Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

The driving forces for twisted or planar intramolecular charge transfers

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Further discussion on excited state energy decomposition

The first excited state energy can be decomposed as follows:

$$E_{S1} = E_G + E_t + E_R \quad (1)$$

E_t is the vertical transition energy from ground state to Frank -Condon first excited state. The vertical transition energy can be decomposed as follows:

$$E_t = \sum_{he} \left(C_h^e\right)^2 (\varepsilon_e - \varepsilon_h) + E_{he} \quad (2)$$

ε_h and ε_e are the energy of the occupied (hole) and virtual (electron) orbitals, respectively, included in the transition. C_h^e is the coefficient for a particular pair of orbitals that contribute to the transition. E_{he} can be considered to be the energy of the hole and electron interactions.

To improve understanding and facilitate energy term calculation, we imposed a further simplification. In excited states with a multi-determinant character, the orbital pairs other than HOMO and LUMO have larger gaps. Therefore, they increase the $\sum_{he} C_h^e (E_e - E_h)$ term. These orbital pairs were incorporated because they can lower the excited state energy by lowering E_{he}, the hole-electron interactions, by changing the hole-electron distribution. Therefore, the contribution of other orbitals can be combined with hole-electron interaction term to single out the HOMO-LUMO gap.

$$\sum_{he} \left(C_h^e\right)^2 (\varepsilon_e - \varepsilon_h) + E_{he} = E_{gap} + E_{he}' \quad (3)$$

$$E_{he}' = \sum_{he \neq H,L} \left(C_h^e\right)^2 (\Delta\varepsilon_{he} - E_{gap}) + E_{he} \quad (4)$$

The transition energy then becomes:

$$E_t = E_{gap} + E_{he}' \quad (5)$$

$$E_{he} \leq E_{he}' \leq E_{HL} \quad (6)$$

where $\Delta\varepsilon_{he}$ is the gap between orbital pairs corresponding to a transition. E_{gap} is the HOMO-LUMO gap. $E_{he}^{'}$ is the modified hole-electron interaction term which is computed in this manuscript by subtracting E_{gap} from vertical transition energy. This term is larger than the original E_{he} (hole-electron interaction energy with multiple orbital pairs taken into consideration, thus the hole-electron distribution is optimized and transition energy is reduced), and smaller than the E_{HL} with only HOMO and LUMO taken into consideration.

To give further insight on this term, we refer to CIS theory in its simplest form by considering only the HOMO and LUMO. The excited Frank-Condon state energy in a vacuum can be written as follows:

$$E_t = E_{gap} - J_{HL} + K_{HL} \qquad 7$$

Alternatively, we can consider TDDFT theory in its simplest form, the SPA (single-pole approximation):

$$E_t = E_{gap} + K_{HL} + (1 - c_{HF})(hl|f_{xc}|lh) - c_{HF} J_{HL} \qquad 8$$

$$K_{HL} = (hl|lh) \text{ and } J_{HL} = (hh|ll) \qquad 9$$

J_{HL} is the Coulomb interaction between the hole in the HOMO and the electron in the LUMO. The K_{HL} can be considered the exchange interaction between the hole and electron. The c_{HF} is the Hartree-Fock exchange percent in the xc potential. f_{xc} is the exchange-correlation core. $(hl|f_{xc}|lh)$ is the exchange-correlation interaction between the hole and electron with h representing the HOMO and l the LUMO. By comparing eq 5 to eq 7, the $E_{he}^{'}$ can be written as follows in the CIS framework:

$$E_{he}^{'} \leq E_{HL} = K_{HL} - J_{HL} \qquad 10$$

The TDDFT framework yields the following：

$$E_{he}^{'} \leq E_{HL} = K_{HL} + (1 - c_{HF})(hl|f_{xc}|lh) - c_{HF} J_{HL} \qquad 11$$

This formula shows that the hole - electron interactions are determined by three terms, the exchange and correlation repulsion (the “repulsion” is used here because this term increases the energy, whereas the classical exchange - correlation term is negative because of the interactions between electrons) and Coulomb attraction between the hole and electron. The former term increases with increasing orbital overlap between the HOMO

and LUMO, and the magnitude of the latter term is the inverse of the distance between the hole and electron. Therefore, a larger orbital overlap increases the hole – electron exchange repulsion, whereas smaller hole and electron distances increase their Coulomb attraction.

Quantitative representation of hole and electron distribution

At first, we need to get the density distribution of hole and electrons. In single-electron excitation process, an electron leaves A and goes to B; where A and B are real space functions, and they will be respectively named as "hole" and "electron" in the following texts. If the excitation can be perfectly described as HOMO to LUMO transition, then A and B are just HOMO and LUMO, respectively. However, in most practical cases, this single-orbital pair model is not suitable, and the excitations have to be represented as the transition of multiple MO pairs with proper weighting coefficients. The most straightforward way to deal with electron excitation problem is CIS, the CIS excited state wave function is written as

$$\Psi^{ex} = \sum_{i\in occ}\sum_{l\in vir} w_i^l \Phi_i^l = \sum_{i\to l} w_i^l \Phi_i^l \quad (1)$$

where i and l respectively run over all occupied and all virtual MOs, Φ_i^l is the configuration state wave function corresponding to moving the electron from originally occupied MO i to virtual MO l. w is configuration coefficient.

The excited state density is written as

$$\rho^{ex} = \int \Psi^{ex}\Psi^{ex} d\mathbf{r}_{other} = \sum_{i\to l}\sum_{j\to m} w_i^l w_j^m \int \Phi_i^l \Phi_j^m d\mathbf{r}_{other} = \rho_{self}^{ex} + \rho_{cross}^{ex} \quad (2)$$

The ρ_{self}^{ex} term represents the contribution to excited state density from each orbital pairs.

$$\rho_{self}^{ex} = \sum_{i\to l} (w_i^l)^2 \int \Phi_i^l \Phi_i^l d\mathbf{r}_{other} \quad (3)$$

The ρ_{cross}^{ex} term represents multi-configuration character of the excited state

$$\rho_{cross}^{ex} = \sum_{i\to l}\sum_{j\to m} w_i^l w_j^m \int \Phi_i^l \Phi_j^m d\mathbf{r}_{other} \quad j \neq i \text{ or } m \neq l \quad (4)$$

The density difference between excited state and ground state is written as

$$\Delta\rho = \rho^{\mathrm{exc}} - \rho^0 = \sum_{i\to l} (w_i^l)^2 \int \Phi_i^l \Phi_i^l d\mathbf{r}_{\mathrm{other}} - \int \Phi^0 \Phi^0 d\mathbf{r}_{\mathrm{other}} + \rho_{\mathrm{cross}}^{\mathrm{exc}} \quad (5)$$

For CIS or TDDFT with TDA approximation we have

$$\sum_{i\to l} (w_i^l)^2 = 1 \quad (6)$$

Put 5 in to 4 we get

$$\begin{aligned}\Delta\rho &= \sum_{i\to 1}(w_i^1)^2\int \Phi_i^1\Phi_i^1 d\mathbf{r}_{\text{other}} - \sum_{i\to 1}(w_i^1)^2\int \Phi^0\Phi^0 d\mathbf{r}_{\text{other}} + \rho_{\text{cross}}^{\text{exc}} \\ &= \sum_{i\to 1}(w_i^1)^2\left(\int \Phi_i^1\Phi_i^1 d\mathbf{r}_{\text{other}} - \int \Phi^0\Phi^0 d\mathbf{r}_{\text{other}}\right) + \rho_{\text{cross}}^{\text{exc}} \\ &= \sum_{i\to 1}(w_i^1)^2(\rho_1 - \rho_i) + \rho_{\text{cross}}^{\text{exc}}\end{aligned} \quad 7$$

We also have

$$\Delta\rho = \rho^{ele} - \rho^{hole} \quad 8$$

Combine 7 and 8 we get

$$\rho^{ele} - \rho^{hole} = \sum_{i\to 1}(w_i^1)^2\rho_1 - \sum_{i\to 1}(w_i^1)^2\rho_i + \rho_{\text{cross}}^{\text{exc}} \quad 9$$

