencies, and non-covalent interactions for large systems.[5, 6] The GFN1-xTB total energy is partitioned as:

$$E = E_{el} + E_{rep} + E_{disp} + E_{XB} \tag{S1}$$

where E_{el} represents the electronic energy, E_{rep} is the atom pairwise repulsion energy, E_{disp} represents for dispersionn energy, and E_{XB} is the halogen bonding energy.

1.1.2 Excited States: sTDA-xTB Method

Excited-state calculations employ the simplified Tamm-Dancoff approximation method

(sTDA) coupled with xTB (sTDA-xTB).[7] The Tamm-Dancoff approximation (TDA) simplifies the full time-dependent DFT (TDDFT) problem by solving the eigenvalue equation:

$$\mathbf{AX} = \omega_{TDA}\mathbf{X} \qquad (S2)$$

Where $\mathbf{X}$ contains the excitation vectors, and ω_{TDA} is the excitation energy, and the orbital rotation Hermitian matrix $\mathbf{A}$ is defined from occupied i, j to unoccupied a, b orbitals:

$$A_{ia,jb} = \delta_{ij}\delta_{ab}(\epsilon_a - \epsilon_i) + 2(ia|jb) - a_x(ij|ab) + (1 - a_x)(ia|f_{XC}|jb) \qquad (S3)$$

here, ϵ_i is the energy of the ith orbital, $(ia|jb)$ and $(ij|ab)$ represent two-electron integrals,. f_{XC} is the exchange-correlation kernel, and a_x is the fraction of exact Hartree-Fock exchange.

The sTDA method introduces key approximations to Eq. S3 for computational efficiency:[8] 1) The term $(ia|f_{XC}|jb)$ is omitted; 2) Two-electron integrals are approximated using a short-range damped Coulomb interactions to reduce the computational costs; and 3) The excitation space is truncated based on an energy cutoff. These approximations, combined with the underlying xTB Hamiltonian for ground-state orbitals and energies, constitute the sTDA-xTB method. More details can be found in refs[1, 2].

Key parameters in sTDA-xTB calculations have demonstrated reasonable for simulating H2TPP@P-CNT(6,5):[9] (1) Exact exchange ($a_x = 0.29$) in Eq. S3; (2) Shift constant for virtual KS orbital eigenvalues set to 3.25 eV (for sTDA calculations);

1.2 Nonadiabatic Dynamics: Trajectory-Based Surface Hopping

To model the ultrafast photoinduced dynamics involving multiple electronic states, we

implement Tully's trajectory-based surface hopping (TSH) method.[10, 11] In TSH, treated

classically by integrating Newton's equations:

$$F_{\boldsymbol{R}} = m_{\boldsymbol{R}} \frac{d^2 \boldsymbol{R}}{dt^2} \tag{S4}$$

where $F_{\boldsymbol{R}}$ represents the atomic forces of the system. $\boldsymbol{R}$ is the coordinates of the nucleus,

and $m_{\boldsymbol{R}}$ is the atomic mass. The time-dependent wave function $\Phi(\mathbf{R}, \mathbf{r}, t)$ can be

expanded as a linear combination of time-independent adiabatic electronic wave functions:

$$\Phi(\boldsymbol{R}, \boldsymbol{r}, t) = \sum_{K=1}^{N} c_K(t) \Phi_K(\boldsymbol{R}, \boldsymbol{r}) \tag{S5}$$

The time-dependent coefficients $c_K(t)$ evolve according to the time-dependent

Schrödinger equation under the classical nuclear trajectory:

$$i\hbar \frac{dc_J(t)}{dt} = c_J(t) E_J(R) - i\hbar \sum_K^{N} c_K(t) \tau_{KJ}(t) \tag{S6}$$

Where E_J is the energy of adiabatic state, and τ_{KJ} is the nonadiabatic coupling (NAC)

vector:

$$\tau_{KJ} = \langle \Psi_J | \partial \Psi_K / \partial t \rangle \tag{S7}$$

Electronic states transition between the Kth and Jth state occur based on the probability:

$$p_{KJ}(t)dt = 2 \frac{Re(c_K^* c_J \tau_{KJ})}{c_K^* c_K} dt \tag{S8}$$

1.3 Numerical Algorithms for NACs

Efficient computation of NACs is crucial for TSH.[12-18] Within the sTDA-xTB framework,

the wavefunction for the Kth excited state is:

$$\Phi_K = \sum_{ia} \omega_{ia}^K \Phi_i^a \tag{S9}$$

where $\omega_{ia}^K \equiv N_K^{-1/2} (\mathbf{X})_{ia}^K$ is the normalized configuration interaction coefficients from occupied orbital i to unoccupied orbital a. The NAC between states K and J, τ_{KJ} is computed using an efficient numerical algorithm adapted to sTDA-xTB:

$$\tau_{KJ} = \sum_{ia} \omega_{ia}^K \partial_t \omega_{ia}^J + \sum_{iab} \omega_{ia}^K \omega_{ib}^J \langle \phi_a \mid \partial_t \phi_b \rangle - \sum_{ija} P_{ij} \omega_{ia}^K \omega_{ja}^J \langle \phi_j | \partial_t \phi_i \rangle \quad (S10)$$

The time derivative $\langle \phi_p \mid \partial_t \phi_q \rangle$ is computed via finite difference scheme:

$$\langle \phi_p \mid \partial_t \phi_q \rangle = \frac{\langle \phi_p(t) | \phi_q(t + \Delta t) \rangle}{\Delta t} \quad (S11)$$

More details can be found in previous works.[19, 20] The algorithm has been independently developed into a standalone module within the generalized trajectory-based surface hopping (GTSH) package.[21, 22]

1.4 Semiclassical Absorption Spectrum

The linear absorption spectrum is simulated using a semiclassical approach based on an ensemble of N ground-state configurations $\mathbf{R}_k$.[23, 24] The optical absorption cross section is calculated as:

$$\sigma(E) = \frac{\pi e^2}{2mc\epsilon_0} \sum_{l \neq i} \left[\frac{1}{N} \sum_k^N f_{il}(\mathbf{R}_k) g(E - \Delta E_{il}(\mathbf{R}_k), \delta) \right] \quad (S12)$$

where ϵ_0, c, e, and m are the vacuum permittivity, speed of light, elementary charge, and electron mass, respectively. f_{il} is the oscillator strength, ΔE_{il} is the excitation energy, and $g(E - \Delta E_{il}(\mathbf{R}_k), \delta)$ is a Gaussian lineshape function with the phenomenological constant δ is:

$$g_{Gauss}(E - \Delta E_{il}(\mathbf{R}_k), \delta) = \left(\frac{2}{\pi} \right)^{\frac{1}{2}} \frac{\hbar}{\delta} \exp \left(- \frac{2 \left(E - \Delta E_{il}(\mathbf{R}_k) \right)^2}{\delta^2} \right) \quad (S13)$$

1.5 Fragment-Based Exciton Analysis

To characterize the properties (local excitation, LE; charge transfer, CT) and spatial location of excitons, we implement a fragment-based analysis at the sTDA-xTB level.[19, 20] The system is partitioned into fragments (here: SV-CNT(6,5) and H2TPP). The one-electron transition density in the Löwdin atomic orbital (AO) is:

$$\mathbf{T}_{LO}^K = (\mathbf{S}_{AO})^{\frac{1}{2}}\mathbf{T}_{AO}^K(\mathbf{S}_{AO})^{\frac{1}{2}} = (\mathbf{S}_{AO})^{\frac{1}{2}}(\mathbf{C}\mathbf{T}_{MO}^K\mathbf{C}^{\mathrm{T}})(\mathbf{S}_{AO})^{\frac{1}{2}} \tag{S14}$$

where $\mathbf{C}$ is the molecular orbital (MO) coefficient matrix and $\mathbf{S}_{AO}$ is the AO overlap matrix, $\mathbf{T}_{MO}^K$ is the one-electron transition density matrix in the MO representation of the Kth state, $\mathbf{T}_{AO}^K$ is the one-electron transition density matrix in the AO representation of the Kth state. Thus, the contribution of the transition from the mth atom to the nth atom in the Kth electronic state is expressed as:

$$D_{mn}^K = \sum_{i\in m, j\in n} (\mathbf{T}_{LO}^K)_{ij}^2 \tag{S15}$$

The fragment transition contribution is:

$$\Omega_{MN}^K = \sum_{m\in M, n\in N} D_{mn}^K \tag{S16}$$

Specifically, if $M = N$, it indicates the LE of the Mth or the Nth fragment. Otherwise, if $M \neq N$, it means CT excitation from the Mth fragment to the Nth fragment. In addition, the amount of electron and hole transferred from the Mth fragment to the Kth state from all other fragments can be obtained from Ω_{MN}^K $(M \neq N)$:

$$e_M^K = \sum_{m\in M} D_{mn}^K = \sum_N \Omega_{DA}^K , \quad h_N^K = \sum_{n\in N} D_{mn}^K = \sum_M \Omega_{DA}^K \tag{S17}$$

2. Additional Figures
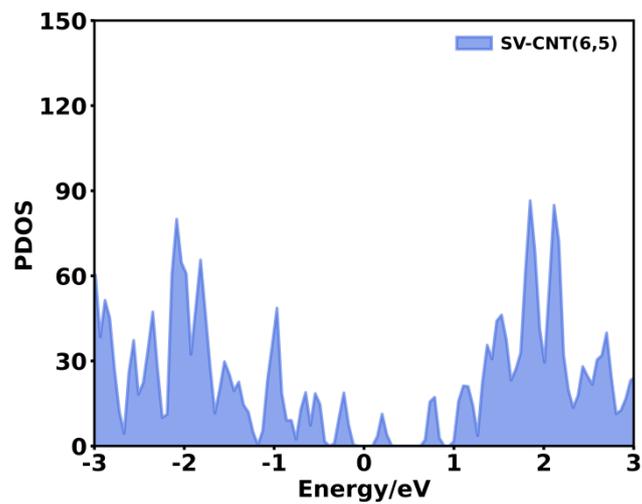
Figure S1. PDOS of SV-CNT(6,5) at PBE level.

S_{11} S_{12} S_{13} S_{14} S_{15}

S_{16} S_{17} S_{18} S_{19} S_{20}

S_{21} S_{22} S_{23} S_{24} S_{25}

S_{26} S_{27} S_{28} S_{29} S_{30}

S_{31} S_{32} S_{33} S_{34} S_{35}

S_{36} S_{37} S_{38} S_{39} S_{40}

S_{41} S_{42} S_{43} S_{44} S_{45}

S_{46} S_{47} S_{48} S_{49} S_{50}

S_{51} S_{52} S_{53} S_{54} S_{55}

S_{56} S_{57} S_{58} S_{59} S_{60}

S_{61} S_{62} S_{63} S_{64} S_{65}

S_{66} S_{67} S_{68} S_{69} S_{70}
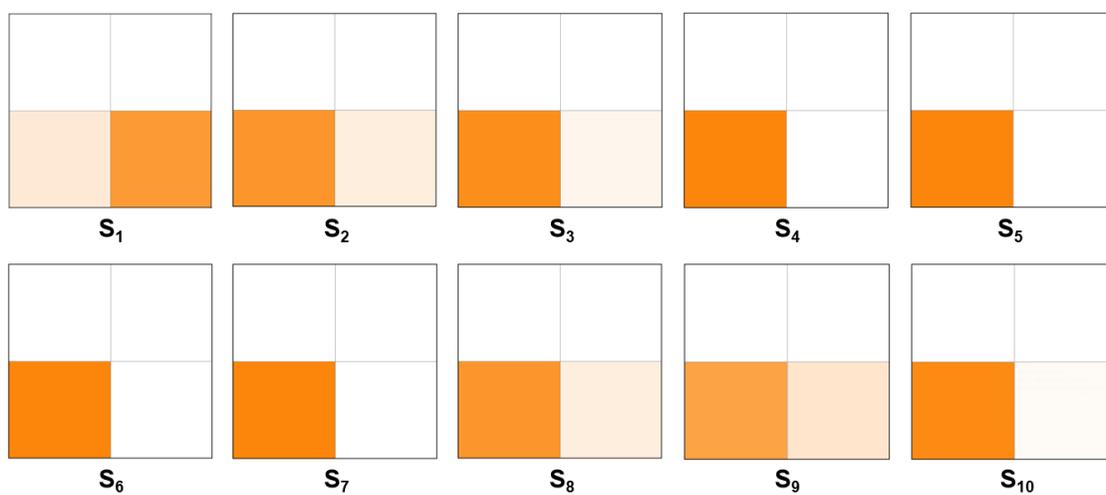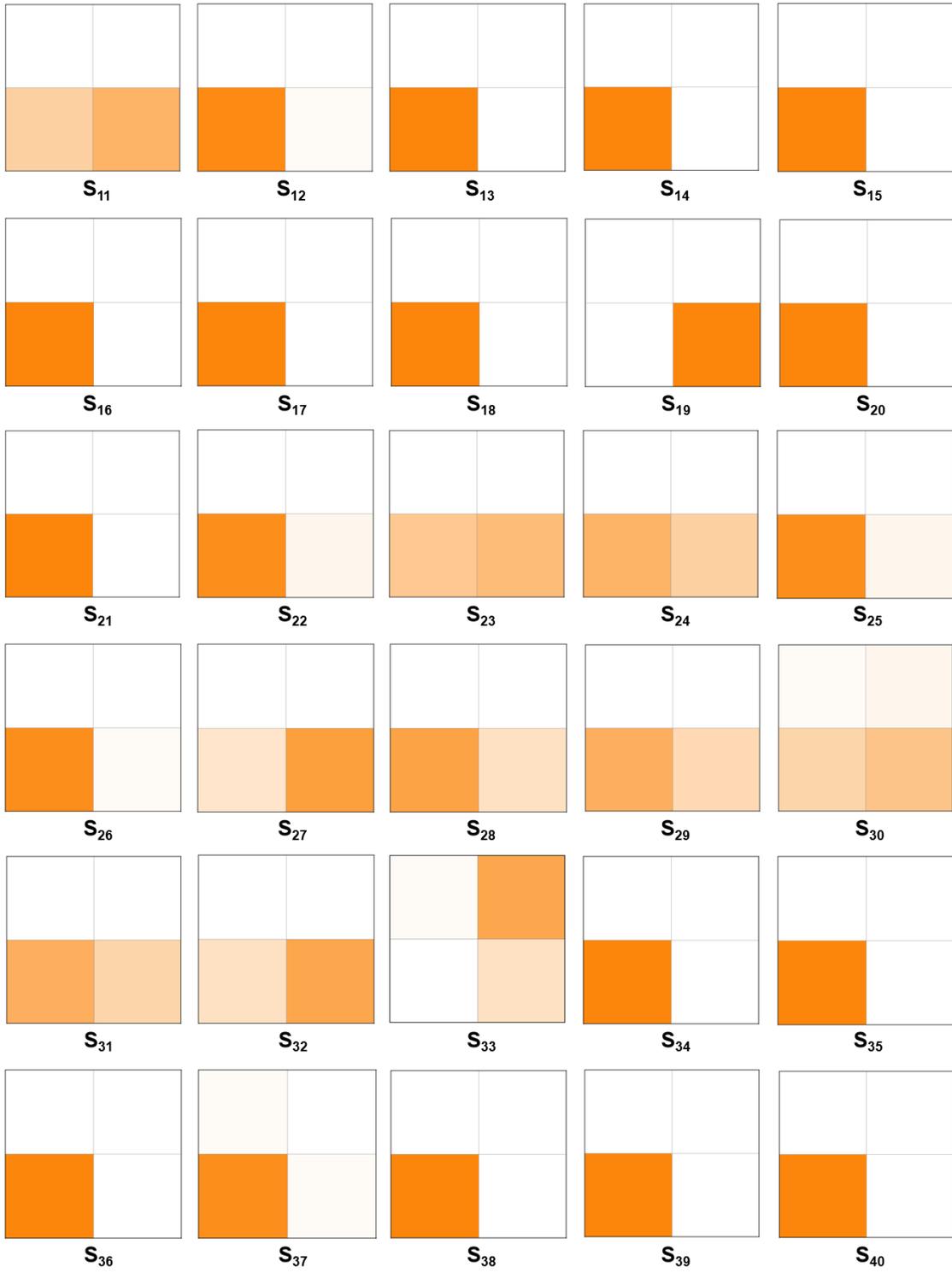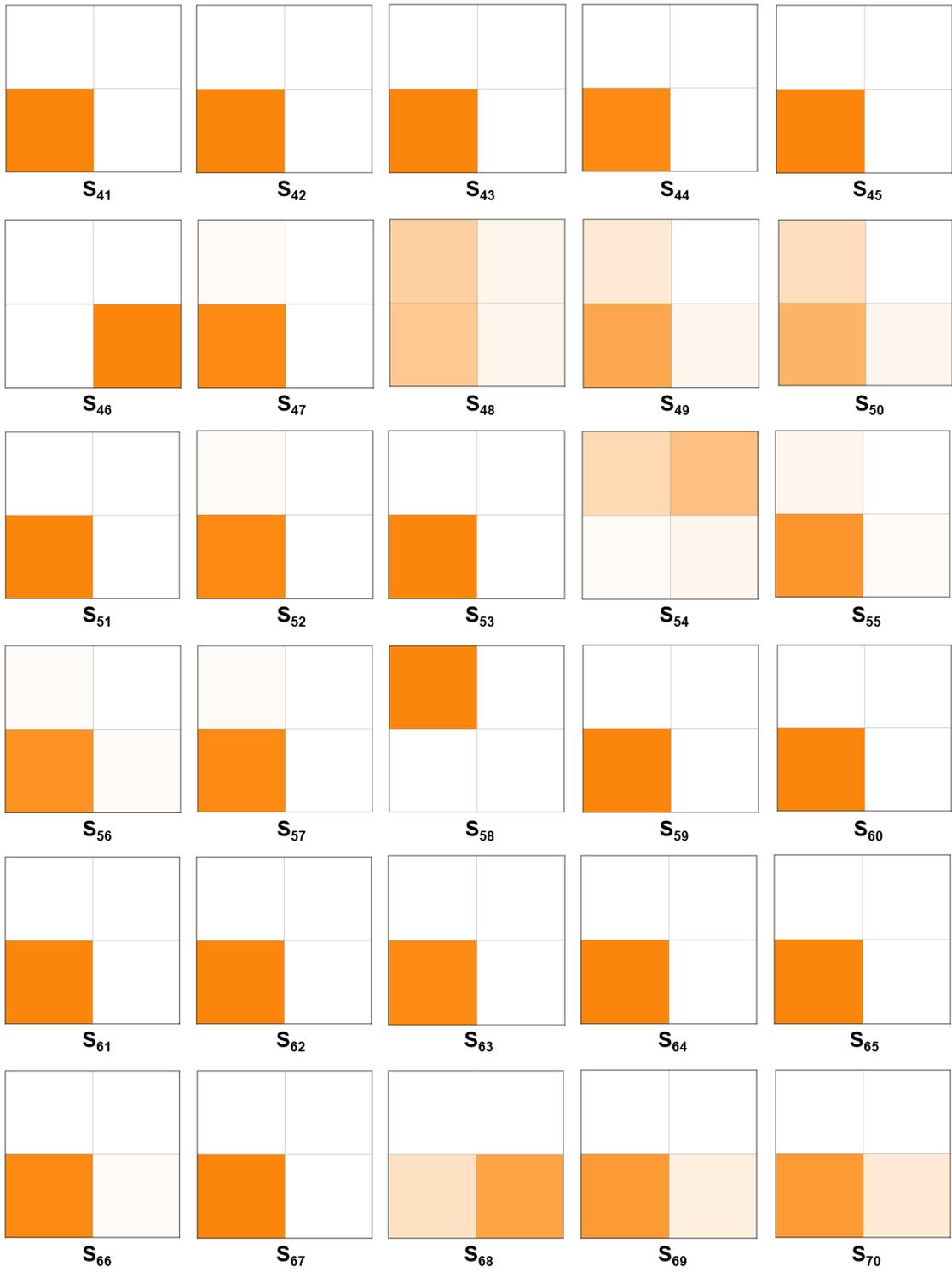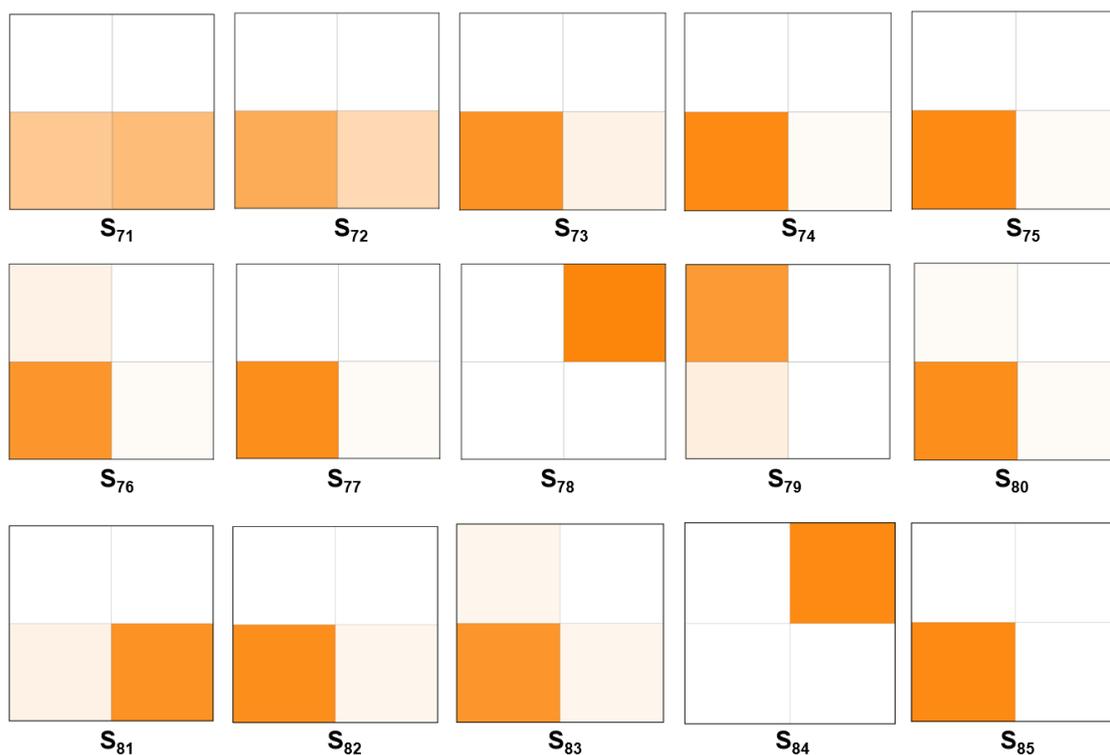
Figure S2. CT matrix of the H2TPP@SV-CNT(6,5), where the x-axis labels represent the donor fragment and the y-axis labels represent the acceptor fragment.

