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Electronic Supporting Information

Evaluating the Nature of Vertical Excited-States of Fused-Ring Electron Acceptors Using TD-DFT and Density-Based Charge Transfer

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S1. Comparison of the energies of vertical excited states with experiment

The $E_{ver\text{-}absorb}$ values (in nm) for all FREAs strictly obey the order RSH < GH < GGA as shown in Table S1. This depicts that $E_{ver\text{-}absorb}$ is inversely proportional to the exact exchange ratio in a functional except for LC-ωPBE and LC-PBE but the difference in the values given by both functionals is small. Generally, PBE0 provides the excellent quantitative agreement with experimentally measured λ_{max}, as well as shows a regular methodical change of λ_{max} values and thus approves the utmost predictive competence. We first analyze the quantitative agreements of $E_{ver\text{-}absorb}$ with experimental λ_{max} and then discuss the patterns in the change of all molecule excitation energies.

Table S1. Experimental λ_{max} and calculated $E_{ver\text{-}absorb}$ values of FREAs[a]

FREA	$E_{ver\text{-}absorb}$												λ_{max}	
	B3LYP		PBE0		CAM-B3LYP		PBE		LC-PBE		LC-ωPBE		Exp.	
	nm	eV	nm	eV	nm	eV	nm	eV	nm	eV	nm	eV	nm	eV
CBM[21]	618	2.01	571	2.17	463	2.67	918	1.35	402	3.08	410	3.02	497	2.49
FBR[22]	591	2.09	558	2.22	468	2.64	775	1.6	408	3.03	416	2.98	488	2.54
IDSe-T-IC[16]	776	1.59	733	1.69	600	2.06	995	1.24	518	2.39	525	2.36	680	1.82
IDTIDSe-IC[15]	756	1.64	709	1.74	568	2.18	964	1.28	496	2.5	503	2.46	701	1.76
IDTIDT-IC[14]	746	1.66	699	1.77	557	2.22	1000	1.24	484	2.56	491	2.52	696	1.78
O-IDTBR[19]	752	1.65	704	1.76	561	2.21	966	1.28	466	2.66	476	2.60	650	1.91
EH-IDTBR[19]	756	1.64	708	1.75	563	2.20	972	1.27	469	2.64	478	2.59	650	1.91
IDT-NTI-2EH[23]	792	1.57	734	1.69	556	2.23	1065	1.16	457	2.71	466	2.66	696	1.78
A2[24]	795	1.56	744	1.66	593	2. 09	1051	1.17	495	2.50	506	2.45	707	1.75
BTCN-M[18]	725	1.71	679	1.82	543	2.28	1043	1.18	470	2.63	478	2.59	622	1.99
MeIC[20]	699	1.77	666	1.86	562	2.20	858	1.44	493	2.51	500	2.48	674	1.83
ITTIC[17]	781	1.58	730	1.69	581	2.13	1048	1.18	495	2.50	503	2.46	700	1.77

[a] X in PCM-TD-X/6-31G(d,p) represents the functional used. $E_{ver\text{-}absorb}$ and λ_{max} are the computed and experimental vertical transition energy of the first excited state, respectively. All the experimental and calculated values are in chloroform solutions.

The $E_{ver\text{-}absorb}$ values calculated using GHs are the furthermost accurate ones among three methods with MAEs of 0.23 and 0.12 eV for B3LYP and PBE0, respectively (see Table S2 and

Fig. S1a). A moderate quantity of exact-exchange seems to be essential to accurately predict the experimental excitation energies of FREAs. The PBE0 outperforms B3LYP in any statistical parameter (see Table S2). The $E_{ver\text{-}absorb}$ values calculated using PBE0 are in better agreement with the experimentally measured data for all compounds. The B3LYP trends also agree well with the experimental results as well, but the variations are larger as compared to those from PBE0. For example, PBE0 provides the lowest error of 0.01 eV for IDTIDT-IC, whereas the B3LYP gives 0.12 eV for the same molecule as shown in Table S3. The minimum deviation given by B3LYP is 0.06 for MeIC while -0.03 through PBE0. For an individual compound, the amounts of errors from B3LYP and PBE0 follow a common pattern. As both give a large error for a specific FREA (i.e. 0.32 and 0.48 eV for CBM through PBE0 and B3LYP respectively) but with a larger deviation by B3LYP (see Table S3). The errors are mostly positive for both B3LYP and PBE0 (see Table S3). A positive deviation indicates a more outstanding approach than one providing a negative deviation if vibronic effects are to be taken into consideration, as reported by Ferrer and co-workers.[1] The bathochromic shift (9 nm red-shifted) provided by the experimental result going from FBR to CBM, is successfully reproduced by GHs and more accurately by PBE0 (13 nm). All the methods provide an accurate validation for IDTIDSe-IC > MeIC, and ITTIC > BTCN-M while IDTIDT-IC > IDSe-T-IC is only valid for PBE. CBM > FBR is valid for GHs and GGA functionals but not for RSHs. One essential finding in Table S1 is that for the same experimental value of λ_{max} (650 nm) for two candidates (ca. O-IDTBR, and EH-IDTBR), all functionals follow the same order EH-IDTBR > O-IDTBR but no proper order for another pair (ca. IDTIDT-IC, and IDT-NTI-2EH) of the same experimental value.

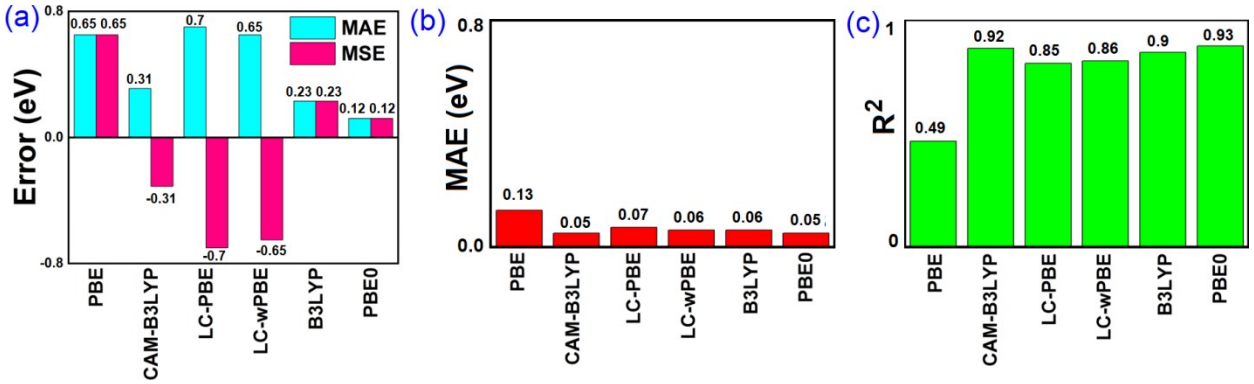

Fig. S1. Comparison between MAEs obtained from (a) unmodified data calculated with PCM-TD/6-31G(d,p) using each functional and (b) the linearly corrected data, (c) Comparison of determination coefficients (R^2) obtained by relating the actual data calculated with PCM-TD/6-31G(d,p) using each functional and the experimental results.

The CAM-B3LYP functional with MAE 0.31 eV gives a superior quantitative agreement than LC-ωPBE with 0.65 eV among RSHs as given in Table S2 and Fig. S1a. The RSHs functionals overestimate and produce a significant variance as a function of their exact-exchange percentage and range-separation parameter ω. The default values of ω for CAMY-B3LYP and LC-ωPBE are 0.34 and 0.4 $Bohr^{-1}$, respectively. A high value of ω would result in more region in space where an exact-exchange is incorporated than DFT exchange.[2] Moreover, LC-ωPBE and LC-PBE contain the maximum amount of exact-exchange (100% at long range) amongst the used functionals. Consequently, a higher value of ω and a greater fraction of exact-exchange in both LC-PBE and LC-ωPBE result in severely overestimated transition energies.

The PBE, on the other hand, significantly underestimates the excitation energies with MAE 0.65 eV (see Table S1 and Fig. S1a), which is consistent with their well-known findings for π-conjugated systems.[3] The primary cause of such large underestimations is an improper depiction of CT or delocalized transitions, particularly in the case of CBM (MAX. DEV. (+) = 1.14 eV). The GHs help to reduce the CT deviation through adding a specific amount of the exact-exchange over the inter-electronic space lowering the deviation from 1.14 for PBE to 0.32 eV for

PBE0 (see Table S3). This suggests that a greater exact-exchange fraction would be needed for correct characterization of CT excitation.

The RSH functional CAM-B3LYP has the lowest CT excitation error of -0.10 eV for FBR. This functional diminishes the underestimation of the transition energy associated with the CT excited-state by concurrently adding a larger percentage of exact-exchange at long-range and a smaller amount at short-range to describe well the particle-hole interaction. A balance in the exact-exchange and the DFT-exchange at an intermediate distance completes the picture. The conclusion is in agreement with the previous research, showing that CAM-B3LYP has the ability to reliably replicate the response properties and electronic excitation spectra of robust CT donor-acceptor systems.[4-6] So far, we have focused on reliably regenerating λ_{max}, which has resulted in a certain rating of the functionals that have been checked. Nonetheless, such a rating may obscure the comparative performance of the functionals established on the methodical shift of λ_{max} for the FREAs. For instance, the MAE standard hints that GHs to be the furthermost accurate ones while the relatively larger inconsistency of the calculated excitation energies may propose differently. This system-dependent performance of GHs is revealed in the incomparable MAE and MSE as shown in Table S2. In this regard, CAM-B3LYP also displays the superior performance to other RSHs (see Table S2). Its stable and systematic overestimation of λ_{max} produces a brilliant R^2 value of 0.92 with the experimental data. The reasonable correlation for CAM-B3LYP (R^2 = 0.92) means that the calculated transition energies might be efficiently calibrated to correctly calculate λ_{max} of new FREAs based on their mother molecules considered in this work. The R^2 values for GHs, PBE0 (R^2 = 0.93), and B3LYP (R^2 = 0.90) are all outstanding, with PBE being the worst (R^2 = 0.49). The performance of the LC-PBE (R^2 = 0.85) and LC-ωPBE (R^2 = 0.86) are lying between GGAs and GHs.

Table S2. Statistical analysis for the whole set of transitions without fitting

Parameter	PBE	B3LYP	PBE0	CAM-B3LYP	LC-PBE	LC-ωPBE
R^2	0.49	0.90	0.93	0.92	0.85	0.86
MSE	0.65	0.23	0.12	-0.31	-0.70	-0.65
MAE	0.65	0.23	0.12	0.31	0.70	0.65
RMS	0.68	0.26	0.16	0.33	0.70	0.66
MAX. DEV. (+)	1.14	0.48	0.32	-	-	-
MAX. DEV. (-)	-	-	-0.03	-0.45	-0.93	-0.88

Note: R^2, determination coefficient; MSE, the mean signed error; MAE, mean absolute error; RMS, root mean squared error; MAX. DEV. (+) and MAX. DEV. (-) are maximum positive deviation and maximum negative deviation obtained by relating the theoretical and experimental results, respectively. All the values are in eV except R^2.

Table S3. $E_{ver\text{-}absorb}$, λ_{max} and deviation (λ_{max} - $E_{ver\text{-}absorb}$) of theoretical value from experimental one for all molecules using B3LYP, PBE0, CAM-B3LYP and PBE for all 12 NFAs [a]

Substance	$E_{ver\text{-}absorb}$ (ev)				λ_{max}	Deviation (λ_{max} - $E_{ver\text{-}absorb}$) (ev)			
	B3LYP	PBE0	CAM-B3LYP	PBE	(ev)	B3LYP	PBE0	CAM-B3LYP	PBE
CBM	2.01	2.17	2.67	1.35	2.49	0.48	0.32	-0.18	1.14
FBR	2.09	2.22	2.64	1.6	2.54	0.45	0.32	-0.1	0.94
IDSe-T-IC	1.59	1.69	2.06	1.24	1.82	0.23	0.13	-0.24	0.58
IDTIDSe-IC	1.64	1.74	2.18	1.28	1.76	0.12	0.02	-0.42	0.48
IDTIDT-IC	1.66	1.77	2.22	1.24	1.78	0.12	0.01	-0.44	0.54
O-IDTBR	1.65	1.76	2.21	1.28	1.91	0.26	0.15	-0.3	0.63
EH-IDTBR	1.64	1.75	2.20	1.27	1.91	0.27	0.16	-0.29	0.64
IDT-NTI-2EH	1.57	1.69	2.23	1.16	1.78	0.21	0.09	-0.45	0.62
A2	1.56	1.66	2.09	1.17	1.75	0.19	0.09	-0.34	0.58
BTCN-M	1.71	1.82	2.28	1.18	1.99	0.28	0.17	-0.29	0.81
MeIC	1.77	1.86	2.20	1.44	1.83	0.06	-0.03	-0.37	0.39
ITTIC	1.58	1.69	2.13	1.18	1.77	0.19	0.08	-0.36	0.59

[a] $E_{ver\text{-}absorb}$ and λ_{max} are the computed vertical and experimental maximum excitation energy of the first excited state, respectively. All the experimental and calculated values are in chloroform solution.

S2. Calibration of vertical excitation energy

The comparatively worthy correlation presented by GHs and RSHs with the experimental data allows one to calibrate the computed excitation energy to provide a more accurate calculation of λ_{max} of a newly designed compound. In this respect, Equations S1 to S4 have been developed based on the linear fitting of calculated $E_{ver\text{-}absorb}$ values with the experimental λ_{max} in chloroform

solution when applying the linear regression analysis. The results for calibrated data are plotted in Fig. S1b and Fig. S1-S2. Simple linear regression involves the calculation of a linear polynomial that determines the best fit between the value of $E_{vert\text{-}absorb}$ and experimental λ_{max}. Statistical analysis of the linearly corrected data using Equations S1-S4 for numerous functionals is given in Table S4. The calibrated MSEs and MAEs improve significantly as compared to the actual TDDFT data. This is true for all functionals, but RSHs show the most significant improvement. This is, of course, a direct result of the RSH functionals already having a high R^2 correlation coefficient between TDDFT and experimental results, and the fit effectively omitted the systemic error. In terms of every statistical descriptor, the calibrated CAM-B3LYP functional represented by Equation S3, outperforms all other functionals (see Table S4). This equation is a useful method for predicting the vertical excitation energies of unknown molecules. As shown, PBE gives a much smaller R^2 as compared to the GHs and RSHs (Fig. S1c), indicating its unsuitability for FREAs analysis or new molecule design. The R^2 value obtained with RSHs is at least 0.85 as shown in Fig. S1c, confirming the significance of these functionals for FREAs analysis. Thus, a linear correction improves the results given by the two RSH functionals. Applying Equation S3 for CAM-B3LYP gives an MAE and RMS limited to 0.05 and 0.07 eV, respectively. Similarly, calibrated PBE0 and B3LYP results indicate their significance for investigating the excited-state nature of FREAs.