Since ρ_1 stands for density on virtual orbital and ρ_i stands for density on occupied orbital, we define

$$\rho_{self}^{\text{hole}} = \sum_{i\to 1}(w_i^1)^2\rho_i \qquad \rho_{self}^{\text{ele}} = \sum_{i\to 1}(w_i^1)^2\rho_1 \quad 10$$

Now we decompose the $\rho_{\text{cross}}^{\text{exc}}$ term

$$\begin{aligned}\rho_{\text{cross}}^{\text{exc}} &= \rho_{\text{cross}}^{\text{ele}} - \rho_{\text{cross}}^{\text{hole}} \\ \rho_{\text{cross}}^{\text{hole}} &= \sum_{i\to 1}\sum_{j\neq i\to 1} w_i^1 w_j^1 \varphi_i\varphi_j \\ \rho_{\text{cross}}^{\text{ele}} &= \sum_{i\to 1}\sum_{i\to m\neq 1} w_i^1 w_i^m \varphi_1\varphi_m\end{aligned} \quad 11$$

Put 11 and 10 into 9 we get

$$\rho^{ele} - \rho^{hole} = \rho_{self}^{\text{ele}} + \rho_{\text{cross}}^{\text{ele}} - \rho_{self}^{\text{hole}} - \rho_{\text{cross}}^{hole} \quad 12$$

So the ρ^{hole} and ρ^{ele} can be defined as

$$\rho^{hole} = \rho_{self}^{hole} + \rho_{cross}^{hole} = \sum_{i\to 1}(w_i^1)^2\int \varphi_i\varphi_i d\mathbf{r} + \sum_{i\to 1}\sum_{j\neq i\to 1} w_i^1 w_j^m \int \varphi_i\varphi_j d\mathbf{r} \quad 13$$

$$\rho^{ele} = \rho_{self}^{ele} + \rho_{cross}^{ele} = \sum_{i\to 1}(w_i^1)^2\int \varphi_1\varphi_1 d\mathbf{r} + \sum_{i\to 1}\sum_{i\to m\neq 1} w_i^1 w_i^m \int \varphi_1\varphi_m d\mathbf{r} \quad 14$$

Where φ denotes MO. "self" and "cross" stand for the contribution of local term and cross term to the hole/electron distribution.

After generalization, above definitions can also be applied to TDHF and TDDFT cases, where de-excitation occurs. The generalized local terms are

$$\rho_{self}^{hole} = \sum_{i\to 1}(w_i^1)^2\int \varphi_i\varphi_i d\mathbf{r} - \sum_{i\leftarrow 1}(w_i^1)^2\int \varphi_i\varphi_i d\mathbf{r} \quad 15$$

$$\rho_{self}^{ele} = \sum_{i\to 1}(w_i^1)^2\int \varphi_1\varphi_1 d\mathbf{r} - \sum_{i\leftarrow 1}(w_i^1)^2\int \varphi_1\varphi_1 d\mathbf{r} \quad 16$$

The generalized cross terms are

$$\rho_{cross}^{hole} = \sum_{i\to 1}\sum_{j\neq i\to 1} w_i^1 w_j^1\int \varphi_i\varphi_j d\mathbf{r} - \sum_{i\leftarrow 1}\sum_{j\neq i\leftarrow 1} w_i^1 w_j^1\int \varphi_i\varphi_j d\mathbf{r} \quad 17$$

$$\rho_{cross}^{ele} = \sum_{i\to 1}\sum_{i\to m\neq 1} w_i^1 w_i^m\int \varphi_1\varphi_m d\mathbf{r} - \sum_{i\leftarrow 1}\sum_{i\leftarrow m\neq 1} w_i^1 w_i^m\int \varphi_1\varphi_m d\mathbf{r} \quad 18$$

Note that the ρ^{hole} is simply the summation of occupied orbitals' contribution to the hole and the ρ^{ele} is the virtual orbitals' contribution to the electron. The integration of ρ^{hole} or ρ^{ele} over the whole space is exactly 1. During transition, one electron transit from the ρ^{hole} area to the ρ^{ele} area. So they do not correspond to the density difference between the ground state and the excited state. But their difference correspond to the unrelaxed density difference between excited state and ground state:

$$\Delta\rho = \rho^{ele} - \rho^{hole}$$

The distribution of hole and electron can be quantitatively represented in following ways.

The overlapping extent of hole and electron (O_{he}) is characterized by:

$$\int \min(\rho^{hole}(r), \rho^{ele}(r))dr$$

The min(a,b) is the smaller of a and b. Centroid of hole and electron can be calculated. For example, X coordinate of centroid of electron is

$$X_{ele} = \int x\rho^{ele}(r)dr$$

where x is X component of r. The distance between the two centroids measures the distance between hole and electron (D_{he})

$$D_{CT,x} = \left|X_{ele} - X_{hole}\right|$$

$$D_{CT} = \sqrt{D_{CT,x}^2 + D_{CT,y}^2 + D_{CT,z}^2}$$

Excited state energy decomposition Data calculated at CAM-B3LYP level

Table S1. Energy terms needed to perform excited state energy decomposition calculated at CAM-B3LYP level

	Conf.	Ground state(a.u.)	HOMO(eV)	LUMO(eV)	H-L gap (eV)	FC state (a.u.)	hole-elec.(eV)	Relaxed S1 state(a.u.)
BN	Planar	-82.0220	-10.1591	0.5698	10.7289	-81.7550	-3.4628	-81.7866
	Twist	-81.9644	-7.7916	-0.4596	7.3320	-81.8550	-4.3545	-81.8561
MABN	Planar	-419.0517	-7.3826	0.1361	7.5187	-418.8792	-2.8258	-418.8854
	Twist	-419.0333	-8.0398	-0.4795	7.5603	-418.8718	-3.1652	-418.8811
DMABN	Planar	-458.3405	-7.2305	0.1856	7.4161	-458.1687	-2.7427	-458.1741
	Twist	-458.3214	-7.4787	-0.4465	7.0321	-458.1755	-3.0619	-458.1857
35DCDMA	Planar	-550.5635	-7.7894	-1.0096	6.7799	-550.4164	-2.7780	-550.4220
	Twist	-550.5456	-7.8890	-1.2224	6.6666	-550.4046	-2.8299	-550.4172
DCS	Planar	-766.6995	-6.5761	-0.9483	5.6277	-766.5673	-2.0302	-766.5767
	Twist	-766.6826	-7.2291	-1.2352	5.9940	-766.5396	-2.1053	-766.5497
MP2BN	Planar	-572.6247	-7.3726	-0.6866	6.6860	-572.4655	-2.3251	-572.4764
	Twist	-572.6219	-7.5802	-0.6213	6.9589	-572.4568	-2.4675	-572.4726
THT	Planar	-1166.5459	-9.9558	-4.3177	5.6381	-1166.4190	-2.1836	-1166.4235
	Twist	-1166.5403	-9.7977	-4.1985	5.5991	-1166.4202	-2.3299	-1166.4299

Table S2. Excited state energy decomposition data calculated at CAM-B3LYP level

	ΔE_G (eV)	ΔE_{gap} (eV)	ΔE_{he} (eV)	ΔE_R (eV)	ΔE_{SI} (eV)
BN	1.5659	-3.3969	-0.8917	0.8325	-1.8902
MABN	0.4989	0.0416	-0.3394	-0.0842	0.1169
DMABN	0.5176	-0.3840	-0.3192	-0.1313	-0.3169
35DCDMA	0.4865	-0.1132	-0.0519	-0.1910	0.1304
DCS	0.4618	0.3663	-0.0751	-0.0196	0.7334
MP2BN	0.0770	0.2729	-0.1119	-0.2149	0.1042
THT	0.1526	-0.0389	-0.1463	-0.1418	-0.1744

Table S3. Dipole moments of all the states calculated at CAM-B3LYP level

	Ground state (D)	PICT state (D)	TICT state (D)	FC state (D)	ΔDM (D)
BN	1.8877	2.6686	4.3451	1.6265	1.6765
MABN	7.6092	9.2094	13.8514	9.0208	4.642
DMABN	7.829	9.9153	15.0947	9.7265	5.1794
35DCDMA	7.3381	11.7051	15.2919	11.3841	3.5868
DCS	9.58	16.0514	23.5519	17.7181	7.5005
MP2BN	5.4051	10.6312	17.7501	12.7666	7.1189
THT	2.0975	6.3763	15.1687	6.9568	8.7924