Note: diagonal elements (X = Y) represent LE excitons localized on a single fragment, while off-diagonal elements (X ≠ Y) represent CT excitons between distinct fragments. The upper left panel shows the electron in H2TPP, with the hole located in SV-CNT(6,5). The upper right panel illustrates both the electron and the hole being located in H2TPP. The lower left panel represents both the electron and the hole being situated in SV-CNT(6,5).The lower right panel depicts the electron in SV-CNT(6,5), while the hole is located in H2TPP.
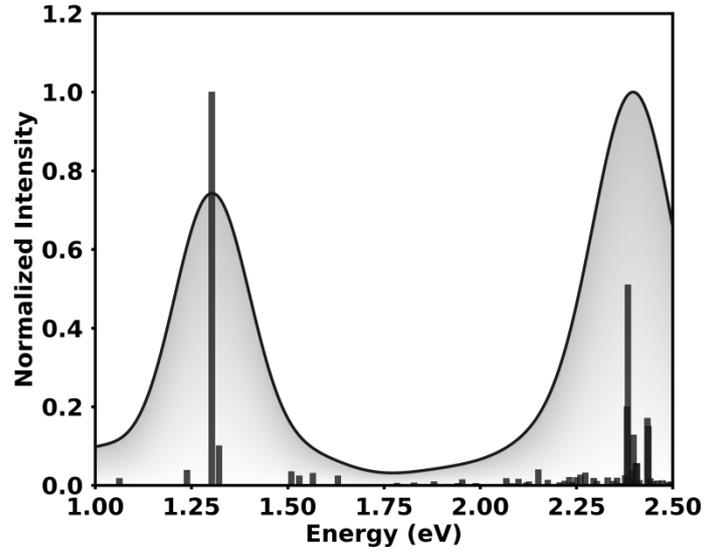
Figure S3. The broadened and discrete spectra at the optimized ground-state geometry.
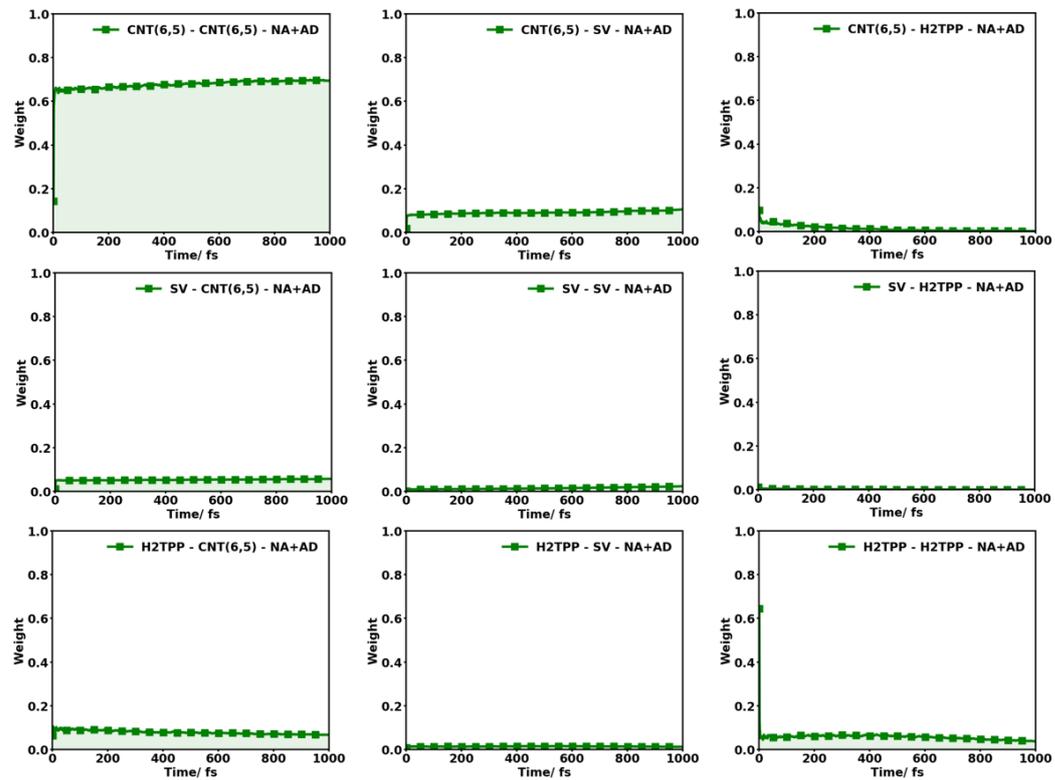
Figure S4. Time-dependent weights of different excitons.
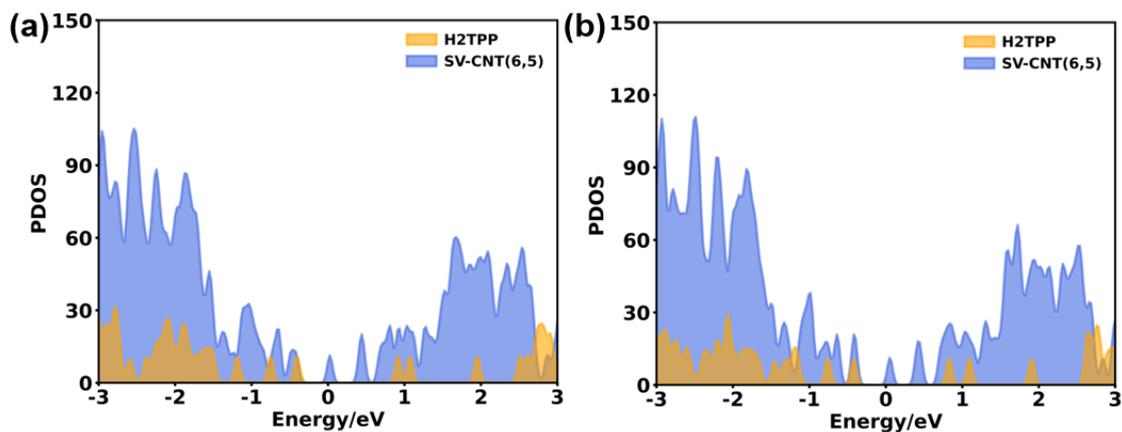
Figure S5. PDOS of H2TPP@SV-CNT(6,5) NVE dynamics simulation snapshots at (a) 0 fs, (b) 2000 fs at xTB level.
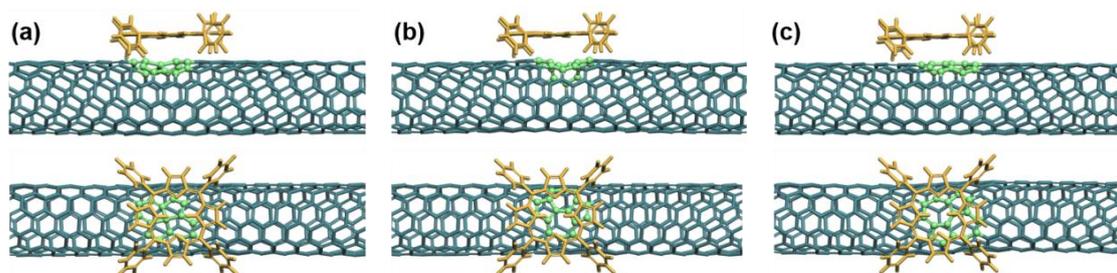
Figure S6. Optimized structure front view and top view of the (a) H2TPP@SV1-CNT(6,5), (b) H2TPP@SW1-CNT(6,5) and (c) H2TPP@SW2-CNT(6,5).

3. Additional Tables

Table S1. Excited state properties, oscillator strengths and excitation energies of H2TPP@SV-CNT(6,5) at sTDA-xTB level.

state	properties	oscillator strengths	excitation energy (eV)
S_1	H2TPP$^+$@SV-CNT(6,5) -	0.1493	0.95518
S_2	H2TPP@SV@-CNT(6,5)*	0.7203	0.99757
S_3	H2TPP@SV-CNT(6,5)*	0.1238	1.06292
S_4	H2TPP@SV-CNT(6,5)*	0.2673	1.23849
S_5	H2TPP@SV-CNT(6,5)*	6.9750	1.30282
S_6	H2TPP@SV-CNT(6,5)*	0.7033	1.32164
S_7	H2TPP@SV-CNT(6,5)*	0.0106	1.38136
S_8	H2TPP@SV-CNT(6,5)*	0.0104	1.47041
S_9	H2TPP@SV-CNT(6,5)*	0.2419	1.50967
S_{10}	H2TPP@SV-CNT(6,5)*	0.0071	1.52028
S_{11}	H2TPP$^+$@SV-CNT(6,5) -	0.1697	1.53021
S_{12}	H2TPP@SV-CNT(6,5)*	0.2123	1.56524
S_{13}	H2TPP@SV-CNT(6,5)*	0.0162	1.60239
S_{14}	H2TPP@SV-CNT(6,5)*	0.1694	1.63046
S_{15}	H2TPP@SV-CNT(6,5)*	0.0105	1.7255
S_{16}	H2TPP@SV-CNT(6,5)*	0.0124	1.77087
S_{17}	H2TPP@SV-CNT(6,5)*	0.0400	1.78409
S_{18}	H2TPP@SV-CNT(6,5)*	0.0027	1.79982
S_{19}	H2TPP$^+$@SV-CNT(6,5) -	0.0000	1.81509

S_{20}	H2TPP@SV-CNT(6,5)*	0.0449	1.82831
S_{21}	H2TPP@SV-CNT(6,5)*	0.0226	1.83797
S_{22}	H2TPP@SV-CNT(6,5)*	0.0188	1.871
S_{23}	H2TPP+@SV-CNT(6,5) -	0.0647	1.8799
S_{24}	H2TPP@SV-CNT(6,5)*	0.0214	1.88572
S_{25}	H2TPP@SV-CNT(6,5)*	0.0240	1.91529
S_{26}	H2TPP@SV-CNT(6,5)*	0.0056	1.92375
S_{27}	H2TPP+@SV-CNT(6,5) -	0.0014	1.93295
S_{28}	H2TPP@SV-CNT(6,5)*	0.0339	1.94121
S_{29}	H2TPP@SV-CNT(6,5)*	0.1001	1.95327
S_{30}	H2TPP+@SV-CNT(6,5) -	0.0051	1.96237
S_{31}	H2TPP@SV-CNT(6,5)*	0.0107	1.97077
S_{32}	H2TPP+@SV-CNT(6,5) -	0.0160	1.97628
S_{33}	H2TPP*@SV-CNT(6,5)	0.0339	1.98864
S_{34}	H2TPP@SV-CNT(6,5)*	0.0090	2.00461
S_{35}	H2TPP@SV-CNT(6,5)*	0.0068	2.0083
S_{36}	H2TPP@SV-CNT(6,5)*	0.0042	2.02896
S_{37}	H2TPP@SV-CNT(6,5)*	0.0005	2.03461
S_{38}	H2TPP@SV-CNT(6,5)*	0.0021	2.0422
S_{39}	H2TPP@SV-CNT(6,5)*	0.0097	2.06377
S_{40}	H2TPP@SV-CNT(6,5)*	0.1220	2.06772
S_{41}	H2TPP@SV-CNT(6,5)*	0.0326	2.0826
S_{42}	H2TPP@SV-CNT(6,5)*	0.1102	2.09958
S_{43}	H2TPP@SV-CNT(6,5)*	0.0448	2.11908

S_{44}	H2TPP@SV-CNT(6,5)*	0.0631	2.1264
S_{45}	H2TPP@SV-CNT(6,5)*	0.0038	2.13815
S_{46}	H2TPP$^+$@SV-CNT(6,5)$^-$	0.0021	2.14857
S_{47}	H2TPP@SV-CNT(6,5)*	0.2764	2.15087
S_{48}	H2TPP@SV-CNT(6,5)*	0.0106	2.16705
S_{49}	H2TPP@SV-CNT(6,5)*	0.0037	2.17193
S_{50}	H2TPP@SV-CNT(6,5)*	0.0915	2.17566
S_{51}	H2TPP@SV-CNT(6,5)*	0.0454	2.20663
S_{52}	H2TPP@SV-CNT(6,5)*	0.0747	2.21908
S_{53}	H2TPP@SV-CNT(6,5)*	0.1427	2.23147
S_{54}	H2TPP*@SV-CNT(6,5)	0.0525	2.23928
S_{55}	H2TPP@SV-CNT(6,5)*	0.1373	2.24916
S_{56}	H2TPP@SV-CNT(6,5)*	0.1844	2.26036
S_{57}	H2TPP@SV-CNT(6,5)*	0.2244	2.27314
S_{58}	H2TPP$^-$@SV-CNT(6,5)$^+$	0.0232	2.29073
S_{59}	H2TPP@SV-CNT(6,5)*	0.1273	2.29509
S_{60}	H2TPP@SV-CNT(6,5)*	0.0725	2.30345
S_{61}	H2TPP@SV-CNT(6,5)*	0.1330	2.33109
S_{62}	H2TPP@SV-CNT(6,5)*	0.0716	2.3478
S_{63}	H2TPP@SV-CNT(6,5)*	0.1312	2.35542
S_{64}	H2TPP@SV-CNT(6,5)*	0.0348	2.36435
S_{65}	H2TPP@SV-CNT(6,5)*	0.1732	2.3765
S_{66}	H2TPP@SV-CNT(6,5)*	1.3961	2.38122
S_{67}	H2TPP@SV-CNT(6,5)*	3.5565	2.38355

S_{68}	H2TPP$^+$@SV-CNT(6,5) -	0.0962	2.39
S_{69}	H2TPP@SV-CNT(6,5)*	0.2610	2.39548
S_{70}	H2TPP@SV-CNT(6,5)*	0.8930	2.39809
S_{71}	H2TPP$^+$@SV-CNT(6,5) -	0.3887	2.40445
S_{72}	H2TPP@SV-CNT(6,5)*	0.3889	2.4076
S_{73}	H2TPP@SV-CNT(6,5)*	0.0870	2.41379
S_{74}	H2TPP@SV-CNT(6,5)*	0.0175	2.42155
S_{75}	H2TPP@SV-CNT(6,5)*	1.1912	2.43433
S_{76}	H2TPP@SV-CNT(6,5)*	1.0469	2.43687
S_{77}	H2TPP@SV-CNT(6,5)*	0.1185	2.44259
S_{78}	H2TPP*@SV-CNT(6,5)	0.0006	2.44543
S_{79}	H2TPP - @SV-CNT(6,5)$^+$	0.0621	2.44782
S_{80}	H2TPP@SV-CNT(6,5)*	0.0791	2.4605
S_{81}	H2TPP$^+$@SV-CNT(6,5) -	0.0020	2.47067
S_{82}	H2TPP@SV-CNT(6,5)*	0.0864	2.47366
S_{83}	H2TPP@SV-CNT(6,5)*	0.0569	2.48758
S_{84}	H2TPP*@SV-CNT(6,5)	0.0080	2.48807
S_{85}	H2TPP@SV-CNT(6,5)*	0.0650	2.49634

Table S2. The start time and population, highest time and population, end time and population of individual excited states calculated from the NAMD simulations at the sTDA-xTB level for the H2TPP@SV-CNT(6,5) system.

state	start time	start population	highest time	highest population	end time	end population
S_1	1	0.0000	1000	0.0548	1000	0.0548
S_2	1	0.0000	1000	0.0194	1000	0.0194
S_3	1	0.0000	1000	0.0313	1000	0.0313
S_4	1	0.0000	1000	0.0135	1000	0.0135
S_5	1	0.0000	1000	0.0097	1000	0.0097
S_6	1	0.0000	1000	0.0080	1000	0.0076
S_7	1	0.0000	1000	0.0215	1000	0.0215
S_8	1	0.0000	1000	0.0164	1000	0.0161
S_9	1	0.0000	1000	0.0131	1000	0.0131
S_{10}	1	0.0000	1000	0.0123	1000	0.0121
S_{11}	1	0.0000	1000	0.0125	1000	0.0125
S_{12}	1	0.0000	1000	0.0117	1000	0.0109
S_{13}	1	0.0000	1000	0.0257	1000	0.0257
S_{14}	1	0.0000	1000	0.0249	1000	0.0243
S_{15}	1	0.0000	1000	0.0242	1000	0.0240
S_{16}	1	0.0000	1000	0.0240	1000	0.0240
S_{17}	1	0.0000	1000	0.0226	1000	0.0220
S_{18}	1	0.0000	1000	0.0228	1000	0.0228
S_{19}	1	0.0000	1000	0.0230	1000	0.0225
S_{20}	1	0.0000	1000	0.0226	1000	0.0223
S_{21}	1	0.0000	1000	0.0225	1000	0.0218
S_{22}	1	0.0000	1000	0.0232	1000	0.0228
S_{23}	1	0.0000	1000	0.0244	1000	0.0239
S_{24}	1	0.0000	1000	0.0233	1000	0.0223
S_{25}	1	0.0000	1000	0.0238	1000	0.0222
S_{26}	1	0.0000	1000	0.0232	1000	0.0231
S_{27}	1	0.0000	1000	0.0224	1000	0.0210
S_{28}	1	0.0000	1000	0.0222	1000	0.0216
S_{29}	1	0.0000	1000	0.0228	1000	0.0204
S_{30}	1	0.0000	886	0.0220	1000	0.0203