Table S4. Statistical analysis for the whole set of transitions with linear fitting

Parameter	PBE	B3LYP	PBE0	CAM-B3LYP	LC-PBE	LC-ωPBE
R^2	0.70	0.90	0.93	0.92	0.85	0.86
MSE	0.00	0.00	0.00	0.00	0.00	0.00
MAE	0.13	0.06	0.05	0.05	0.07	0.06

RMS	0.18	0.08	0.06	0.07	0.10	0.09
MAX. DEV. (+) (eV)	0.451	0.09	0.06	0.14	0.17	0.17
MAX. DEV. (-) (eV)	-0.348	-0.20	-0.164	-0.11	-0.24	-0.23

Note: R^2, determination coefficient; MSE, the mean signed error; MAE, mean absolute error; RMS, root mean squared error; MAX. DEV. (+) and MAX. DEV. (-) are maximum positive deviation and maximum negative deviation obtained by relating the theoretical and experimental results, respectively. All the values are in eV except R^2.

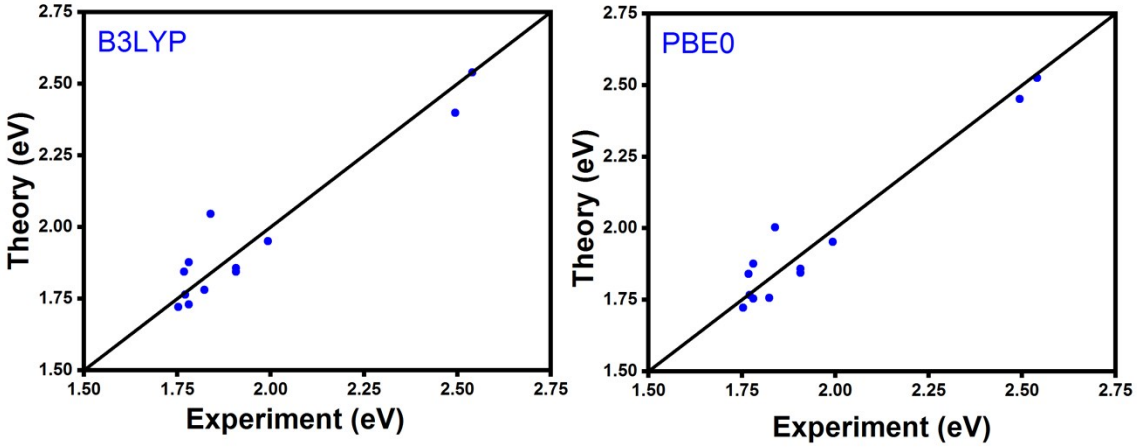

Figure S2. Comparison between the experimental λ_{max} and the linearly corrected theoretical data using PBE0 (right side) and B3LYP (left side). The solid line shows the theory-experiment perfect match.

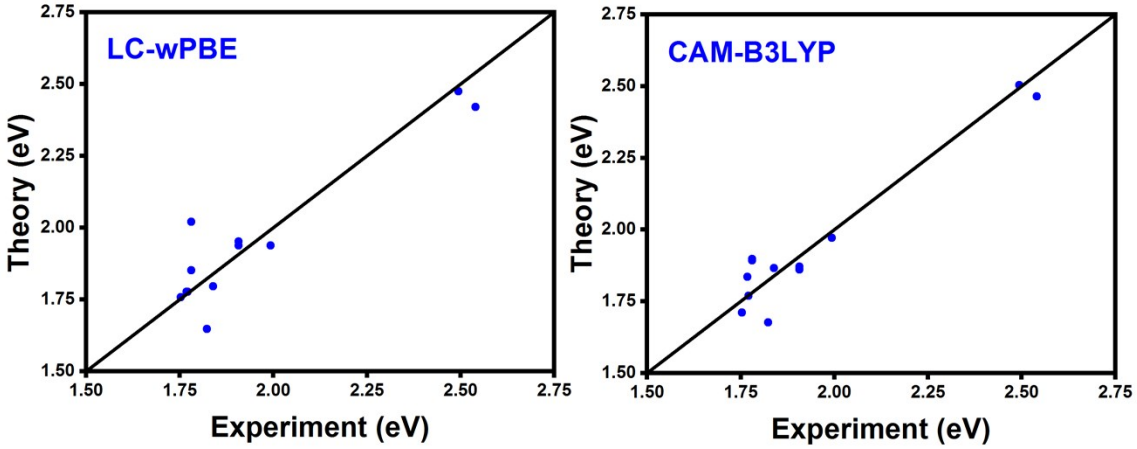

Figure S3. Comparison between the experimental λ_{max} and the linearly corrected theoretical data using LC-ωPBE (left side) and CAM-B3LYP (right side). The solid line shows the theory-experiment perfect match.

$$\lambda_{best} = 1.45 \times \lambda_{PBE0} - 0.6866 \quad \text{(S1)}$$

$$\lambda_{best} = 1.52 \times \lambda_{B3LYP} - 0.6435 \quad \text{(S2)}$$

$$\lambda_{best} = 1.35 \times \lambda_{CAM\text{-}B3LYP} - 1.11 \quad \text{(S3)}$$

$$\lambda_{best} = 1.25 \times \lambda_{LC\text{-}\omega PBE} - 1.3 \quad \text{(S4)}$$

Table S5. Calculated q_{CT} values (using PCM-TD-X/6-31G(d,p)) associated with first effective transition of NFAs [a]

Molecule	PBE0	B3LYP	CAM-B3LYP	PBE
CBM	0.973	0.963	0.602	0.578
FBR	0.602	0.597	0.549	0.469
IDSe-T-IC	0.691	0.632	0.612	0.487
IDTIDSe-IC	0.742	0.727	0.695	0.613
IDTIDT-IC	0.753	0.702	0.662	0.605
O-IDTBR	0.672	0.627	0.581	0.521
EH-IDTBR	0.666	0.651	0.516	0.483
IDT-NTI-2EH	0.788	0.774	0.764	0.581
A2	0.971	0.661	0.612	0.480
BTCN-M	0.696	0.610	0.522	0.498
MeIC	0.578	0.565	0.543	0.424
ITTIC	0.729	0.721	0.693	0.579

[a] X in PCM-TD-X/6-31G(d,p) represents the functional used. The q_{CT} is the intra-molecular charge transfer calculated for the first excited state respectively.

Table S6. Experimental λ_{max}, calculated vertical transition energy (E), and oscillator strength of first ten excited-states (f) of FREAs using PCM-TD-CAM-B3LYP/6-31G(d,p) [a]

	CAM-B3LYP																				λmax
Excited States	1		2		3		4		5		6		7		8		9		10		
Parameters	E	f	E	f	E	f	E	f	E	f	E	f	E	f	E	f	E	f	E	f	
CBM	2.67	2.27	2.96	0.02	3.05	0.02	3.29	0.00	3.83	0.06	3.86	0.08	4.19	0.31	4.19	0.24	4.27	0.18	4.29	0.09	2.49
FBR	2.64	2.49	2.86	0.38	3.27	0.00	3.27	0.00	3.64	0.09	3.70	0.16	3.93	0.17	3.93	0.05	4.28	0.04	4.28	0.00	2.54
IDSe-T-IC	2.06	3.63	2.39	0.00	3.13	0.00	3.23	0.00	3.33	0.00	3.39	0.14	3.66	0.00	3.76	0.13	3.86	0.00	3.93	0.39	1.82
IDTIDSe-IC	2.18	3.99	2.42	0.00	3.10	0.01	3.23	0.00	3.31	0.14	3.36	0.00	3.68	0.00	3.69	0.05	3.72	0.04	3.72	0.04	1.76
IDTIDT-IC	2.22	3.98	2.47	0.00	3.15	0.02	3.31	0.00	3.39	0.19	3.40	0.00	3.67	0.00	3.67	0.00	3.75	0.19	3.87	0.00	1.78
O-IDTBR	2.21	2.85	2.52	0.05	3.30	0.00	3.30	0.00	3.40	0.11	3.42	0.07	3.62	0.05	3.64	0.23	3.84	0.39	4.01	0.02	1.91
EH-IDTBR	2.20	2.82	2.51	0.04	3.30	0.00	3.30	0.00	3.39	0.14	3.42	0.07	3.61	0.06	3.63	0.24	3.82	0.35	3.99	0.02	1.91
IDT-NTI-2EH	2.23	2.46	2.46	0.00	3.01	0.75	3.09	0.00	3.36	0.21	3.51	0.00	3.65	0.31	3.77	0.00	3.92	0.00	3.92	0.00	1.78
A2	2.09	2.39	2.33	0.04	3.09	0.02	3.14	0.03	3.32	0.16	3.33	0.29	3.69	0.52	3.79	0.17	3.84	0.02	3.86	0.01	1.75
BTCN-M	2.28	2.70	2.64	0.00	3.09	0.54	3.37	0.07	3.38	0.00	3.42	0.00	3.64	0.00	3.64	0.00	3.74	0.02	3.79	0.00	1.99
MeIC	2.20	3.44	2.62	0.00	3.46	0.05	3.51	0.00	3.58	0.00	3.64	0.16	3.65	0.00	3.65	0.00	3.66	0.11	3.7	0.00	1.83
ITTIC	2.13	3.35	2.34	0.16	3.09	0.28	3.28	0.07	3.31	0.01	3.38	0.16	3.65	0.09	3.66	0.00	3.71	0.04	3.77	0.15	1.77

[a] E, f and λ_{max} are the computed vertical transition energy, oscillator strength and experimental maximum excitation energy. All the experimental and calculated values are in chloroform solution. E and λ_{max} are in eV, while f is in a.u.

Table S7. Experimental λ_{max}, calculated vertical transition energy (E), and oscillator strength of first ten excited-states (f) of FREAs using PCM-TD-B3LYP/6-31G(d,p) [a]

B3LYP																					
Excited States	1		2		3		4		5		6		7		8		9		10		λ_{max}
Parameters	E	f	E	f	E	f	E	f	E	f	E	f	E	f	E	f	E	f	E	f	
CBM	2.01	0.00	2.10	1.61	2.15	0.04	2.36	0.01	2.92	0.02	3.06	0.29	3.29	0.00	3.29	0.02	3.32	0.20	3.35	0.02	2.49
FBR	2.09	1.85	2.33	0.12	2.62	0.18	2.70	0.00	2.70	0.00	2.76	0.31	3.00	0.01	3.07	0.09	3.09	0.28	3.17	0.07	2.54
IDSe-T-IC	1.59	2.90	1.86	0.00	2.27	0.02	2.27	0.22	2.37	0.00	2.46	0.39	2.70	0.05	2.74	0.00	2.77	0.11	2.89	0.00	1.82
IDTIDSe-IC	1.64	2.89	1.86	0.00	2.26	0.38	2.29	0.00	2.35	0.00	2.43	0.47	2.70	0.05	2.71	0.00	2.73	0.05	2.84	0.00	1.76
IDTIDT-IC	1.66	2.83	1.88	0.00	2.31	0.41	2.32	0.00	2.40	0.00	2.46	0.49	2.74	0.05	2.74	0.00	2.75	0.09	2.86	0.00	1.78
O-IDTBR	1.65	2.33	1.92	0.02	2.39	0.03	2.56	0.16	2.63	0.02	2.65	0.23	2.76	0.00	2.76	0.00	2.91	0.26	3.09	0.03	1.91
EH-IDTBR	1.64	2.29	1.91	0.02	2.38	0.03	2.55	0.17	2.62	0.02	2.64	0.23	2.76	0.00	2.76	0.00	2.91	0.29	3.08	0.03	1.91
IDT-NTI-2EH	1.57	1.77	1.74	0.00	2.28	0.00	2.38	0.15	2.58	0.12	2.59	0.12	2.61	0.00	2.67	0.00	2.69	1.13	2.74	0.00	1.78
A2	1.56	1.95	1.80	0.02	2.15	0.03	2.31	0.22	2.46	0.09	2.46	0.07	2.55	0.06	2.62	0.00	2.65	0.00	2.71	0.02	1.75
BTCN-M	1.71	1.43	1.96	0.00	2.19	1.07	2.41	0.00	2.42	0.11	2.44	0.00	2.51	0.00	2.63	0.20	2.66	0.00	2.71	0.00	1.99
MeIC	1.77	2.92	2.14	0.00	2.49	0.00	2.64	0.01	2.68	0.00	2.75	0.07	2.75	0.41	2.83	0.04	2.84	0.00	2.89	0.00	1.83
ITTIC	1.59	2.49	1.79	0.10	2.19	0.02	2.27	0.57	2.33	0.32	2.36	0.00	2.69	0.14	2.76	0.00	2.79	0.03	2.83	0.04	1.77

[a] E, f and λ_{max} are the computed vertical transition energy, oscillator strength and experimental maximum excitation energy. All the experimental and calculated values are in chloroform solution. E and λ_{max} are in eV, while f is in a.u.