Excited state energy decomposition data calculated at B3LYP level

Table S4. Energy terms needed to perform excited state energy decomposition calculated at B3LYP level

	Conf.	Ground state(a.u.)	HOMO(eV)	LUMO(eV)	H-L gap(eV)	FC state (a.u.)	hole-elec.(eV)	Relaxed S1 state(a.u.)
BN	Planar	-82.0554	-8.3427	-0.1720	8.1707	-81.7957	-1.1028	-81.8049
	Twist	-81.9982	-6.0767	-1.7067	4.3700	-81.8936	-1.5229	-81.8968
MABN	Planar	-419.1879	-5.9994	-1.0888	4.9107	-419.0246	-0.4666	-419.0308
	Twist	-419.1689	-6.3366	-1.7372	4.5994	-419.0365	-0.9967	-419.0443
DMABN	Planar	-458.4939	-5.8672	-1.0471	4.8201	-458.3323	-0.4208	-458.3385
	Twist	-458.4745	-5.8302	-1.7095	4.1207	-458.3585	-0.9635	-458.3677
35DCDMA	Planar	-550.7331	-6.3910	-2.2208	4.1702	-550.6008	-0.5710	-550.6085
	Twist	-550.7149	-6.2367	-2.4586	3.7781	-550.6079	-0.8686	-550.6202
DCS	Planar	-766.9732	-5.3200	-2.0692	3.2508	-766.8604	-0.1808	-766.8633
	Twist	-766.9569	-5.6519	-2.4113	3.2407	-766.8584	-0.5595	-766.8671
MP2BN	Planar	-572.8164	-5.9687	-1.8725	4.0962	-572.6788	-0.3515	-572.6814
	Twist	-572.8128	-6.0607	-1.8839	4.1768	-572.6870	-0.7515	-572.6982
THT	Planar	-1166.8009	-8.7046	-5.4421	3.2624	1166.6883	-0.1989	-1166.6936
	Twist	-1166.7939	-8.4205	-5.4794	2.9411	1166.7115	-0.6989	-1166.7181

Table S5. Excited state energy decomposition data calculated at B3LYP level

	ΔE_G (eV)	ΔE_{gap} (eV)	ΔE_{he} (eV)	ΔE_R (eV)	ΔE_{S1} (eV)
BN	1.5562	-3.8007	-0.4202	0.1640	-2.5006
MABN	0.5191	-0.3113	-0.5301	-0.0455	-0.3677
DMABN	0.5285	-0.6994	-0.5426	-0.0826	-0.7960
35DCDMA	0.4962	-0.3921	-0.2975	-0.1234	-0.3168
DCS	0.4435	-0.0101	-0.3787	-0.1572	-0.1025
MP2BN	0.0979	0.0806	-0.4000	-0.2349	-0.4564
THT	0.1916	-0.3214	-0.5000	-0.0365	-0.6663

Excited state energy decomposition Data calculated at BHandHLYP level

Table S6. Energy terms needed to perform excited state energy decomposition calculated at BHandHLYP level

	Conf.	Ground state(a.u.)	HOMO(eV)	LUMO(eV)	H-L gap(eV)	FC state (a.u.)	hole-elec.(eV)	Relaxed S1 state(a.u.)
BN	Planar	-81.9996	-9.8807	0.4759	10.3566	-81.7219	-2.8017	-81.9996
	Twist	-81.9439	-7.6308	-0.4275	7.2033	-81.8167	-3.7414	-81.9439
MABN	Planar	-418.9276	-7.0270	0.1404	7.1674	-418.7464	-2.2383	-418.9276
	Twist	-418.9099	-7.9443	-0.4849	7.4594	-418.7332	-2.6508	-418.9099
DMABN	Planar	-458.2065	-6.8882	0.1886	7.0767	-458.0253	-2.1466	-458.2065
	Twist	-458.1885	-7.3671	-0.4449	6.9222	-458.0277	-2.5458	-458.1885
35DCDMA	Planar	-550.3941	-7.4523	-1.0469	6.4054	-550.2385	-2.1714	-550.3941
	Twist	-550.3777	-7.7875	-1.2322	6.5554	-550.2199	-2.2611	-550.3777
DCS	Planar	-766.4928	-6.1758	-0.9701	5.2057	-766.3595	-1.5785	-766.4928
	Twist	-766.4783	-7.0422	-1.2694	5.7728	-766.3314	-1.7755	-766.4783
MP2BN	Planar	-572.4629	-6.9192	-0.7056	6.2136	-572.3026	-1.8528	-572.4629
	Twist	-572.4599	-7.1323	-0.6408	6.4914	-572.2939	-1.9740	-572.4599
THT	Planar	-1166.3006	-9.6380	-4.3659	5.2721	-1166.1696	-1.7075	-1166.3006
	Twist	-1166.2943	-9.4807	-4.2445	5.2361	-1166.1720	-1.9096	-1166.2943

Table S7. Excited state energy decomposition data calculated at BHandHLYP level

	ΔE_G (eV)	ΔE_{gap} (eV)	ΔE_{he} (eV)	ΔE_R (eV)	ΔE_{S1} (eV)
BN	1.5153	-3.1533	-0.9397	0.2567	-2.3211
MABN	0.4799	0.2920	-0.4125	-0.0812	0.2782
DMABN	0.4887	-0.1546	-0.3991	-0.1351	-0.2001
35DCDMA	0.4456	0.1499	-0.0897	-0.1905	0.3153
DCS	0.3959	0.5671	-0.1970	-0.0646	0.7013
MP2BN	0.0805	0.2778	-0.1212	-0.1456	0.0915
THT	0.1720	-0.0359	-0.2021	-0.1525	-0.2185

Excited state energy decomposition Data calculated at HF level

Table S8. Energy terms needed to perform excited state energy decomposition calculated at HF level

	Conf.	Ground state(a.u.)	HOMO(eV)	LUMO(eV)	H-L gap(eV)	FC state (a.u.)	hole-elec.(eV)	Relaxed S1 state(a.u.)
BN	Planar	-81.5038	-11.9150	1.5478	13.4628	-81.2069	-5.3851	-81.2183
	Twist	-81.4518	-9.7626	1.4022	11.1648	-81.2897	-6.7541	-81.2917
MABN	Planar	-416.5234	-8.2393	2.4019	10.6412	-416.3268	-5.2896	-416.3360
	Twist	-416.5084	-9.6039	1.8404	11.4443	-416.2991	-5.7483	-416.3103
DMABN	Planar	-455.5471	-8.1100	2.5553	10.6653	-455.3491	-5.2755	-455.3525
	Twist	-455.5334	-9.5003	1.9574	11.4576	-455.3242	-5.7641	-455.3355
35DCDMA	Planar	-547.2748	-8.6986	1.3519	10.0505	-547.0951	-5.1630	-547.1023
	Twist	-547.2637	-9.9327	1.2409	11.1735	-547.0585	-5.5884	-547.0664
DCS	Planar	-761.9986	-7.1897	1.3791	8.5688	-761.8458	-4.4122	-761.8625
	Twist	-761.9886	-8.0262	1.1201	9.1462	-761.8278	-4.7717	-761.8456
MP2BN	Planar	-569.1580	-8.0882	1.6703	9.7586	-568.9715	-4.6830	-568.9970
	Twist	-569.1566	-8.3685	1.7394	10.1079	-568.9477	-4.4235	-568.9592
THT	Planar	-1161.0922	-10.7574	-1.8746	8.8828	-1160.9352	-4.6109	-1160.9454
	Twist	-1161.0877	-10.7561	-1.5808	9.1754	-1160.9084	-4.2964	-1160.9317

Table S9. Excited state energy decomposition data calculated at HF level

	ΔE_G (eV)	ΔE_{gap} (eV)	ΔE_{he} (eV)	ΔE_R (eV)	ΔE_{S1} (eV)
BN	1.4139	-2.2980	-1.3690	0.2556	-1.9975
MABN	0.4089	0.8032	-0.4586	-0.0555	0.6979
DMABN	0.3742	0.7923	-0.4886	-0.2155	0.4623
35DCDMA	0.2998	1.1230	-0.4255	-0.0194	0.9780
DCS	0.2724	0.5774	-0.3595	-0.0297	0.4607
MP2BN	0.0369	0.3493	0.2596	0.3831	1.0289
THT	0.1216	0.2926	0.3146	-0.3557	0.3731

