Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Influence of non-covalent interactions in dictating the polarity and mobility of charge carriers in a series of crystalline NDIs: A computational case study

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Table of contents

1. Frontier Molecular Orbitals of NDIs

Frontier molecular orbitals are generated at the isosurface value (0.03) from the optimized geometry. The geometries are optimized using B3LYP-D3/6-31+G* level of theory. All the calculations are carried out using Gaussian16 program unless stated otherwise. [1]

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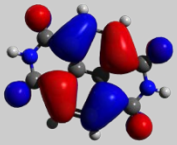
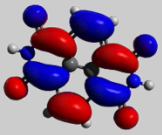
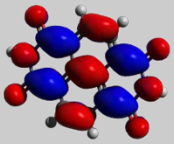
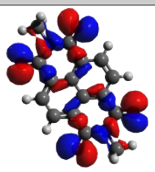
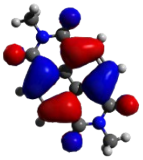
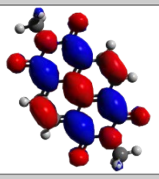
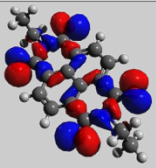
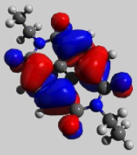
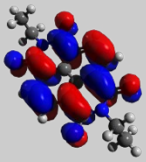
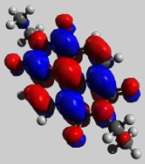
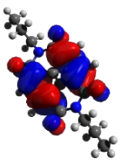
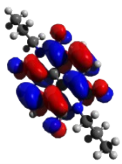
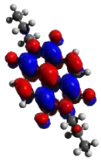
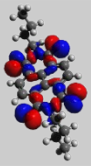
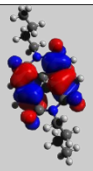
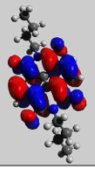
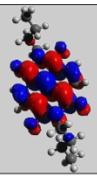
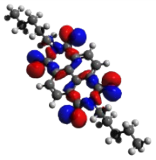
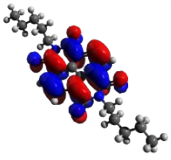
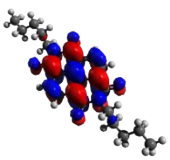
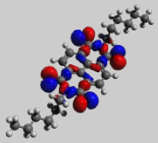
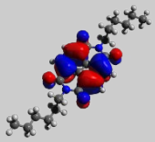
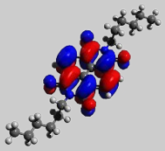
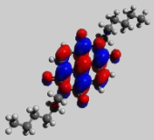
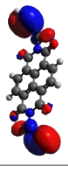
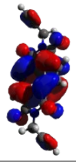
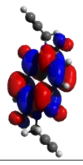
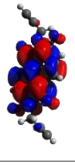
IH				
I				
II				
III				
IV				
V				
VI				
IIIp				

Fig S1: Frontier molecular orbitals of the monomeric NDIs (visualized at the isosurface value of 0.03)

1.1. Ionization potential (IP) and electron affinity (EA) of monomeric NDIs

For the calculation of ionization potential (IP) and electron affinity (EA), optimization of all the neutral structures were carried out using B3LYP-D3/6-31+G* level of theory whereas optimization of all the charged species were done at uB3LYP-D3/6-31+G* level of theory.

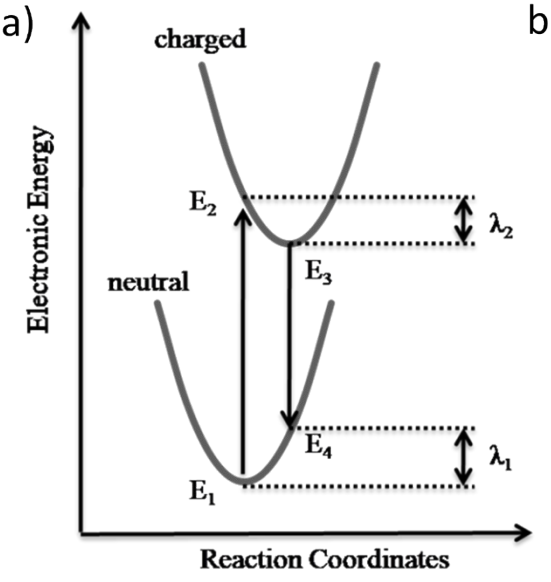
Code	$IP_{vertical}$	$EA_{vertical}$	$IP_{adiabatic}$	$EA_{adiabatic}$	$IP_{Koopmans'}$	$EA_{Koopmans'}$
IH	9.13	2.46	9.03	2.63	7.76	3.97
I	8.88	2.30	8.78	2.47	7.35	3.78
II	8.81	2.28	8.71	2.46	7.30	3.74
III	8.78	2.29	8.68	2.46	7.28	3.72
IV	8.76	2.30	8.66	2.47	7.28	3.72
V	8.74	2.29	8.64	2.46	7.27	3.71
VI	8.73	2.29	8.64	2.46	7.27	3.70
IIIp	8.79	2.44	8.74	2.61	7.43	3.87