Table S8. Experimental λ_{max}, calculated vertical transition energy (E), and oscillator strength of first ten excited-states (f) of FREAs using PCM-TD-PBE0/6-31G(d,p) [a]

	PBE0																				
Excited States	1		2		3		4		5		6		7		8		9		10		λ_{max}
Parameters	E	f	E	f	E	f	E	f	E	f	E	f	E	f	E	f	E	f	E	f	
CBM	2.17	0.00	2.23	1.77	2.33	0.01	2.51	0.01	3.06	0.02	3.24	0.31	3.53	0.28	3.54	0.01	3.56	0.01	3.56	0.02	2.49
FBR	2.22	2.04	2.47	0.18	2.78	0.14	2.85	0.00	2.85	0.00	2.93	0.25	3.20	0.00	3.26	0.11	3.26	0.23	3.37	0.04	2.54
IDSe-T-IC	1.69	3.10	1.99	0.00	2.40	0.00	2.44	0.19	2.52	0.00	2.61	0.39	2.88	0.04	2.92	0.00	2.94	0.08	3.07	0.00	1.82
IDTIDSe-IC	1.74	3.15	1.99	0.00	2.43	0.00	2.44	0.31	2.52	0.00	2.58	0.47	2.86	0.01	2.87	0.00	2.91	0.04	3.00	0.00	1.76
IDTIDT-IC	1.77	3.10	2.01	0.00	2.46	0.00	2.49	0.34	2.58	0.00	2.61	0.49	2.90	0.02	2.90	0.00	2.94	0.08	3.03	0.00	1.78
O-IDTBR	1.76	2.47	2.05	0.02	2.54	0.03	2.74	0.19	2.83	0.02	2.84	0.19	2.90	0.00	2.90	0.00	3.09	0.19	3.26	0.04	1.91
EH-IDTBR	1.75	2.43	2.04	0.02	2.53	0.03	2.73	0.21	2.82	0.02	2.83	0.20	2.91	0.00	2.91	0.00	3.08	0.21	3.24	0.04	1.91
IDT-NTI-2EH	1.69	1.91	1.88	0.00	2.42	0.00	2.53	0.12	2.74	0.56	2.78	0.00	2.78	0.00	2.83	0.74	2.83	0.06	2.95	0.00	1.78
A2	1.66	2.07	1.92	0.02	2.28	0.03	2.46	0.19	2.64	0.09	2.64	0.08	2.72	0.02	2.80	0.00	2.82	0.00	2.88	0.02	1.75
BTCN-M	1.82	1.65	2.10	0.00	2.33	1.07	2.56	0.00	2.60	0.09	2.61	0.00	2.70	0.00	2.81	0.17	2.82	0.00	2.90	0.00	1.99
MeIC	1.86	3.06	2.27	0.00	2.61	0.00	2.80	0.00	2.83	0.00	2.89	0.33	2.92	0.06	2.98	0.00	2.99	0.02	3.05	0.00	1.83
ITTIC	1.69	2.73	1.92	0.10	2.34	0.03	2.45	0.55	2.49	0.24	2.54	0.03	2.87	0.08	2.94	0.01	2.96	0.03	3.01	0.04	1.77

[a] E, f and λ_{max} are the computed vertical transition energy, oscillator strength and experimental maximum excitation energy. All the experimental and calculated values are in chloroform solution. E and λ_{max} are in eV, while f is in a.u.

Table S9. Orbitals (computed through PCM-TD-PBE0/6-31G(d,p)) contributing the most to the effective electronic transitions of all 12 NFAs

Molecule	No.	Composition	Molecule	No	Composition
CBM	2	Homo-1 → Lumo (97%)	IDTIDT-IC	1	Homo → Lumo (94%)
	6	Homo-2 → Lumo+1 (92%)		4	Homo → Lumo+2 (91%)
	7	Homo-1 → Lumo+2 (84%)		6	Homo-1 → Lumo+1 (85%)
FBR	1	Homo → Lumo (93%)		9	Homo-2 → Lumo (80%)
	2	Homo → Lumo+1 (90%)	IDSe-T-IC	1	Homo → Lumo (95%)
	3	Homo-1 → Lumo (86%)		4	Homo → Lumo+2 (92%)
	6	Homo-1 → Lumo+1 (86%)		6	Homo-1 → Lumo+1(92%)
	8	Homo → Lumo+3 (84%)		9	Homo-4 → Lumo (87%)
	9	Homo → Lumo+2 (83%)	IDTIDSe-IC	1	Homo → Lumo (94%)
BTCN-M	1	Homo → Lumo (97%)		4	Homo → Lumo+2 (91%)
	3	Homo-1 → Lumo (94%)		6	Homo-1 → Lumo+1 (85%)
	5	Homo → Lumo+2 (93%)		9	Homo-2 → Lumo (67%)
	8	Homo-2 → Lumo+1 (68%)	A2	1	Homo → Lumo (95%)
MeIC	1	Homo → Lumo (96%)		4	Homo-1 → Lumo+1 (84%)
	6	Homo-4 → Lumo (56%) Homo-1 → Lumo+1 (33%)		5	Homo → Lumo+2 (86%)
	7	Homo-4 → Lumo (27%) Homo-1 → Lumo+1 (60%)		6	Homo → Lumo+3 (86%)
EH-IDTBR	1	Homo → Lumo (96%)	O-IDTBR	1	Homo → Lumo (96%)
	4	Homo-1 → Lumo+1 (84%)		4	Homo-1 → Lumo+1 (83%)
	6	Homo → Lumo+2 (18%) Homo → Lumo+3 (71%)		6	Homo → Lumo+3 (92%)
	9	Homo-2 → Lumo (82%)		9	Homo-2 → Lumo (82%)
ITTIC	1	Homo → Lumo (93%)	IDT-NTI-2EH	1	Homo → Lumo (97%)
	2	Homo → Lumo+1 (94%)		4	Homo-1 → Lumo+1 (77%)
	4	Homo → Lumo+2 (87%)		5	Homo-3 → Lumo (34%) Homo → Lumo+2 (21%)
	5	Homo-1 → Lumo+1 (86%)		8	Homo → Lumo+2 (73%)
	7	Homo-2 → Lumo (78%)		9	Homo-5 → Lumo (18%) Homo-4 → Lumo (51%) Homo-2 → Lumo+2 (22%)

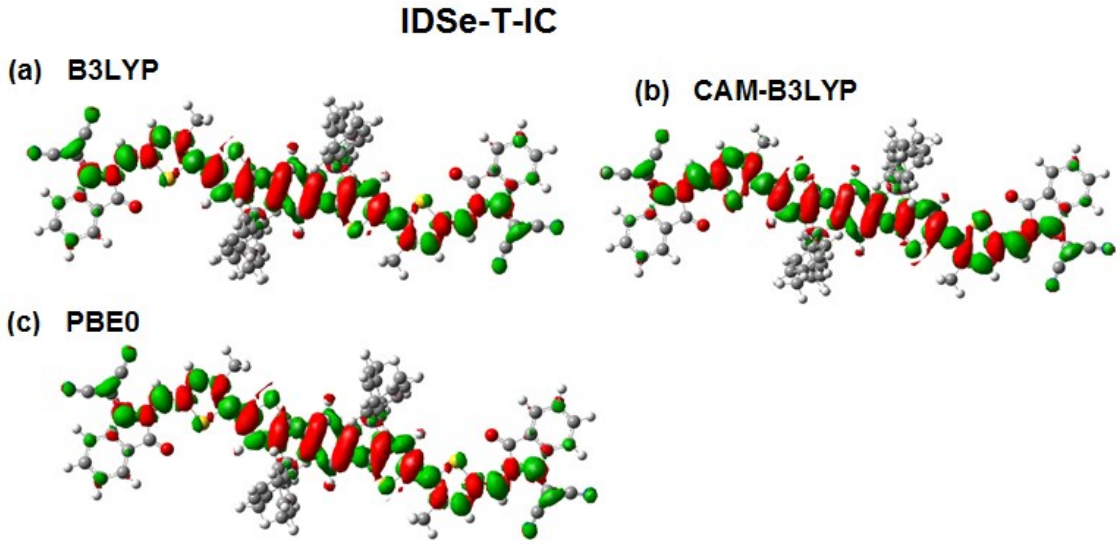

Fig. S4. Plot of the density difference between the ground and first excited states computed for IDSe-T-IC through PCM-TD-DFT (contour threshold: 0.0004 a.u.)

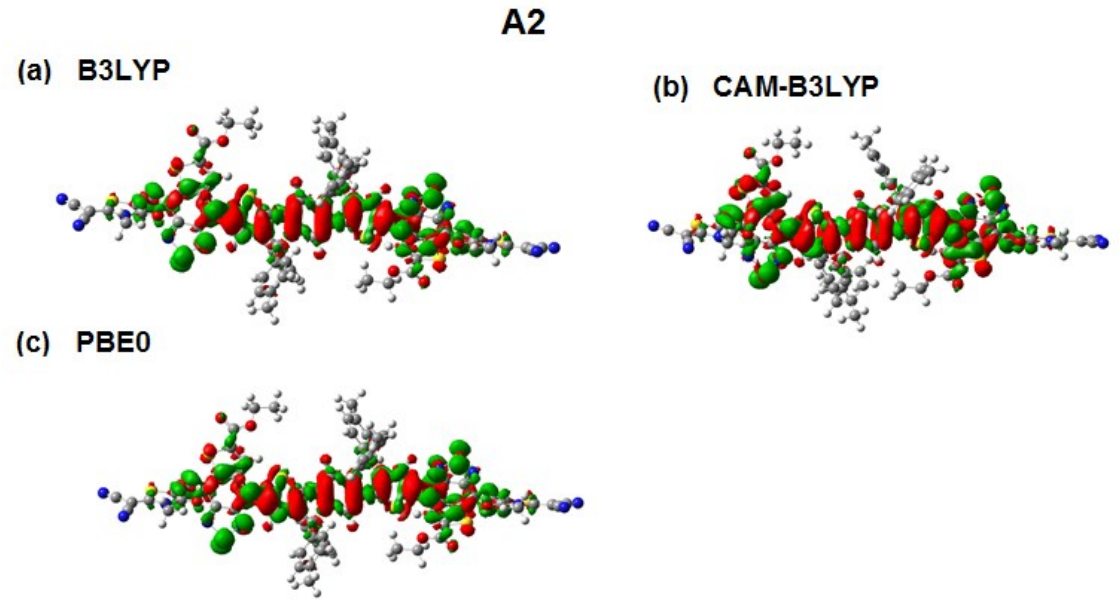

Fig. S5. Plot of the density difference between the ground and first excited states computed for A2 through PCM-TD-DFT (contour threshold: 0.0004 a.u.)

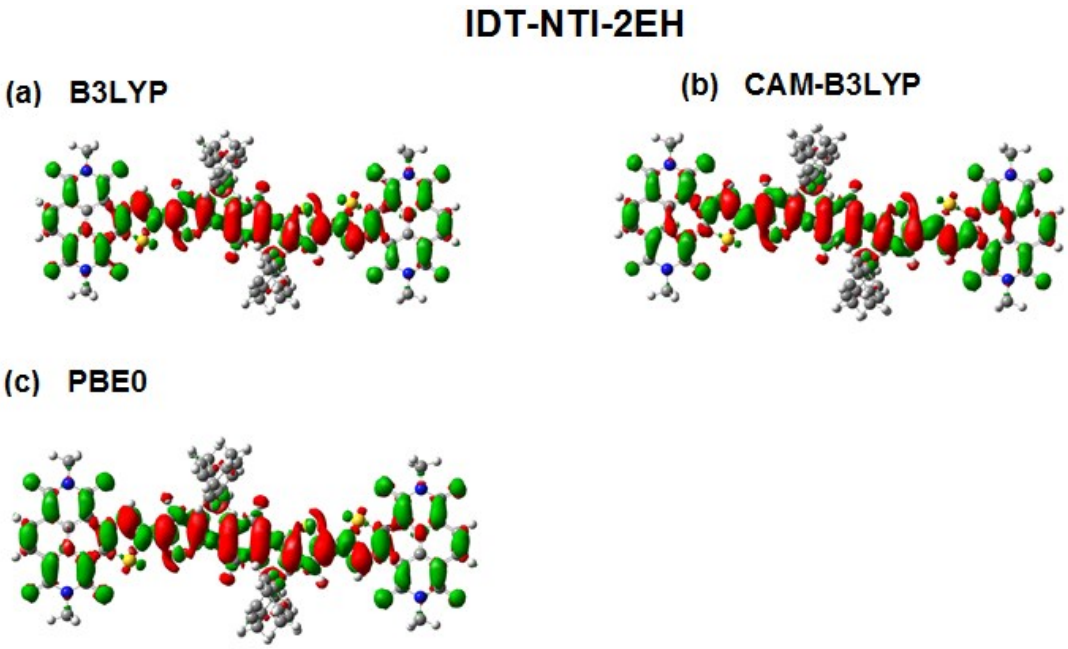

Fig. S6. Plot of the density difference between the ground and first excited states computed for IDT-NTI-2EH through PCM-TD-DFT (contour threshold: 0.0004 a.u.)

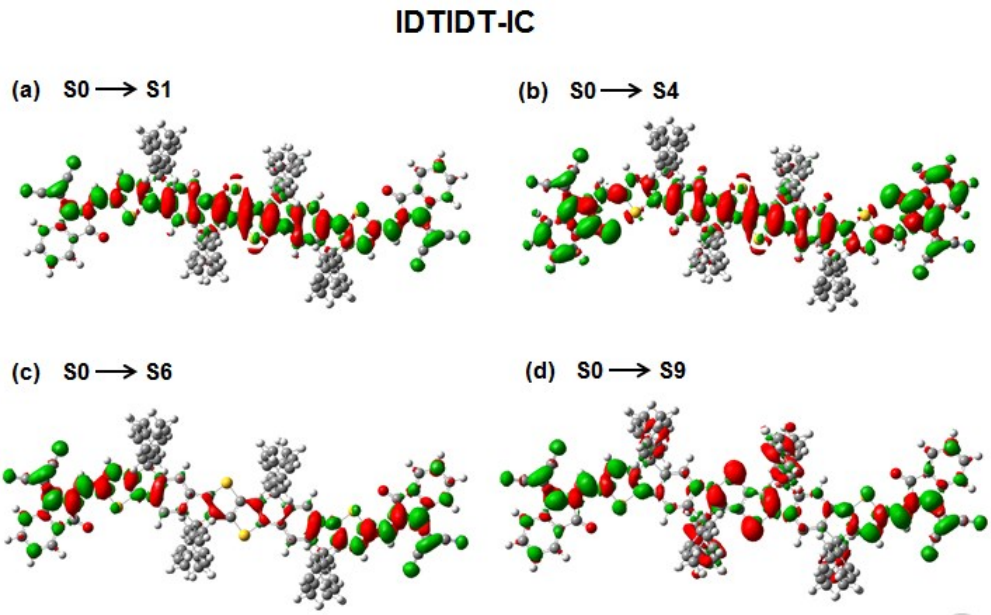

Fig. S7. Plot of the density difference between the ground and excited states computed for IDTIDT-IC through PCM-TD-PBE0 (contour threshold: 0.0004 a.u.)