Excited state energy decomposition Data calculated at BLYP level

Table S10. Energy terms needed to perform excited state energy decomposition calculated at BLYP level

	Conf.	Ground state(a.u.)	HOMO(eV)	LUMO(eV)	H-L gap(eV)	FC state (a.u.)	hole-elec.(eV)	Relaxed S1 state(a.u.)
BN	Planar	-82.0058	-7.0612	-0.7119	6.3494	-81.7634	0.2480	-81.7715
	Twist	-81.9477	-4.8073	-2.4156	2.3917	-81.8595	0.0086	-81.8668
MABN	Planar	-419.0212	-5.0729	-1.6540	3.4189	-418.8735	0.6024	-418.8809
	Twist	-419.0012	-5.0383	-2.3228	2.7155	-418.9014	-0.0001	-418.9094
DMABN	Planar	-458.3002	-4.9499	-1.6082	3.3416	-458.1552	0.6053	-458.1646
	Twist	-458.2799	-4.5860	-2.2989	2.2872	-458.1959	-0.0010	-458.2057
35DCDMA	Planar	-550.5302	-5.4351	-2.7373	2.6978	-550.4168	0.3881	-550.4283
	Twist	-550.5111	-4.9833	-3.0113	1.9721	-550.4378	0.0219	-550.4499
DCS	Planar	-766.6404	-4.5341	-2.4981	2.0360	-766.5444	0.5762	-766.5616
	Twist	-766.6229	-4.4326	-2.8826	1.5500	-766.5659	0.0010	-766.5743
MP2BN	Planar	-572.5861	-5.0987	-2.3740	2.7247	-572.4657	0.5517	-572.4670
	Twist	-572.5820	-5.0835	-2.4556	2.6279	-572.4853	0.0028	-572.4952
THT	Planar	-1166.4308	-7.8596	-5.8324	2.0273	-1166.3315	0.6754	-1166.3394
	Twist	-1166.4231	-7.4819	-5.9978	1.4841	-1166.3685	0.0029	-1166.3758

Table S11. Excited state energy decomposition data calculated at BLYP level

	ΔE_G (eV)	ΔE_{gap} (eV)	ΔE_{he} (eV)	ΔE_R (eV)	ΔE_{S1} (eV)
BN	1.5812	-3.9577	-0.2394	0.0216	-2.5944
MABN	0.5450	-0.7034	-0.6026	-0.0164	-0.7773
DMABN	0.5516	-1.0545	-0.6063	-0.0085	-1.1177
35DCDMA	0.5217	-0.7257	-0.3662	-0.0175	-0.5877
DCS	0.4750	-0.4860	-0.5752	0.2420	-0.3441
MP2BN	0.1119	-0.0969	-0.5489	-0.2329	-0.7668
THT	0.2090	-0.5432	-0.6725	0.0165	-0.9900

Transitions and corresponding orbitals calculated at CAM-B3LYP level

Table S12. Calculated wavelength, osillator strength, and orbitals of first three excited state transitions. For each compound, the transition data of all four geometries are listed. P for planar. T for Twisted. G for ground state. S1 for first singlet excited state.

	Wavelength(nm)	osillator strength	orbitals
BN-P-G	170.63	0.0000	H-1->L+1 (84%), H-1->L+4 (15%)
	167.71	0.0605	HOMO->LUMO (95%)
	152.02	0.1972	HOMO->L+1 (88%)
BN-P-S1	249.59	0.0000	HOMO->L+1 (88%), HOMO->L+4 (12%)
	201.37	0.0182	HOMO->LUMO (96%)
	181.98	0.0849	HOMO->L+2 (97%)
BN-T-G	416.40	0.0000	HOMO->LUMO (96%)
	236.70	0.0188	HOMO->L+1 (96%)
	190.19	0.0000	HOMO->L+4 (87%)
BN-T-S1	427.76	0.0000	HOMO->LUMO (96%)
	239.66	0.0212	HOMO->L+1 (95%)
	191.72	0.0000	HOMO->L+4 (87%)
MABN-P-G	264.20	0.0603	HOMO->LUMO (25%), HOMO->L+2 (64%)
	245.93	0.4558	HOMO->LUMO (69%), HOMO->L+2 (23%)
	241.70	0.0003	HOMO->L+1 (89%)
MABN-P-S1	285.18	0.0796	HOMO->LUMO (75%), HOMO->L+2 (17%)
	250.90	0.3758	HOMO->LUMO (20%), HOMO->L+2 (69%)
	247.79	0.0005	HOMO->L+1 (89%)
MABN-T-G	282.10	0.0000	HOMO->LUMO (94%)
	236.12	0.0004	HOMO->L+1 (98%)
	235.32	0.0079	H-2->LUMO (58%), H-1->L+1 (39%)
MABN-T-S1	319.60	0.0000	HOMO->LUMO (94%)
	241.15	0.0064	H-2->LUMO (57%), H-1->L+1 (40%)
	239.19	0.0480	H-1->LUMO (16%), HOMO->L+1 (82%)
DMABN-P-G	265.30	0.0358	H-1->LUMO (10%), HOMO->L+2 (89%)
	250.97	0.5549	HOMO->LUMO (94%)
	238.75	0.0278	HOMO->L+1 (88%)
DMABN-P-S1	283.10	0.0385	HOMO->LUMO (91%)
	253.50	0.4839	HOMO->L+1 (93%)
	241.08	0.0291	HOMO->L+2 (88%)
DMABN-T-G	312.22	0.0000	HOMO->LUMO (94%)
	260.28	0.0001	HOMO->L+1 (99%)
	237.78	0.0087	HOMO->L+2 (80%)
DMABN-T-S1	363.86	0.0000	HOMO->LUMO (95%)
	266.09	0.0003	HOMO->L+1 (99%)
	246.51	0.0119	HOMO->L+2 (83%)
35DCDMA-P-G	309.82	0.0670	HOMO->LUMO (95%)
	246.58	0.1554	H-1->LUMO (10%), HOMO->L+1 (87%)

	227.84	0.0269	HOMO->L+2 (87%)
35DCDMA-P-S1	335.87	0.0623	HOMO->LUMO (96%)
	252.45	0.0811	H-1->LUMO (17%), HOMO->L+1 (80%)
	230.39	0.0275	HOMO->L+2 (87%)
35DCDMA-T-G	323.14	0.0001	HOMO->LUMO (99%)
	305.87	0.0000	HOMO->L+1 (92%)
	246.04	0.0066	H-2->LUMO (60%), H-1->L+1 (37%)
35DCDMA-T-S1	395.89	0.0001	HOMO->LUMO (99%)
	318.75	0.0000	HOMO->L+1 (91%)
	253.78	0.0144	H-2->LUMO (65%), H-1->L+1 (32%)
DCS-P-G	344.65	1.2917	HOMO->LUMO (91%)
	278.98	0.0884	HOMO->L+1 (14%), HOMO->L+3 (55%), HOMO->L+6 (15%)
	255.83	0.0213	HOMO->L+2 (84%)
DCS-P-S1	400.54	1.3704	HOMO->LUMO (96%)
	289.42	0.0986	HOMO->L+2 (51%), HOMO->L+3 (18%), HOMO->L+6 (15%)
	276.82	0.0166	H-3->LUMO (18%), HOMO->L+2 (19%), HOMO->L+3 (45%)
DCS-T-G	318.84	0.0000	HOMO->LUMO (71%), HOMO->L+2 (19%)
	310.76	1.2492	H-1->LUMO (96%)
	254.42	0.0002	HOMO->L+2 (14%), HOMO->L+4 (78%)
DCS-T-S1	372.58	0.0000	HOMO->LUMO (77%), HOMO->L+2 (13%)
	345.17	1.3142	H-1->LUMO (97%)
	262.42	0.0004	HOMO->L+1 (10%), HOMO->L+4 (86%)
MP2BN-P-G	286.31	0.6604	HOMO->LUMO (96%)
	257.82	0.0091	H-2->LUMO (19%), HOMO->L+1 (74%)
	228.45	0.0205	H-1->LUMO (92%)
MP2BN-P-S1	328.91	0.7237	HOMO->LUMO (97%)
	272.15	0.0155	H-2->LUMO (15%), HOMO->L+1 (77%)
	238.26	0.0084	HOMO->L+2 (76%)
MP2BN-T-G	276.05	0.0023	HOMO->LUMO (95%)
	236.76	0.0088	HOMO->L+1 (97%)
	235.92	0.0000	H-3->LUMO (58%), H-2->L+1 (37%)
MP2BN-T-S1	342.13	0.0000	HOMO->LUMO (96%)
	252.09	0.0096	HOMO->L+1 (97%)
	243.75	0.0094	H-3->LUMO (61%), H-2->L+1 (35%)
THT-P-G	358.91	0.9203	HOMO->LUMO (95%)
	274.82	0.0141	H-3->LUMO (17%), HOMO->L+2 (69%)
	261.29	0.0348	H-2->LUMO (38%), H-1->LUMO (46%)
THT-P-S1	390.49	0.8691	HOMO->LUMO (95%)
	279.27	0.0202	H-2->LUMO (14%), H-1->LUMO (51%), HOMO->L+2 (16%)
	277.61	0.0277	H-3->LUMO (19%), H-1->LUMO (18%), HOMO->L+2 (40%)
THT-T-G	379.25	0.0000	HOMO->LUMO (92%)
	273.98	0.0314	HOMO->L+1 (11%), HOMO->L+3 (29%), HOMO->L+6 (53%)
	258.07	0.6995	H-3->LUMO (23%), H-2->LUMO (29%),
THT-T-S1	451.80	0.0000	HOMO->LUMO (93%)
	281.28	0.3663	H-1->LUMO (92%)
	272.93	0.2453	H-3->LUMO (29%), H-2->LUMO (58%)