Table S1: Vertical, adiabatic and Koopman's ionization potential (IP) and electron affinity (EA) values of NDI monomers (all energies are in electron volt)

2. Internal reorganization energy of monomeric NDIs

Internal reorganization energy (λ) is computed using the "four point energy" approach at B3LYP-D3/6-31+G* level of theory. Optimization and single point of all the neutral structures were carried out using B3LYP-D3/6-31+G* level of theory whereas optimization and single point of all the charged species were done at uB3LYP-D3/6-31+G* level of theory.

a)



b)

Sl No.	λ_h	λ_e
IH	207.9	331.4
I	207.4	332.7
II	206.8	338.5
III	205.5	339.3
IV	205.4	341.1
V	199.9	341.4
VI	197.8	342.1
IIIp	106.1	349.7

Fig S2: a) Adiabatic potential energy surfaces for the neutral state and the charged state, showing vertical transitions b) Internal hole and electron reorganization energy values of the NDIs (all energies are in meV)

Details of the four point energy method used to calculate reorganization energy:

$\lambda = \lambda_1 + \lambda_2$

$\lambda_1 = E_4 - E_1$

$\lambda_2 = E_2 - E_3$

Here, λ is the reorganization energy; E_1 is the lowest energy of neutral species; E_3 is the the lowest energy of cationic species for hole reorganization energy (λ_h), or anionic species for electron reorganization energy (λ_e).
For hole reorganization energy (λ_h), E_4 is the single point energy of a neutral molecule with the optimized cation geometry, while for the electron reorganization energy (λ_e), is the single point energy of a neutral molecule with optimized anion geometry. And E_2 is the single point energy of the charged (cationic for λ_h and anionic for λ_e) molecule with the optimized geometry of the neutral species.

3. Crystal structure and Molecular packing:

To obtain a clear idea on the intermolecular interaction leading to the 3-D packing in single crystals for each derivative, a detailed analysis has been carried out. It was revealed that in the case of both **I** and **II**; the single crystals belong to the monoclinic unit cell and the space group is P2(1)/c and for **VI** triclinic unit cell with $P\bar{1}$ space group with γ motif molecular packing for all three (**Fig. S3**). Non-classical C-H···O hydrogen bonding ($d_{C\text{-}H\cdots O}$ =2.69, 2.41 and 2.60 Å for **I** and 2.81, 2.53 and 2.40 Å for **II** and 2.84 Å for **VI** are the most prevailing interactions. The packing densities (ρ = 1.55 g cm^{-3} (**I**) and 1.56 g cm^{-3} (**II**)) are very similar without solvent molecules insertion, with eight and five molecules respectively in the unit cell for **I** and **II**; and for **VI** ρ = 1.25 g cm^{-3} with eight molecules in the unit cell. **I**, **II** and **VI** are packed with slipped π – stacking with an interplanar nearest neighbour separation of 3.35, 3.25 Å and 3.34 Å. Molecule **I** is slipped along the short axis with a slip angle of 47.35° and the corresponding long axis displacement angle was 74.79°. For **II**, the angles are 43.31° and 72.02° respectively and for **VI** 44.84° and 70.74° (Fig. S3). The crystalline packing of **I**, **II** are regulated by noncovalent intermolecular interactions of C···C (varies 3.28 to 3.46 Å), C···O (ranging 3.10 to 3.30 Å), C···H mainly. For **I**, O···H interactions (30.1 %), along with

H···H (29.4 %), C···H (17.6 %), C···C (9.1 %), C···O (8.8 %) interactions, control the packing, similarly for **II** crystal packing was influenced by O···H (25.5 %), H···H (38.6 %), C···H (17.7 %), C···C (6.7 %), C···O (8.2 %), and interactions for **VI**, 17 % (O···H interaction), 59.1 % (H···H), 11.9 % (C···H), 4.4 % (C···C) and 5.3 % (C···O).