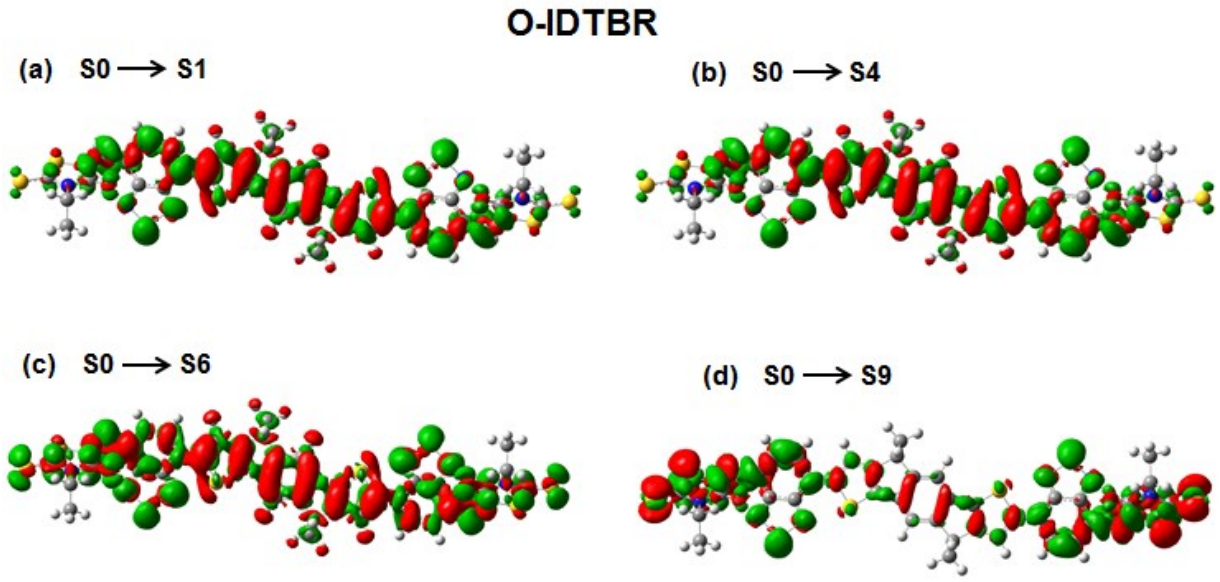

Fig. S8. Plot of the density difference between the ground and excited states computed for O-IDTBR through PCM-TD-PBE0 (contour threshold: 0.0004 a.u.)

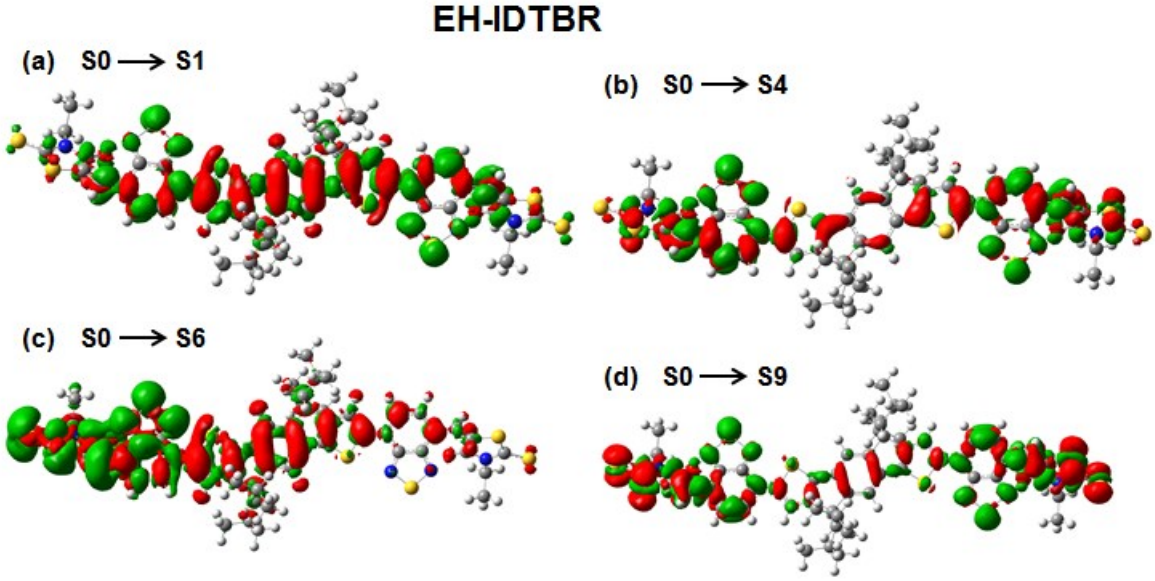

Fig. S9. Plot of the density difference between the ground and excited states computed for EH-IDTBR through PCM-TD-PBE0 (contour threshold: 0.0004 a.u.)

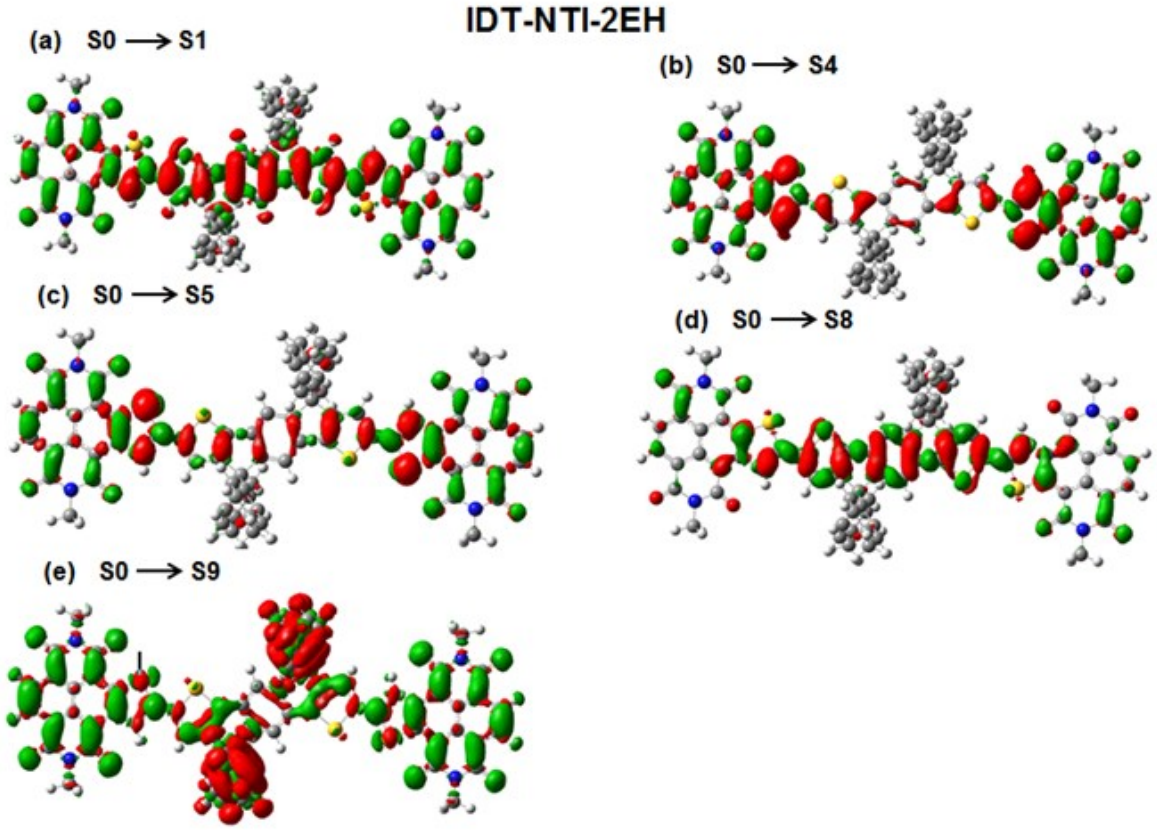

Fig. S10. Plot of the density difference between the ground and excited states computed for IDT-NTI-2EH through PCM-TD-PBE0 (contour threshold: 0.0004 a.u.)

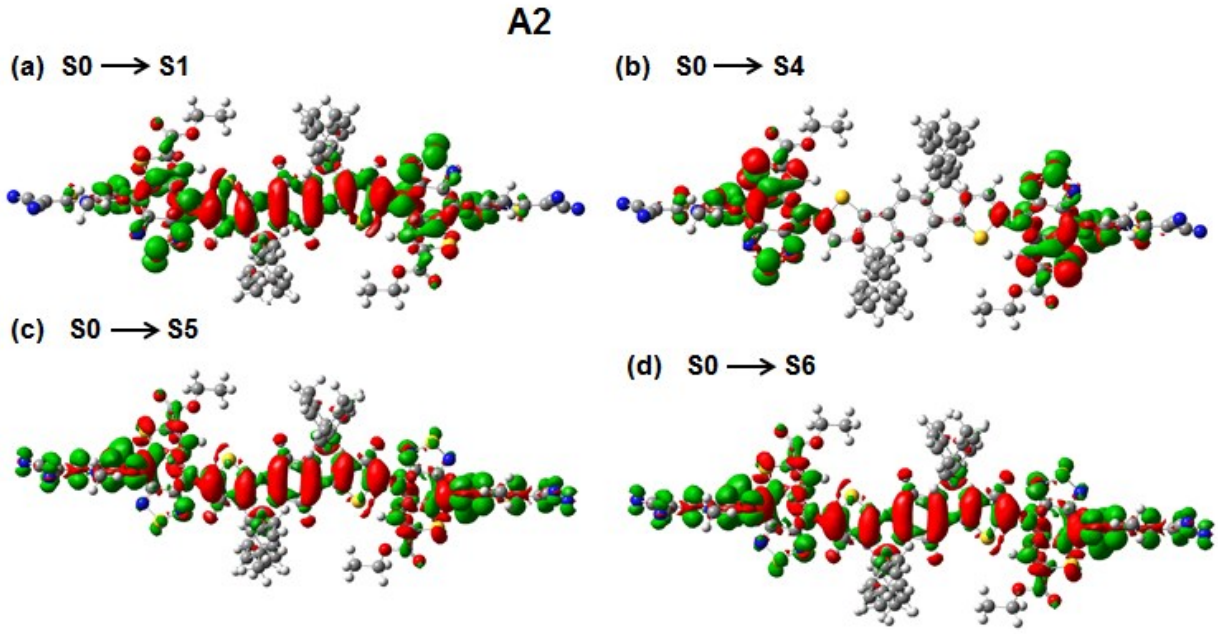

Fig. S11. Plot of the density difference between the ground and excited states computed for A2 through PCM-TD-PBE0 (contour threshold: 0.0004 a.u.)

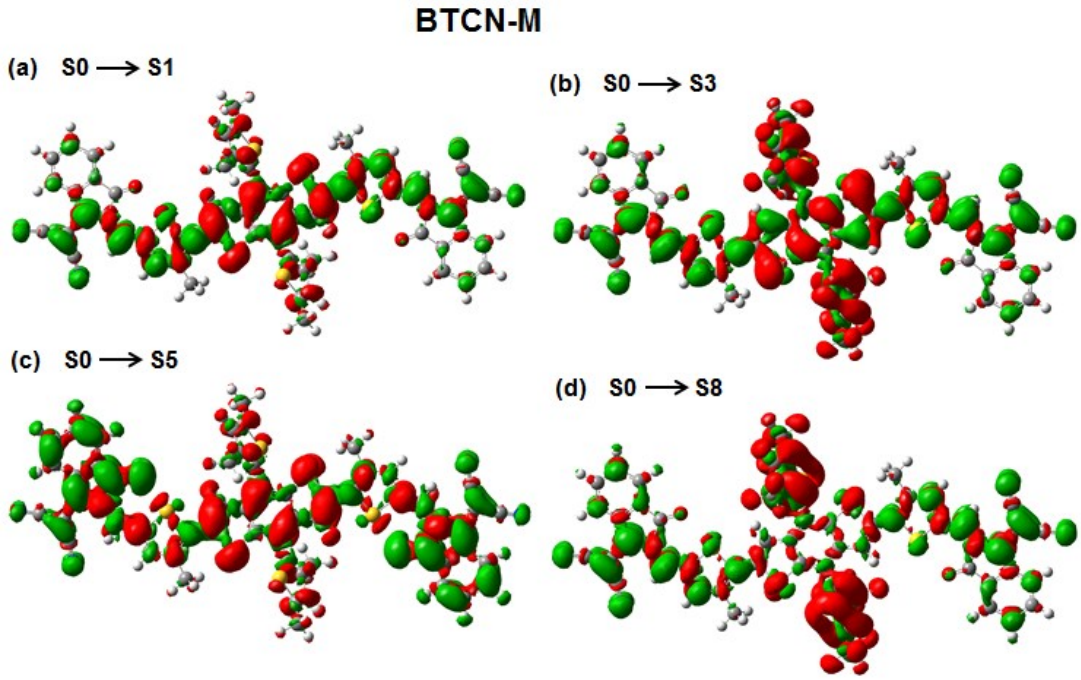

Fig. S12. Plot of the density difference between the ground and excited states computed for BTCN-M through PCM-TD-PBE0 (contour threshold: 0.0004 a.u.)

Cartesian Coordinates

Below are the Cartesian coordinates of all NFAs chemical structures optimized in chloroform solution using DFT-PBE0/6-31G(d,p) and PCM solvent model. All data is in Å.