S_{31}	1	0.0000	878	0.0227	1000	0.0205
S_{32}	1	0.0000	819	0.0220	1000	0.0198
S_{33}	1	0.0000	759	0.0219	1000	0.0191
S_{34}	1	0.0000	786	0.0211	1000	0.0187
S_{35}	1	0.0000	847	0.0223	1000	0.0185
S_{36}	1	0.0000	810	0.0214	1000	0.0180
S_{37}	1	0.0000	766	0.0223	1000	0.0174
S_{38}	1	0.0000	748	0.0254	1000	0.0171
S_{39}	1	0.0000	722	0.0263	1000	0.0170
S_{40}	1	0.0000	673	0.0258	1000	0.0157
S_{41}	1	0.0000	586	0.0251	1000	0.0159
S_{42}	1	0.0000	579	0.0263	1000	0.0147
S_{43}	1	0.0000	576	0.0260	1000	0.0134
S_{44}	1	0.0000	486	0.0285	1000	0.0130
S_{45}	1	0.0000	514	0.0292	1000	0.0117
S_{46}	1	0.0037	465	0.0322	1000	0.0114
S_{47}	1	0.0028	420	0.0337	1000	0.0125
S_{48}	1	0.0033	509	0.0353	1000	0.0111
S_{49}	1	0.0067	491	0.0375	1000	0.0100
S_{50}	1	0.0033	334	0.0406	1000	0.0097
S_{51}	1	0.0100	318	0.0403	1000	0.0083
S_{52}	1	0.0167	367	0.0435	1000	0.0074
S_{53}	1	0.0233	284	0.0454	1000	0.0072
S_{54}	1	0.0267	222	0.0456	1000	0.0059
S_{55}	1	0.0567	2	0.0567	1000	0.0048
S_{56}	1	0.0333	211	0.0468	1000	0.0045
S_{57}	1	0.0367	189	0.0455	1000	0.0037
S_{58}	1	0.0300	162	0.0456	1000	0.0032
S_{59}	1	0.0367	136	0.0428	1000	0.0027
S_{60}	1	0.0533	1	0.0533	1000	0.0021
S_{61}	1	0.0167	98	0.0412	1000	0.0017
S_{62}	1	0.0267	78	0.0397	1000	0.0014
S_{63}	1	0.0200	119	0.0386	1000	0.0013
S_{64}	1	0.0367	72	0.0403	1000	0.0007
S_{65}	1	0.0267	65	0.0411	1000	0.0007
S_{66}	1	0.0300	44	0.0407	1000	0.0006
S_{67}	1	0.0367	6	0.0432	1000	0.0005
S_{68}	1	0.0433	1	0.0433	1000	0.0004

S_{69}	1	0.0300	19	0.0456	1000	0.0003
S_{70}	1	0.0467	17	0.0541	1000	0.0002
S_{71}	1	0.0467	9	0.0537	1000	0.0002
S_{72}	1	0.0533	9	0.0586	1000	0.0001
S_{73}	1	0.0733	1	0.0733	1000	0.0001
S_{74}	1	0.0233	13	0.0407	1000	0.0000
S_{75}	1	0.0367	5	0.0385	1000	0.0001
S_{76}	1	0.0433	1	0.0433	1000	0.0000
S_{77}	1	0.0167	6	0.0319	1000	0.0000
S_{78}	1	0.0167	11	0.0224	1000	0.0000
S_{79}	1	0.0133	14	0.0157	1000	0.0000
S_{80}	1	0.0167	2	0.0170	1000	0.0000
S_{81}	1	0.0033	9	0.0075	1000	0.0000
S_{82}	1	0.0000	54	0.0032	1000	0.0000
S_{83}	1	0.0000	40	0.0026	1000	0.0000
S_{84}	1	0.0000	46	0.0014	1000	0.0000
S_{85}	1	0.0000	85	0.0010	1000	0.0000

Table S3. Excited state properties, oscillator strengths and excitation energies of H2TPP@SV1-CNT(6,5) at sTDA-xTB level.

state	properties	oscillator strengths	excitation energy (eV)
S_1	H2TPP@SV1-CNT(6,5)*	5.4013	1.2263
S_2	H2TPP@SV1-CNT(6,5)*	0.0007	1.2534
S_3	H2TPP@SV1-CNT(6,5)*	0.0002	1.3094
S_4	H2TPP@SV1-CNT(6,5)*	3.6419	1.3622
S_5	H2TPP@SV1-CNT(6,5)*	0.0007	1.5566
S_6	H2TPP@SV1-CNT(6,5)*	0.3196	1.5608
S_7	H2TPP@SV1-CNT(6,5)*	0.0249	1.5702
S_8	H2TPP@SV1-CNT(6,5)*	0.0001	1.6230
S_9	H2TPP@SV1-CNT(6,5)*	0.0232	1.6662
S_{10}	H2TPP@SV1-CNT(6,5)*	0.0004	1.7484
S_{11}	H2TPP@SV1-CNT(6,5)*	0.0125	1.7889
S_{12}	H2TPP@SV1-CNT(6,5)*	0.2422	1.7976
S_{13}	H2TPP$^+$@SV1-CNT(6,5)$^-$	0.0100	1.8232
S_{14}	H2TPP@SV1-CNT(6,5)*	0.0027	1.8333
S_{15}	H2TPP@SV1-CNT(6,5)*	0.0217	1.8402
S_{16}	H2TPP@SV1-CNT(6,5)*	0.0082	1.9124
S_{17}	H2TPP@SV1-CNT(6,5)*	0.0718	1.9260
S_{18}	H2TPP@SV1-CNT(6,5)*	0.0018	1.9273
S_{19}	H2TPP@SV1-CNT(6,5)*	0.0002	1.9339
S_{20}	H2TPP@SV1-CNT(6,5)*	0.2386	1.9756

S_{21}	H2TPP$^+$@SV1-CNT(6,5) $^-$	0.0475	1.9823
S_{22}	H2TPP*@SV1-CNT(6,5)	0.0011	1.9899
S_{23}	H2TPP@SV1-CNT(6,5)*	0.0001	2.0143
S_{24}	H2TPP@SV1-CNT(6,5)*	0.0003	2.0297
S_{25}	H2TPP@SV1-CNT(6,5)*	0.0226	2.0344
S_{26}	H2TPP@SV1-CNT(6,5)*	0.4203	2.0558
S_{27}	H2TPP@SV1-CNT(6,5)*	0.0031	2.0594
S_{28}	H2TPP@SV1-CNT(6,5)*	0.0155	2.0782
S_{29}	H2TPP@SV1-CNT(6,5)*	0.0001	2.0834
S_{30}	H2TPP@SV1-CNT(6,5)*	0.0042	2.0925
S_{31}	H2TPP$^+$@SV1-CNT(6,5) $^-$	0.0012	2.0951
S_{32}	H2TPP@SV1-CNT(6,5)*	0.0004	2.1094
S_{33}	H2TPP@SV1-CNT(6,5)*	0.0320	2.1190
S_{34}	H2TPP@SV1-CNT(6,5)*	0.0008	2.1220
S_{35}	H2TPP@SV1-CNT(6,5)*	0.0020	2.1452
S_{36}	H2TPP@SV1-CNT(6,5)*	0.3506	2.1553
S_{37}	H2TPP@SV1-CNT(6,5)*	0.0014	2.1814
S_{38}	H2TPP@SV1-CNT(6,5)*	0.3489	2.1926
S_{39}	H2TPP@SV1-CNT(6,5)*	0.7930	2.2295
S_{40}	H2TPP*@SV1-CNT(6,5)	0.3370	2.2336
S_{41}	H2TPP@SV1-CNT(6,5)*	0.0205	2.2407
S_{42}	H2TPP@SV1-CNT(6,5)*	0.0178	2.2413
S_{43}	H2TPP@SV1-CNT(6,5)*	0.0018	2.2639
S_{44}	H2TPP@SV1-CNT(6,5)*	0.0551	2.2993

S_{45}	H2TPP$^+$@SV1-CNT(6,5) -	0.0055	2.3245
S_{46}	H2TPP@SV1-CNT(6,5)*	0.0577	2.3593
S_{47}	H2TPP@SV1-CNT(6,5)*	0.1285	2.3647
S_{48}	H2TPP@SV1-CNT(6,5)*	0.7890	2.3678
S_{49}	H2TPP@SV1-CNT(6,5)*	0.5078	2.3737
S_{50}	H2TPP@SV1-CNT(6,5)*	0.8004	2.3751
S_{51}	H2TPP@SV1-CNT(6,5)*	0.1228	2.3836
S_{52}	H2TPP@SV1-CNT(6,5)*	0.0006	2.3942
S_{53}	H2TPP@SV1-CNT(6,5)*	0.1420	2.4024
S_{54}	H2TPP@SV1-CNT(6,5)*	5.3316	2.4091
S_{55}	H2TPP - @SV1-CNT(6,5)$^+$	0.0694	2.4161
S_{56}	H2TPP@SV1-CNT(6,5)*	0.4694	2.4309
S_{57}	H2TPP$^+$@SV1-CNT(6,5) -	0.1733	2.4332
S_{58}	H2TPP@SV1-CNT(6,5)*	0.2769	2.4446
S_{59}	H2TPP@SV1-CNT(6,5)*	0.0160	2.4465
S_{60}	H2TPP@SV1-CNT(6,5)*	0.0894	2.4546
S_{61}	H2TPP*@SV1-CNT(6,5)	0.0003	2.4587
S_{62}	H2TPP@SV1-CNT(6,5)*	0.0011	2.4752
S_{63}	H2TPP$^+$@SV1-CNT(6,5) -	0.0214	2.4820
S_{64}	H2TPP@SV1-CNT(6,5)*	0.0889	2.4924
S_{65}	H2TPP*@SV1-CNT(6,5)	0.0022	2.4960
S_{66}	H2TPP@SV1-CNT(6,5)*	0.0036	2.4972
S_{67}	H2TPP - @SV1-CNT(6,5)$^+$	0.0085	2.5016
S_{68}	H2TPP@SV1-CNT(6,5)*	1.2291	2.5084

S_{69}	H2TPP@SV1-CNT(6,5)*	0.0026	2.5209
S_{70}	H2TPP@SV1-CNT(6,5)*	0.0021	2.5244
S_{71}	H2TPP@SV1-CNT(6,5)*	0.0397	2.5506
S_{72}	H2TPP*@SV1-CNT(6,5)	0.0083	2.5526
S_{73}	H2TPP@SV1-CNT(6,5)*	0.0084	2.5590
S_{74}	H2TPP@SV1-CNT(6,5)*	0.0175	2.5615
S_{75}	H2TPP‐@SV1-CNT(6,5)$^+$	0.0028	2.5661
S_{76}	H2TPP@SV1-CNT(6,5)*	0.0214	2.5745
S_{77}	H2TPP@SV1-CNT(6,5)*	0.0299	2.5786
S_{78}	H2TPP@SV1-CNT(6,5)*	0.0017	2.5793
S_{79}	H2TPP@SV1-CNT(6,5)*	0.0513	2.5855
S_{80}	H2TPP@SV1-CNT(6,5)*	0.0024	2.5902
S_{81}	H2TPP@SV1-CNT(6,5)*	0.0019	2.5971
S_{82}	H2TPP@SV1-CNT(6,5)*	0.0272	2.6086
S_{83}	H2TPP‐@SV1-CNT(6,5)$^+$	0.0173	2.6100
S_{84}	H2TPP@SV1-CNT(6,5)*	0.0375	2.6144
S_{85}	H2TPP@SV1-CNT(6,5)*	0.0575	2.6164

Table S4. Excited state properties, oscillator strengths and excitation energies of H2TPP@SW1-CNT(6,5) at sTDA-xTB level.

state	properties	oscillator strengths	excitation energy (eV)
S_1	H2TPP@SW1-CNT(6,5)*	0.0005	1.1948
S_2	H2TPP@SW1-CNT(6,5)*	5.5616	1.2390
S_3	H2TPP@SW1-CNT(6,5)*	0.0003	1.2760
S_4	H2TPP@SW1-CNT(6,5)*	3.7269	1.2888
S_5	H2TPP@SW1-CNT(6,5)*	0.0002	1.4309
S_6	H2TPP@SW1-CNT(6,5)*	0.0723	1.4733
S_7	H2TPP@SW1-CNT(6,5)*	0.0001	1.5660
S_8	H2TPP$^+$@SW1-CNT(6,5) $^-$	0.0005	1.5734
S_9	H2TPP@SW1-CNT(6,5)*	0.0006	1.5958
S_{10}	H2TPP@SW1-CNT(6,5)*	0.0006	1.7095
S_{11}	H2TPP@SW1-CNT(6,5)*	0.0033	1.7438
S_{12}	H2TPP@SW1-CNT(6,5)*	0.0070	1.7460
S_{13}	H2TPP@SW1-CNT(6,5)*	0.0662	1.7672
S_{14}	H2TPP@SW1-CNT(6,5)*	0.0246	1.8301
S_{15}	H2TPP@SW1-CNT(6,5)*	0.0302	1.8319
S_{16}	H2TPP$^+$@SW1-CNT(6,5) $^-$	0.0034	1.8355
S_{17}	H2TPP@SW1-CNT(6,5)*	0.0034	1.8954
S_{18}	H2TPP@SW1-CNT(6,5)*	0.0167	1.9066
S_{19}	H2TPP@SW1-CNT(6,5)*	0.0061	1.9147
S_{20}	H2TPP@SW1-CNT(6,5)*	0.0598	1.9232

S_{21}	H2TPP@SW1-CNT(6,5)*	0.0017	1.9353
S_{22}	H2TPP@SW1-CNT(6,5)*	0.0109	1.9400
S_{23}	H2TPP@SW1-CNT(6,5)*	0.2860	1.9521
S_{24}	H2TPP*@SW1-CNT(6,5)	0.0070	1.9893
S_{25}	H2TPP@SW1-CNT(6,5)*	0.0089	2.0045
S_{26}	H2TPP@SW1-CNT(6,5)*	0.0126	2.0177
S_{27}	H2TPP@SW1-CNT(6,5)*	0.0064	2.0198
S_{28}	H2TPP@SW1-CNT(6,5)*	0.0963	2.0472
S_{29}	H2TPP@SW1-CNT(6,5)*	0.0016	2.0529
S_{30}	H2TPP@SW1-CNT(6,5)*	0.0004	2.0668
S_{31}	H2TPP@SW1-CNT(6,5)*	0.0264	2.0821
S_{32}	H2TPP@SW1-CNT(6,5)*	0.0990	2.1008
S_{33}	H2TPP@SW1-CNT(6,5)*	0.0029	2.1045
S_{34}	H2TPP$^+$@SW1-CNT(6,5)$^-$	0.0019	2.1095
S_{35}	H2TPP$^+$@SW1-CNT(6,5)$^-$	0.0010	2.1288
S_{36}	H2TPP@SW1-CNT(6,5)*	0.0023	2.1473
S_{37}	H2TPP@SW1-CNT(6,5)*	0.0038	2.1544
S_{38}	H2TPP@SW1-CNT(6,5)*	0.1977	2.1739
S_{39}	H2TPP@SW1-CNT(6,5)*	0.0191	2.1813
S_{40}	H2TPP@SW1-CNT(6,5)*	0.0027	2.1964
S_{41}	H2TPP*@SW1-CNT(6,5)	0.0506	2.2134
S_{42}	H2TPP@SW1-CNT(6,5)*	0.0831	2.2197
S_{43}	H2TPP@SW1-CNT(6,5)*	0.0005	2.2306
S_{44}	H2TPP@SW1-CNT(6,5)*	0.3567	2.2550

S_{45}	H2TPP@SW1-CNT(6,5)*	1.8011	2.2674
S_{46}	H2TPP@SW1-CNT(6,5)*	0.0717	2.2772
S_{47}	H2TPP@SW1-CNT(6,5)*	0.0011	2.3002
S_{48}	H2TPP@SW1-CNT(6,5)*	0.0156	2.3094
S_{49}	H2TPP@SW1-CNT(6,5)*	1.9346	2.3259
S_{50}	H2TPP$^+$@SW1-CNT(6,5)$^-$	0.0080	2.3357
S_{51}	H2TPP@SW1-CNT(6,5)*	0.3630	2.3363
S_{52}	H2TPP@SW1-CNT(6,5)*	1.0023	2.3419
S_{53}	H2TPP@SW1-CNT(6,5)*	0.9960	2.3488
S_{54}	H2TPP@SW1-CNT(6,5)*	0.0766	2.3604
S_{55}	H2TPP@SW1-CNT(6,5)*	0.0957	2.3771
S_{56}	H2TPP@SW1-CNT(6,5)*	0.2510	2.3892
S_{57}	H2TPP@SW1-CNT(6,5)*	1.7758	2.3906
S_{58}	H2TPP@SW1-CNT(6,5)*	0.0306	2.4000
S_{59}	H2TPP@SW1-CNT(6,5)*	0.5045	2.4125
S_{60}	H2TPP$^-$@SW1-CNT(6,5)$^+$	0.0473	2.4163
S_{61}	H2TPP@SW1-CNT(6,5)*	0.1015	2.4269
S_{62}	H2TPP@SW1-CNT(6,5)*	0.4373	2.4382
S_{63}	H2TPP$^+$@SW1-CNT(6,5)$^-$	0.0763	2.4386
S_{64}	H2TPP@SW1-CNT(6,5)*	1.3984	2.4431
S_{65}	H2TPP@SW1-CNT(6,5)*	0.1380	2.4558
S_{66}	H2TPP*@SW1-CNT(6,5)	0.0005	2.4605
S_{67}	H2TPP@SW1-CNT(6,5)*	0.0032	2.4777
S_{68}	H2TPP@SW1-CNT(6,5)*	0.2123	2.4939

S_{69}	H2TPP@SW1-CNT(6,5)*	0.0237	2.4945
S_{70}	H2TPP*@SW1-CNT(6,5)	0.0038	2.5038
S_{71}	H2TPP@SW1-CNT(6,5)*	0.1127	2.5071
S_{72}	H2TPP@SW1-CNT(6,5)*	0.0121	2.5229
S_{73}	H2TPP@SW1-CNT(6,5)*	0.2133	2.5257
S_{74}	H2TPP$^+$@SW1-CNT(6,5)$^-$	0.0250	2.5390
S_{75}	H2TPP@SW1-CNT(6,5)*	0.0153	2.5498
S_{76}	H2TPP@SW1-CNT(6,5)*	0.1499	2.5509
S_{77}	H2TPP$^+$@SW1-CNT(6,5)$^-$	0.0028	2.5573
S_{78}	H2TPP@SW1-CNT(6,5)*	0.2583	2.5594
S_{79}	H2TPP$^-$@SW1-CNT(6,5)$^+$	0.0376	2.5639
S_{80}	H2TPP$^+$@SW1-CNT(6,5)$^-$	0.0074	2.5683
S_{81}	H2TPP@SW1-CNT(6,5)*	0.0020	2.5722
S_{82}	H2TPP$^+$@SW1-CNT(6,5)$^-$	0.0052	2.5792
S_{83}	H2TPP@SW1-CNT(6,5)*	0.0419	2.5840
S_{84}	H2TPP@SW1-CNT(6,5)*	0.0051	2.5856
S_{85}	H2TPP@SW1-CNT(6,5)*	0.0019	2.5892

Table S5. Excited state properties, oscillator strengths and excitation energies of H2TPP@SW2-CNT(6,5) at sTDA-xTB level.