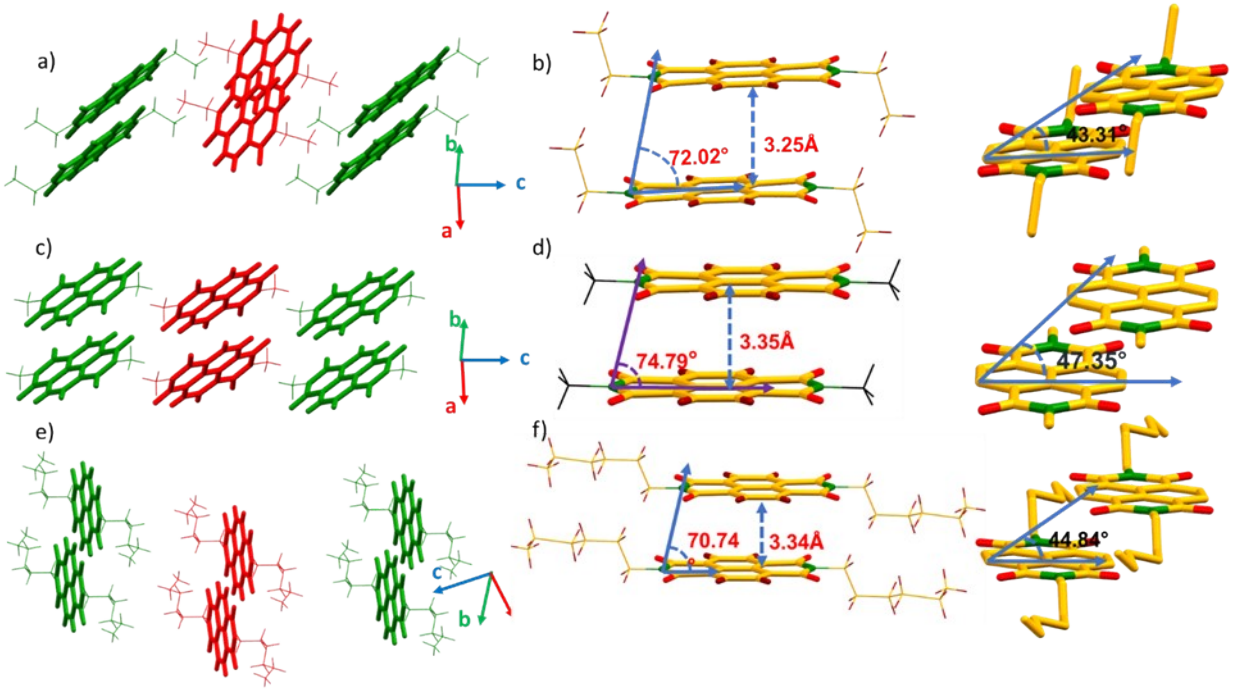


Fig S3: Molecular packing type a) **I**, c) **II**, e) **VI** and slipping angle and π – stacking distances b) **I**, d) **II**, f) **VI**.