CBM

0 1

C	0.71765400	-1.38152200	0.76638300
C	-0.71767300	-1.38149700	0.76643300
C	-1.11985200	-0.17248100	0.14349600
N	-0.00001100	0.54905600	-0.21417000
C	1.11983000	-0.17250900	0.14343900
C	2.46088500	0.14871400	-0.03973700
C	3.42659600	-0.75834800	0.41168000
C	3.02708600	-1.96087500	1.04489800
C	1.69252400	-2.27211500	1.22563200
C	-1.69254200	-2.27204400	1.22577700
C	-3.02710500	-1.96079000	1.04508100
C	-3.42661700	-0.75829200	0.41181100
C	-2.46091000	0.14874700	-0.03965800
C	0.00000000	1.82014800	-0.89581900
C	-4.85766100	-0.49792700	0.20620900
C	4.85764100	-0.49797200	0.20609400
C	-5.75527900	-1.53123100	-0.01555700
C	-7.13567500	-1.34134500	-0.21593300
C	-7.72878000	-0.08643700	-0.21138000
C	-6.84146200	1.01943900	0.01887100
C	-5.42664700	0.82027600	0.22232700
C	5.42662500	0.82023100	0.22228200
C	6.84144600	1.01940400	0.01888400
C	7.72877500	-0.08645900	-0.21138300
C	7.13566900	-1.34136700	-0.21602000
C	5.75526700	-1.53126300	-0.01570000
N	-7.21121100	2.29741700	0.07977700
S	-5.86389400	3.15794800	0.37631200
N	-4.76898600	1.96289600	0.44040000
N	4.76895600	1.96284500	0.44036600
S	5.86386700	3.15790100	0.37638500
N	7.21119000	2.29738200	0.07984400
C	-9.11970900	0.21002600	-0.41305800
C	9.11971500	0.21002500	-0.41296400
C	-10.18333000	-0.61814800	-0.63939900
C	10.18336200	-0.61810600	-0.63935500
C	-11.48503000	-0.05491500	-0.81073700
N	-12.54548300	0.39950800	-0.95084200
C	-10.11875100	-2.04037300	-0.72402700

N	-10.08643200	-3.20033100	-0.79642600
C	11.48505900	-0.05482700	-0.81055800
N	12.54551300	0.39962900	-0.95055400
C	10.11881900	-2.04032200	-0.72416300
N	10.08660000	-3.20027400	-0.79671300
H	2.76022800	1.06572300	-0.53116500
H	3.78542200	-2.63598900	1.42727200
H	1.40775000	-3.19433600	1.72322400
H	-1.40776500	-3.19422500	1.72344200
H	-3.78543900	-2.63586900	1.42752200
H	-2.76025800	1.06574300	-0.53110800
H	-0.88152900	2.39263200	-0.60167900
H	0.88141000	2.39272300	-0.60149500
H	0.00012200	1.69888500	-1.98452600
H	-5.37756900	-2.54647100	-0.07053100
H	-7.73878600	-2.22413900	-0.39186800
H	7.73878400	-2.22415400	-0.39197200
H	5.37756000	-2.54650100	-0.07073300
H	-9.35868800	1.27021400	-0.37731800
H	9.35868600	1.27021100	-0.37709200

FBR

0 1

C	1.17050600	-0.78255300	-0.07742300
C	0.72766900	-2.11665900	-0.05057200
C	-0.72765100	-2.11665300	0.05050800
C	-1.17047000	-0.78254300	0.07745700
C	0.00002500	0.18415700	0.00005300
C	-1.64405000	-3.16452400	0.12509800
C	-2.99755200	-2.87216000	0.22872200
C	-3.45629900	-1.54230400	0.24877100
C	-2.51924100	-0.49472200	0.17378200
C	2.51928100	-0.49474300	-0.17372700
C	3.45632600	-1.54233200	-0.24878800
C	2.99756000	-2.87218300	-0.22883700
C	1.64405500	-3.16453700	-0.12523700
C	0.08322600	1.06308300	1.25658100
C	-0.08316400	1.06318300	-1.25640600
C	-4.89139700	-1.22917300	0.31463400
C	4.89142800	-1.22921500	-0.31462100
C	-5.82840000	-2.01233500	1.06767700
C	-7.22728200	-1.65577000	1.10957600
C	-7.73708400	-0.51083100	0.40016600
C	-6.79380900	0.21555700	-0.31060300
C	-5.42800700	-0.13867900	-0.34646000
C	5.82843000	-2.01234300	-1.06770200
C	7.22731700	-1.65579500	-1.10956300
C	7.73712500	-0.51090400	-0.40008200
C	6.79385300	0.21545200	0.31072600
C	5.42804700	-0.13877000	0.34654800
N	-5.54193500	-3.08890600	1.80471900

S	-6.93621700	-3.59035900	2.46801800
N	-7.95606600	-2.47510500	1.86650800
N	5.54195900	-3.08886600	-1.80481200
S	6.93624400	-3.59030100	-2.46812000
N	7.95610000	-2.47509600	-1.86653400
C	-9.15320000	-0.26168800	0.51731100
C	9.15324900	-0.26178200	-0.51717300
C	-9.99816200	0.68622000	0.02886600
C	9.99818600	0.68615700	-0.02874500
C	-9.75548000	1.85292700	-0.83703200
N	-10.95311700	2.53767400	-1.07524200
C	-12.08434200	2.05546500	-0.48507700
S	-11.71510300	0.62158900	0.43954900
C	9.75544800	1.85294400	0.83702600
N	10.95305700	2.53775700	1.07518900
C	12.08431700	2.05550300	0.48512800
S	11.71515100	0.62150500	-0.43933700
O	-8.70152900	2.23384800	-1.31731000
S	-13.60735200	2.68150400	-0.59224800
O	8.70147300	2.23388400	1.31723900
S	13.60730500	2.68160300	0.59226700
C	-10.93764100	3.74315900	-1.90168200
C	10.93751500	3.74333500	1.90149100
C	-10.66445000	4.99275600	-1.08151900
C	10.66422200	4.99281900	1.08118900
H	-1.31388400	-4.19908400	0.10147200
H	-3.71644000	-3.68082800	0.28578700
H	-2.86041300	0.53610300	0.22325500
H	2.86046600	0.53608100	-0.22312400
H	3.71643800	-3.68085700	-0.28595900
H	1.31387400	-4.19909400	-0.10168500
H	-0.79905600	1.70650200	1.33375500
H	0.14409700	0.45233000	2.16163000
H	0.96688200	1.70796700	1.21530000
H	0.79912600	1.70659700	-1.33352800
H	-0.14404200	0.45250200	-2.16150300
H	-0.96681200	1.70807400	-1.21507600
H	-7.12193400	1.08414400	-0.86792800
H	-4.77070200	0.47341000	-0.95626100
H	7.12198400	1.08400000	0.86810600
H	4.77074400	0.47328600	0.95638500
H	-9.63679000	-1.01046600	1.14407300
H	9.63686500	-1.01059300	-1.14387500
H	-10.15843200	3.58693600	-2.65034700
H	-11.90762500	3.79770800	-2.39957600
H	10.15833500	3.58714500	2.65019400
H	11.90750800	3.79800700	2.39935500
H	-10.65539800	5.86640600	-1.73899600
H	-11.43975100	5.14124600	-0.32542500
H	-9.69223200	4.92745200	-0.58617800
H	10.65512900	5.86654500	1.73856500
H	11.43949600	5.14127100	0.32506000

H	9.69199700	4.92739500	0.58587800

IDSe-T-IC

0 1

C	-2.76549700	2.38883400	1.20718900
C	-2.55926500	2.34681600	-1.33952500
C	-3.84140100	3.28473300	1.20012000
C	-4.18387600	3.99987200	2.34061800
C	-3.46728700	3.85067200	3.53259300
C	-2.40068000	2.95090100	3.53743700
C	-2.05417700	2.23021100	2.39690400
C	-2.08476300	3.66044500	-1.39932900
C	-2.08100100	4.36368200	-2.59905100
C	-2.55008500	3.78441600	-3.78118100
C	-3.01558400	2.46885700	-3.71751400
C	-3.02045100	1.76045300	-2.52022300
C	-3.82246400	4.64971800	4.75451000
C	-2.57865300	4.55873800	-5.06858200
C	-11.37111900	-0.52330100	-0.03651100
C	-10.99933100	0.90320700	-0.01328800
C	-12.25850200	1.67218900	0.00784100
C	-13.34453800	0.78463400	-0.00461000
C	-12.82535800	-0.60242900	-0.03627700
O	-9.87254100	1.37738800	-0.01079400
C	-13.62109700	-1.73239000	-0.06327700
C	-12.41696600	3.04695200	0.03691500
C	-13.71443400	3.55422200	0.05488400
C	-14.80692000	2.68469300	0.04306600
C	-14.64140100	1.29959100	0.01310900
C	11.37111200	0.52339600	0.03922600
C	10.99936900	-0.90314500	0.01721700
C	12.25856800	-1.67210900	-0.00288500
C	13.34457600	-0.78451100	0.00909400
C	12.82535000	0.60256100	0.03949200
O	9.87259400	-1.37736100	0.01489900
C	13.62104900	1.73256100	0.06602700
C	12.41708200	-3.04689100	-0.03071700
C	13.71457100	-3.55413800	-0.04790800
C	14.80702700	-2.68456700	-0.03657700
C	14.64145900	-1.29944400	-0.00786000
C	-1.10788700	0.84288200	-0.00135600
C	-1.25570300	-0.56492300	-0.00825700
C	-2.47231400	1.54278000	-0.03581700
C	-3.39692800	0.33511800	-0.03431200
C	-2.66848000	-0.83717000	-0.02038800
C	-4.78885600	0.17716700	-0.03950600
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C	-15.90433000	-4.18724100	-0.02783800
C	-14.80835500	-5.05219300	-0.04702600
C	-13.51292800	-4.53940700	-0.04135500
C	-7.05930000	2.42721300	-0.01047700
C	-8.20841500	1.43242600	0.01822300
C	-7.73319600	0.12606200	0.00522200
C	5.86769500	-1.45843300	0.02135000
C	6.29469400	-0.10885000	0.00755200
C	7.05928000	-2.42722000	0.01061900
C	8.20840700	-1.43244800	-0.01817500
C	7.73319900	-0.12607700	-0.00526200
C	-9.59455700	1.48624100	0.01838000
C	-10.19745700	0.21498600	0.01304300
S	-8.96996700	-1.05455100	-0.00206000
C	9.59454700	-1.48627600	-0.01833600
C	10.19745900	-0.21502600	-0.01309400
S	8.96998200	1.05452500	0.00192800
C	5.38122300	0.95337800	-0.00243900
C	4.03664800	0.64239800	0.01041000

C	3.60820400	-0.70938800	0.01611700
C	4.51891500	-1.76992700	0.01607100
C	2.84025900	1.60614500	-0.00343300
C	1.69519100	0.60898900	-0.00982500
C	2.16710000	-0.68600100	0.01406900
C	2.73659200	2.45254200	1.27296700
C	2.90640700	2.45232200	-1.27933100
C	3.68241600	3.61594800	-1.31945900
C	3.81371800	4.34516700	-2.49512300
C	3.17440000	3.94510300	-3.67274200
C	2.40537600	2.78100700	-3.62869300
C	2.27262400	2.04535000	-2.45433300
C	1.93553200	3.59905200	1.29604400
C	1.76171100	4.32618400	2.46854300
C	2.37989200	3.93908000	3.66044100
C	3.17093400	2.78827700	3.63496100
C	3.34668500	2.05629200	2.46492600
C	3.29042700	4.75628100	-4.93214500
C	2.22089000	4.74738200	4.91688600
C	0.28681900	0.64124100	-0.00794600
C	-0.28681600	-0.64121500	0.00795700
S	0.92291600	-1.89168500	0.03241700
S	-0.92291500	1.89170800	-0.03247400
C	-2.16709900	0.68602300	-0.01417500
C	-1.69518800	-0.60896600	0.00973500
C	-3.60820600	0.70940500	-0.01617900
C	-4.03664200	-0.64238300	-0.01049200
C	-2.84025100	-1.60612500	0.00334600
C	-2.90639800	-2.45229700	1.27924800
C	-2.73658100	-2.45252400	-1.27305100
C	-3.34665800	-2.05627600	-2.46501200
C	-3.17088800	-2.78826300	-3.63505100
C	-2.37984700	-3.93905800	-3.66052300
C	-1.76168400	-4.32617100	-2.46861000
C	-1.93552100	-3.59904300	-1.29611800
C	-3.68237700	-3.61594900	1.31936100
C	-3.81368200	-4.34516900	2.49502000
C	-3.17440200	-3.94507900	3.67265700
C	-2.40541200	-2.78096700	3.62862000
C	-2.27265300	-2.04530600	2.45425800
C	-2.22077700	-4.74736600	-4.91695600
C	-3.29047700	-4.75626000	4.93205400
C	-4.51892300	1.76994000	-0.01608100
C	-5.86770300	1.45843800	-0.02133300
C	-6.29469100	0.10885100	-0.00759800
C	-5.38121500	-0.95337200	0.00234300
C	-16.15936200	0.18971600	0.06804200
N	-17.32288800	0.21537700	0.07502700
C	-14.24615200	1.57114600	0.09468100
N	-13.89780600	2.68162400	0.12420700
C	16.15937500	-0.18969600	-0.06826300
N	17.32290200	-0.21532300	-0.07524100

C	14.24619500	-1.57116800	-0.09487300
N	13.89787900	-2.68165600	-0.12438900
H	5.79564500	-4.83899100	-0.32003300
H	5.52456700	-6.16349800	-2.36909000
H	7.84906600	-3.28963200	-4.53889300
H	8.10756900	-1.95251900	-2.49800900
H	8.63659300	-4.60472200	0.44120800
H	8.98791100	-5.87797600	2.50862800
H	6.12141100	-3.40693100	4.52064100
H	5.78014500	-2.11820900	2.46143100
H	-8.63675300	4.60465900	-0.44077800
H	-8.98814100	5.87817300	-2.50803700
H	-6.12147000	3.40758200	-4.52036300
H	-5.78014700	2.11859500	-2.46132800
H	5.58361800	-6.19160700	-4.88515000
H	6.63171600	-5.05846000	-5.75616500
H	7.33034000	-6.43139200	-4.89636700
H	8.82586300	-5.77903500	5.09522600
H	7.39204500	-5.01904600	5.80615400
H	7.23763900	-6.50702900	4.86767600
H	-8.82547900	5.78255600	-5.09298700
H	-7.23492600	6.50632800	-4.86812100
H	-7.39480100	5.01860600	-5.80603200
H	-6.63426000	5.05811900	5.75665800
H	-5.58233000	6.18877400	4.88703200
H	-7.32849200	6.43256900	4.89568300
H	-8.10771000	1.95227300	2.49806500
H	-7.84916600	3.28911700	4.53912700
H	-5.52439400	6.16308100	2.36975100
H	-5.79550800	4.83885300	0.32052600
H	12.05951000	-1.08520500	-0.03205700
H	16.62153900	2.16826400	-0.01203800
H	16.90879900	4.59890100	0.03242300
H	14.96999600	6.12543500	0.06603700
H	12.63970500	5.18414900	0.05550000
H	-12.05950800	1.08516000	0.03202900
H	-16.62156000	-2.16825700	0.01178600
H	-16.90884900	-4.59888900	-0.03277100
H	-14.97006400	-6.12544300	-0.06645200
H	-12.63976200	-5.18418400	-0.05588000
H	-10.18984900	2.39299500	0.02158500
H	10.18983200	-2.39303500	-0.02148100
H	5.72343400	1.98375700	-0.02191200
H	4.17863400	-2.80113300	0.00911500
H	4.18102700	3.96368100	-0.41910900
H	4.42442000	5.24498600	-2.49721300
H	1.89914400	2.43982000	-4.52850800
H	1.67171700	1.14067100	-2.45882200
H	1.45185100	3.93831200	0.38430800
H	1.13314500	5.21343000	2.45501600
H	3.66113200	2.45634700	4.54713800
H	3.96730300	1.16577200	2.48453700