state	properties	oscillator strengths	excitation energy (eV)
S_1	H2TPP@SW2-CNT(6,5)*	0.0001	1.2040
S_2	H2TPP@SW2-CNT(6,5)*	3.4034	1.2534
S_3	H2TPP@SW2-CNT(6,5)*	4.6081	1.2653
S_4	H2TPP@SW2-CNT(6,5)*	1.3424	1.2727
S_5	H2TPP@SW2-CNT(6,5)*	0.0019	1.4544
S_6	H2TPP@SW2-CNT(6,5)*	0.0111	1.5067
S_7	H2TPP$^+$@SW2-CNT(6,5)$^-$	0.0011	1.5230
S_8	H2TPP@SW2-CNT(6,5)*	0.0090	1.5457
S_9	H2TPP@SW2-CNT(6,5)*	0.0011	1.5550
S_{10}	H2TPP@SW2-CNT(6,5)*	0.0027	1.6561
S_{11}	H2TPP@SW2-CNT(6,5)*	0.0090	1.6707
S_{12}	H2TPP@SW2-CNT(6,5)*	0.0623	1.7189
S_{13}	H2TPP@SW2-CNT(6,5)*	0.0045	1.7238
S_{14}	H2TPP@SW2-CNT(6,5)*	0.0002	1.7880
S_{15}	H2TPP@SW2-CNT(6,5)*	0.0042	1.8252
S_{16}	H2TPP@SW2-CNT(6,5)*	0.0024	1.8267
S_{17}	H2TPP$^+$@SW2-CNT(6,5)$^-$	0.0686	1.8853
S_{18}	H2TPP@SW2-CNT(6,5)*	0.1233	1.9032
S_{19}	H2TPP@SW2-CNT(6,5)*	0.0229	1.9060
S_{20}	H2TPP@SW2-CNT(6,5)*	0.0264	1.9206

S_{21}	H2TPP@SW2-CNT(6,5)*	0.0001	1.9305
S_{22}	H2TPP@SW2-CNT(6,5)*	0.1728	1.9718
S_{23}	H2TPP*@SW2-CNT(6,5)	0.0137	1.9904
S_{24}	H2TPP@SW2-CNT(6,5)*	0.0040	2.0001
S_{25}	H2TPP@SW2-CNT(6,5)*	0.3621	2.0102
S_{26}	H2TPP@SW2-CNT(6,5)*	0.0073	2.0259
S_{27}	H2TPP@SW2-CNT(6,5)*	0.0118	2.0316
S_{28}	H2TPP@SW2-CNT(6,5)*	0.0009	2.0458
S_{29}	H2TPP@SW2-CNT(6,5)*	0.0016	2.0538
S_{30}	H2TPP$^+$@SW2-CNT(6,5) $^-$	0.0002	2.0554
S_{31}	H2TPP@SW2-CNT(6,5)*	0.0508	2.0685
S_{32}	H2TPP@SW2-CNT(6,5)*	0.0036	2.0689
S_{33}	H2TPP$^+$@SW2-CNT(6,5) $^-$	0.0009	2.0799
S_{34}	H2TPP@SW2-CNT(6,5)*	0.0154	2.0962
S_{35}	H2TPP@SW2-CNT(6,5)*	0.0183	2.1091
S_{36}	H2TPP@SW2-CNT(6,5)*	0.0004	2.1176
S_{37}	H2TPP@SW2-CNT(6,5)*	0.0012	2.1187
S_{38}	H2TPP@SW2-CNT(6,5)*	0.1205	2.1444
S_{39}	H2TPP@SW2-CNT(6,5)*	0.0169	2.1517
S_{40}	H2TPP@SW2-CNT(6,5)*	0.5130	2.1754
S_{41}	H2TPP@SW2-CNT(6,5)*	0.4531	2.1919
S_{42}	H2TPP@SW2-CNT(6,5)*	0.0160	2.1970
S_{43}	H2TPP@SW2-CNT(6,5)*	0.0039	2.2068
S_{44}	H2TPP*@SW2-CNT(6,5)	0.0893	2.2263

S_{45}	H2TPP@SW2-CNT(6,5)*	0.0039	2.2359
S_{46}	H2TPP@SW2-CNT(6,5)*	0.3570	2.2575
S_{47}	H2TPP@SW2-CNT(6,5)*	0.2138	2.2901
S_{48}	H2TPP@SW2-CNT(6,5)*	0.7220	2.3072
S_{49}	H2TPP$^+$@SW2-CNT(6,5)$^-$	0.2108	2.3313
S_{50}	H2TPP@SW2-CNT(6,5)*	0.0048	2.3338
S_{51}	H2TPP@SW2-CNT(6,5)*	2.4888	2.3371
S_{52}	H2TPP@SW2-CNT(6,5)*	0.0604	2.3475
S_{53}	H2TPP@SW2-CNT(6,5)*	0.4032	2.3544
S_{54}	H2TPP@SW2-CNT(6,5)*	0.0164	2.3617
S_{55}	H2TPP$^+$@SW2-CNT(6,5)$^-$	0.0232	2.3683
S_{56}	H2TPP$^+$@SW2-CNT(6,5)$^-$	0.1041	2.3708
S_{57}	H2TPP@SW2-CNT(6,5)*	0.0652	2.3783
S_{58}	H2TPP@SW2-CNT(6,5)*	0.6093	2.3919
S_{59}	H2TPP$^-$@SW2-CNT(6,5)$^+$	0.0429	2.3950
S_{60}	H2TPP@SW2-CNT(6,5)*	0.2048	2.3987
S_{61}	H2TPP@SW2-CNT(6,5)*	0.0255	2.4179
S_{62}	H2TPP@SW2-CNT(6,5)*	0.2570	2.4236
S_{63}	H2TPP@SW2-CNT(6,5)*	0.3374	2.4346
S_{64}	H2TPP@SW2-CNT(6,5)*	0.0596	2.4395
S_{65}	H2TPP*@SW2-CNT(6,5)	0.0016	2.4563
S_{66}	H2TPP$^-$@SW2-CNT(6,5)$^+$	0.0023	2.4706
S_{67}	H2TPP@SW2-CNT(6,5)*	1.2062	2.4780
S_{68}	H2TPP$^+$@SW2-CNT(6,5)$^-$	0.1703	2.4867

S_{69}	H2TPP@SW2-CNT(6,5)*	0.1711	2.4891
S_{70}	H2TPP@SW2-CNT(6,5)*	0.3318	2.4910
S_{71}	H2TPP*@SW2-CNT(6,5)	0.1337	2.4987
S_{72}	H2TPP⁺@SW2-CNT(6,5)⁻	0.1523	2.5036
S_{73}	H2TPP@SW2-CNT(6,5)*	0.1583	2.5074
S_{74}	H2TPP@SW2-CNT(6,5)*	0.4257	2.5086
S_{75}	H2TPP⁺@SW2-CNT(6,5)⁻	0.0003	2.5315
S_{76}	H2TPP@SW2-CNT(6,5)*	0.0148	2.5386
S_{77}	H2TPP@SW2-CNT(6,5)*	0.0311	2.5399
S_{78}	H2TPP⁻@SW2-CNT(6,5)⁺	0.0168	2.5429
S_{79}	H2TPP@SW2-CNT(6,5)*	0.1279	2.5500
S_{80}	H2TPP⁺@SW2-CNT(6,5)⁻	0.0202	2.5561
S_{81}	H2TPP@SW2-CNT(6,5)*	0.0064	2.5602
S_{82}	H2TPP*@SW2-CNT(6,5)	0.0112	2.5614
S_{83}	H2TPP@SW2-CNT(6,5)*	0.0724	2.5684
S_{84}	H2TPP@SW2-CNT(6,5)*	0.0022	2.5714
S_{85}	H2TPP@SW2-CNT(6,5)*	0.0637	2.5727

4. Cartesian Coordinates

4.1 Cartesian Coordinates of H2TPP@SV-CNT(6,5)

C	0.118722419	13.974568019	9.945488406
C	1.316392831	13.229646168	10.140547908
C	1.251494870	11.814691178	10.085863421
C	2.449907664	11.087219718	9.833969278
C	2.579903378	13.872459330	9.984935523
C	3.776961683	13.121067294	10.157188373
C	5.039620326	13.769007057	10.025328850
C	6.236503945	13.013401825	10.179004334
C	1.118716509	9.526319160	8.492142984
C	2.384197563	9.939028764	9.005910198
C	3.582325921	9.476425783	8.389299347
C	3.713657666	11.708731783	10.059059824
C	4.912907599	10.990045110	9.785543105
C	6.175927346	11.605122694	10.032924794
C	7.377645399	10.899963297	9.732926292
C	7.498197540	13.667016107	10.072953438
C	8.695556712	12.908167896	10.205884253
C	9.955594657	13.567780444	10.125888964
C	11.154274033	12.807059643	10.239081939
C	0.893679491	9.482793043	4.440221229
C	1.047736299	8.986024169	7.183933823
C	2.241770935	8.919829347	6.411091555
C	3.509701839	8.982859506	7.062449598
C	4.702735862	8.946066712	6.286335527
C	4.848156678	9.871974735	8.916855061
C	6.047242674	9.437214472	8.281322625
C	7.313683487	9.817697465	8.819809290
C	8.513208201	9.414570524	8.164591453
C	8.640279068	11.506400465	10.005481312
C	9.846149330	10.818419790	9.675784719
C	11.109097241	11.413882524	9.977984983
C	12.321371020	10.752102276	9.609750748
C	12.409242212	13.475995742	10.187780518
C	13.609418846	12.713293362	10.283076773
C	14.852603129	13.397353236	10.299299841
C	16.069346766	12.632615739	10.368662282
C	17.362980493	14.495121889	9.776699908
C	19.723515284	13.940142661	9.555787115

C	0.811304995	10.445717493	3.403772349
C	1.996153232	11.124501472	3.007584598
C	2.162456972	9.194434666	5.022854988
C	3.349994937	9.568209658	4.334629896
C	4.619722642	9.265034742	4.907587732
C	5.804961692	9.659680892	4.227615639
C	5.971900801	8.991729184	6.937578071
C	7.162830385	8.985176953	6.157867909
C	8.433463701	9.016956981	6.806202716
C	9.621117090	9.035477793	6.022558668
C	9.780628151	9.778392729	8.714605954
C	10.979826609	9.410723793	8.038574280
C	12.248016242	9.765671795	8.593272160
C	13.442919786	9.442751238	7.889080378
C	13.585032885	11.340703142	9.935952573
C	14.811546623	10.749380271	9.485358153
C	16.076558458	11.346102054	9.794482253
C	17.334381805	10.890210207	9.239973877
C	17.243110086	13.344888115	10.530240850
C	19.587375851	12.565575612	9.935274527
C	20.910966511	11.987996140	10.179582010
C	22.231305721	13.991756322	9.798529006
C	24.706412012	13.934449289	9.905689139
C	0.644293643	13.147119420	2.701405259
C	1.912033368	12.499061727	2.672807967
C	3.096843304	13.283698937	2.709657023
C	3.264809701	10.561457800	3.326943311
C	4.447970871	11.251534573	2.947042456
C	5.717041956	10.678412869	3.246113229
C	6.899443044	11.376517551	2.878890395
C	7.075962659	9.341062130	4.788227709
C	8.257858826	9.750660621	4.112107083
C	9.530151390	9.418715640	4.660609330
C	10.708625216	9.838971284	3.985678028
C	10.892796643	9.053722071	6.667887782
C	12.073539393	9.088155807	5.877020864
C	13.346711947	9.101406044	6.516213847
C	14.520405342	9.133102386	5.718597095
C	14.712231835	9.812256661	8.427043603
C	15.898014202	9.506816049	7.716681288
C	17.178349064	9.862568312	8.246937771
C	18.295422622	9.340554837	7.541056535
C	18.689461177	11.365594886	9.509391016
C	19.647432278	10.343943168	9.227661812

C	20.933557536	10.659802802	9.719751459
C	22.096097778	10.019671290	9.263813624
C	22.166966036	12.645847102	10.225525925
C	23.383040288	11.879890279	10.180612710
C	24.646207911	12.550734840	10.211688827
C	25.852074854	11.791883303	10.128960959
C	27.175465462	13.850073791	9.958556456
C	29.642047825	13.754771422	10.001866199
C	0.404865216	16.258343338	5.299369428
C	0.562480650	14.492830285	3.138923557
C	1.750356098	15.138975711	3.580443972
C	3.017094953	14.613751235	3.192951483
C	4.207165755	15.240170715	3.656483097
C	4.363749898	12.635762694	2.655335021
C	5.550243481	13.416851713	2.714103304
C	6.816368214	12.769703602	2.631434280
C	8.004576967	13.546231023	2.716891539
C	8.168481545	10.793141784	3.156050655
C	9.351129671	11.500222732	2.804490561
C	10.619942631	10.906102738	3.056547724
C	11.803320062	11.622364486	2.723993420
C	11.980585661	9.492218360	4.521344552
C	13.157601077	9.922829390	3.847955389
C	14.428769442	9.553405201	4.366254782
C	15.605988376	9.995827618	3.700094998
C	15.792099052	9.130968962	6.352196709
C	16.953426010	9.129133529	5.533924597
C	18.213646642	9.035583824	6.164801711
C	19.406474525	9.063931550	5.396058087
C	19.553479576	9.444100323	8.153308842
C	20.739365651	9.048722938	7.465829530
C	22.008478084	9.221728415	8.088470047
C	23.197226208	8.978373306	7.351857466
C	23.350646673	10.559796157	9.666753878
C	24.541159219	9.970444128	9.158406813
C	25.799822315	10.489158656	9.570861112
C	26.993859364	9.909875067	9.058009833
C	27.114785399	12.454198400	10.195588287
C	28.316982783	11.694974952	10.086064702
C	29.580043650	12.350195248	10.181720008
C	30.779197185	11.592791915	10.045464077
C	30.906658413	14.364170468	9.744437863
C	32.106327413	13.653431528	10.038298717
C	33.370913142	14.270406024	9.801618268

C	34.569371470	13.547791337	10.067566672
C	0.328984792	16.417150818	6.706120257
C	1.523296824	16.283365041	7.469140315
C	1.672266890	16.015384071	4.691931063
C	2.864736279	16.302942639	5.413811501
C	4.131652044	16.076889860	4.798260167
C	5.325495915	16.335767900	5.528975841
C	5.472758130	14.727574553	3.247728548
C	6.664931222	15.332712714	3.733447111
C	7.929322521	14.834157581	3.303552317
C	9.123279327	15.416337151	3.812889482
C	9.270243561	12.901387610	2.607035850
C	10.460185465	13.672116229	2.720814563
C	11.724935995	13.030328792	2.583338348
C	12.917657299	13.792542061	2.730579999
C	13.072467309	11.017196533	2.950814795
C	14.259362230	11.742526665	2.646865087
C	15.527937568	11.127671162	2.853187863
C	16.723246823	11.860646710	2.598029426
C	16.874243161	9.596663430	4.203367762
C	18.069761548	10.062960541	3.589733430
C	19.332230686	9.639858203	4.100927031
C	20.528071343	10.151961246	3.527043714
C	20.665678447	8.931939093	6.051985229
C	21.860278807	9.065523076	5.291469752
C	23.123930074	8.921623687	5.935663058
C	24.317808231	9.096837552	5.181636993
C	24.464261597	9.184901997	7.979394674
C	25.655173889	8.959368452	7.236172902
C	26.921364372	9.149466141	7.864398604
C	28.114441357	8.935893673	7.118445991
C	28.256350349	10.411942853	9.487156500
C	29.450739016	9.842117288	8.963384210
C	30.714661097	10.329614548	9.406254076
C	31.910035394	9.774005745	8.868211061
C	32.042572393	12.243255301	10.165959077
C	33.240403155	11.489393328	10.005363112
C	34.504292730	12.134239367	10.147326985
C	35.701711769	11.385133980	9.965299047
C	35.833542632	14.172475606	9.851795116
C	37.031389680	13.441289075	10.093610982
C	38.295349866	14.073466232	9.899692122
C	39.492997288	13.335596443	10.119559339
C	0.186923616	15.184760664	9.210197837

C	1.451552573	15.637020215	8.728957276
C	2.647792570	15.104880983	9.287978379
C	2.789699837	16.415941883	6.825024138
C	3.984579676	16.255532293	7.582348949
C	5.251498266	16.404156015	6.943050284
C	6.445408985	16.217594176	7.695696517
C	6.591519263	16.125381281	4.906331710
C	7.786013143	16.353287485	5.645596920
C	9.051392942	16.161853171	5.016260876
C	10.245533542	16.361822847	5.763600342
C	10.386773617	14.934108701	3.362341026
C	11.581477134	15.490985693	3.896672586
C	12.844460713	15.025441384	3.426299789
C	14.038950575	15.560351209	3.981651207
C	14.182834388	13.155887635	2.567735082
C	15.377170402	13.907781635	2.751028884
C	16.645023066	13.276132552	2.572006670
C	17.837830293	14.023215651	2.783086103
C	17.991962125	11.236960969	2.796164359
C	19.185234380	11.981477926	2.582269897
C	20.452298419	11.351949544	2.775103833
C	21.645367514	12.102866237	2.583367279
C	21.789053793	9.711501939	4.028163149
C	22.982769032	10.243599501	3.469106169
C	24.246633815	9.784848480	3.944519994
C	25.441255924	10.333305231	3.401204832
C	25.582300304	8.932545296	5.819617322
C	26.775675831	9.127311953	5.071058251
C	28.041149890	8.944416892	5.703157571
C	29.234874966	9.162058428	4.960398808
C	29.379945333	9.109317851	7.751920899
C	30.573499714	8.915027690	7.001216912
C	31.839693679	9.072773044	7.638651380
C	33.034498069	8.897561337	6.884689689
C	33.174461327	10.246522374	9.327211570
C	34.370402249	9.703936042	8.776951962
C	35.635015405	10.162122718	9.251884223
C	36.832143285	9.637561469	8.686939600
C	36.965455912	12.025876951	10.129456457
C	38.163488148	11.283362744	9.926642740
C	39.427137655	11.919553195	10.110686007
C	40.625603543	11.184909077	9.882573261
C	3.912396155	15.571575692	8.821911295
C	5.107069583	15.022208627	9.366978053

C	6.371907022	15.501389737	8.916575381
C	7.565131495	14.938262017	9.449860427
C	7.712273461	16.379941794	7.060725431
C	8.904867515	16.173782202	7.809486761
C	10.171926833	16.349964662	7.179272962
C	11.363024084	16.124541066	7.924613662
C	11.510046241	16.188590057	5.128616811
C	12.703770260	16.360613920	5.883365571
C	13.966592243	16.212418141	5.239359394
C	15.159489390	16.359098311	5.998313001
C	15.301685791	15.114119020	3.491961675
C	16.495401876	15.634437671	4.063556319
C	17.759382103	15.209615352	3.557455944
C	18.952141316	15.709650089	4.148254730
C	19.106367771	13.397704511	2.594193197
C	20.299145224	14.138312962	2.833567463
C	21.568165636	13.517815365	2.632866172
C	22.759618635	14.247936256	2.903514745
C	22.910060551	11.467059932	2.755462728
C	24.103973157	12.222974003	2.588201470
C	25.368942297	11.582235680	2.734630820
C	26.560897617	12.345973953	2.597155447
C	26.704664242	9.856456552	3.857297359
C	27.899090448	10.426847424	3.335608686
C	29.163076424	9.934062756	3.773687078
C	30.356908660	10.525188789	3.274913633
C	30.500542491	8.961433898	5.586461468
C	31.695311967	9.203981825	4.851519230
C	32.961563547	8.986078594	5.471651673
C	34.156109763	9.257306879	4.746339996
C	34.300417906	9.037821662	7.527500277
C	35.496262654	8.888684805	6.769098238
C	36.761850281	9.011690623	7.416784821
C	37.957517291	8.890979017	6.653484582
C	38.096616966	10.082977742	9.175390950
C	39.294113714	9.579449538	8.592105676
C	40.558997878	10.010101193	9.092390380
C	8.829556961	15.429968450	9.013543919
C	10.021584340	14.855187151	9.536838662
C	11.285654031	15.359891309	9.115698876
C	12.475651566	14.778969845	9.636109070
C	12.630725600	16.307766892	7.298541873
C	13.821155469	16.061205072	8.039465923
C	15.085193780	16.250976450	7.410855225