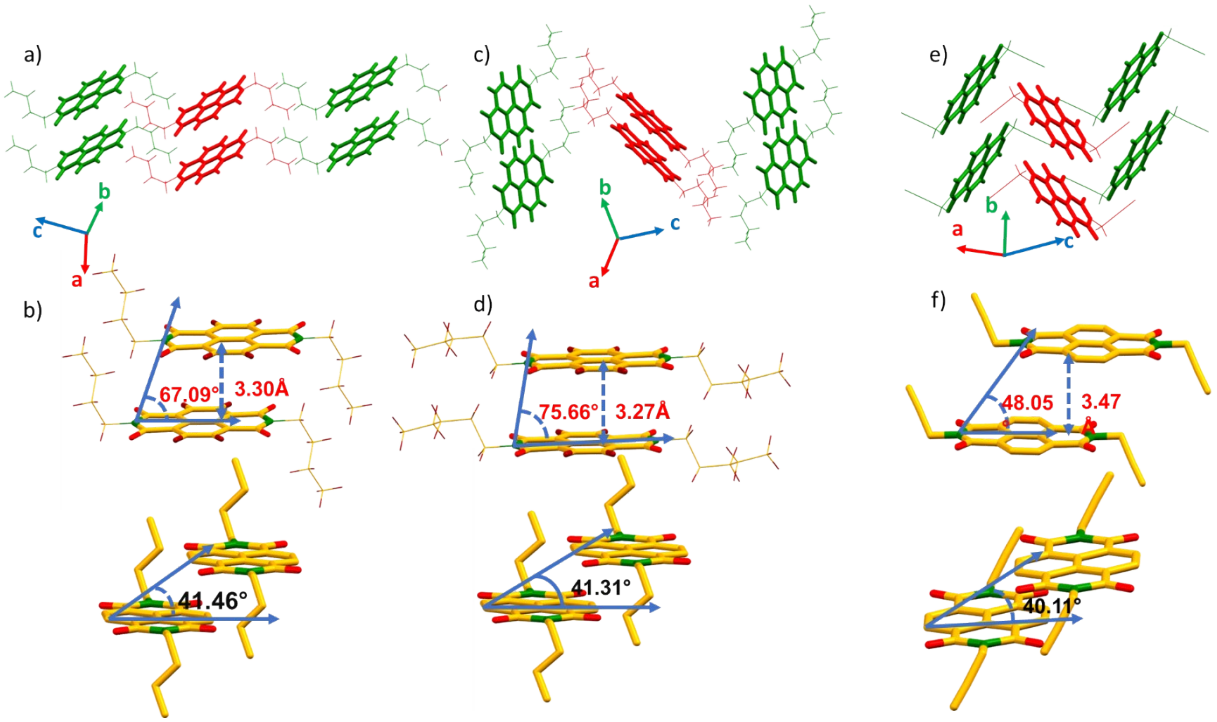


Fig S4: Molecular packing type a) **IIIp**, c) **IV**, e) **V** and slipping angle and π – stacking distances b) **IIIp**, d) **IV**, f) **V**.

In the case of **III**, the supramolecular arrangement leads to X-type pattern crystal packing (β motif) with relatively large inter layer molecular overlap with high π – stacking along the a-axis. It falls in to orthorhombic system with 'Pbca' space group and packing density of 1.41 g cm^{-3} with eight molecules in a unit cell without any solvent molecule inclusion. Along with weak C-H···O ($d_{C-H\cdots O}$ =2.50 Å) hydrogen bonding interactions, H···H interactions (2.27 Å and 2.31 Å) stimulate the crystal packing. The noncovalent intermolecular interactions like C···C (varies 3.31 to 3.39 Å), C···O (3.21 Å) also control the crystalline packing of **III**. The % of noncovalent interactions regulating the crystal packing of **III** are, 25.3 % (O···H interaction), 49.9 % (H···H), 4.7 % (C···H), 13.9 % (C···C) and 1.4 % (C···O). Two nearby molecules (along the π – stacking) are 52.96° crossed (fig S5) and the nearest neighbour interplanar separation of 3.33 Å through π – stacking.