H	4.27903300	5.21569200	-5.02149900
H	3.11681500	4.14204300	-5.81979800
H	2.55321800	5.56784500	-4.94634800
H	2.97786900	5.53868700	4.97332700
H	1.24136700	5.23194800	4.95870900
H	2.33369900	4.12502000	5.80883100
H	-3.96727600	-1.16575700	-2.48463300
H	-3.66107400	-2.45633200	-4.54723300
H	-1.13311900	-5.21341800	-2.45507500
H	-1.45185500	-3.93830300	-0.38437400
H	-4.18095600	-3.96369700	0.41899900
H	-4.42435500	-5.24500800	2.49709600
H	-1.89920700	-2.43976400	4.52844400
H	-1.67176500	-1.14061500	2.45875900
H	-2.33499900	-4.12528900	-5.80891500
H	-1.24068400	-5.23073100	-4.95941600
H	-2.97680000	-5.53963300	-4.97270400
H	-2.55406000	-5.56855000	4.94575100
H	-3.11576800	-4.14226900	5.81966000
H	-4.27947800	-5.21472500	5.02193700
H	-4.17864600	2.80114600	-0.00909200
H	-5.72342000	-1.98375300	0.02178500

O-IDTBR

0 1

C	-0.67317500	1.22027800	-0.80648200
C	-1.37884300	-0.00927900	-0.80655100
C	-0.71045200	-1.23866800	-0.80647800
C	0.67320700	-1.22024100	-0.80649800
C	1.37887300	0.00931600	-0.80662200
C	0.71048300	1.23870500	-0.80653400
C	1.62946000	-2.41002300	-0.80557200
C	2.96220100	-1.69527400	-0.81013300
C	2.78287300	-0.32576200	-0.80905600
C	-1.62942600	2.41006000	-0.80553000
C	-2.96216700	1.69531300	-0.81002500
C	-2.78284200	0.32580000	-0.80893100
C	1.45385100	-3.26474900	0.45810500
C	1.44791900	-3.27366800	-2.06215100
C	-1.44793800	3.27369500	-2.06212500
C	-1.45375800	3.26479700	0.45813200
C	4.31299600	-2.06590400	-0.80428300
C	5.17276900	-0.97290400	-0.80091300
S	4.26658500	0.53423800	-0.78997800
C	-4.31296100	2.06594600	-0.80414700
C	-5.17273900	0.97295000	-0.80075700
S	-4.26655600	-0.53419500	-0.78981100
C	6.61902900	-1.02145700	-0.81758700
C	-6.61899800	1.02150900	-0.81742700
C	7.30978400	-2.20585900	-1.04398100

C	8.71361400	-2.29232400	-1.03131300
C	9.54524500	-1.21752700	-0.75806000
C	8.88999300	0.04396000	-0.59873700
C	7.44781600	0.13602200	-0.62519000
C	-7.30975300	2.20592300	-1.04376700
C	-8.71358300	2.29238000	-1.03112900
C	-9.54521800	1.21756400	-0.75795700
C	-8.88996800	-0.04392600	-0.59867900
C	-7.44779000	-0.13597700	-0.62508800
N	9.48752000	1.22874800	-0.47974300
S	8.31027600	2.34173800	-0.37490300
N	7.00114600	1.38426200	-0.49304900
N	-9.48748600	-1.22872900	-0.47978200
S	-8.31024600	-2.34172000	-0.37489200
N	-7.00112300	-1.38421700	-0.49292600
C	10.98322100	-1.40082800	-0.75220000
C	-10.98319000	1.40087100	-0.75210200
C	11.90743000	-0.82024900	0.04835400
C	-11.90742200	0.82027700	0.04840700
S	-13.63928600	1.01210700	-0.20314500
C	-14.03345300	0.07570600	1.22474800
N	-12.89753800	-0.31460500	1.86429000
C	-11.67005700	0.07418900	1.30087600
S	13.63930000	-1.01199400	-0.20318500
C	14.03339900	-0.07570000	1.22479200
N	12.89746300	0.31449000	1.86435900
C	11.67000400	-0.07430400	1.30089000
S	15.59051800	0.24122900	1.67201500
S	-15.59058800	-0.24128500	1.67185900
O	10.60910800	0.14081700	1.84860000
O	-10.60918900	-0.14099000	1.84862000
C	-12.90112500	-1.09735400	3.09755100
C	12.90101000	1.09707700	3.09771900
C	12.84539500	2.59012400	2.82095400
C	-12.84554600	-2.59036400	2.82058500
H	-1.26368200	-2.17446500	-0.80580400
H	1.26371500	2.17450200	-0.80590600
H	2.19308400	-4.07196000	0.47769600
H	0.45775800	-3.71799000	0.47968000
H	1.57790600	-2.66148100	1.36154200
H	1.56869500	-2.67722300	-2.97060900
H	2.18639800	-4.08166200	-2.07865100
H	0.45148700	-3.72646000	-2.07648600
H	-2.18642100	4.08168600	-2.07860000
H	-0.45150900	3.72649000	-2.07650600
H	-1.56875000	2.67724000	-2.97057100
H	-0.45766200	3.71803300	0.47966000
H	-2.19298600	4.07201200	0.47774700
H	-1.57777700	2.66153900	1.36158100
H	4.66533900	-3.09079800	-0.78635100
H	-4.66529600	3.09084300	-0.78623600
H	6.75510100	-3.11447100	-1.24922100

H	9.16387600	-3.26370400	-1.21714200
H	-6.75507400	3.11455600	-1.24892600
H	-9.16384300	3.26377000	-1.21691700
H	11.35461300	-2.10913300	-1.49250700
H	-11.35455900	2.10923400	-1.49236800
H	-12.02610400	-0.77032800	3.66319900
H	-13.80546700	-0.82684700	3.64581500
H	12.02599400	0.76994900	3.66331400
H	13.80535400	0.82651900	3.64595600
H	12.83640200	3.13780000	3.76733700
H	13.71674300	2.91324300	2.24554300
H	11.93881000	2.84832500	2.26713800
H	-12.83654000	-3.13816800	3.76689400
H	-13.71691700	-2.91338800	2.24515400
H	-11.93898100	-2.84851000	2.26671300

EH-IDTBR

0 1

C	0.67461000	1.22487200	0.61536500
C	1.37199200	-0.00717500	0.67140500
C	0.69948200	-1.23359700	0.69349300
C	-0.68478900	-1.21409200	0.66086500
C	-1.38027400	0.01642100	0.60797400
C	-0.70911000	1.24452000	0.58628000
C	-1.64155800	-2.41044700	0.65126300
C	-2.97948200	-1.68349600	0.64152400
C	-2.78222200	-0.31403500	0.59380400
C	1.63497500	2.41281900	0.63330700
C	2.96898000	1.68960200	0.64114000
C	2.77568000	0.32106900	0.69197500
C	-1.37105300	-3.19295000	-0.67566900
C	-1.40310500	-3.33132100	1.87118300
C	1.42533300	3.16159800	1.98068800
C	1.41530700	3.36878700	-0.55982900
C	-4.34441600	-2.01125900	0.66565300
C	-5.18001000	-0.90089000	0.63363800
S	-4.24240800	0.58149100	0.56111300
C	4.32926700	2.03361500	0.62073500
C	5.17246500	0.92853200	0.66082600
S	4.24438900	-0.56223500	0.70817300
C	-6.62668300	-0.91861500	0.66349800
C	6.61931000	0.95549600	0.67063100
C	-7.34294400	-2.08260900	0.91646400
C	-8.74827900	-2.13620100	0.91918600
C	-9.55784400	-1.04716300	0.63532600
C	-8.87508800	0.19576800	0.44896400
C	-7.43093300	0.25438500	0.45969400
C	7.33027800	2.13641400	0.84692500
C	8.73530700	2.19921400	0.82377800
C	9.54810500	1.10082600	0.59035000

C	8.87168900	-0.15524000	0.48548800
C	7.42839500	-0.22222900	0.52163500
N	-9.44609100	1.39213600	0.31672600
S	-8.24454500	2.47548100	0.18160700
N	-6.95691400	1.48956000	0.30247100
N	9.44912900	-1.35360500	0.41213200
S	8.25333800	-2.45035200	0.35728100
N	6.96079100	-1.46724200	0.44195600
C	-10.99930400	-1.19725600	0.64443300
C	10.98885000	1.25974100	0.57118400
C	-11.91756300	-0.60591900	-0.15537500
C	11.89976100	0.62985600	-0.20697600
S	13.63570200	0.80042200	0.03161700
C	14.00756100	-0.20838900	-1.35239300
N	12.86260500	-0.60416200	-1.97217200
C	11.64462000	-0.16459900	-1.42575600
S	-13.65087100	-0.75367300	0.11587400
C	-14.03759600	0.17344200	-1.32001600
N	-12.89957200	0.52772800	-1.97627600
C	-11.67569000	0.11719100	-1.42014200
S	-15.59135400	0.52255800	-1.75535000
S	15.55679800	-0.57740400	-1.78676300
O	-10.61598000	0.29965500	-1.98188800
O	10.57845500	-0.38042200	-1.96281000
C	12.84784400	-1.44185700	-3.16869400
C	-12.89755400	1.29483500	-3.21929300
C	-12.80362400	2.78937300	-2.96162300
C	12.76872500	-2.91967200	-2.82392400
C	2.32035500	4.38897600	2.25445000
C	1.60159900	5.70665500	1.96147700
C	2.81970700	4.37306500	3.69885900
C	1.33072000	2.78275400	-1.97700400
C	0.76889100	3.84745400	-2.92018800
C	2.66193900	2.26237100	-2.51666600
C	-1.32511800	-2.70755700	3.27279700
C	-2.67191000	-2.23307100	3.81662600
C	-0.70798200	-3.72449900	4.23411700
C	-1.81039700	-4.65732500	-0.82798000
C	-3.31332300	-4.90340700	-0.73263600
C	-1.28389900	-5.17487400	-2.16855500
H	1.25205100	-2.16901200	0.73590700
H	-1.26109200	2.18013500	0.54412800
H	-0.28424000	-3.18698400	-0.82176400
H	-1.78702000	-2.60451500	-1.50429100
H	-2.17274800	-4.11425600	1.87715400
H	-0.45290400	-3.85030400	1.68444400
H	0.37133800	3.46436000	2.03700200
H	1.56922400	2.42021200	2.77590000
H	0.47383000	3.89928500	-0.36335400
H	2.20177700	4.13560000	-0.54034500
H	-4.73368200	-3.01941400	0.69787600
H	4.70651100	3.04607400	0.54217200

H	-6.80837600	-3.00135500	1.12975900
H	-9.21901200	-3.09376600	1.12516100
H	6.79159900	3.06129100	1.01950800
H	9.20229200	3.16974100	0.96826200
H	-11.38013300	-1.88692000	1.39738100
H	11.37534600	1.99179500	1.27987700
H	11.97583400	-1.12599400	-3.74521600
H	13.75415800	-1.21204000	-3.73201800
H	-12.03649200	0.94005000	-3.78961000
H	-13.81381100	1.03912100	-3.75476800
H	-12.79219600	3.32529000	-3.91469100
H	-13.66061000	3.14001900	-2.38074800
H	-11.88507700	3.03247500	-2.42083700
H	12.74394300	-3.50979800	-3.74415300
H	13.63843600	-3.23112000	-2.23966700
H	11.86167700	-3.13672300	-2.25341400
H	3.20292500	4.33615500	1.60347200
H	1.24702300	5.76411700	0.92858700
H	0.73122100	5.82045100	2.61873100
H	1.97725700	4.39392900	4.40053000
H	3.40476100	3.47103500	3.90636400
H	0.61914300	1.94606300	-1.95505100
H	1.43230500	4.72014100	-2.96280900
H	0.67020200	3.45743000	-3.93842200
H	3.42137400	3.05408600	-2.50646600
H	3.04832400	1.42180800	-1.93652900
H	-0.65074600	-1.84200800	3.22355400
H	-3.10465300	-1.42929400	3.21756500
H	-3.39303700	-3.05971800	3.84033600
H	-0.61950800	-3.30814900	5.24286300
H	-1.33031100	-4.62544100	4.30136100
H	-1.32296100	-5.24463000	-0.03788300
H	-3.54696900	-5.93899200	-1.00155400
H	-3.69200200	-4.74372900	0.28047900
H	-1.51056400	-6.23857500	-2.29321200
H	-1.74645800	-4.63533300	-3.00368200
H	-2.55982000	-1.86363800	4.84169400
H	0.29109000	-4.03305000	3.90824200
H	-3.86877300	-4.24884100	-1.41409200
H	-0.19922500	-5.04959300	-2.25119600
H	-0.21786700	4.19439200	-2.59532200
H	2.54747900	1.92806500	-3.55344000
H	3.44979600	5.24348300	3.91086200
H	2.26318400	6.56176700	2.13659800

IDT-NTI-2EH

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C	1.35970000	-0.20806700	-0.01997200
C	0.84457200	1.11074900	-0.01375300