C	16.274858824	15.954186410	8.132537146
C	16.420604197	16.238386257	5.344910950
C	17.613726586	16.344289115	6.108576895
C	18.874232005	16.248296721	5.455628824
C	20.063553178	16.293153556	6.233107306
C	20.220601709	15.299203952	3.641682507
C	21.411150822	15.768112818	4.266823290
C	22.679961492	15.374114343	3.759868108
C	23.860474038	15.816044696	4.421346848
C	24.027629556	13.634065854	2.689552960
C	25.215309474	14.356011857	2.996164477
C	26.482840960	13.752116624	2.758138481
C	27.668149360	14.463939047	3.092038389
C	27.826003262	11.701419735	2.720296527
C	29.016627459	12.472345354	2.615212686
C	30.281664143	11.824127006	2.712452412
C	31.470507289	12.600606435	2.636730767
C	31.622144516	10.017723960	3.693189661
C	32.814506249	10.631265662	3.217757500
C	34.080597523	10.111906954	3.617677278
C	35.270953288	10.746660796	3.165559348
C	35.422970579	9.022966460	5.359616336
C	36.616308984	9.323533882	4.644247013
C	37.883139067	9.073163832	5.249731843
C	39.074363154	9.400972928	4.543523983
C	39.223740729	8.995564674	7.302550864
C	40.418515443	8.902100461	6.533909640
C	13.741519256	15.291287578	9.228784390
C	14.926552071	14.702471840	9.754273522
C	16.192176797	15.169321994	9.305014134
C	17.537666659	16.145535538	7.510568712
C	18.716634252	15.735123945	8.187296703
C	19.979922104	15.970535816	7.601980025
C	21.133118938	15.561066877	8.319343537
C	21.330859017	16.241215658	5.598510708
C	22.499500823	16.262494754	6.406023416
C	23.771613797	16.245990866	5.769261569
C	24.949928997	16.272743971	6.564337276
C	25.131265280	15.447409036	3.896763409
C	26.311045867	15.874942390	4.565427383
C	27.581862711	15.526007633	4.026435424
C	28.762986398	15.940690466	4.700665091
C	28.936271630	13.871270985	2.829155004
C	30.120269011	14.573699396	3.183480019

C	31.388536776	13.990871487	2.899596784
C	32.572468580	14.684095101	3.271441730
C	32.736582557	11.951089832	2.706398752
C	33.923512297	12.732060572	2.656491677
C	35.190879969	12.083572490	2.701530161
C	36.376074741	12.868825273	2.674669666
C	36.538277083	10.217271254	3.546581582
C	37.726168681	10.870124101	3.114964283
C	38.994294715	10.329890096	3.476045942
C	40.180596932	10.997067909	3.063079479
C	40.342079494	9.131591764	5.137519054
C	18.624505296	14.800800634	9.237101605
C	21.018307703	14.556265227	9.321065400
C	22.404233205	15.912057569	7.779174115
C	23.589281670	15.562187367	8.478308701
C	24.859855311	15.916769210	7.933879285
C	26.048701353	15.550993288	8.623702563
C	26.220966522	16.276424420	5.922300556
C	27.403115380	16.291688618	6.712428422
C	28.674002851	16.311027438	6.066256745
C	29.860407482	16.308499185	6.850716155
C	30.033288462	15.608770413	4.148038106
C	31.216474665	16.007296121	4.828153173
C	32.486392453	15.692439385	4.263747833
C	33.670943062	16.075544308	4.950493542
C	33.840505708	14.112500113	2.966274252
C	35.024187823	14.797172224	3.354516233
C	36.292734329	14.239221689	3.026635566
C	37.477398427	14.914073968	3.430652901
C	37.644344802	12.221293727	2.694487871
C	38.829015898	13.008124196	2.688731983
C	40.097516348	12.360719173	2.685603774
C	23.500534470	14.580734672	9.495961285
C	25.971532521	14.527502193	9.603774318
C	27.317844133	15.907227138	8.074597030
C	28.512404874	15.512830711	8.742022663
C	29.780203673	15.883238194	8.200821080
C	30.975828743	15.461024936	8.849461170
C	31.130319609	16.342934752	6.202545714
C	32.319621421	16.317500648	6.983641816
C	33.588329266	16.372163637	6.334117677
C	34.779858481	16.320607878	7.110844448
C	34.939806612	15.777276943	4.374620968
C	36.126780087	16.140274362	5.069016091

C	37.395026714	15.861124678	4.481918684
C	38.583895515	16.201841833	5.185298065
C	38.746039234	14.367071890	3.083253954
C	39.932126245	15.028331785	3.506608249
C	28.441058697	14.450412501	9.677888490
C	32.243064179	15.847980901	8.318946417
C	33.439478021	15.401172012	8.949396381
C	34.705431068	15.805027025	8.429138519
C	35.901704343	15.332129043	9.039900005
C	36.047599979	16.393369053	6.461237400
C	37.240206426	16.313774304	7.233994365
C	38.506941657	16.407684288	6.585427864
C	39.700665136	16.301791981	7.353261593
C	39.851766590	15.942269316	4.587154746
C	37.167240720	15.752612491	8.533267855
C	38.363610837	15.259794735	9.127104477
C	39.628494669	15.697850852	8.633664058
N	21.152728664	13.045933905	13.266505194
N	16.947644096	13.019014522	13.363879017
N	19.008496381	15.065398149	13.164881302
N	19.092366346	10.994542363	13.237282626
C	21.907833975	14.186537287	13.247741490
C	21.954257783	11.938564753	13.318430422
C	16.148542911	14.129303903	13.308695189
C	16.190489024	11.879140432	13.362277419
C	21.431122668	15.498312894	13.204904659
C	21.521662038	10.608588931	13.313397461
C	16.580849302	15.451349757	13.162432460
C	16.666258503	10.566054821	13.290602645
C	20.090010237	15.884892716	13.152972586
C	20.186517206	10.192056892	13.277982291
C	17.915551393	15.866030212	13.105008503
C	18.009921043	10.177318174	13.256037752
C	23.270108713	13.774868845	13.291972616
C	23.298715357	12.409647683	13.326127315
C	14.803638105	13.662100608	13.319863815
C	14.828980879	12.296786935	13.352862552
C	22.461605660	16.573467806	13.239552434
C	22.582268044	9.569830834	13.343805404
C	15.517278210	16.478841186	13.031253812
C	15.633112918	9.501543186	13.225664011
C	19.666821157	17.272059098	13.070437551
C	19.781639507	8.798218429	13.339111791
C	18.318736370	17.260684795	13.038575151

C	18.433500605	8.788431509	13.316782123
C	22.622358355	17.350049504	14.386849215
C	23.481701248	9.500101720	14.408914143
C	23.281270676	16.811655236	12.137976468
C	22.703168333	8.653891315	12.297692112
C	14.583225620	16.675818634	14.049171360
C	15.565058221	8.660162534	12.113641819
C	15.421827746	17.246091742	11.868887536
C	14.705669837	9.338828297	14.255659336
C	23.590787392	18.342181312	14.430013750
C	24.483806311	8.541179901	14.420221580
C	24.243674138	17.809576878	12.180913054
C	23.714231671	7.705360066	12.305127926
C	13.571196522	17.612617237	13.901859577
C	14.583032261	7.684758444	12.030491506
C	14.402584487	18.174222367	11.720197194
C	13.727728445	8.359122624	14.171179432
C	24.402387874	18.575168619	13.327849044
C	24.608004308	7.646739185	13.365716243
C	13.473535194	18.358801131	12.735210595
C	13.661170293	7.532783167	13.057582500
H	20.138986630	13.020827841	13.237408203
H	17.959490989	13.039080826	13.292699656
H	24.115403698	14.443668194	13.287563845
H	24.173580869	11.780488077	13.339322011
H	13.929337277	14.290268076	13.272496816
H	13.978004713	11.635927837	13.334156273
H	20.329530721	18.121757546	13.041451887
H	20.451196715	7.957075982	13.415206812
H	17.646173525	18.101955497	12.997890473
H	17.773724848	7.937920715	13.372287135
H	21.992688357	17.165174956	15.250063512
H	23.381141293	10.188670097	15.240653355
H	23.154651278	16.218112906	11.240277491
H	22.011524441	8.701207654	11.464490732
H	14.663455730	16.102966973	14.966397010
H	16.276653514	8.785680502	11.304961638
H	16.138917828	17.096212116	11.069472834
H	14.764529541	9.972686146	15.133595232
H	23.713379369	18.935459428	15.329531656
H	25.171385846	8.492063765	15.257452398
H	24.871046335	17.988818532	11.314479085
H	23.804802181	7.010104407	11.477774136
H	12.854599587	17.759852029	14.702372064

H	14.536316353	7.041052796	11.158967796
H	14.332012810	18.753748115	10.806215040
H	13.014701343	8.240300321	14.979635409
H	25.156926328	19.352965315	13.363347402
H	25.396802663	6.902989027	13.372963822
H	12.677039498	19.085118774	12.619198893
H	12.893826545	6.769652785	12.992334828

4.2 Cartesian Coordinates of H2TPP@SV1-CNT(6,5)

C	0.144082945	13.951073750	10.019836250
C	1.337474931	13.191074500	10.214030250
C	1.256157474	11.777346250	10.153311000
C	2.449186564	11.037373750	9.891614500
C	2.614089880	13.813798750	10.060976250
C	3.807804123	13.047926500	10.230297750
C	5.085248083	13.675460500	10.098996750
C	6.279838478	12.905175500	10.245136750
C	1.093062134	9.508357500	8.541772250
C	2.368696493	9.899863250	9.049650250
C	3.561145681	9.434433500	8.416904000
C	3.725546714	11.637454500	10.118058500
C	4.918767615	10.909106000	9.827226750
C	6.194895723	11.500181750	10.079171750
C	7.387478610	10.786063750	9.756103000
C	7.559179410	13.535430250	10.134661750
C	8.755744395	12.761276750	10.255922250
C	10.039598968	13.391862000	10.163624750
C	11.238791594	12.613758500	10.262545250
C	0.856082803	9.478008250	4.486029250
C	1.014624678	8.979016250	7.229401500
C	2.205445510	8.906288750	6.447019000
C	3.479981835	8.956272000	7.084806750
C	4.667783685	8.916609000	6.295388000
C	4.836871069	9.809482000	8.936536750
C	6.027877209	9.375433750	8.280730750
C	7.302968241	9.729654000	8.814859000
C	8.491242708	9.326459750	8.137309500
C	8.664119567	11.364909000	10.034522000
C	9.854816860	10.665086000	9.678325000
C	11.132090954	11.227740750	9.985681500
C	12.318081577	10.543911750	9.592235250
C	12.532051379	13.242678750	10.191742750
C	13.738409667	12.457671750	10.284594000
C	15.057100182	13.081197750	10.220387000
C	16.281101371	12.304705500	10.289704000
C	17.538609646	14.028501000	9.272132000
C	19.794009577	14.351302500	9.739701750
C	0.781212940	10.435517500	3.444409750
C	1.967570522	11.105573250	3.035583000
C	2.125801518	9.183412000	5.059427500

C	3.311675104	9.546380000	4.358175000
C	4.584160846	9.236224500	4.916973500
C	5.767614857	9.619959250	4.221628250
C	5.943507447	8.949869000	6.931111500
C	7.128259837	8.939217250	6.137648750
C	8.403656871	8.953411750	6.772763250
C	9.585421975	8.969050000	5.976322250
C	9.766321142	9.657534500	8.684916750
C	10.950378218	9.284912000	7.986484000
C	12.225370906	9.591666500	8.545556000
C	13.401089513	9.236048500	7.823892500
C	13.596184682	11.090886500	9.929156750
C	14.766958887	10.444512250	9.462566750
C	16.028680895	11.030793250	9.764529750
C	17.177064892	10.504524250	9.147174500
C	17.910831168	12.691579250	9.921745750
C	19.542588385	13.086525750	10.291417250
C	20.764000947	12.305301250	10.232618250
C	22.225774717	14.282459250	9.885083500
C	24.691169261	14.146680000	9.944146000
C	0.635745058	13.137352000	2.738876250
C	1.896013046	12.480288750	2.699829250
C	3.085810618	13.257821750	2.731953500
C	3.232872720	10.534897500	3.345794000
C	4.418188756	11.215533750	2.950032000
C	5.685715467	10.635803750	3.236464250
C	6.870602774	11.329354500	2.858829500
C	7.041805762	9.296984500	4.768630000
C	8.223419694	9.702157500	4.081886250
C	9.497996251	9.366153000	4.618306750
C	10.678301645	9.791607500	3.941826000
C	10.859794937	8.961717250	6.609123750
C	12.037446683	8.995489750	5.807791000
C	13.311264939	8.953522750	6.435581500
C	14.484077130	8.994452250	5.625899250
C	14.674173443	9.525214250	8.381838750
C	15.836168665	9.168126000	7.639300500
C	17.105073810	9.503968250	8.164492250
C	18.280891573	9.236788000	7.445299500
C	18.285592554	11.342027000	9.298825000
C	19.511150577	10.671446500	9.026884750
C	20.763581971	11.049300500	9.578081250
C	21.960991410	10.390158750	9.170828750
C	22.083680992	12.926498500	10.272066500

C	23.290901614	12.139969250	10.195649750
C	24.584730735	12.768398750	10.253316750
C	25.783601509	11.988457250	10.176451500
C	27.157293660	14.015165000	10.002475750
C	29.626193621	13.884938500	10.054688500
C	0.439001213	16.224252000	5.368188750
C	0.569827702	14.480223500	3.187171500
C	1.763732130	15.111959750	3.634133000
C	3.022006833	14.582139500	3.232774250
C	4.218360502	15.191789250	3.702050000
C	4.345536497	12.601201250	2.662036500
C	5.536736886	13.376113500	2.718684000
C	6.797310470	12.724157750	2.619008000
C	7.988944058	13.497595250	2.701105250
C	8.140547841	10.745136750	3.125946000
C	9.325783820	11.451905000	2.769312500
C	10.597162588	10.862938250	3.018036500
C	11.784247587	11.580973000	2.686114750
C	11.952135750	9.435927500	4.463960250
C	13.133710669	9.878278750	3.798342000
C	14.405305631	9.491481000	4.300550250
C	15.592021232	9.955408500	3.654827500
C	15.757443087	8.915098750	6.247175000
C	16.937763111	8.986957000	5.444001500
C	18.211246918	8.933913500	6.068876500
C	19.402800449	9.055807750	5.310586750
C	19.496641663	9.651044000	8.035757250
C	20.702013672	9.286572000	7.385794250
C	21.936953745	9.550033750	8.024412000
C	23.140484455	9.230709000	7.340181000
C	23.234554460	10.840372750	9.637821000
C	24.437436997	10.221707000	9.164233000
C	25.712316306	10.693566000	9.603970500
C	26.913374612	10.095486000	9.107052750
C	27.066197529	12.623603500	10.253367500
C	28.263556171	11.848684000	10.151367000
C	29.541724296	12.483612500	10.250061250
C	30.737606973	11.712460750	10.121623250
C	30.902348956	14.472371750	9.792814000
C	32.096306620	13.752177000	10.100593500
C	33.372592809	14.348717250	9.861571750
C	34.566769917	13.615427750	10.137580750
C	0.372078884	16.378498000	6.775699000
C	1.569003920	16.227443250	7.537434000

C	1.702134572	15.973292500	4.758253750
C	2.900256797	16.237942000	5.482166500
C	4.160885242	16.006301250	4.860464250
C	5.360505377	16.239297500	5.592052000
C	5.474701252	14.677787250	3.275213250
C	6.672165552	15.267459000	3.765567750
C	7.926901922	14.775409750	3.309817750
C	9.125513020	15.347461500	3.818098750
C	9.252186732	12.853448250	2.574894250
C	10.444683874	13.624411000	2.680834750
C	11.710887418	12.987595500	2.535420500
C	12.905280719	13.754600250	2.669600500
C	13.056398068	10.983784250	2.915367000
C	14.247260757	11.711414500	2.616718500
C	15.519107266	11.104347000	2.827928250
C	16.714136549	11.844402750	2.567858000
C	16.864275745	9.540179750	4.139828500
C	18.056249472	10.037987000	3.528826750
C	19.330436312	9.623520500	4.016495500
C	20.525990635	10.149594500	3.446346500
C	20.652400608	9.019014750	5.993667500
C	21.851599329	9.143104250	5.248115500
C	23.096793943	9.067580500	5.931854250
C	24.299408271	9.202888500	5.188701250
C	24.391906812	9.430686250	7.987018000
C	25.594408167	9.155712000	7.273732750
C	26.855149179	9.332535750	7.913815000
C	28.056745124	9.088853500	7.184288250
C	28.188061298	10.568796500	9.547677250
C	29.386521630	9.984920000	9.033478500
C	30.660725944	10.450263500	9.481892750
C	31.857585960	9.880135500	8.950056000
C	32.014592945	12.344072250	10.241015500
C	33.209458051	11.576809500	10.085682000
C	34.486062434	12.203138000	10.226002250
C	35.679842104	11.440285250	10.045110500
C	35.843112593	14.219375250	9.920666250
C	37.036756533	13.475591000	10.168529500
C	38.312850912	14.086872250	9.973811000
C	39.505775563	13.333851250	10.194751250
C	0.222844285	15.157872750	9.280724500
C	1.497121341	15.588094500	8.800437250
C	2.692523272	15.043606250	9.360691000
C	2.837663207	16.341261500	6.894571000

C	4.035851672	16.162850000	7.648544750
C	5.303107736	16.293859000	7.007091750
C	6.502854254	16.088703500	7.751850250
C	6.618157103	16.031330750	4.958000500
C	7.819232477	16.234738500	5.693947000
C	9.072967532	16.055976000	5.044479000
C	10.274986516	16.229056000	5.784137750
C	10.380348140	14.879182250	3.336170750
C	11.578776775	15.435020750	3.861512000
C	12.836954354	14.989563000	3.361460250
C	14.033798927	15.536563750	3.900255500
C	14.174371986	13.123423750	2.514306500
C	15.369348846	13.885143000	2.681868000
C	16.642661973	13.260465000	2.522984750
C	17.837941585	14.015784000	2.727487500
C	17.984998404	11.226495250	2.755425000
C	19.180477141	11.977546500	2.535599500
C	20.453827655	11.356470500	2.707502500
C	21.648443245	12.115459750	2.524621750
C	21.789407239	9.730397250	3.958481500
C	22.986258315	10.267554250	3.409681750
C	24.244082751	9.832499000	3.920083500
C	25.442530892	10.378393500	3.384595250
C	25.547853910	9.073758500	5.858135750
C	26.750046011	9.233800500	5.115833000
C	28.004196791	9.065949750	5.767890500
C	29.205100674	9.257375250	5.028271750
C	29.321269108	9.250522500	7.822920750
C	30.520987586	9.033483750	7.082043750
C	31.788309077	9.178632000	7.720498750
C	32.986129770	8.986979250	6.969255000
C	33.131791900	10.334003000	9.408663500
C	34.327110524	9.779446500	8.858138250
C	35.601267698	10.219896000	9.328742250
C	36.795620362	9.683495000	8.759632250
C	36.956015320	12.061101250	10.207257250
C	38.148913556	11.303906000	10.001265500
C	39.424844165	11.918770250	10.184069000
C	40.617568471	11.169524750	9.949781250
C	3.966910863	15.486563500	8.892190500
C	5.163164156	14.924921250	9.434810500
C	6.437969911	15.378101500	8.976657250
C	7.635337492	14.801106000	9.501858250
C	7.767348979	16.236207500	7.110384500