XYZ coordinates of all the geometries

Table S13. Xyz coordinates of all the geometries calculated at CAM-B3LYP level

		Ground state				S1 state		
		x	y	z		x	y	z
BN-P	H	-0.84300	-1.15975	0.00000	H	-0.84375	-1.21824	0.00000
	B	0.00003	0.77514	0.00000	B	0.00002	0.73748	0.00000
	H	-1.04243	1.35231	0.00000	H	-0.76231	1.72754	0.00000
	H	1.04226	1.35263	0.00000	H	0.76210	1.72768	0.00000
	H	0.84288	-1.15994	0.00000	H	0.84378	-1.21824	0.00000
	N	0.00003	-0.60871	0.00000	N	0.00002	-0.67231	0.00000
BN-T	H	-1.19540	0.00000	0.83985	H	-1.21592	0.00003	0.83914
	B	0.80541	0.00000	0.00000	B	0.82876	0.00000	0.00001
	H	1.43181	-1.02581	0.00000	H	1.38169	-1.06188	-0.00006
	H	1.43181	1.02581	0.00000	H	1.38169	1.06188	-0.00002
	H	-1.19546	0.00000	-0.83981	H	-1.21592	-0.00003	-0.83913
	N	-0.64283	0.00000	0.00000	N	-0.63933	0.00000	0.00001
MABN-P	C	-0.37381	1.39968	0.00000	C	0.39010	1.42779	-0.00009
	C	0.98963	1.24599	0.00000	C	-0.99814	1.26261	-0.00008
	C	1.56071	-0.02892	0.00000	C	-1.54586	-0.02664	-0.00016
	C	0.72302	-1.13904	0.00000	C	-0.74483	-1.20181	-0.00029
	C	-0.64848	-0.99244	0.00000	C	0.66122	-1.04182	-0.00022
	C	-1.22566	0.28340	-0.00002	C	1.20394	0.24351	-0.00017
	H	-0.80270	2.39497	0.00001	H	0.85409	2.40407	-0.00004
	H	1.63117	2.11744	0.00001	H	-1.66026	2.11611	0.00006
	H	1.15502	-2.13128	0.00001	H	-1.20507	-2.17628	-0.00021
	H	-1.27397	-1.87353	0.00001	H	1.30631	-1.90793	-0.00011
	C	2.98024	-0.18842	0.00000	C	-2.96080	-0.16381	0.00012
	N	4.12078	-0.31525	0.00000	N	-4.10327	-0.29285	0.00035
	C	-3.53475	-0.61777	0.00000	C	3.55375	-0.57329	0.00032
	H	-4.53750	-0.19601	-0.00003	H	4.53224	-0.10056	0.00042
	H	-3.43486	-1.25027	-0.88695	H	3.46513	-1.20428	0.88701
	H	-3.43491	-1.25026	0.88696	H	3.46542	-1.20452	-0.88622
	N	-2.57848	0.45978	0.00001	N	2.53852	0.45017	0.00000
	H	-2.92373	1.40232	0.00001	H	2.83912	1.41295	0.00006
MABN-T	C	0.51299	-1.19790	-0.21162	C	0.50993	-1.24164	-0.20893
	C	-0.86120	-1.20502	-0.06945	C	-0.84249	-1.21946	-0.07563
	C	-1.55353	0.00023	0.00273	C	-1.56757	0.00001	-0.00322
	C	-0.86114	1.20523	-0.06937	C	-0.84245	1.21944	-0.07563
	C	0.51317	1.19806	-0.21154	C	0.50997	1.24160	-0.20896
	C	1.21804	0.00008	-0.28610	C	1.22234	-0.00002	-0.27868
	H	1.06123	-2.12928	-0.27250	H	1.04280	-2.18146	-0.26216
	H	-1.40449	-2.13915	-0.01711	H	-1.38170	-2.15609	-0.01317
	H	-1.40416	2.13954	-0.01698	H	-1.38163	2.15610	-0.01323

	H	1.06131	2.12946	-0.27233	H	1.04285	2.18142	-0.26231
	C	-2.97980	0.00001	0.14817	C	-2.96836	0.00003	0.14441
	N	-4.12017	-0.00030	0.26448	N	-4.11650	0.00002	0.26571
	C	3.49770	-0.00017	0.71047	C	3.49965	0.00002	0.69509
	H	4.53131	-0.00164	0.36652	H	4.53841	-0.00084	0.36845
	H	3.35886	0.88599	1.33996	H	3.28017	0.87524	1.31561
	H	3.35681	-0.88509	1.34121	H	3.27893	-0.87395	1.31686
	N	2.62155	-0.00011	-0.43466	N	2.60334	-0.00007	-0.41407
	H	3.01201	-0.00006	-1.35732	H	3.04607	-0.00001	-1.34231
	C	-0.18517	1.20320	-0.00001	C	0.20469	-1.23402	-0.00042
	C	1.19074	1.19734	0.00000	C	-1.21179	-1.23081	-0.00048
	C	1.90212	0.00001	0.00000	C	-1.88800	0.00000	-0.00002
	C	1.19074	-1.19734	0.00000	C	-1.21179	1.23082	0.00039
	C	-0.18517	-1.20320	-0.00001	C	0.20470	1.23402	0.00036
	C	-0.91500	0.00000	-0.00002	C	0.89595	0.00000	0.00001
	H	-0.69813	2.15270	0.00000	H	0.73378	-2.17163	-0.00084
	H	1.72862	2.13645	0.00000	H	-1.77041	-2.15371	-0.00086
	H	1.72863	-2.13644	0.00001	H	-1.77040	2.15372	0.00079
	H	-0.69813	-2.15270	0.00001	H	0.73379	2.17164	0.00083
DMABN-P	C	3.33051	0.00000	0.00001	C	-3.31334	0.00001	0.00002
	N	4.47811	-0.00001	0.00001	N	-4.46196	-0.00001	0.00006
	C	-3.00951	-1.25017	0.00001	C	3.01158	1.24351	-0.00076
	H	-4.07591	-1.04239	-0.00002	H	4.07352	1.02098	-0.00082
	H	-2.78441	-1.85156	-0.88600	H	2.77687	1.83517	-0.88659
	H	-2.78445	-1.85153	0.88605	H	2.77718	1.83616	0.88451
	C	-3.00951	1.25016	0.00001	C	3.01157	-1.24352	0.00080
	H	-2.78440	1.85156	0.88601	H	2.77685	-1.83518	0.88663
	H	-2.78447	1.85153	-0.88603	H	2.77718	-1.83617	-0.88446
	H	-4.07592	1.04239	0.00006	H	4.07352	-1.02099	0.00086
	N	-2.28239	0.00000	0.00000	N	2.26149	0.00000	0.00002
	C	-0.18665	1.19813	-0.00007	C	-0.19281	0.87681	0.87677
	C	1.19487	1.20541	-0.00006	C	1.16595	0.86381	0.86376
	C	1.89079	0.00000	-0.00001	C	1.89679	-0.00004	-0.00004
	C	1.19487	-1.20541	0.00005	C	1.16592	-0.86388	-0.86382
	C	-0.18666	-1.19812	0.00005	C	-0.19284	-0.87685	-0.87682
	C	-0.89534	0.00000	-0.00003	C	-0.90699	-0.00001	-0.00002
	H	-0.73682	2.13087	-0.00011	H	-0.72743	1.54247	1.54242
	H	1.74087	2.13943	-0.00010	H	1.70878	1.52600	1.52592
DMABN-T	H	1.74087	-2.13942	0.00010	H	1.70873	-1.52608	-1.52598
	H	-0.73682	-2.13087	0.00009	H	-0.72748	-1.54251	-1.54245
	C	3.32449	0.00000	0.00000	C	3.30345	-0.00008	-0.00002
	N	4.47079	0.00000	0.00001	N	4.45890	-0.00010	-0.00002
	C	-2.99770	0.00010	1.26685	C	-3.02328	-0.88238	0.88233
	H	-4.07234	0.00004	1.09008	H	-4.10116	-0.78156	0.78149
	H	-2.76209	-0.88450	1.87116	H	-2.70645	-1.90647	0.66833
	H	-2.76216	0.88482	1.87100	H	-2.70647	-0.66841	1.90643
	C	-2.99776	-0.00010	-1.26682	C	-3.02331	0.88236	-0.88230