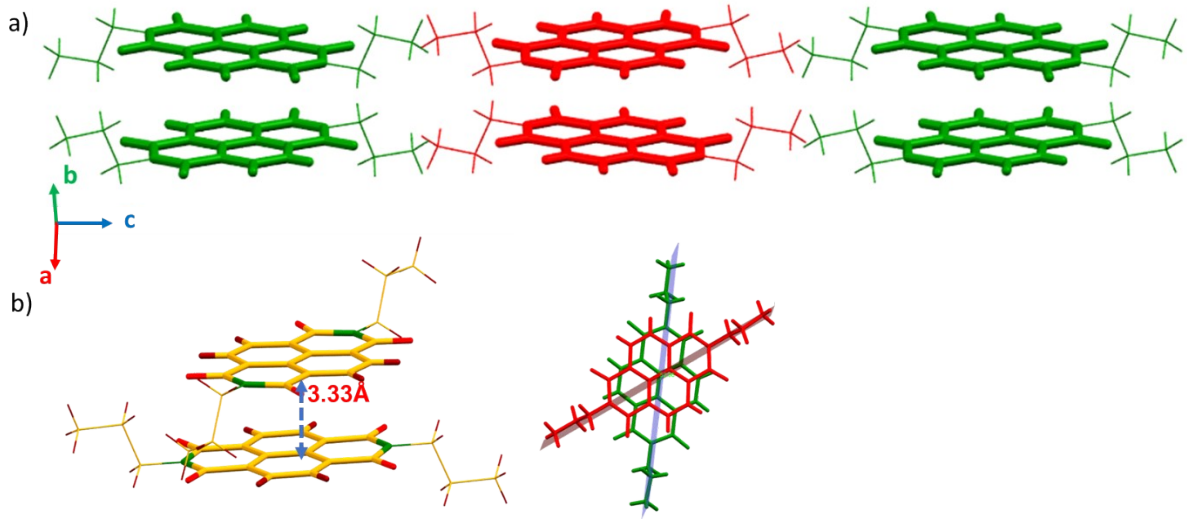


Fig S5: Molecular packing type a) **III** and and π – stacking distances b) **III**

IH follows a sheet like molecular packing in its single crystal along the a-axis with a relatively lower intermolecular overlap along π – stacking. The crystal belongs to the triclinic system with '$P\bar{1}$' space group and six molecules in its unit cell. **IH** crystals are found to be packed with highest packing density (ρ = 1.70 g cm^{-3}) among the eight molecules. Non-classical weak C-H···O hydrogen bonding ($d_{C-H\cdots O}$ =1.99, 2.48, 2.38 and 2.60 Å) interactions are the determining factor for **IH** crystal packing. The major intermolecular noncovalent interactions- C···C (varies 3.27 to 3.49 Å), C···O (ranging 3.04 to 3.23 Å) guide the crystal packing. The crystalline packing of **IH** is controlled by noncovalent intermolecular interactions- O···H (38.5 %), H···H (11.9 %), C···H (13.8 %), C···C (11.1 %), C···O (15.9 %) interactions. The nearest

π – stacking distance of 3.30 Å with large slip along short axis (fig S6) is observed. A summary of unit cell characteristics of all the derivatives are summarized in the **Table S2**.

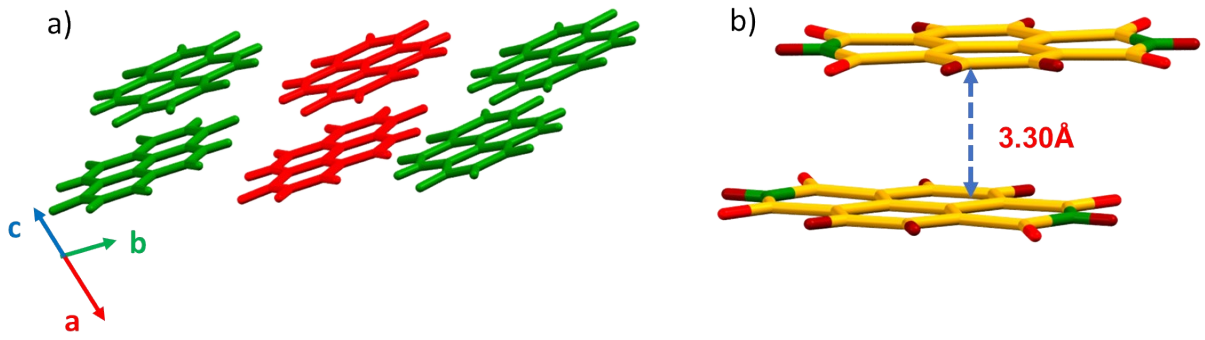


Fig S6: Molecular packing type a) **IH** and π – stacking distances b) **IH**.