C	8.968667774	16.002945250	7.843677000
C	10.228936574	16.168851500	7.200761750
C	11.430934833	15.905047500	7.919075000
C	11.523540658	16.088674000	5.117657250
C	12.725864426	16.237310000	5.858904250
C	13.971574328	16.148904500	5.177984250
C	15.170764108	16.285718000	5.921437000
C	15.296833130	15.106203250	3.396673250
C	16.492246440	15.643642750	3.955849000
C	17.766202457	15.220337250	3.475416000
C	18.958035170	15.731445500	4.074973750
C	19.108678682	13.394279500	2.551828000
C	20.303104087	14.140562250	2.795057250
C	21.574989609	13.529434000	2.596701250
C	22.765650734	14.264508750	2.877996500
C	22.917951862	11.488552000	2.693230500
C	24.112066794	12.253097500	2.543572750
C	25.378204506	11.619199500	2.702735500
C	26.570749193	12.387663500	2.580353250
C	26.697200210	9.919985250	3.876727000
C	27.895853978	10.481847250	3.357102250
C	29.150932112	9.999468250	3.822020500
C	30.348046113	10.580811750	3.320742250
C	30.462843835	9.062205000	5.666312250
C	31.662153090	9.283923000	4.930838500
C	32.923179786	9.064529250	5.555430500
C	34.120308823	9.315472500	4.825034750
C	34.255154797	9.115180250	7.608095500
C	35.451425564	8.950870250	6.847935500
C	36.721316989	9.060502000	7.488683500
C	37.915963057	8.923745000	6.721361250
C	38.069567845	10.108140750	9.244299750
C	39.262915942	9.592023000	8.655171000
C	40.537568492	10.001295250	9.151228250
C	8.910442747	15.261652500	9.050396750
C	10.110717557	14.672109750	9.559256000
C	11.385576953	15.135110250	9.110456000
C	12.588419259	14.529347750	9.600100000
C	12.681935370	16.097096750	7.269623250
C	13.885045479	15.790900750	7.960292250
C	15.120680864	16.043896000	7.318032000
C	16.326393418	15.692610000	7.974585500
C	16.420265924	16.235613500	5.238949750
C	17.611956811	16.370975250	5.994518500

C	18.884796915	16.307299250	5.369416750
C	20.065107592	16.394202500	6.170362750
C	20.229894684	15.307595750	3.596356250
C	21.416619632	15.785922750	4.231101500
C	22.688379583	15.389551500	3.736252500
C	23.870278386	15.844563250	4.393492250
C	24.038201091	13.662864250	2.661882750
C	25.225635981	14.387555500	2.978681500
C	26.497224034	13.793018250	2.744954250
C	27.682275924	14.506855000	3.088323500
C	27.833900432	11.746700750	2.721944500
C	29.025281660	12.518744250	2.623814500
C	30.286170593	11.870582250	2.737495250
C	31.476693550	12.645320000	2.663323750
C	31.604449853	10.076956500	3.757922250
C	32.799885920	10.678067250	3.275627750
C	34.058102105	10.155219500	3.685013500
C	35.252180463	10.775896500	3.223379750
C	35.384139120	9.075537250	5.437599000
C	36.579307384	9.356327500	4.714502000
C	37.844696141	9.099295750	5.316665500
C	39.037405005	9.412484750	4.603327500
C	39.186646106	9.013819250	7.363372250
C	40.379944219	8.909305000	6.588925250
C	13.859484710	14.971188500	9.121237250
C	15.057766642	14.322594500	9.540599500
C	16.311889787	14.691120250	8.984630500
C	17.542855077	16.094610500	7.376689250
C	18.718400160	15.842128250	8.101765500
C	19.986535625	16.167694750	7.567655000
C	21.148321155	15.823501750	8.315825500
C	21.337484019	16.305823250	5.547937250
C	22.510493709	16.360369750	6.355927000
C	23.784801650	16.308558750	5.729391250
C	24.962451771	16.357237750	6.530531500
C	25.144572510	15.477706250	3.880193000
C	26.324507695	15.915155250	4.550194000
C	27.599534519	15.568538500	4.022848500
C	28.780690056	15.987222750	4.702213000
C	28.952284386	13.918095250	2.833713000
C	30.136711673	14.620550750	3.196085500
C	31.404586650	14.036824250	2.920613250
C	32.590176584	14.726292000	3.300779750
C	32.736564100	11.991251750	2.746724750

C	33.926891589	12.767300750	2.697069500
C	35.186641038	12.109869250	2.749280250
C	36.375822135	12.888680000	2.723299000
C	36.512798748	10.239329750	3.607570250
C	37.704137712	10.881353500	3.168265750
C	38.966763911	10.335088750	3.530066000
C	40.155062355	10.993639500	3.108002750
C	40.304684639	9.137699500	5.192388250
C	18.647388449	14.863786750	9.107572750
C	21.054960686	14.926896000	9.416350250
C	22.420268040	16.099996250	7.748385250
C	23.597261454	15.755432500	8.472593500
C	24.872408566	16.056145000	7.912632500
C	26.055417594	15.697854500	8.620383500
C	26.237306291	16.338611000	5.899985250
C	27.418283429	16.368873500	6.697717750
C	28.694102283	16.371131750	6.063876500
C	29.878577116	16.375009750	6.857680250
C	30.054645668	15.655525500	4.160717500
C	31.238046850	16.053215250	4.847991750
C	32.510726841	15.733877000	4.294364750
C	33.696483797	16.109862000	4.989350750
C	33.855858746	14.149131000	3.003185250
C	35.042452841	14.826120750	3.400310250
C	36.306144156	14.258916000	3.077759500
C	37.494387739	14.924225500	3.488706750
C	37.636304283	12.231828750	2.744216000
C	38.824399944	13.012870750	2.737289500
C	40.085239706	12.356796000	2.727580750
C	23.505052661	14.820540250	9.534228250
C	25.967051510	14.706605750	9.630247500
C	27.330640292	16.021031750	8.068978750
C	28.518393783	15.630037500	8.754769750
C	29.793818857	15.974672500	8.215075000
C	30.984499082	15.553117000	8.879237250
C	31.153946110	16.396269750	6.220778750
C	32.341688222	16.370451500	7.010588250
C	33.616413920	16.410867750	6.372140750
C	34.807077890	16.354175000	7.156501500
C	34.967009578	15.804598750	4.422627250
C	36.155905397	16.157270750	5.124052250
C	37.423729983	15.868648750	4.542715000
C	38.616109275	16.196532500	5.250010500
C	38.756469392	14.370345750	3.137957250

C	39.947213418	15.021734250	3.564140250
C	28.433496948	14.590768750	9.715081750
C	32.260112715	15.917729250	8.351513250
C	33.452803293	15.467316500	8.994366750
C	34.728366535	15.850334750	8.479060000
C	35.922331514	15.371535750	9.099072750
C	36.080334938	16.412972000	6.515945500
C	37.273570061	16.324824500	7.293216250
C	38.544910630	16.402892500	6.650436500
C	39.740237382	16.282855000	7.419773750
C	39.881146515	15.927045750	4.652790000
C	37.197374186	15.771852500	8.595956000
C	38.391800810	15.268181000	9.194515000
C	39.666090871	15.684212000	8.702480750
N	21.159523778	13.087332000	13.284420750
N	16.962462360	12.992912000	13.249994250
N	19.024340618	15.072802250	13.123513250
N	19.096679153	11.003046000	13.179277000
C	21.915125150	14.228052750	13.300400250
C	21.960676467	11.979057500	13.312059250
C	16.165503898	14.103037000	13.188068250
C	16.201508989	11.856023250	13.289916000
C	21.434667286	15.537973250	13.254654250
C	21.532456868	10.649259750	13.261245500
C	16.594149787	15.425078250	13.044679000
C	16.679638308	10.542467750	13.248601250
C	20.092502752	15.909152000	13.153978750
C	20.202536911	10.217390750	13.211932500
C	17.923030229	15.857044250	13.020546500
C	18.026603790	10.168614000	13.207141750
C	23.276358971	13.815809250	13.354657750
C	23.304766012	12.450402750	13.350791500
C	14.819460893	13.640219750	13.217700500
C	14.841325655	12.276498000	13.284066000
C	22.457549971	16.619537750	13.311428250
C	22.596883983	9.614490750	13.275670750
C	15.522909745	16.445814000	12.915117250
C	15.649643195	9.474885750	13.207552500
C	19.652898068	17.289586000	13.051932750
C	19.818644618	8.817048500	13.268287500
C	18.307605237	17.257682250	12.965180000
C	18.471027711	8.786990750	13.264364000
C	22.610408243	17.387356750	14.465070250
C	23.471114002	9.509059750	14.358189250

C	23.280979489	16.870881000	12.215933250
C	22.737056353	8.733415750	12.202577500
C	14.631079495	16.675042500	13.963105500
C	15.585665887	8.610383000	12.113301000
C	15.386568707	17.174191250	11.733150750
C	14.711952781	9.339447000	14.232361000
C	23.576589006	18.381605250	14.519071500
C	24.465967984	8.542889000	14.364183750
C	24.242195125	17.868582000	12.269748500
C	23.738398566	7.774506000	12.207962750
C	13.621734073	17.616630500	13.830177000
C	14.591838416	7.646936250	12.035656500
C	14.372166724	18.110714250	11.601955500
C	13.724403443	8.368713000	14.155587750
C	24.394237390	18.624699250	13.423563500
C	24.604672110	7.676298500	13.288493750
C	13.488430711	18.334242250	12.649263000
C	13.656520843	7.525873500	13.054446500
H	20.146561592	13.067160000	13.236027750
H	17.976202353	13.006645750	13.219377750
H	24.121044091	14.485247500	13.376634250
H	24.179595846	11.820832750	13.356096750
H	13.947177831	14.271372000	13.168563750
H	13.988566211	11.617645750	13.290558500
H	20.304973426	18.148051500	13.048618500
H	20.501492950	7.985502000	13.333895250
H	17.623378471	18.087433500	12.892831500
H	17.824066214	7.926944500	13.327814000
H	21.977282697	17.194917250	15.324020000
H	23.354848444	10.174639750	15.206464000
H	23.158332577	16.286010750	11.313003750
H	22.066010457	8.814450000	11.354697750
H	14.742085303	16.122681000	14.889769500
H	16.307712628	8.712007750	11.310904750
H	16.070172496	16.991345000	10.911186000
H	14.768845701	9.988273000	15.099432750
H	23.693358879	18.969094750	15.423033750
H	25.134393554	8.465097750	15.214586000
H	24.872912475	18.053439000	11.406913750
H	23.841779503	7.100424500	11.364842750
H	12.937065981	17.790629500	14.652984000
H	14.545347147	6.991000750	11.173354250
H	14.270805485	18.668058250	10.677311250
H	13.002707813	8.271565750	14.959191000

H	25.147844666	19.402791750	13.468884750
H	25.384129903	6.922801750	13.294702750
H	12.697468357	19.068583500	12.546760750
H	12.877976588	6.773960500	12.992407500

4.3 Cartesian Coordinates of H2TPP@SW1-CNT(6,5)

C	0.119493825	13.937192500	9.787564000
C	1.298849515	13.177922000	9.983906750
C	1.230440249	11.763593500	9.933720500
C	2.412148460	11.020851000	9.688234750
C	2.551916891	13.820497250	9.833434000
C	3.730826783	13.055799750	10.010347000
C	4.983465430	13.705023000	9.888817000
C	6.161894578	12.935832250	10.048669750
C	1.090671819	9.455005500	8.351678250
C	2.346819133	9.865854250	8.870066250
C	3.535629613	9.389633500	8.257993000
C	3.664826526	11.643549750	9.915713250
C	4.849473663	10.910499750	9.652880750
C	6.100394551	11.526970500	9.907284250
C	7.288747449	10.805573250	9.624954250
C	7.413462419	13.590746500	9.955510500
C	8.592154087	12.817969500	10.094915250
C	9.840710260	13.478863750	10.026748500
C	11.018258787	12.702536500	10.143832500
C	0.876461441	9.440698000	4.304351750
C	1.021370146	8.913627500	7.043940250
C	2.212190166	8.845461500	6.270664250
C	3.471773000	8.896212250	6.931028500
C	4.666137042	8.858003500	6.161243500
C	4.789853541	9.783490750	8.795930250
C	5.982995197	9.332342250	8.172224250
C	7.235431468	9.709869750	8.727841500
C	8.433136750	9.284780500	8.092203250
C	8.538509346	11.414279250	9.904581250
C	9.730830119	10.705365000	9.600802750
C	10.978546310	11.305901750	9.906165750
C	12.179485141	10.615071750	9.581769750
C	12.261266275	13.371322000	10.107093000
C	13.438464504	12.596391500	10.212211500
C	14.667882306	13.280082750	10.239767000
C	15.836973699	12.485713250	10.337845750
C	17.114278678	14.542532000	9.941354250
C	19.151784010	13.639552250	9.836086750
C	0.802017461	10.418622500	3.280439500
C	1.994993316	11.097327500	2.897779250
C	2.142269173	9.138175500	4.885428000

C	3.336048437	9.519704000	4.210695000
C	4.599750725	9.199784000	4.787210250
C	5.795215238	9.605610500	4.131127000
C	5.923808680	8.887358500	6.827896250
C	7.121462758	8.879371500	6.062215000
C	8.378221672	8.888232000	6.732776500
C	9.578602140	8.909963500	5.970900250
C	9.685049606	9.643385250	8.663393750
C	10.888646556	9.249465500	8.015851250
C	12.141210023	9.591955750	8.601251250
C	13.349800139	9.235245250	7.938765000
C	13.424245338	11.207643250	9.917494250
C	14.636179539	10.545349000	9.558255750
C	15.881416823	11.132203000	9.922205750
C	17.126977178	10.554861250	9.507047000
C	17.036410964	13.179271250	10.361861000
C	18.271661509	12.552003750	10.177783000
C	20.474127862	13.554419250	9.849581500
C	21.213705344	12.367581250	10.172699000
C	22.590680216	14.217462250	10.059548500
C	24.959013001	14.076527750	10.020764750
C	0.648870255	13.122021750	2.585791250
C	1.919094503	12.474295500	2.568364500
C	3.109816992	13.255672500	2.614669500
C	3.263632284	10.530998500	3.219721250
C	4.456582537	11.223599250	2.864796000
C	5.723911748	10.648214750	3.173388500
C	6.915900917	11.353455750	2.844284000
C	7.057352158	9.267793500	4.700729500
C	8.253221424	9.695341500	4.060340000
C	9.514586632	9.340987750	4.621981000
C	10.709657772	9.788315000	3.994817500
C	10.835948676	8.902144750	6.642911250
C	12.037655968	8.954024250	5.883474500
C	13.296330547	8.935041500	6.554485000
C	14.497182820	9.015277750	5.797344500
C	14.603578270	9.572715250	8.531005250
C	15.820784413	9.264300000	7.856740000
C	17.079908446	9.611176500	8.444390750
C	18.282722306	9.316410750	7.741481250
C	18.388935698	11.203828750	9.791505500
C	19.629321236	10.600893000	9.351144750
C	20.943714709	11.057093250	9.737779250
C	22.125263214	10.312304000	9.356643000

C	22.513986935	12.832693250	10.391203250
C	23.632169325	12.016010500	10.320276000
C	24.883190181	12.684154750	10.311426500
C	26.032283307	11.883827750	10.167880000
C	27.364563508	13.929475750	9.945747000
C	29.784865130	13.799293750	9.929631500
C	0.415595059	16.254981000	5.155890750
C	0.572244025	14.472374750	3.010900250
C	1.760969979	15.120075000	3.453495000
C	3.031143836	14.590733750	3.085078250
C	4.217392916	15.224553750	3.554037250
C	4.380359028	12.610431000	2.580465500
C	5.569421462	13.391697000	2.657179000
C	6.839739584	12.748647750	2.605536500
C	8.028110769	13.527072750	2.712125250
C	8.181902898	10.768034000	3.136416000
C	9.373113040	11.483439000	2.830117000
C	10.637661407	10.887231750	3.102365750
C	11.827463450	11.612136000	2.815596000
C	11.971478936	9.420798500	4.546820000
C	13.164364168	9.884474000	3.928638750
C	14.426929817	9.505690000	4.469317750
C	15.615557833	9.980115500	3.850958750
C	15.758680508	8.991585750	6.465769750
C	16.950614815	9.078086750	5.696481000
C	18.213475901	9.043211500	6.354578750
C	19.403236899	9.126125000	5.577948750
C	19.552996539	9.640140500	8.318471500
C	20.746877803	9.264333750	7.622054250
C	22.023689033	9.460343500	8.224140000
C	23.206654985	9.120885250	7.493678000
C	23.440555189	10.726503500	9.760425250
C	24.606894185	10.089779750	9.248276000
C	25.896208853	10.575043500	9.632237250
C	27.063282174	9.960920250	9.104512000
C	27.288765883	12.534916250	10.187171500
C	28.453310720	11.746422500	10.060095500
C	29.710039968	12.396586500	10.121497500
C	30.880704045	11.615587250	9.980069500
C	31.031995730	14.404340500	9.648765250
C	32.211525349	13.671976500	9.925909250
C	33.461749704	14.284887250	9.670345500
C	34.641083449	13.544873500	9.927791000
C	0.339650732	16.411129000	6.562400000

C	1.521468260	16.268798750	7.335354750
C	1.681586068	16.007095000	4.556272750
C	2.865115666	16.300037750	5.288356000
C	4.133791615	16.073649000	4.685844750
C	5.314741931	16.341296000	5.432414750
C	5.489374343	14.709769250	3.172722000
C	6.673846331	15.327169250	3.667802250
C	7.947072901	14.826114500	3.273301000
C	9.130332664	15.424555250	3.795043000
C	9.297715292	12.886011250	2.638956250
C	10.485132301	13.660355250	2.775516500
C	11.752842696	13.020755500	2.676346500
C	12.939778960	13.788775000	2.844537750
C	13.091036509	11.005827250	3.064691500
C	14.278712788	11.739389750	2.795527500
C	15.541472686	11.122639250	3.017099250
C	16.728868564	11.862941500	2.766444000
C	16.878635925	9.585953000	4.375140750
C	18.065289757	10.071093250	3.761511750
C	19.329521962	9.662587000	4.272113500
C	20.518696963	10.162124000	3.671407000
C	20.668304617	9.043435500	6.226827750
C	21.856639635	9.131685500	5.447381000
C	23.122653807	9.000688500	6.082260250
C	24.309103231	9.131236750	5.301411250
C	24.493580963	9.289965250	8.085030250
C	25.671992230	9.010803250	7.328940750
C	26.954903599	9.179713250	7.926214000
C	28.131995763	8.939600500	7.158875000
C	28.342834829	10.451313750	9.495828500
C	29.513431447	9.852647250	8.961337500
C	30.784872391	10.338352750	9.372994750
C	31.957947103	9.757845250	8.824210750
C	32.137686873	12.263655250	10.069834250
C	33.311361398	11.488561500	9.906933000
C	34.568012215	12.132892250	10.024208000
C	35.744949549	11.366257500	9.841659750
C	35.892685832	14.167221500	9.700475000
C	37.072173188	13.421324500	9.940716500
C	38.324729341	14.051806750	9.742029250
C	39.504394284	13.299760250	9.962286250
C	0.190112975	15.151888250	9.061236500
C	1.445522307	15.608363750	8.586904250
C	2.624310287	15.060027750	9.150759000

C	2.783255695	16.408090000	6.699176000
C	3.962205819	16.238980000	7.471444000
C	5.227005328	16.399972500	6.845808000
C	6.402943378	16.203761250	7.616463750
C	6.586498631	16.135940000	4.828516500
C	7.765075294	16.376397750	5.588691750
C	9.040237035	16.191270250	4.983927750
C	10.217058145	16.404121250	5.755901000
C	10.404153764	14.936328750	3.387647500
C	11.587449288	15.510157500	3.937698750
C	12.861026968	15.035605250	3.514302500
C	14.045086483	15.578765500	4.093011000
C	14.204791411	13.152122000	2.714107500
C	15.392463220	13.910000250	2.914920250
C	16.654958159	13.277502500	2.745481250
C	17.843120466	14.023841750	2.974289500
C	17.991366348	11.237638750	2.962023500
C	19.179740378	11.986114000	2.738166250
C	20.443999404	11.355337000	2.913753250
C	21.632305975	12.111954500	2.718241750
C	21.781170770	9.729869250	4.164823250
C	22.969339986	10.253016500	3.584547000
C	24.232617609	9.797466750	4.052939750
C	25.419918801	10.345459750	3.490684250
C	25.581635300	8.962179250	5.915403000
C	26.765355083	9.136580250	5.140010500
C	28.039836548	8.944478000	5.744629500
C	29.222654171	9.158970500	4.978145000
C	29.411635790	9.101755250	7.763458000
C	30.588201695	8.893395750	6.989773500
C	31.863613358	9.044505500	7.603451000
C	33.041814934	8.865236750	6.826342000
C	33.225055651	10.231666500	9.257568750
C	34.401097328	9.671188250	8.694774500
C	35.664825624	10.132346000	9.149464250
C	36.843587189	9.593362250	8.572059250
C	37.000553536	12.007009250	9.988168250
C	38.179553238	11.248516500	9.784477250
C	39.434062443	11.884512000	9.959074250
C	40.614514134	11.134459250	9.732692500
C	3.881166731	15.533622750	8.697894500
C	5.057547733	14.966898250	9.248052500
C	6.315673703	15.457296000	8.818149000
C	7.488566763	14.873220250	9.356169500