	H	-2.76219	0.88450	-1.87113	H	-2.70647	1.90645	-0.66832
	H	-2.76223	-0.88482	-1.87098	H	-2.70653	0.66839	-1.90641
	H	-4.07239	-0.00006	-1.09000	H	-4.10119	0.78154	-0.78144
	N	-2.30796	0.00000	0.00000	N	-2.30921	-0.00001	0.00000
	C	0.24999	1.19878	-0.00001	C	0.28128	-1.22650	0.00022
	C	-1.13729	1.18698	0.00000	C	-1.14305	-1.21886	0.00010
	C	-1.85602	0.00000	0.00000	C	-1.82671	0.00000	-0.00009
	C	-1.13730	-1.18698	-0.00001	C	-1.14305	1.21886	-0.00024
	C	0.24999	-1.19878	-0.00001	C	0.28128	1.22650	-0.00031
	C	0.97933	0.00000	-0.00002	C	0.95940	0.00000	-0.00002
	H	0.75523	2.15183	0.00000	H	0.80037	-2.16916	0.00045
	H	-2.93575	0.00000	0.00000	H	-2.90878	0.00000	-0.00008
	H	0.75522	-2.15183	-0.00002	H	0.80037	2.16916	-0.00044
	C	-1.83968	2.43926	0.00001	C	-1.86096	-2.43789	0.00014
	N	-2.39447	3.44160	0.00002	N	-2.42032	-3.44491	0.00012
35DCDMA-P	C	-1.83969	-2.43926	0.00000	C	-1.86096	2.43789	-0.00010
	N	-2.39449	-3.44159	0.00000	N	-2.42031	3.44491	0.00007
	C	3.07090	-1.25228	0.00003	C	3.08555	1.24253	0.00054
	H	4.13730	-1.04608	0.00008	H	4.14759	1.02324	0.00019
	H	2.84565	-1.85300	0.88653	H	2.84468	1.83367	-0.88414
	H	2.84574	-1.85301	-0.88649	H	2.84506	1.83263	0.88603
	C	3.07090	1.25227	-0.00001	C	3.08555	-1.24253	-0.00049
	H	2.84568	1.85300	-0.88651	H	2.84459	-1.83370	0.88415
	H	2.84572	1.85299	0.88651	H	2.84515	-1.83260	-0.88602
	H	4.13730	1.04606	-0.00003	H	4.14759	-1.02324	-0.00002
	N	2.34626	-0.00001	-0.00001	N	2.33825	0.00000	0.00001
	C	0.25701	-1.19529	-0.00002	C	0.31394	-1.22399	0.00002
	C	-1.13474	-1.19627	-0.00001	C	-1.13143	-1.21538	-0.00002
	C	-1.83899	0.00001	-0.00001	C	-1.80037	0.00001	-0.00002
	C	-1.13472	1.19628	0.00000	C	-1.13142	1.21539	0.00001
	C	0.25703	1.19528	-0.00001	C	0.31396	1.22398	-0.00004
	C	0.96519	-0.00001	-0.00003	C	0.93790	-0.00001	-0.00003
	H	0.79888	-2.13203	-0.00002	H	0.86298	-2.15260	0.00005
	H	-2.91998	0.00002	0.00000	H	-2.88295	0.00002	-0.00002
	H	0.79891	2.13201	0.00001	H	0.86301	2.15258	-0.00004
	C	-1.84624	-2.44196	-0.00001	C	-1.83899	-2.43795	-0.00006
35DCDMA-P	N	-2.40981	-3.43935	-0.00001	N	-2.38409	-3.45346	-0.00009
	C	-1.84621	2.44199	0.00001	C	-1.83895	2.43797	0.00006
	N	-2.40976	3.43938	0.00003	N	-2.38404	3.45349	0.00011
	C	3.06440	-0.00007	1.26866	C	3.06174	-0.00003	1.25034
	H	4.13848	-0.00002	1.09095	H	4.13811	0.00001	1.11051
	H	2.82931	0.88499	1.87167	H	2.74065	0.87522	1.82235
	H	2.82936	-0.88520	1.87158	H	2.74072	-0.87535	1.82230
	C	3.06446	0.00004	-1.26862	C	3.06180	0.00001	-1.25031
	H	2.82937	-0.88499	-1.87167	H	2.74071	-0.87521	-1.82237
	H	2.82948	0.88519	-1.87154	H	2.74084	0.87535	-1.82225
	H	4.13854	-0.00003	-1.09086	H	4.13816	-0.00007	-1.11043