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C	-1.35966800	0.21314700	-0.03197800
C	-0.84443900	-1.10564700	-0.03943900
C	-2.79598100	0.09084200	-0.02349800
C	-3.18616500	-1.23354900	-0.01099000
C	-1.97207300	-2.14895600	-0.03321800
C	2.79599800	-0.08604200	-0.02117600
C	3.18657600	1.23821300	-0.03389800
C	1.97248900	2.15386900	-0.01752000
S	-4.13071900	1.16434800	-0.03026700
C	-5.25113900	-0.18532500	-0.00950600
C	-4.57880700	-1.39939100	-0.00660200
S	4.13020100	-1.15993300	-0.00289700
C	5.25117900	0.18945700	-0.01222000
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C	-1.83694800	-3.00495000	1.23142500
C	-2.02793700	-2.99238300	-1.31297300
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C	2.02418400	2.99949600	1.26088300
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C	-1.43824500	-4.50559000	3.60234500
C	-2.25674200	-3.37422300	3.59091300
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C	-1.36713200	-2.61540700	-2.48182600
C	1.01594900	4.13637400	-1.29704300
C	0.82479500	4.86754700	-2.46390900
C	1.45180700	4.50395200	-3.65925000
C	2.27155500	3.37356700	-3.64242200
C	2.46375800	2.63653700	-2.47772700
C	1.36216700	2.62259400	2.42918100
C	1.49558700	3.36947500	3.59766200
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C	2.96377200	4.88185100	2.47066300
C	2.83322000	4.14154600	1.30302600
C	-1.25342400	-5.32139200	4.85050700
C	-2.43110400	-5.32224800	-4.94835500
C	1.27169800	5.31763700	-4.90948000
C	2.41419600	5.33582200	4.89354900
C	-6.67299000	0.02257200	0.00735300
C	6.67294400	-0.01960000	-0.00905200
C	-7.64505900	-0.94208400	-0.06601300
C	-8.96389300	-0.41193400	-0.01434900
C	-8.95136600	1.02160600	0.09877100
S	-7.33617300	1.65114400	0.14436600
C	7.64516700	0.94201000	-0.11396900
C	8.96388300	0.41029100	-0.07567100
C	8.95082000	-1.02126200	0.06045100

S	7.33570200	-1.64689000	0.14374700
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C	-11.39686600	-0.32484000	0.00483400
C	-11.35705300	1.09130700	0.11742200
C	-10.11630400	1.76124900	0.16414000
C	-12.65954300	-0.96051400	-0.03971700
C	-13.82637100	-0.22082500	0.02409400
C	-13.77996100	1.17423400	0.13564900
C	-12.56039900	1.82508600	0.18219900
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N	-11.27764400	3.90380000	0.34294700
C	-10.07002100	3.22524100	0.28198300
C	-10.27738000	-2.54146200	-0.17518800
N	-11.54676700	-3.11996900	-0.21330300
C	-12.75315200	-2.43058800	-0.15596900
C	-11.19876400	5.35459900	0.46057800
C	-11.58220600	-4.57255800	-0.32673100
O	-13.55658100	3.96530400	0.36223000
O	-9.01057000	3.83720500	0.32649700
O	-13.82520500	-3.01407500	-0.19916600
O	-9.29481100	-3.26764500	-0.23758100
C	10.20138400	1.06870800	-0.15434600
C	11.39670300	0.31843300	-0.09737300
C	11.35629800	-1.09572300	0.03791600
C	10.11536100	-1.76226200	0.11654300
C	12.65957200	0.95068800	-0.17338400
C	13.82600100	0.20968300	-0.11791200
C	13.77899800	-1.18344200	0.01554600
C	12.55924600	-1.83097300	0.09278700
C	10.27823000	2.53388900	-0.29697500
N	11.54785100	3.10930300	-0.36348500
C	12.75382300	2.41855200	-0.31450600
C	12.53414900	-3.30468100	0.23380700
N	11.27562700	-3.90451400	0.30529800
C	10.06838500	-3.22434600	0.25579500
O	9.29598800	3.26056000	-0.35911200
O	13.82602200	2.99913500	-0.38467000
O	13.55443000	-3.97056600	0.28563700
O	9.00873700	-3.83345400	0.32678700
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C	11.19602900	-5.35335100	0.44448200
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H	-5.09179300	-2.35375400	0.00632000
H	5.09244500	2.35804200	-0.01703800
H	-0.52529400	-4.45282800	0.32134400
H	-0.16968100	-5.74160700	2.37966200
H	-2.75131800	-3.06301600	4.50805900
H	-3.09360600	-1.75847500	2.45732600
H	-3.36534000	-4.45213800	-0.45954600
H	-3.61073000	-5.75264100	-2.52562400
H	-0.97557900	-3.04301900	-4.54674800

H	-0.73865800	-1.73045300	-2.48799900
H	0.52444000	4.45534800	-0.38224000
H	0.17644300	5.74043500	-2.44412300
H	2.77060700	3.06152300	-4.55685300
H	3.10540600	1.76068200	-2.50255900
H	0.73576100	1.73617100	2.43543500
H	0.96599400	3.05204700	4.49276100
H	3.59884200	5.76473200	2.47274900
H	3.36023800	4.46076500	0.40799200
H	-1.98116100	-6.14033900	4.89654900
H	-0.25714000	-5.77086000	4.88983800
H	-1.39042000	-4.71316300	5.74876800
H	-3.46799700	-5.62513500	-5.12343000
H	-2.08507700	-4.76829700	-5.82479200
H	-1.83482400	-6.23971800	-4.88066800
H	1.99930200	6.13679000	-4.95389700
H	1.41261200	4.70801000	-5.80618600
H	0.27540100	5.76663200	-4.95359800
H	2.08490400	4.77595200	5.77270500
H	3.44652500	5.65793800	5.06067300
H	1.80029100	6.24195400	4.83025800
H	-7.44984600	-1.99972900	-0.16077900
H	7.45004500	1.99824900	-0.22341500
H	-14.77413300	-0.74684500	-0.01404000
H	-14.68942100	1.76271100	0.18691900
H	-12.21488300	5.73977000	0.48977800
H	-10.66354100	5.62363300	1.37315700
H	-10.65961600	5.76607400	-0.39462000
H	-11.09703700	-4.88537300	-1.25332200
H	-11.04950700	-5.02259700	0.51283500
H	-12.62534200	-4.87833200	-0.32354100
H	14.77391100	0.73312900	-0.18014400
H	14.68810700	-1.77300900	0.06006200
H	11.09134800	4.85757000	-1.42962200
H	11.05861800	5.02418300	0.33434800
H	12.62732500	4.86426400	-0.51288800
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H	10.67427000	-5.60844500	1.36875900
H	10.64324900	-5.77580200	-0.39656000

A2

0 1

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C	-0.57677200	1.30568800	-0.30164000
C	-1.36712000	0.15240900	-0.29929300
C	-0.79696300	-1.14325300	-0.28994100
C	0.57674500	-1.30567100	-0.30159100
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C	-3.13120900	-1.36859200	-0.34218200

C	-1.87998000	-2.23269800	-0.30182100
C	2.79751900	0.03068000	-0.32463600
C	3.13118600	1.36860000	-0.34217500
C	1.87996000	2.23271000	-0.30183100
C	-1.69407400	-3.09473300	-1.55539200
C	-1.91285100	-3.06961000	0.98338700
C	1.69410000	3.09478700	-1.55537400
C	1.91284100	3.06957800	0.98341500
C	0.82444100	4.19011100	-1.53942400
C	0.58101800	4.92530300	-2.69398000
C	1.19880100	4.60008600	-3.90508000
C	2.06475700	3.50460100	-3.91636100
C	2.30848200	2.76297500	-2.76415600
C	1.25253800	2.67876700	2.14767900
C	1.36802500	3.42515900	3.31887000
C	2.14501700	4.58222400	3.36937400
C	2.81292300	4.96625500	2.20100700
C	2.70020900	4.22672100	1.03156400
C	-0.82439300	-4.19004300	-1.53944900
C	-0.58087900	-4.92516500	-2.69402600
C	-1.19857700	-4.59987700	-3.90515500
C	-2.06457800	-3.50443200	-3.91642100
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C	-1.25245300	-2.67890400	2.14763200
C	-1.36790700	-3.42536300	3.31878400
C	-2.14496100	-4.58238700	3.36927000
C	-2.81296800	-4.96630900	2.20092300
C	-2.70027900	-4.22671300	1.03151800
C	-0.95955200	-5.41796600	-5.14268400
C	-2.24999800	-5.40255800	4.62384400
C	2.25009900	5.40228900	4.62401300
S	4.17522200	-0.98397100	-0.33735000
C	5.24615400	0.41251600	-0.37983200
C	4.51711200	1.59295400	-0.35770700
S	-4.17526300	0.98397000	-0.33739900
C	-5.24618100	-0.41252700	-0.37984200
C	-4.51713400	-1.59295700	-0.35769700
C	0.96000900	5.41827800	-5.14258600
C	-7.38397300	0.78945900	-0.98509000
C	-8.81246200	0.92033300	-0.85673500
C	7.38391200	-0.78956500	-0.98500700
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C	-6.86000300	1.82335200	-1.83288900
C	-7.80607100	2.69077100	-2.27234000
S	-9.41018300	2.33428500	-1.68314800
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S	9.41006600	-2.33454600	-1.68288200
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C	7.64597000	-3.85419100	-3.15861600
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C	11.91844400	0.00098900	0.88478800
C	-11.57554200	-0.15437700	2.31084600
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S	-13.66425400	0.03740200	0.67813900
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N	12.75369400	0.29217900	3.07358300
C	13.92015500	0.21636400	2.38872200
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C	-12.64124700	-0.43599700	4.51743100
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C	-8.94691000	-1.07851000	0.41018200
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C	-6.68728300	-0.26280100	-0.36827800
N	-9.53651300	-2.10030000	1.03233300
S	-8.35481900	-3.11843000	1.47772400
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N	9.53655400	2.10034200	1.03209000
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O	-8.57162800	4.56737600	-3.49120500
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N	-17.16775300	-0.07541100	1.21146700
C	15.56433200	0.55576300	4.23638200
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C	16.29141500	0.18487900	1.96958500
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C	6.13150100	-5.14283800	-4.41081900
C	-4.65523200	5.15945300	-4.71718600
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 H                 -3.22480300   -4.55725600    0.13912400
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BTCN-M

0 1
 C                 -1.38835900    0.12739700   -0.10177700
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C	-0.76312400	-1.14260200	0.04563100
C	0.61701200	-1.31056000	0.13938300
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C	2.79927300	-0.00853800	0.23903500
C	3.25653700	1.28420200	0.19021700
S	1.93844300	2.43023700	-0.02096400
C	-2.79929300	0.00846800	-0.23898800
C	-3.25656600	-1.28426900	-0.19016800
S	-1.93847200	-2.43031800	0.02094300
C	-1.25080100	2.62913000	-0.27249500
C	1.25081000	-2.62921400	0.27237500
C	4.63567000	1.70395900	0.26048500
C	-4.63570500	-1.70401100	-0.26039000
C	-2.13430900	3.24370800	0.58512400
C	-2.55163600	4.51840200	0.09380200
C	-2.00531200	4.87081700	-1.10737300
S	-0.94735400	3.62235500	-1.67437100
C	5.17222300	2.96469500	0.54537700
C	6.57005900	2.91876300	0.54246600
C	7.13148700	1.67284000	0.25688400
S	5.86323900	0.51329000	-0.03150800
C	2.13444300	-3.24364900	-0.58522600
C	2.55172800	-4.51840700	-0.09404100
C	2.00526000	-4.87101100	1.10701500
S	0.94720900	-3.62265500	1.67406200
C	-5.17228100	-2.96475100	-0.54522600
C	-6.57011600	-2.91880000	-0.54229700
C	-7.13152100	-1.67285800	-0.25675300
S	-5.86325400	-0.51331500	0.03158200
C	-4.40126300	-4.21368700	-0.84465700
C	4.40118300	4.21360700	0.84485200
C	-2.22393000	6.11997200	-1.89450600
C	-2.59585500	2.68359800	1.89540800
C	2.59618200	-2.68330700	-1.89534500
C	2.22378300	-6.12029000	1.89397500
C	8.53974400	1.51349700	0.23428800
C	9.37009100	0.44414000	-0.00029300
C	-8.53977400	-1.51349000	-0.23413400
C	-9.37008800	-0.44410000	0.00041400
C	10.82968400	0.44957000	0.02946700
C	11.28254200	-0.92579900	-0.27663900
C	10.15726700	-1.73677000	-0.48742600
C	8.93445600	-0.92799500	-0.32811500
C	-10.82968200	-0.44947700	-0.02933400
C	-11.28248200	0.92595300	0.27658200
C	-10.15717600	1.73689500	0.48731000
C	-8.93439800	0.92804700	0.32812000
C	12.55496600	-1.49070500	-0.37704600
C	12.65761400	-2.84724000	-0.68448300
C	11.52679100	-3.64059900	-0.89156300

C	10.25399100	-3.08373800	-0.79341600
C	-12.55488200	1.49093500	0.37686300
C	-12.65747500	2.84751300	0.68412700
C	-11.52662100	3.64084100	0.89115700
C	-10.25384500	3.08390600	0.79312900
C	11.67341500	1.51041400	0.29066900
O	7.78752700	-1.33132400	-0.44976300
O	-7.78745300	1.33133200	0.44976500
C	-11.67346600	-1.51032800	-0.29033800
C	13.09406300	1.40470200	0.29317700
N	14.25720800	1.37846200	0.30897900
C	11.23687400	2.83331000	0.58795400
N	10.93263100	3.92917000	0.83550900
C	-13.09410800	-1.40454300	-0.29284800
N	-14.25725200	-1.37824000	-0.30862000
C	-11.23699700	-2.83330300	-0.58737200
N	-10.93282200	-3.92922000	-0.83476400
H	3.44714300	-0.86339600	0.39570300
H	-3.44716200	0.86333900	-0.39559000
H	-3.24048500	5.16307700	0.63105600
H	7.19100300	3.78316900	0.75676200
H	3.24064500	-5.16299500	-0.63131300
H	-7.19107500	-3.78320600	-0.75654900
H	-3.64442900	-4.04923700	-1.61727100
H	-3.88810100	-4.59577700	0.04435300
H	-5.07733200	-4.99647300	-1.19540800
H	3.64432700	4.04910600	1.61743300
H	5.07723400	4.99638100	1.19566800
H	3.88804600	4.59574200	-0.04415200
H	-2.91788100	6.77314100	-1.36000200
H	-1.29070000	6.67117300	-2.04959800
H	-2.64953300	5.90947400	-2.88115300
H	-2.03885100	1.78561000	2.16992200
H	-2.46953600	3.42128000	2.69432100
H	-3.66011900	2.42339800	1.86268000
H	2.03848300	-1.78588000	-2.17029500
H	3.66018100	-2.42207400	-1.86209200
H	2.47100400	-3.42123400	-2.69420600
H	2.91789200	-6.77332100	1.35950900
H	2.64915500	-5.90994100	2.88075300
H	1.29055300	-6.67157700	2.04876500
H	9.02746700	2.45771200	0.45618600
H	-9.02752200	-2.45770300	-0.45598300
H	13.45707300	-0.91321200	-0.22459900
H	13.64393600	-3.29370900	-0.76394000
H	11.64456900	-4.69321900	-1.12910100
H	9.35575600	-3.67309600	-0.94836600
H	-13.45701100	0.91346800	0.22444500
H	-13.64377800	3.29404200	0.76348500
H	-11.64435700	4.69349700	1.12855900
H	-9.35558700	3.67323800	0.94803800