C	7.670893129	16.386313000	7.002567750
C	8.843679718	16.165815500	7.771285250
C	10.115472179	16.369878500	7.169283750
C	11.285539693	16.126870500	7.935141000
C	11.496240997	16.233684750	5.152924750
C	12.673419719	16.415421250	5.935724750
C	13.955709737	16.254272000	5.335672250
C	15.134224224	16.395740250	6.128758250
C	15.316599356	15.119720750	3.649126500
C	16.503152000	15.628004500	4.254889750
C	17.767921030	15.192371500	3.772587250
C	18.956015878	15.664339250	4.398422000
C	19.105102962	13.399134750	2.771817000
C	20.294081276	14.136353000	3.030440750
C	21.558193193	13.523733750	2.801379750
C	22.744725518	14.255641000	3.078175500
C	22.895160965	11.475963500	2.873340750
C	24.082399168	12.239842750	2.704871000
C	25.345699955	11.598237250	2.832658750
C	26.533168168	12.366283500	2.684051000
C	26.685788709	9.866752250	3.927673750
C	27.872335257	10.440316250	3.388236750
C	29.140787291	9.942840750	3.799933750
C	30.327918617	10.537986250	3.284457250
C	30.497317693	8.947665000	5.576229500
C	31.680078424	9.196861000	4.821349000
C	32.953841818	8.968287750	5.415488000
C	34.137830623	9.246683000	4.673950250
C	34.313376979	8.998766750	7.450229500
C	35.493783156	8.848727500	6.671208750
C	36.761977140	8.963870750	7.304910750
C	37.945220241	8.841614500	6.526201000
C	38.104292439	10.040570250	9.047427500
C	39.285923033	9.523298500	8.456640500
C	40.544056723	9.953159750	8.953616750
C	8.746943467	15.380537000	8.947355000
C	9.916765122	14.780816250	9.470317500
C	11.174393278	15.305157250	9.084169500
C	12.338311480	14.691851750	9.597874000
C	12.565239457	16.345483250	7.347748500
C	13.731934440	16.086408250	8.115290000
C	15.021975306	16.302626000	7.537261250
C	16.188543499	16.019529250	8.304255000
C	16.420187493	16.239538250	5.532737250

C	17.602600364	16.317771000	6.334414250
C	18.877663355	16.180494500	5.713265250
C	20.071457249	16.211398000	6.502261500
C	20.220422013	15.263977500	3.879821000
C	21.410163505	15.730712000	4.505399000
C	22.672749879	15.367065500	3.954846000
C	23.864849582	15.833657000	4.571922250
C	24.007976320	13.648756250	2.830055750
C	25.196447881	14.374144750	3.116172500
C	26.459470299	13.772405500	2.846626750
C	27.652234837	14.488446250	3.139162750
C	27.797433290	11.719622500	2.782485250
C	28.987089849	12.489523500	2.654438500
C	30.252283950	11.839398750	2.727564750
C	31.443454268	12.611415750	2.622544500
C	31.598310700	10.025975000	3.674667750
C	32.786518115	10.640344750	3.183629000
C	34.057371030	10.115422500	3.556765000
C	35.246311145	10.747702000	3.090634250
C	35.409948593	8.999727250	5.264455500
C	36.595891670	9.304877000	4.537152750
C	37.865901758	9.038864500	5.124801500
C	39.054541153	9.369304250	4.413498250
C	39.210501714	8.936555750	7.168960250
C	40.397029163	8.840543250	6.391880250
C	13.595294308	15.238151250	9.246145250
C	14.744323226	14.623875750	9.779243500
C	15.997313390	15.203607750	9.451254750
C	17.501849911	16.164740000	7.743740000
C	18.682309323	15.720949500	8.453253500
C	19.995015108	15.912893000	7.880874500
C	21.237443508	15.623342750	8.563617750
C	21.341051205	16.198493250	5.839207500
C	22.544750156	16.304394250	6.592233250
C	23.803078095	16.305168500	5.908655000
C	25.020218810	16.383352000	6.645291000
C	25.126014040	15.474028500	4.007429750
C	26.326726925	15.929060500	4.617824000
C	27.585608351	15.572367000	4.049820500
C	28.786888134	16.004986750	4.677070500
C	28.914776103	13.890977500	2.854434000
C	30.109636739	14.597403750	3.164288500
C	31.371849245	14.006333000	2.864793000
C	32.567384468	14.702504500	3.196938250

C	32.710149123	11.960379500	2.672662500
C	33.902037104	12.735557000	2.593999750
C	35.169918990	12.084466750	2.624641250
C	36.362752612	12.861868500	2.575871750
C	36.517099446	10.211493250	3.450118750
C	37.707767074	10.859702250	3.010994250
C	38.977999450	10.312278750	3.357560000
C	40.170192620	10.975873250	2.946091750
C	40.322653455	9.084949000	4.997657250
C	18.413719473	14.826890750	9.508000250
C	21.354858304	14.661809000	9.582760250
C	22.499257358	16.035998500	7.987119500
C	23.744513335	15.756871250	8.639906250
C	24.988468904	16.073326750	8.025825000
C	26.200100353	15.687008000	8.673014250
C	26.273142735	16.372802000	5.962766250
C	27.481589806	16.403849500	6.714089000
C	28.733872466	16.403723750	6.035818500
C	29.937150003	16.397419250	6.793798250
C	30.044834077	15.657299250	4.103376000
C	31.244655775	16.065829500	4.748374500
C	32.502362362	15.732472500	4.168392250
C	33.699543823	16.118048000	4.831548000
C	33.830419483	14.121708250	2.882077750
C	35.025536137	14.806957500	3.239262250
C	36.290081660	14.237930250	2.909281250
C	37.483616284	14.911580750	3.294795750
C	37.631786985	12.211433750	2.590000250
C	38.824709604	12.990710750	2.572499250
C	40.094510814	12.341238250	2.570813750
C	23.790928612	14.807199000	9.692868500
C	26.186860964	14.649199000	9.642076500
C	27.443769018	16.023948000	8.079044750
C	28.645213384	15.599627250	8.711129250
C	29.891820162	15.962616250	8.141774750
C	31.084528214	15.512112750	8.766047250
C	31.189133568	16.417632500	6.120008000
C	32.386622657	16.379051000	6.884086000
C	33.639555522	16.422303250	6.214513250
C	34.832641911	16.355443250	6.981842750
C	34.958294801	15.803760250	4.244835250
C	36.152387383	16.165780250	4.926649750
C	37.413087756	15.872411000	4.334720250
C	38.603722467	16.210362000	5.034822750

C	38.750058372	14.354757250	2.951922250
C	39.941531035	15.015352750	3.366418000
C	28.606497752	14.523181000	9.631683500
C	32.333494016	15.895270250	8.214994500
C	33.522237038	15.422700250	8.827554500
C	34.772797874	15.825105000	8.294601750
C	35.957992403	15.332208500	8.896465000
C	36.087671280	16.420771000	6.319283750
C	37.276547593	16.326508500	7.089686000
C	38.533701912	16.415242750	6.435368500
C	39.718282404	16.296404250	7.208261000
C	39.866785116	15.939432500	4.438640000
C	37.210833832	15.752757250	8.383708500
C	38.392948422	15.241733750	8.975752500
C	39.647231274	15.680235750	8.482286000
N	21.153702819	13.081714750	13.316127500
N	16.949791087	13.018562500	13.345620750
N	19.010742397	15.083740250	13.185262000
N	19.093105465	11.011220000	13.227926500
C	21.907328382	14.224391500	13.336716500
C	21.955718655	11.974016750	13.361302000
C	16.151042530	14.128796000	13.282937500
C	16.192766985	11.877984250	13.348866000
C	21.428753267	15.535091500	13.280843750
C	21.527317812	10.643194250	13.308427250
C	16.580255723	15.453481750	13.146598750
C	16.670540723	10.564218250	13.288106000
C	20.086896768	15.911099500	13.189667500
C	20.194569057	10.218360500	13.255913000
C	17.913240990	15.876456500	13.104192750
C	18.016959628	10.184502500	13.248829500
C	23.268524410	13.813840250	13.409502750
C	23.298743490	12.447924000	13.414959500
C	14.806279616	13.660500500	13.279345500
C	14.831458391	12.295364750	13.321537750
C	22.451617258	16.619837250	13.332746500
C	22.588119629	9.603849750	13.323319500
C	15.513336699	16.478998000	13.022380250
C	15.641041391	9.495560000	13.232596500
C	19.656113331	17.294211000	13.090012250
C	19.800986681	8.820608000	13.304296750
C	18.309025935	17.273490000	13.036665750
C	18.453090999	8.799595750	13.297243750
C	22.625425535	17.369804000	14.495384500

C	23.477420989	9.508948250	14.394957750
C	23.249288507	16.898685500	12.225100000
C	22.713696933	8.705865750	12.261671750
C	14.574004111	16.656776750	14.039274250
C	15.589261926	8.625555250	12.141381250
C	15.421296145	17.267613250	11.874125750
C	14.695430264	9.357216750	14.250122000
C	23.589603261	18.366366250	14.547368500
C	24.473528240	8.543814250	14.398520000
C	24.211292110	17.895949750	12.277601250
C	23.717220583	7.749033000	12.263184000
C	13.560555085	17.593880750	13.903723000
C	14.601621154	7.655812750	12.059994500
C	14.399221746	18.194181500	11.735789000
C	13.714562187	8.379894500	14.170177750
C	24.386749469	18.630672000	13.441613500
C	24.600208454	7.665099000	13.331218750
C	13.465236280	18.359471500	12.749491000
C	13.660040076	7.531407500	13.072640750
H	20.140734132	13.057724250	13.263419000
H	17.963966311	13.037291750	13.319713500
H	24.111976172	14.484521500	13.436574500
H	24.174685987	11.820410000	13.434106000
H	13.932178013	14.287639250	13.217637000
H	13.980682072	11.634544250	13.295435750
H	20.314765104	18.147276250	13.066057750
H	20.477049314	7.983467500	13.367196000
H	17.632558550	18.110558000	12.979390500
H	17.801837338	7.942565750	13.354957250
H	22.008235697	17.163571000	15.362669500
H	23.372196720	10.182102000	15.238643750
H	23.107769807	16.335350250	11.312656750
H	22.031240349	8.772142250	11.421741500
H	14.651450818	16.068720000	14.947162500
H	16.316663916	8.725476500	11.343516250
H	16.142526067	17.135916750	11.075601000
H	14.742127973	10.008415500	15.116056250
H	23.720301334	18.940477500	15.457987250
H	25.152783784	8.476180000	15.241192500
H	24.823267306	18.097876500	11.404933000
H	23.809300555	7.064980750	11.426607500
H	12.841248144	17.726516250	14.704338250
H	14.566188243	6.995311500	11.200496750
H	14.331597196	18.788791500	10.831292750

H	12.988765390	8.280624000	14.969847500
H	25.141390571	19.408002500	13.486670250
H	25.382416613	6.914222750	13.334250250
H	12.666776658	19.085089000	12.642011750
H	12.887528503	6.773235750	13.008743750

4.4 Cartesian Coordinates of H2TPP@SW2-CNT(6,5)

C	0.141652805	13.963928500	9.956671750
C	1.324409878	13.188981000	10.153299750
C	1.235103436	11.776111750	10.089107250
C	2.418191708	11.022496500	9.824399750
C	2.603709360	13.799242000	10.007807250
C	3.786780970	13.017115000	10.173388750
C	5.066477077	13.632865500	10.052491750
C	6.250400455	12.845871000	10.186540000
C	1.056417404	9.503467750	8.479316000
C	2.332571114	9.885019000	8.983801000
C	3.517565705	9.402147750	8.351346000
C	3.696802379	11.608496000	10.050752500
C	4.879954452	10.866469500	9.756314250
C	6.158329424	11.443327500	10.007270250
C	7.340553736	10.713961000	9.681691250
C	7.531308382	13.465373000	10.088998250
C	8.716206254	12.674735500	10.191318250
C	9.998821374	13.297336750	10.114710500
C	11.183424217	12.502114250	10.184882500
C	0.828835971	9.469652500	4.425086250
C	0.977060721	8.970010500	7.168866750
C	2.165295770	8.881534000	6.384127500
C	3.437458035	8.916949000	7.022270750
C	4.625187956	8.855896500	6.233650250
C	4.793510943	9.764061000	8.870184000
C	5.977427412	9.305699750	8.219067500
C	7.252635887	9.647659750	8.752141000
C	8.435516499	9.214648500	8.082973250
C	8.618996979	11.280790500	9.955598750
C	9.798596495	10.563315500	9.601873500
C	11.076704477	11.118041250	9.898801750
C	12.250420859	10.408546000	9.518438750
C	12.470194552	13.123891500	10.123015750
C	13.653483574	12.324408000	10.155145000
C	14.949610356	12.936585750	10.094789000
C	16.138667508	12.138787000	10.113373750
C	17.546814011	14.106626500	9.654136000
C	20.096746151	14.397285000	9.799969000
C	0.768063360	10.431818750	3.386887000
C	1.964538942	11.093975750	2.987268000
C	2.094705473	9.158824000	4.996273250

C	3.287343627	9.511726250	4.298386250
C	4.554678935	9.181802000	4.856236750
C	5.747355695	9.559436000	4.170493000
C	5.897270165	8.869498000	6.872859500
C	7.085226845	8.838685500	6.082477750
C	8.357296862	8.829936000	6.721141750
C	9.545750136	8.829047750	5.930659500
C	9.709207559	9.534524500	8.631003500
C	10.890260689	9.123310750	7.947047000
C	12.162379878	9.415671000	8.511020250
C	13.342292306	9.022925250	7.814251000
C	13.527393014	10.951851250	9.829499000
C	14.691453042	10.248842500	9.429227000
C	15.966350638	10.772949000	9.771993250
C	17.098206022	10.008489000	9.397494750
C	17.461537213	12.746112500	10.115286000
C	18.565945015	11.837828750	10.185048500
C	20.707932974	13.145122250	10.218249250
C	20.027789494	11.960646000	10.198213750
C	22.402498349	14.609311500	9.872078000
C	24.772866275	14.354823250	9.847554250
C	0.650516898	13.134059750	2.691701000
C	1.908480723	12.471488250	2.661069500
C	3.106146992	13.240201750	2.710358500
C	3.225193802	10.512006250	3.296823250
C	4.421324368	11.188773250	2.920427750
C	5.683179262	10.596282250	3.206440000
C	6.878671816	11.288785500	2.856123250
C	7.015353398	9.212527250	4.717208750
C	8.208211403	9.619039250	4.046938250
C	9.477039744	9.256050000	4.580996250
C	10.671068117	9.692393000	3.931255750
C	10.815779323	8.793756750	6.571012000
C	12.006338447	8.826421000	5.783363500
C	13.274456032	8.758771000	6.423260500
C	14.468411258	8.835752000	5.642450500
C	14.610817081	9.282910750	8.395859500
C	15.793643239	8.907736000	7.686832250
C	17.053413007	9.113593250	8.299931500
C	18.261357389	8.842158250	7.585440250
C	18.334970325	10.504469750	9.804072000
C	19.547738414	9.911125000	9.355856250
C	20.642097706	10.729381250	9.725259000
C	21.938148090	10.409174500	9.215953250

C	22.170548353	13.264926250	10.198556000
C	23.280081800	12.365547500	10.102736750
C	24.601666132	12.975017000	10.135556750
C	25.791195088	12.179889000	10.085632000
C	27.210629147	14.178377000	9.897166000
C	29.661446100	14.014235000	9.955951000
C	0.466250077	16.231136500	5.310025000
C	0.595489253	14.477286750	3.139107000
C	1.791811631	15.101925500	3.595605000
C	3.051071801	14.564501750	3.211178500
C	4.247061355	15.170353750	3.691311500
C	4.363805220	12.578747750	2.651101000
C	5.560994808	13.345354750	2.729535500
C	6.819139877	12.688164750	2.641105750
C	8.014858377	13.453793500	2.747907750
C	8.142675636	10.689757000	3.120688500
C	9.337653715	11.398153000	2.798455250
C	10.604205119	10.796541000	3.045601000
C	11.797892542	11.520188000	2.750489250
C	11.940154914	9.313046500	4.454003500
C	13.134691666	9.782061250	3.827747500
C	14.403973930	9.389003250	4.340211250
C	15.600244291	9.890382250	3.741882000
C	15.735633186	8.736041500	6.282879250
C	16.938024819	8.872634250	5.523171000
C	18.205076068	8.768506500	6.170880750
C	19.404588106	8.966295250	5.420129750
C	19.519714587	9.121376000	8.200315250
C	20.735548798	9.052014250	7.479694250
C	21.944337633	9.498736250	8.105024000
C	23.148571783	9.267904750	7.386324000
C	23.195589718	11.028406000	9.584259750
C	24.412134277	10.406903500	9.135066500
C	25.700596771	10.872738750	9.555392000
C	26.900420094	10.237013250	9.095139500
C	27.085809738	12.792926000	10.166307750
C	28.270577570	11.998374000	10.090761750
C	29.556372191	12.618694000	10.177626250
C	30.741553309	11.829674250	10.069054750
C	30.938210596	14.585318000	9.686973500
C	32.118355065	13.853551000	10.006551750
C	33.395842101	14.435333250	9.762605750
C	34.578285857	13.692135250	10.053316250
C	0.395958062	16.392025000	6.716275750

C	1.584486515	16.235847000	7.490938250
C	1.731614858	15.969831750	4.714221750
C	2.924243259	16.234500000	5.449103000
C	4.188185716	15.994591250	4.842518750
C	5.381123778	16.230667000	5.585984500
C	5.505020302	14.647982500	3.284377750
C	6.700231642	15.235231000	3.786967000
C	7.957141322	14.732676750	3.355090250
C	9.151406614	15.303929750	3.876963500
C	9.274845963	12.804243000	2.633571500
C	10.468197311	13.570250000	2.764939500
C	11.731076277	12.930409250	2.629053500
C	12.921784542	13.697424750	2.782079000
C	13.066628634	10.917121250	2.981583000
C	14.258191918	11.655567000	2.714064000
C	15.529295975	11.052783750	2.933466000
C	16.717645623	11.803489250	2.684871750
C	16.870145469	9.486168750	4.245717750
C	18.061593343	10.014736250	3.662677500
C	19.332932286	9.601122500	4.152598000
C	20.517061698	10.145855250	3.568154250
C	20.672715038	8.915536000	6.070772500
C	21.856747731	9.119330000	5.316133500
C	23.107071243	9.066702750	5.984984250
C	24.298998236	9.218994000	5.229115250
C	24.390744571	9.541576500	8.008628500
C	25.591185183	9.240568500	7.301607750
C	26.850785086	9.434065000	7.928394750
C	28.047220436	9.167093750	7.198808500
C	28.181304451	10.703070750	9.523590500
C	29.375649393	10.092106250	9.024390500
C	30.654199107	10.553562500	9.459585500
C	31.844444914	9.963995000	8.932783750
C	32.022805031	12.449895250	10.174983000
C	33.207984118	11.666421500	10.035073500
C	34.487530271	12.282374500	10.163393750
C	35.671511355	11.503594250	9.992056000
C	35.856249981	14.282101750	9.833323250
C	37.039392301	13.527086750	10.092369750
C	38.317947298	14.124403750	9.897682750
C	39.500927879	13.358728250	10.126476500
C	0.228520573	15.171953500	9.220948750
C	1.505720706	15.594256750	8.752105250
C	2.690809170	15.034558250	9.319004500