	N	2.37450	-0.00002	0.00000	N	2.37221	-0.00002	0.00000
	C	-3.52044	-1.28508	0.00005	C	3.52080	-1.30820	-0.00029
	C	-2.14529	-1.39016	0.00004	C	2.16776	-1.45731	-0.00025
	C	-1.31099	-0.27390	-0.00001	C	1.27558	-0.35051	-0.00004
	C	-1.93611	0.97468	-0.00006	C	1.88331	0.93958	0.00014
	C	-3.30569	1.10327	-0.00005	C	3.24264	1.09702	0.00019
	C	-4.14345	-0.02787	0.00002	C	4.11317	-0.01509	-0.00006
	H	-4.11104	-2.18888	0.00008	H	4.14384	-2.18992	-0.00045
	H	-1.70052	-2.37910	0.00007	H	1.74700	-2.45588	-0.00034
	H	-1.33977	1.87828	-0.00012	H	1.26201	1.82402	0.00033
	H	-3.73203	2.09532	-0.00011	H	3.64697	2.09837	0.00039
	C	0.13442	-0.46132	-0.00001	C	-0.11765	-0.56326	0.00021
	C	1.07595	0.48597	0.00000	C	-1.07501	0.45294	0.00004
	H	0.44463	-1.50188	-0.00001	H	-0.44667	-1.59461	0.00059
	H	0.77584	1.52855	0.00002	H	-0.73036	1.48053	-0.00004
	C	2.52193	0.27272	-0.00001	C	-2.47284	0.27868	-0.00008
	C	3.36527	1.38622	0.00010	C	-3.33215	1.41040	-0.00016
	C	3.11767	-0.99297	-0.00011	C	-3.09403	-1.00648	0.00008
DCS-P	C	4.73845	1.25401	0.00011	C	-4.69163	1.28324	-0.00014
	H	2.92871	2.37755	0.00018	H	-2.88802	2.39912	-0.00024
	C	4.48666	-1.13749	-0.00010	C	-4.45751	-1.13143	0.00022
	H	2.50275	-1.88255	-0.00020	H	-2.48632	-1.90067	0.00021
	C	5.31165	-0.01314	0.00000	C	-5.28351	0.00168	0.00004
	H	5.37334	2.13009	0.00019	H	-5.32512	2.16032	-0.00025
	H	4.93069	-2.12420	-0.00019	H	-4.91215	-2.11386	0.00037
	C	-6.12040	1.40516	-0.00009	C	6.05131	1.46209	-0.00004
	H	-7.20148	1.29471	-0.00002	H	7.13377	1.37541	-0.00004
	H	-5.84271	1.98559	0.88554	H	5.75476	2.03106	-0.88617
	H	-5.84281	1.98543	-0.88586	H	5.75477	2.03112	0.88606
	C	-6.34185	-1.08421	0.00011	C	6.33871	-1.01849	0.00009
	H	-6.16960	-1.70426	-0.88546	H	6.18263	-1.63991	0.88648
	H	-6.16966	-1.70406	0.88582	H	6.18280	-1.63994	-0.88631
	H	-7.38664	-0.78544	0.00004	H	7.37215	-0.68498	0.00019
	C	6.73505	-0.16342	0.00001	C	-6.69624	-0.13950	-0.00002
	N	7.87550	-0.28473	0.00001	N	-7.84192	-0.25110	-0.00006
	N	-5.50932	0.09615	0.00000	N	5.46645	0.13790	0.00000
	C	3.52052	1.28440	0.00010	C	3.52210	1.32302	-0.00010
	C	2.14221	1.40544	0.00007	C	2.16163	1.42369	-0.00023
	C	1.31706	0.28217	-0.00005	C	1.30230	0.29417	-0.00026
	C	1.92641	-0.97413	-0.00016	C	1.94081	-0.98501	-0.00013
	C	3.30111	-1.09349	-0.00013	C	3.29517	-1.11788	0.00010
DCS-T	C	4.12226	0.03269	0.00002	C	4.11460	0.03341	0.00006
	H	4.14764	2.16786	0.00018	H	4.13951	2.21288	-0.00015
	H	1.69246	2.39167	0.00013	H	1.71565	2.41177	-0.00035
	H	1.32261	-1.87225	-0.00029	H	1.33810	-1.88281	-0.00014
	H	3.76278	-2.07374	-0.00023	H	3.74416	-2.10460	0.00018
	C	-0.13424	0.47640	-0.00005	C	-0.10336	0.46833	-0.00028

	C	-1.07012	-0.47295	-0.00004	C	-1.06571	-0.50006	-0.00024
	H	-0.44267	1.51692	-0.00003	H	-0.42693	1.50472	-0.00030
	H	-0.76544	-1.51404	-0.00003	H	-0.76198	-1.54109	-0.00028
	C	-2.51936	-0.26751	-0.00003	C	-2.48523	-0.28845	-0.00008
	C	-3.35373	-1.38628	0.00005	C	-3.35112	-1.40001	-0.00041
	C	-3.11936	0.99495	-0.00009	C	-3.09360	0.98378	0.00036
	C	-4.72810	-1.26181	0.00008	C	-4.71761	-1.26124	-0.00025
	H	-2.91123	-2.37490	0.00010	H	-2.92048	-2.39434	-0.00073
	C	-4.48939	1.13203	-0.00007	C	-4.45901	1.12913	0.00033
	H	-2.50875	1.88745	-0.00016	H	-2.47977	1.87415	0.00068
	C	-5.30673	0.00240	0.00002	C	-5.29732	0.01012	0.00006
	H	-5.35848	-2.14100	0.00014	H	-5.35416	-2.13675	-0.00044
	H	-4.93941	2.11590	-0.00012	H	-4.89780	2.11881	0.00064
	C	6.21833	-0.16208	-1.26494	C	6.22432	-0.16139	-1.24737
	H	7.28864	-0.26311	-1.08889	H	7.29826	-0.24504	-1.10439
	H	5.90113	-1.02013	-1.87083	H	5.84011	-1.01397	-1.81412
	H	6.06681	0.74090	-1.86951	H	5.97613	0.73055	-1.82852
	C	6.21825	-0.16221	1.26506	C	6.22424	-0.16108	1.24766
	H	6.06659	0.74067	1.86973	H	5.97614	0.73110	1.82848
	H	5.90108	-1.02039	1.87077	H	5.83987	-1.01341	1.81467
	H	7.28859	-0.26310	1.08906	H	7.29817	-0.24490	1.10477
	C	-6.73152	0.14491	0.00004	C	-6.71432	0.16448	0.00025
	N	-7.87236	0.25984	0.00006	N	-7.85666	0.28924	0.00041
	N	5.53035	-0.09818	0.00003	N	5.51771	-0.09603	0.00011
	C	-1.94359	0.99108	-0.56784	C	0.10289	-0.15215	0.00958
	C	-0.56640	0.90220	-0.58443	C	-0.60191	1.03718	-0.35430
	C	0.09164	-0.20625	-0.04858	C	-1.96301	1.07605	-0.37509
	C	-0.68426	-1.23203	0.49617	C	-2.72515	-0.07320	-0.01790
	C	-2.06101	-1.15727	0.50752	C	-2.04945	-1.27012	0.30323
	H	-2.44007	1.85363	-0.99214	C	-0.68766	-1.32478	0.29607
	H	0.00315	1.69449	-1.05003	H	-0.05941	1.91755	-0.66475
	H	-0.19119	-2.09214	0.92910	H	-2.47842	1.97989	-0.66984
	H	-2.64831	-1.95851	0.93596	H	-2.62709	-2.15055	0.55223
	C	1.54720	-0.34970	-0.08375	H	-0.19143	-2.24884	0.55822
	C	2.27792	-1.47935	-0.37790	C	1.50773	-0.30053	-0.01410
MP2BN-P	N	2.44179	0.67006	0.15973	C	2.24649	-1.52385	-0.14044
	C	3.64443	-1.13901	-0.31793	N	2.45635	0.71633	0.07071
	H	1.85950	-2.43651	-0.64409	C	3.59125	-1.21321	-0.14741
	C	3.70993	0.18482	0.02174	H	1.79977	-2.49488	-0.26752
	H	4.48519	-1.78675	-0.50334	C	3.69853	0.16654	-0.01256
	H	4.56112	0.82299	0.19316	H	4.42146	-1.89328	-0.24351
	C	2.14557	2.01772	0.60090	H	4.57814	0.78808	0.04032
	H	1.97723	2.69158	-0.24067	C	-4.13592	-0.02247	-0.01562
	H	1.26356	2.02126	1.23738	N	-5.28902	0.02578	-0.01387
	H	2.98831	2.39005	1.17974	C	2.22705	2.10612	0.41336
	C	-2.70148	-0.03928	-0.02039	H	1.95857	2.70041	-0.46041
	C	-4.13089	0.04963	-0.00190	H	1.43261	2.17838	1.15353