Code	R	CCDC	Crystal system	Colour	Shape	a	b	c	α	β	γ
IH	H	189606	Triclinic	colourless	plate	7.867	5.305	12.574	90	72.73	90
I	CH_3	1029338	Monoclinic	light yellow	needle/flexible plastic	4.621	8.019	17.024	90	93.99	90
II	C_2H_5	1029339	Monoclinic	light yellow	needle/flexible elastic	4.844	7.736	18.315	90	90.12	90
III	C_3H_7	1029340	Orthorhombic	yellow	needle	6.962	17.242	27.580	90	90	90
IV	C_4H_9	819749	Triclinic	colourless	prismatic	5.223	7.840	11.132	103.72	94.28	93.86
V	C_5H_{11}	238148	Monoclinic	orange	acicular	5.028	8.107	24.026	90	90.79	90
VI	C_6H_{13}	671518	Triclinic	pink	plate	4.898	8.284	14.524	96.33	98.10	93.59
IIIp	CH_2-C≡CH	100718	Monoclinic	pink	needle	9.746	6.310	12.867	90	111.78	90

Table S2: Crystal structure data of the studied NDIs. (*a*, *b*, *c* are in A^0 and α, β, γ are in degree)

3.1. Hirschfield surface analysis and percentage of interactions

Important intermolecular interactions within the crystal structure of NDIs were identified through Hirshfeld surface analysis using Crystal Explorer 17.5. [2] The Hirshfeld surface is defined as a set of points in 3D space where the ratio of promolecule and procrystal electron densities is equal to 0.5. The exploration of intermolecular contacts is provided by mapping normalized contact distances (d_{norm}), which is a function of a closest distance from the point to the nuclei interior (d_i) and exterior (d_e) to the surface as well as on the van der Waals radii (r_{vdw}). The percentage of interactions obtained from the Hirshfeld surface analysis are visualized in the following pi-charts. (**Fig. S7**)

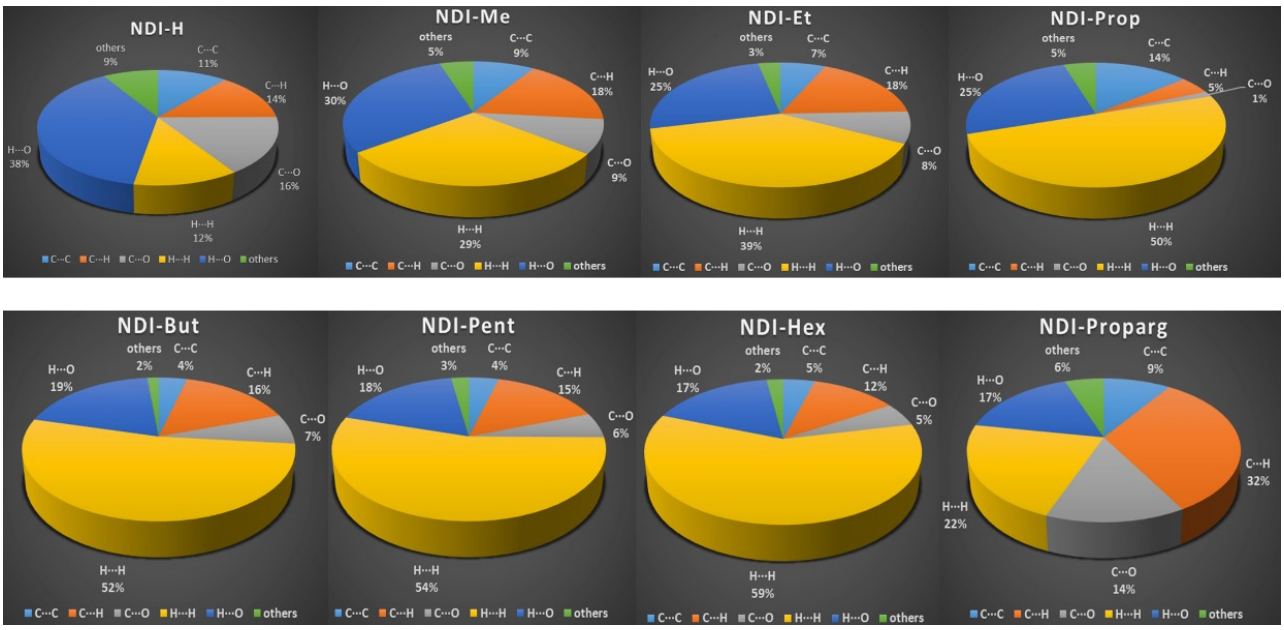


Fig S7: Pi-charts showing percentage of interactions in the crystal structure of NDIs

4. Charge transfer integral by dimer orbital projection method

Before discussing our results, we would like to discuss about the methodology we used here to calculate the charge transfer integral (J). The charge transfer integral is written mathematically as:

$$J_{AB} = \ < \psi_A | \hat{\mathrm{H}} | \psi_B >$$

Here, ψ_A and ψ_B represent the wave functions of two different quantum states A and B which are orthogonal and $\hat{\mathrm{H}}$ represents the Hamiltonian operator. Here J measures the extent of electronic coupling between states. The larger the value of J, the larger the probability that a charge in state A will move to state B and vice versa.