C	2.856350499	16.343391500	6.860355500
C	4.045744944	16.158799750	7.627441750
C	5.316793327	16.288267750	7.000242500
C	6.506641697	16.075697250	7.759256000
C	6.643368794	16.013281250	4.969633500
C	7.836824987	16.221732500	5.719686000
C	9.096563871	16.032701500	5.090790250
C	10.290812501	16.214651500	5.844939750
C	10.407978593	14.825194750	3.419728250
C	11.601266953	15.383250500	3.957816500
C	12.858261972	14.931299500	3.476104750
C	14.049423349	15.476985750	4.030407500
C	14.187430130	13.068152250	2.626889500
C	15.375564397	13.836987750	2.799278250
C	16.644527248	13.217998750	2.632099750
C	17.830617434	13.985718500	2.830168750
C	17.989306824	11.199293250	2.886123750
C	19.174957309	11.962717500	2.656280500
C	20.445924010	11.352364000	2.828039500
C	21.632443331	12.122858750	2.626866250
C	21.789301988	9.729852750	4.042684500
C	22.976074482	10.280592000	3.478135500
C	24.239472393	9.849238500	3.962127750
C	25.428607162	10.410672250	3.418156250
C	25.548002238	9.114330750	5.890763250
C	26.743142462	9.275943750	5.136254500
C	27.996814934	9.122913750	5.782456250
C	29.191160689	9.315283000	5.031770500
C	29.311688746	9.335821250	7.827706750
C	30.505663885	9.105898250	7.080082000
C	31.772914665	9.250898750	7.710413500
C	32.964527934	9.050176250	6.951515000
C	33.121525979	10.413580250	9.379561250
C	34.308848709	9.842726500	8.828584000
C	35.585189353	10.276261250	9.289466750
C	36.770981257	9.725083250	8.716854250
C	36.950141939	12.113992500	10.144544750
C	38.133370817	11.341508750	9.942044500
C	39.411913623	11.944368750	10.119783250
C	40.594818212	11.180047000	9.887081250
C	3.967987765	15.472090750	8.864272250
C	5.153570385	14.892751750	9.410194250
C	6.431081397	15.346199250	8.971440750
C	7.618446797	14.748124000	9.494172500

C	7.776265319	16.227483000	7.135045250
C	8.967948485	15.988337250	7.882982750
C	10.235038340	16.163569500	7.260199250
C	11.429489347	15.896124500	7.994545250
C	11.547519398	16.059036250	5.202164000
C	12.742247148	16.212831500	5.960459000
C	13.994799643	16.094087000	5.304940250
C	15.190888353	16.215224500	6.064944500
C	15.307559071	15.049993000	3.528026500
C	16.496944169	15.584471250	4.096979000
C	17.759434232	15.178755750	3.589000000
C	18.946524920	15.701643500	4.177969250
C	19.103067008	13.377798500	2.654045750
C	20.289679390	14.139004500	2.887260750
C	21.560737932	13.536603250	2.688971500
C	22.746994733	14.289060250	2.950800500
C	22.904936794	11.507656250	2.775593750
C	24.091523167	12.282846500	2.609785250
C	25.360691646	11.656826500	2.747626250
C	26.549541138	12.431965000	2.608842250
C	26.687647076	9.958368250	3.895612750
C	27.879004327	10.530241250	3.367635750
C	29.136803161	10.054261000	3.823917500
C	30.330363388	10.638129750	3.313523500
C	30.448825013	9.126669000	5.664172250
C	31.643088679	9.347062000	4.920026250
C	32.903342443	9.126555750	5.538223250
C	34.096817330	9.373127250	4.799784000
C	34.233894725	9.172698250	7.582584000
C	35.423812992	8.998775000	6.814530500
C	36.694141679	9.098996750	7.448268750
C	37.883678763	8.953005250	6.673984000
C	38.047061819	10.141361750	9.193593750
C	39.232549753	9.610626750	8.601295500
C	40.508744507	10.010037500	9.092120250
C	8.896501137	15.216675000	9.069303750
C	10.087029783	14.601190500	9.566395000
C	11.366056179	15.081686500	9.152696000
C	12.560659171	14.445272500	9.619015000
C	12.693120518	16.096199250	7.372898250
C	13.890316608	15.790846000	8.085689000
C	15.149192345	16.013787500	7.467059750
C	16.350628583	15.673588500	8.154240500
C	16.438365593	16.146682250	5.395538000

C	17.631169144	16.258319500	6.156103500
C	18.879555045	16.243931250	5.481853750
C	20.063983957	16.407412500	6.244465250
C	20.218432793	15.310648250	3.681239000
C	21.402972240	15.826429000	4.290323000
C	22.674536317	15.437490500	3.779781250
C	23.866867656	15.936564250	4.386997250
C	24.018861562	13.693806000	2.723302250
C	25.208021933	14.432388250	3.003731500
C	26.479266190	13.839348750	2.758357250
C	27.671535760	14.564375500	3.058947500
C	27.815490290	11.796099250	2.733868250
C	29.006838601	12.568966000	2.615806000
C	30.270162551	11.923769250	2.721046250
C	31.464147035	12.694966500	2.626391500
C	31.587607516	10.136879000	3.744994000
C	32.782162962	10.733557500	3.252330250
C	34.039567204	10.209913750	3.657870500
C	35.235130874	10.821659000	3.185529000
C	35.359240747	9.126051000	5.404892000
C	36.552319008	9.399245250	4.674761250
C	37.816013575	9.130326500	5.269752750
C	39.008955700	9.431294500	4.549989000
C	39.154613767	9.030773250	7.310574000
C	40.343473012	8.912887750	6.530533250
C	13.841226552	14.929207500	9.209757250
C	15.041036872	14.267106750	9.631045250
C	16.330965171	14.750699000	9.234857000
C	17.591112058	15.980225250	7.544561750
C	18.795055242	15.711082250	8.248755250
C	20.001475300	16.192141750	7.643654500
C	21.218806607	16.082189250	8.354700250
C	21.331238395	16.394064500	5.589292250
C	22.531899671	16.550651000	6.347360500
C	23.799163455	16.482499000	5.694583000
C	25.002020797	16.576304000	6.460235500
C	25.137088653	15.556953000	3.864134250
C	26.333856827	16.027463500	4.486520250
C	27.603512959	15.658956250	3.956721750
C	28.798021672	16.096069000	4.606443250
C	28.940558349	13.972198750	2.801711000
C	30.134646866	14.681263000	3.130728500
C	31.401628625	14.091797750	2.857080750
C	32.596897264	14.783957750	3.213556500

C	32.724553598	12.040971250	2.709109500
C	33.920850780	12.810784500	2.640140500
C	35.179406290	12.150430750	2.696420000
C	36.376873841	12.920086750	2.656651000
C	36.493353154	10.279765000	3.566045500
C	37.689724703	10.908844250	3.117522000
C	38.949033232	10.353210750	3.475532250
C	40.145608377	10.999806750	3.051620000
C	40.273812915	9.141683000	5.133725500
C	18.801022090	14.744744500	9.313020250
C	21.190413789	15.228853250	9.463113250
C	22.476244172	16.394066250	7.754541750
C	23.684838758	16.080916750	8.449879000
C	24.944509370	16.323934750	7.851940500
C	26.125531209	15.911366500	8.541732500
C	26.269213872	16.511810750	5.815918250
C	27.462363657	16.545116750	6.601004750
C	28.730864862	16.513268250	5.959186750
C	29.920772563	16.505306250	6.748540250
C	30.067869208	15.742267750	4.067619750
C	31.261595236	16.146054500	4.739475750
C	32.531211137	15.809194000	4.189952250
C	33.723728597	16.182384750	4.880628500
C	33.861404993	14.198230250	2.922408000
C	35.057003205	14.872942750	3.307079750
C	36.319341688	14.295176000	2.994081500
C	37.515477132	14.952534000	3.404366250
C	37.634717377	12.256576250	2.683509250
C	38.832506779	13.026879250	2.673556250
C	40.090538875	12.363715500	2.672042500
C	23.641310798	15.126135250	9.493905500
C	26.045735638	14.897496000	9.529206750
C	27.393617909	16.204277250	7.975192250
C	28.573573007	15.778489000	8.651413000
C	29.845436178	16.103474750	8.105135250
C	31.026825789	15.661128500	8.768582750
C	31.191743734	16.504663500	6.108818750
C	32.379778439	16.464771000	6.899237000
C	33.652781094	16.488679500	6.262513000
C	34.840112764	16.419591000	7.051928750
C	34.992632117	15.862224250	4.319861250
C	36.184865112	16.206231750	5.024481250
C	37.452903860	15.903300750	4.453062000
C	38.645034042	16.221627500	5.168787250

C	38.776543652	14.386564750	3.067783500
C	39.972826204	15.028211750	3.500836000
C	28.486285450	14.737380750	9.608748000
C	32.300660300	16.011134250	8.239578500
C	33.483439724	15.547009000	8.887823000
C	34.759141948	15.916812750	8.374655000
C	35.942901149	15.427706750	9.003786250
C	36.113165404	16.465038250	6.416015250
C	37.300378818	16.365732750	7.202093000
C	38.573552558	16.431852000	6.568335500
C	39.761332870	16.304856750	7.349266250
C	39.911596012	15.938459250	4.584916000
C	37.219493747	15.815641500	8.505572500
C	38.404200216	15.302380750	9.114900250
C	39.681308508	15.708219750	8.632113500
N	21.163070645	13.105403750	13.293795750
N	16.964997752	12.975951500	13.238866000
N	19.033823042	15.073897500	13.157057500
N	19.092676329	11.001822500	13.215717750
C	21.921754395	14.244155250	13.324110250
C	21.961449398	11.995196750	13.292616250
C	16.172377782	14.086894250	13.148249250
C	16.201426494	11.841040750	13.270233500
C	21.438904589	15.554118250	13.317805250
C	21.532549523	10.665324000	13.258962250
C	16.602483380	15.410842750	13.032031500
C	16.679796389	10.526809750	13.272740500
C	20.094658181	15.918075500	13.217621500
C	20.204635447	10.225222250	13.243593250
C	17.928738621	15.851065250	13.044316250
C	18.029192012	10.159400000	13.258139000
C	23.282594841	13.828341250	13.344098500
C	23.307323756	12.462929500	13.311208250
C	14.825266816	13.626054000	13.134746000
C	14.842800401	12.262726000	13.211434750
C	22.454455809	16.641419250	13.400778250
C	22.598383924	9.631198250	13.271336000
C	15.530094102	16.431770500	12.908208250
C	15.650932226	9.458166250	13.246770000
C	19.646196895	17.296204000	13.129041000
C	19.831905139	8.822893500	13.320591250
C	18.303545927	17.255112250	13.015048000
C	18.484396329	8.782617250	13.331903750
C	22.606029113	17.385690250	14.570021750

C	23.469674205	9.526378750	14.356179000
C	23.270016630	16.927709750	12.308171000
C	22.735589735	8.744832250	12.202506750
C	14.637530745	16.645721500	13.958885000
C	15.612312092	8.546097250	12.190547750
C	15.396665981	17.179183500	11.738170500
C	14.683385626	9.369829750	14.249281250
C	23.562738018	18.388619750	14.640287000
C	24.456662740	8.552209250	14.370731500
C	24.221084601	17.933785250	12.377096500
C	23.729717113	7.778328000	12.215816250
C	13.631335973	17.592677000	13.841234750
C	14.611222240	7.589693500	12.121197000
C	14.384160158	18.119863500	11.621135250
C	13.690455844	8.403656500	14.183949000
C	24.371846369	18.665965500	13.546273000
C	24.590632969	7.677809250	13.300603250
C	13.501195450	18.330045250	12.672021000
C	13.644681020	7.518380250	13.115224250
H	20.148892170	13.090748750	13.276703500
H	17.979423711	12.986490500	13.245101250
H	24.128990812	14.495779250	13.363144000
H	24.179947362	11.830507750	13.289248000
H	13.956611083	14.258893500	13.053533000
H	13.989534204	11.604757250	13.195121000
H	20.292331819	18.158961000	13.148183500
H	20.521800065	7.997455250	13.385843500
H	17.614174822	18.080050750	12.936947000
H	17.844741914	7.918665250	13.410513500
H	21.979527529	17.169821000	15.428368250
H	23.356256950	10.198510500	15.199830000
H	23.147383128	16.363497000	11.393488500
H	22.066055159	8.825260500	11.353370500
H	14.746015791	16.076751750	14.875895500
H	16.358467208	8.605694750	11.406489000
H	16.080792372	17.008296250	10.913997250
H	14.720721605	10.052861500	15.090927000
H	23.678407420	18.957824250	15.556194750
H	25.121246820	8.473402250	15.224269000
H	24.843092051	18.143982750	11.513413250
H	23.830083132	7.098457250	11.376752250
H	12.947429433	17.755811250	14.667126000
H	14.583735239	6.900945250	11.283770000
H	14.284472384	18.692028750	10.705187000

H	12.946317582	8.344130000	14.970777000
H	25.117088353	19.451475750	13.604114500
H	25.362321628	6.916251250	13.314662250
H	12.713106595	19.069267000	12.581575250
H	12.859548971	6.772633000	13.059448750

References

1   Grimme, S.; Bannwarth, C. Ultra-Fast Computation of Electronic Spectra for Large Systems by Tight-Binding Based Simplified Tamm-Dancoff Approximation (sTDA-xTB). *J. Chem. Phys.* **2016**, *145,* 054103.

2   Seibert, J.; Pisarek, J.; Schmitz, S.; Bannwarth, C.; Grimme, S. Extension of the Element Parameter Set for Ultra-Fast Excitation Spectra Calculation (sTDA-xTB). *Mol. Phys.* **2019**, *117,* 1104-1116.

3   Hehn, A. S.; Sertcan, B.; Belleflamme, F.; Chulkov, S. K.; Watkins, M. B.; Hutter, J. Excited-State Properties for Extended Systems: Efficient Hybrid Density Functional Methods. *J. Chem. Theory Comput.* **2022**, *18,* 4186-4202.

4   Grimme, S.; Bannwarth, C.; Shushkov, P. A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements (Z = 1–86). *J. Chem. Theory Comput.* **2017**, *13,* 1989-2009.

5   Nurhuda, M.; Perry, C. C.; Addicoat, M. A. Performance of GFN1-xTB for Periodic Optimization of Metal Organic Frameworks. *Phys. Chem. Chem. Phys.* **2022**, *24,* 10906-10914.

6   Vicent-Luna, J. M.; Apergi, S.; Tao, S. Efficient Computation of Structural and Electronic Properties of Halide Perovskites Using Density Functional Tight Binding: GFN1-xTB Method. *J. Chem. Inf. Model.* **2021**, *61,* 4415-4424.

7   Hirata, S.; Head-Gordon, M. Time-Dependent Density Functional Theory within the Tamm–Dancoff Approximation. *Chem. Phys. Lett.* **1999**, *314,* 291-299.

8   Grimme, S. A Simplified Tamm-Dancoff Density Functional Approach for the Electronic Excitation Spectra of Very Large Molecules. *J. Chem. Phys.* **2013**, *138,* 244104.

9   Chen, W.-K.; Zhao, X.; Liu, X.-Y.; Xie, X.-Y.; Zeng, Y.; Cui, G. Photoinduced Nonadiabatic Dynamics of a Single-Walled Carbon Nanotube-Porphyrin Complex. *J. Phys. Chem. A* **2024**, *128,* 8803-8815.

10   Tully, J. C.; Preston, R. K. Trajectory Surface Hopping Approach to Nonadiabatic Molecular Collisions: The Reaction of H^+ with D_2. *J. Chem. Phys.* **1971**, *55,* 562-572.

11   Hammes-Schiffer, S.; Tully, J. C. Proton Transfer in Solution: Molecular Dynamics with Quantum Transitions. *J. Chem. Phys.* **1994**, *101,* 4657-4667.

12   Fang, Y.-G.; Peng, L.-Y.; Liu, X.-Y.; Fang, W.-H.; Cui, G. QM/MM Nonadiabatic Dynamics Simulation on Ultrafast Excited-State Relaxation in Osmium(II) Compounds in Solution. *Comput. Theor. Chem.* **2019**, *1155,* 90-100.

13   Chen, W.-K.; Sun, X.-W.; Fang, Q.; Liu, X.-Y.; Cui, G.-L. GW/BSE Nonadiabatic Dynamics Simulations on Excited-State Relaxation Processes of Zinc Phthalocyanine-Fullerene Dyads: Roles of Bridging Chemical Bonds. *Chin. J. Chem. Phys.* **2021**, *34,* 704-716.

14 Liu, X.-Y.; Chen, W.-K.; Fang, W.-H.; Cui, G. Nonadiabatic Dynamics Simulations for Photoinduced Processes in Molecules and Semiconductors: Methodologies and Applications. *J. Chem. Theory Comput.* **2023**, *19,* 8491-8522.

15 Zhang, Y.; Jia, M.-R.; Liu, X.-Y.; Fang, W.-H.; Cui, G. Photoinduced Dynamics of a Single-Walled Carbon Nanotube with a sp^3 Defect: The Importance of Excitonic Effects. *J. Phys. Chem. A* **2024**, *128,* 3311-3320.

16 Li, Z. W.; Yang, J. J.; Liu, X. Y.; Fang, W. H.; Wang, H.; Cui, G. Chemical Bonding as a New Avenue for Controlling Excited-State Properties and Excitation Energy-Transfer Processes in Zinc Phthalocyanine-Fullerene Dyads. *Chem. - Eur. J.* **2021**, *27,* 4159-4167.

17 Liu, X. Y.; Li, Z. W.; Fang, W. H.; Cui, G. Nonadiabatic Exciton and Charge Separation Dynamics at Interfaces of Zinc Phthalocyanine and Fullerene: Orientation Does Matter. *J. Phys. Chem. A* **2020**, *124,* 7388-7398.

18 Zhang, S.; Zeng, Y. P.; Wan, X. J.; Xu, D. H.; Liu, X. Y.; Cui, G.; Li, L. Ultrafast Exciton Delocalization and Localization Dynamics of a Perylene Bisimide Quadruple Π-Stack: A Nonadiabatic Dynamics Simulation. *Phys. Chem. Chem. Phys.* **2022**, *24,* 7293-7302.

19 Liu, X.-Y.; Zhang, Y.-H.; Fang, W.-H.; Cui, G. Early-Time Excited-State Relaxation Dynamics of Iridium Compounds: Distinct Roles of Electron and Hole Transfer. *J. Phys. Chem. A* **2018**, *122,* 5518-5532.

20 Ryabinkin, I. G.; Nagesh, J.; Izmaylov, A. F. Fast Numerical Evaluation of Time-Derivative Nonadiabatic Couplings for Mixed Quantum-Classical Methods. *J. Phys. Chem. Lett.* **2015**, *6,* 4200-4203.

21 Cui, G.; Thiel, W. Generalized Trajectory Surface-Hopping Method for Internal Conversion and Intersystem Crossing. *J. Chem. Phys.* **2014**, *141,* 124101.

22 Liu, X.-Y.; Xie, X.-Y.; Fang, W.-H.; Cui, G. Photoinduced Relaxation Dynamics of Nitrogen-Capped Silicon Nanoclusters: A TD-DFT Study. *Mol. Phys.* **2018**, *116,* 869-884.

23 Crespo-Otero, R.; Barbatti, M. Spectrum Simulation and Decomposition with Nuclear Ensemble: Formal Derivation and Application to Benzene, Furan and 2-Phenylfuran. *Theor. Chem. Acc.* **2014**, *131,* 89-102.

24 Barbatti, M.; Aquino, A. J. A.; Lischka, H. The UV Absorption of Nucleobases: Semi-Classical Ab Initio Spectra Simulations. *Phys. Chem. Chem. Phys.* **2010**, *12,* 4959−4967.