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C	1.29401300	-0.46248100	-0.01608800
C	1.03768700	0.92995800	-0.01773200
C	0.26066800	-1.40460700	-0.01017300
C	-1.03769300	-0.92991300	-0.01709900
C	-1.29402200	0.46252500	-0.01649000
C	-0.26067300	1.40465500	-0.01121700
C	-2.34169100	-1.74053100	-0.00138500
C	-3.35456000	-0.61032500	0.00894900
C	-2.72685500	0.61957400	-0.01313500
C	-4.75264400	-0.46650100	-0.00034200
C	-5.16137600	0.88369500	-0.02002500
S	-3.79942100	1.97674400	-0.04071100
S	-6.11048100	-1.51306700	0.02151200
C	-7.22914700	-0.13866800	0.00692400
C	-6.54090900	1.07571500	-0.01640600
C	2.34169400	1.74057300	-0.00255700
C	3.35455300	0.61036600	0.00869500
C	2.72684200	-0.61954100	-0.01253400
C	4.75264000	0.46652400	-0.00032600
C	5.16135700	-0.88369200	-0.01898500
S	3.79939400	-1.97674400	-0.03901700
S	6.11049300	1.51308300	0.02087600
C	7.22914200	0.13865800	0.00737000
C	6.54088700	-1.07573000	-0.01513700
C	2.55663000	2.56667400	-1.27850100
C	2.37310100	2.59369200	1.27024700
C	-2.55653700	-2.56759600	-1.27672600
C	-2.37316900	-2.59269700	1.27204800
C	3.51022100	3.58994800	-1.29633700
C	3.78443000	4.29021000	-2.46572500
C	3.11748100	3.99843000	-3.65869800
C	2.17168400	2.97096200	-3.63743000
C	1.89524300	2.26495000	-2.47054500
C	1.74032100	3.84135200	1.29776200
C	1.69051900	4.58964700	2.46729200
C	2.27318600	4.12566900	3.65105400
C	2.90031100	2.87922800	3.61903600
C	2.94998500	2.12353300	2.45058900
C	-3.50997300	-3.59101100	-1.29379600
C	-3.78414600	-4.29212700	-2.46269600
C	-3.11730300	-4.00108800	-3.65589400
C	-2.17163000	-2.97347300	-3.63538600
C	-1.89523700	-2.26661400	-2.46901800
C	-1.74018900	-3.84022500	1.30060600
C	-1.69043600	-4.58763300	2.47070800
C	-2.27336300	-4.12286400	3.65402700

C	-2.90070400	-2.87655400	3.62097000
C	-2.95033000	-2.12174900	2.45195000
C	3.39029300	4.78052400	-4.91209800
C	2.24785300	4.95527400	4.90338300
C	-3.39001800	-4.78403200	-4.90878400
C	-2.24808400	-4.95149800	4.90700000
C	-8.60509700	-0.47414400	0.01682000
C	8.60509900	0.47411300	0.01722000
C	-9.76290500	0.27480600	0.01047400
C	9.76289600	-0.27485700	0.01120500
C	-11.10941500	-0.30271700	0.02420300
C	-12.05285300	0.81389600	0.00675300
C	-11.32939000	2.04196400	-0.01526100
C	-9.88896600	1.76346000	-0.01278800
C	11.10941700	0.30264400	0.02500700
C	12.05284200	-0.81396700	0.00667500
C	11.32936300	-2.04201900	-0.01560100
C	9.88894300	-1.76350900	-0.01239000
C	-13.40891600	1.00285600	0.00556500
S	-13.77323300	2.68700600	-0.02288900
C	-12.10223600	3.16813200	-0.03349000
C	13.40890300	-1.00293900	0.00514900
S	13.77319700	-2.68708300	-0.02394000
C	12.10219200	-3.16819000	-0.03432600
O	-8.99199500	2.59558600	-0.02691400
O	8.99196900	-2.59563600	-0.02626200
C	11.50466700	1.62766100	0.05130000
C	-11.50463700	-1.62776500	0.04949200
C	-11.67955500	4.59506200	-0.05846500
C	11.67949200	-4.59510200	-0.05999500
C	10.63305400	2.75040700	0.07214800
N	9.95698300	3.69825600	0.08982400
C	12.88435500	1.97472400	0.06066800
N	14.01053600	2.26848100	0.06854600
C	-10.63299800	-2.75052000	0.06885700
N	-9.95689300	-3.69836600	0.08529800
C	-12.88431700	-1.97485300	0.05908100
N	-14.01048800	-2.26864200	0.06715100
H	0.47191900	-2.46937700	0.00222100
H	-0.47192400	2.46943500	0.00036600
H	-7.06579000	2.02174300	-0.02963500
H	7.06575300	-2.02177600	-0.02760000
H	4.03548600	3.85496600	-0.38296500
H	4.53172600	5.07978900	-2.44911700
H	1.63968500	2.71551700	-4.55077800
H	1.15595600	1.47021500	-2.49442400
H	1.29220200	4.23965300	0.39176200
H	1.19168600	5.55588800	2.45965100
H	3.36067700	2.48896500	4.52341200
H	3.44060000	1.15465400	2.46557300
H	-4.03514500	-3.85547100	-0.38021000
H	-4.53133400	-5.08179200	-2.44551300

H	-1.63971400	-2.71858300	-4.54893800
H	-1.15606500	-1.47178900	-2.49348700
H	-1.29185300	-4.23913100	0.39498100
H	-1.19143000	-5.55379000	2.46387000
H	-3.36126900	-2.48569000	4.52498700
H	-3.44113100	-1.15295300	2.46611400
H	2.74354700	5.66394400	-4.97242000
H	4.42492400	5.13296400	-4.94479000
H	3.20429800	4.17933700	-5.80628900
H	1.30570600	5.50252200	5.00050900
H	2.37804900	4.33635800	5.79503800
H	3.05463000	5.69767100	4.89846800
H	-2.74039000	-5.66524000	-4.97050100
H	-4.42351900	-5.13991800	-4.93943200
H	-3.20781000	-4.18217400	-5.80331600
H	-1.30619500	-5.49915700	5.00428000
H	-2.37769100	-4.33180800	5.79820500
H	-3.05526000	-5.69346500	4.90291600
H	-8.76326400	-1.54898900	0.03308900
H	8.76328000	1.54896200	0.03305800
H	-14.21449400	0.28296600	0.01891300
H	14.21449100	-0.28306200	0.01861200
H	-12.04871200	5.13618700	0.81845500
H	-10.58919600	4.63927000	-0.06479600
H	-12.05814900	5.10827300	-0.94800400
H	12.05154900	-5.13760000	0.81482600
H	10.58912000	-4.63934600	-0.06299400
H	12.05518600	-5.10687700	-0.95160900

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C	-1.47074300	-0.39211200	-0.19080400
C	-1.28198000	1.00982300	-0.14690400
C	-0.00548600	1.57962500	-0.11167600
C	1.08004300	0.72242200	-0.11088500
C	0.89102700	-0.67910400	-0.16189900
C	-0.38510100	-1.24860700	-0.20763700
C	2.57274800	1.08411500	-0.07983100
C	3.18453200	-0.30467000	-0.12560600
C	2.20489500	-1.27431200	-0.15943800
C	-2.96308100	-0.75473600	-0.23029800
C	-3.57459200	0.63428500	-0.20955500
C	-2.59665300	1.60416000	-0.15105000
C	4.46981000	-0.88004600	-0.10810000
C	4.44038300	-2.28121800	-0.14033000
S	2.80969400	-2.89698600	-0.17680400
S	6.09567700	-0.30263300	-0.07540500
C	6.72334100	-1.94413700	-0.10478000
C	5.70726900	-2.88444700	-0.13797200
C	-4.86107900	1.20677600	-0.19656500

C	-4.83498800	2.60693000	-0.13952000
S	-3.20542300	3.22449000	-0.08527900
S	-6.48486400	0.62655900	-0.25746200
C	-7.11557000	2.26473100	-0.19576600
C	-6.10397300	3.20759200	-0.13663700
C	2.90107500	1.92821300	-1.31595200
C	3.00599800	1.75396600	1.23114500
C	-3.43344300	-1.50184700	1.02553500
C	-3.25236100	-1.52158800	-1.52470900
C	-2.72697100	-1.43039300	2.22808500
C	-3.21577700	-2.03826800	3.38010300
C	-4.42532500	-2.73686900	3.37651500
C	-5.13422800	-2.79762100	2.17389400
C	-4.64954500	-2.19282700	1.01912400
C	-3.04056200	-2.90290400	-1.59227000
C	-3.22476100	-3.59528500	-2.78306900
C	-3.63120100	-2.93889300	-3.94896100
C	-3.83657400	-1.55995700	-3.87759200
C	-3.65000400	-0.86120800	-2.68827000
C	2.70614000	3.31340400	-1.29991700
C	2.92592400	4.07779800	-2.43964900
C	3.35204700	3.49157200	-3.63545400
C	3.54057600	2.10836800	-3.64751400
C	3.31874300	1.33780000	-2.50971000
C	4.23626800	2.41655500	1.30457600
C	4.69050600	2.95045400	2.50497900
C	3.93513100	2.84649000	3.67644600
C	2.71130000	2.17849800	3.59992200
C	2.25298500	1.63998200	2.40104300
C	-3.86726300	-3.69715100	-5.22429000
C	-4.93223400	-3.42187800	4.61394400
C	4.41298900	3.45499500	4.96436200
C	3.62522200	4.32585600	-4.85476500
C	8.13289300	-2.20959400	-0.08676400
C	-8.52652200	2.52551800	-0.20231700
C	8.74313700	-3.45998900	-0.19274200
C	10.12744600	-3.37827500	-0.14065800
C	10.62952700	-2.07736200	0.00386600
S	9.30018700	-0.94075000	0.07946900
C	-9.15242300	3.76148600	-0.34794100
C	-10.54099300	3.67757600	-0.28090600
C	-11.02707700	2.37948200	-0.11894200
S	-9.69296000	1.26305400	-0.00017800
C	12.02196400	-1.85158100	0.06780200
C	-12.39281400	2.07115800	0.08333700
C	12.80022200	-0.72288400	0.20346600
C	-13.09409700	0.90215700	0.23482100
C	14.25490800	-0.66904000	0.24976400
C	14.64024900	0.75233400	0.40799200
C	13.47593400	1.53326800	0.45508000
C	12.29555500	0.65643200	0.33065300
C	-12.81411100	-0.49652700	-0.01192400

C	-13.71908400	-1.28448800	0.85200100
C	-14.68868600	-0.41904600	1.38757800
C	-14.39036600	0.96948100	0.96976900
C	-13.77080800	-2.64535000	1.14730600
C	-14.79786400	-3.10373600	1.97301400
C	-15.76619300	-2.23746100	2.48588800
C	-15.71828700	-0.87558900	2.19347900
C	15.88277900	1.37920200	0.50852100
C	15.91788700	2.76650500	0.65255400
C	14.74914600	3.52936000	0.69736400
C	13.50519200	2.90994900	0.59783700
C	15.15331800	-1.71576900	0.16475500
O	11.12895800	1.02216200	0.33501800
O	-15.03632900	1.97025600	1.22303400
C	-12.04778400	-1.00875100	-1.03979600
C	-11.83863800	-2.40364500	-1.23266500
N	-11.63661300	-3.53594400	-1.40845900
C	-11.54329400	-0.19058900	-2.08961400
N	-11.17167900	0.44416200	-2.99100400
C	16.56639000	-1.54805000	0.22073400
N	17.72703700	-1.47222000	0.26019800
C	14.78476400	-3.08257200	0.01113600
N	14.53573200	-4.21285800	-0.11427700
H	0.12631300	2.65718000	-0.08593500
H	-0.51669000	-2.32545100	-0.25399800
H	5.88329300	-3.95280800	-0.15067000
H	-6.28471200	4.27375100	-0.07857100
H	-1.78397600	-0.89407600	2.27038300
H	-2.64254200	-1.96700600	4.30148700
H	-6.08256600	-3.32834200	2.13714300
H	-5.22019700	-2.27345900	0.09806800
H	-2.74085600	-3.44724600	-0.70110200
H	-3.05294900	-4.66885100	-2.80617400
H	-4.14981500	-1.01908800	-4.76730300
H	-3.81285100	0.21247800	-2.67205500
H	2.39120000	3.80317900	-0.38275000
H	2.76623300	5.15268300	-2.39826700
H	3.86768700	1.62137300	-4.56302600
H	3.46911300	0.26321500	-2.55734800
H	4.84228200	2.53050700	0.40992300
H	5.65173900	3.45819100	2.53044800
H	2.10213800	2.07512600	4.49482700
H	1.29773200	1.12444800	2.38213500
H	-3.18814800	-4.54982800	-5.31368000
H	-4.88989600	-4.09077200	-5.26284500
H	-3.73127800	-3.05713400	-6.10024400
H	-4.60011100	-2.90702200	5.51973500
H	-6.02474200	-3.46695900	4.62629600
H	-4.56319900	-4.45284300	4.67132200
H	5.50187500	3.40025400	5.05131600
H	4.13542000	4.51401600	5.02566700
H	3.97461000	2.95195700	5.83045700

H	4.64947100	4.71704900	-4.84149200
H	3.51144800	3.74142400	-5.77178400
H	2.95099800	5.18530500	-4.91042400
H	8.19504800	-4.38650600	-0.31094500
H	10.78891800	-4.23561300	-0.20814400
H	-8.60813100	4.68479000	-0.50216100
H	-11.20576000	4.53122800	-0.35542500
H	12.55744000	-2.79290100	-0.00963000
H	-13.00687600	2.95276100	0.27814100
H	-13.03357300	-3.34217800	0.76801800
H	-14.84262800	-4.15980700	2.22053200
H	-16.55631300	-2.62998300	3.11833000
H	-16.45718800	-0.18115100	2.58089500
H	16.81257400	0.82671800	0.47851100
H	16.88104000	3.26116200	0.73144600
H	14.81414700	4.60706100	0.81015300
H	12.57853100	3.47442100	0.62917600

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