	N	-5.27504	0.12202	0.01358	H	3.14154	2.50994	0.84297
MP2BN-T	C	0.10052	-0.26114	-0.02002	C	0.13451	-0.27790	-0.03395
	C	-0.61650	0.13994	-1.14386	C	-0.61125	0.12484	-1.19419
	C	-1.99045	0.27952	-1.09721	C	-1.95912	0.28727	-1.12519
	C	-2.67057	0.01940	0.08832	C	-2.67667	0.06080	0.08373
	C	-1.96710	-0.38318	1.21929	C	-1.93949	-0.36596	1.22485
	C	-0.59342	-0.51922	1.15917	C	-0.59148	-0.53523	1.17896
	H	-0.08691	0.33487	-2.06755	H	-0.10184	0.29262	-2.13493
	H	-2.54199	0.58713	-1.97557	H	-2.50449	0.58796	-2.01069
	H	-2.50059	-0.58966	2.13750	H	-2.46981	-0.56807	2.14672
	H	-0.04520	-0.83958	2.03583	H	-0.06692	-0.87576	2.06300
	C	1.56990	-0.41037	-0.07655	C	1.55157	-0.41782	-0.08493
	C	2.33025	-1.50596	-0.39720	C	2.39794	-1.53871	-0.40391
	N	2.42383	0.62616	0.21201	N	2.42461	0.63385	0.20018
	C	3.68975	-1.12362	-0.30425	C	3.69752	-1.14935	-0.30691
	H	1.94263	-2.47620	-0.66286	H	2.00952	-2.50664	-0.67015
	C	3.71181	0.19114	0.06898	C	3.68394	0.21948	0.07399
	H	4.55198	-1.74437	-0.48397	H	4.58773	-1.73142	-0.47660
	H	4.53911	0.85742	0.24957	H	4.51753	0.88070	0.25105
	C	-4.09614	0.16400	0.14414	C	-4.06894	0.23996	0.14511
	N	-5.23535	0.28154	0.18946	N	-5.21446	0.38978	0.19623
	C	2.03659	1.98118	0.54045	C	1.97920	1.96992	0.57749
	H	1.66528	2.51344	-0.33680	H	1.37360	2.39171	-0.21976
	H	1.26043	1.98376	1.30431	H	1.37591	1.91166	1.47901
	H	2.90499	2.50918	0.92781	H	2.85372	2.59168	0.75192
THT-P	C	6.50597	-0.86053	-0.23665	C	-2.47066	0.69977	0.14512
	C	5.10233	-0.34374	-0.11559	C	-2.69179	-0.60649	-0.27760
	C	4.01586	-1.19062	-0.23831	C	-3.94621	-1.18286	-0.22635
	C	4.87576	1.02040	0.12168	C	-5.01941	-0.44452	0.25433
	C	2.73809	-0.66440	-0.12230	C	-4.79334	0.87122	0.65748
	C	3.60996	1.54871	0.24147	C	-3.54065	1.45535	0.60541
	C	2.52950	0.68390	0.11967	C	-0.35755	0.19061	-0.67606
	S	1.20948	-1.48491	-0.26837	H	-4.09524	-2.19985	-0.56704
	N	1.16921	1.00312	0.22782	H	-5.62769	1.46075	1.01718
	C	0.34695	-0.02680	0.03924	H	-3.40931	2.48242	0.91618
	C	0.75320	2.33408	0.66546	C	1.08699	0.10502	-0.39772
	C	-1.09049	-0.00566	0.04902	C	2.03581	0.48816	-1.36908
	C	-1.80413	-1.10857	0.54477	C	1.56930	-0.39761	0.83493
	C	-1.83259	1.04682	-0.50943	C	3.37245	0.38545	-1.14232
	C	-3.17077	-1.14863	0.52235	H	1.67567	0.85722	-2.31950
	C	-3.19978	1.01254	-0.55595	C	2.89695	-0.51045	1.09159
	C	-3.92314	-0.08422	-0.02912	H	0.85106	-0.69073	1.58864
	N	-5.27057	-0.11686	-0.05813	C	3.85714	-0.12426	0.10286
	C	-5.99066	-1.26881	0.46055	H	4.06537	0.66305	-1.92089
	C	-6.02249	0.98817	-0.63016	H	3.22543	-0.87159	2.05369
	H	-5.81055	1.92477	-0.11002	C	6.16515	0.27403	-0.59913
	H	-5.80016	1.11783	-1.69210	H	7.10032	0.40609	-0.06390

	H	-7.08367	0.78346	-0.53157	H	6.32511	-0.43266	-1.41564
	H	-7.05650	-1.10431	0.33958	H	5.86333	1.23645	-1.00171
	H	-5.72615	-2.18129	-0.07852	C	5.68342	-0.88931	1.53626
	H	-5.79074	-1.41852	1.52388	H	5.65787	-0.20515	2.38641
	H	-3.67041	-2.00871	0.93972	H	5.11305	-1.78391	1.76866
	H	-3.72184	1.83394	-1.02123	H	6.71343	-1.17901	1.35302
	H	-1.26952	-1.93933	0.98895	N	-1.14262	1.09758	0.04502
	H	-1.32798	1.88820	-0.96510	C	-0.78061	2.49857	0.12122
	H	0.77355	3.03680	-0.16655	H	-1.19230	2.93647	1.02824
	H	-0.24825	2.27994	1.07793	H	0.30107	2.59622	0.16423
	H	1.43883	2.67001	1.43971	H	-1.14983	3.05487	-0.74538
	H	3.47343	2.60663	0.41691	S	-1.20976	-1.33259	-0.87865
	H	4.16273	-2.24637	-0.42620	C	-6.39249	-1.04812	0.34486
	H	5.72799	1.68248	0.21181	H	-7.15731	-0.33839	0.02877
	H	7.07060	-0.66673	0.67681	H	-6.47830	-1.93625	-0.28011
	H	6.52300	-1.93296	-0.42264	H	-6.62306	-1.34173	1.37123
	H	7.03197	-0.36686	-1.05540	N	5.16412	-0.23762	0.33520
THT-T	C	6.54238	-0.74306	0.00003	C	-6.54450	-0.79853	0.00044
	C	5.11771	-0.27303	-0.00007	C	-5.13008	-0.28992	0.00034
	C	4.06881	-1.17167	-0.00001	C	-4.05329	-1.16865	-0.00002
	C	4.83751	1.10514	-0.00010	C	-4.87007	1.07929	0.00050
	C	2.76811	-0.68412	0.00003	C	-2.76608	-0.67046	-0.00024
	C	3.55439	1.59736	-0.00005	C	-3.58331	1.58788	0.00020
	C	2.50961	0.67923	0.00002	C	-2.51532	0.69913	-0.00017
	S	1.26830	-1.56498	0.00003	S	-1.26616	-1.59640	-0.00055
	N	1.13968	0.95485	0.00003	N	-1.17078	1.01689	-0.00032
	C	0.36605	-0.11691	0.00003	C	-0.35111	-0.11147	-0.00033
	C	0.63630	2.32832	0.00002	C	-0.70859	2.38305	-0.00032
	C	-1.09814	-0.10749	0.00004	C	1.10662	-0.09010	-0.00017
	C	-1.80969	-0.10292	1.19872	C	1.84442	-0.07918	-1.21068
	C	-1.80964	-0.10292	-1.19866	C	1.84417	-0.07939	1.21050
	C	-3.18408	-0.08675	1.20497	C	3.20231	-0.07330	-1.22697
	C	-3.18404	-0.08676	-1.20497	C	3.20206	-0.07348	1.22709
	C	-3.91913	-0.07745	-0.00002	C	3.93804	-0.07689	0.00013
	N	-5.27477	-0.06311	-0.00003	N	5.26939	-0.08589	0.00026
	C	-6.00716	-0.07559	1.25276	C	6.02700	-0.09546	-1.25207
	C	-6.00713	-0.07573	-1.25283	C	6.02678	-0.09568	1.25273
	H	-5.77027	0.79795	-1.86528	H	5.80229	0.79202	1.84318
	H	-5.79605	-0.97652	-1.83536	H	5.79295	-0.98665	1.83473
	H	-7.07183	-0.05564	-1.04196	H	7.08586	-0.09991	1.02381
	H	-7.07185	-0.05528	1.04187	H	7.08604	-0.09922	-1.02297
	H	-5.79627	-0.97641	1.83532	H	5.79363	-0.98659	-1.83403
	H	-5.77015	0.79805	1.86521	H	5.80224	0.79209	-1.84264
	H	-3.69541	-0.08824	2.15495	H	3.72368	-0.06970	-2.17138
	H	-3.69532	-0.08824	-2.15498	H	3.72321	-0.06994	2.17162
	H	-1.28074	-0.11760	2.14431	H	1.29763	-0.08520	-2.14362
	H	-1.28067	-0.11760	-2.14423	H	1.29718	-0.08554	2.14332

	H	0.99553	2.84104	-0.89041	H	-1.06310	2.91405	0.88633
	H	-0.44780	2.30528	0.00005	H	0.37690	2.40929	-0.00036
	H	0.99559	2.84107	0.89041	H	-1.06318	2.91406	-0.88692
	H	3.37238	2.66312	-0.00005	H	-3.42069	2.65698	0.00031
	H	4.25893	-2.23709	-0.00001	H	-4.22578	-2.23764	-0.00010
	H	5.66521	1.80348	-0.00018	H	-5.70306	1.77185	0.00081
	H	7.07142	-0.37337	0.87993	H	-7.08799	-0.45018	-0.87951
	H	6.60642	-1.82963	-0.00145	H	-6.57521	-1.88730	0.00160
	H	7.07244	-0.37087	-0.87819	H	-7.08859	-0.44825	0.87924