There are different methods for calculating the charge transfer integrals (J) that make use of various approximations. The most straightforward, albeit limited, way to calculate the charge transfer integral is the so-called “energy splitting method”. In this method hole transfer integral is quantified as the energy difference between the HOMO and HOMO−1. In contrast, the energy difference between the LUMO+1 and LUMO is defined as the electron transfer integral.

Brédas et al, showed that the neglect of electronic polarization leads to qualitatively incorrect values and trends for the transfer integrals computed with this ‘energy splitting method’.

In this study, to calculate the charge transfer integral between the stacks of the active material, we used the dimer projection, in short DIPRO method proposed by Baumeier et. al. [3] Effect of electronic polarization is considered to estimate the charge transfer integral values. For transfer integral calculations, we used B3LYP-D3/6-31+G* level of theory.

Charge transfer integral is directly related to rate of electron transfer according to Marcus-Hush theory. At room temperature, according to the Marcus-Hush hopping mechanism the charge hopping rate (k) is given by:

$$k = \frac{V^2}{\hbar}\left(\frac{\pi}{\lambda K_B T}\right)^{\frac{1}{2}} \exp\left(-\frac{\lambda}{4K_B T}\right)$$

Here, $\hbar$ is the Planck's constant, K_B is the Boltzman's constant, T is temperature, λ is the reorganization energy.

V is the electronic coupling expressed by:

$$V = \frac{J_{AB} - S_{AB}(t_{AA} - t_{BB})/2}{1 - S_{AB}^2}$$

Where,

$$J_{AB} = \langle \psi_A | \hat{H} | \psi_B \rangle$$

$$S_{AB} = \langle \psi_A | \psi_B \rangle$$

$$t_{AA} = \langle \psi_A | \hat{H} | \psi_A \rangle$$

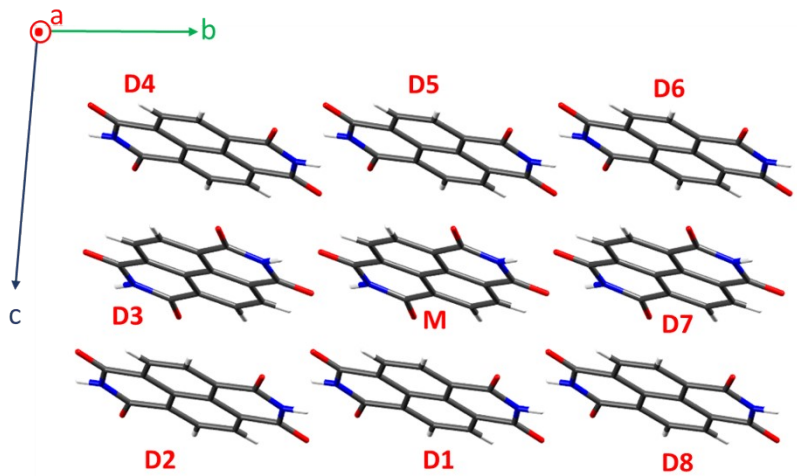
$$t_{BB} = \langle \psi_B | \hat{H} | \psi_B \rangle$$

To calculate the transfer integral, we first choose a reference crystallographic plane and a reference axis. The reference axis must lie on the reference plane. Usually the reference axis is the pi-stacking direction. Then we choose different interacting hoping dimers, and calculated the charge transfer integral using the aforementioned method.

Theta (**θ**) is the angle between any dimer of our interest (vector connecting two centroids) and the reference axis (crystallographic axis such as *a*, *b* or *c*). Gamma (**γ**) is the projection angle of any dimer of our interest to the reference plane we have considered. If the **γ**=0^0 for all the neighbouring dimers, all the interacting molecules lies in a same plane.

4.1. Charge transfer integral of IH

For **IH** we considered *c* as the reference axis and *bc* as the reference plane.

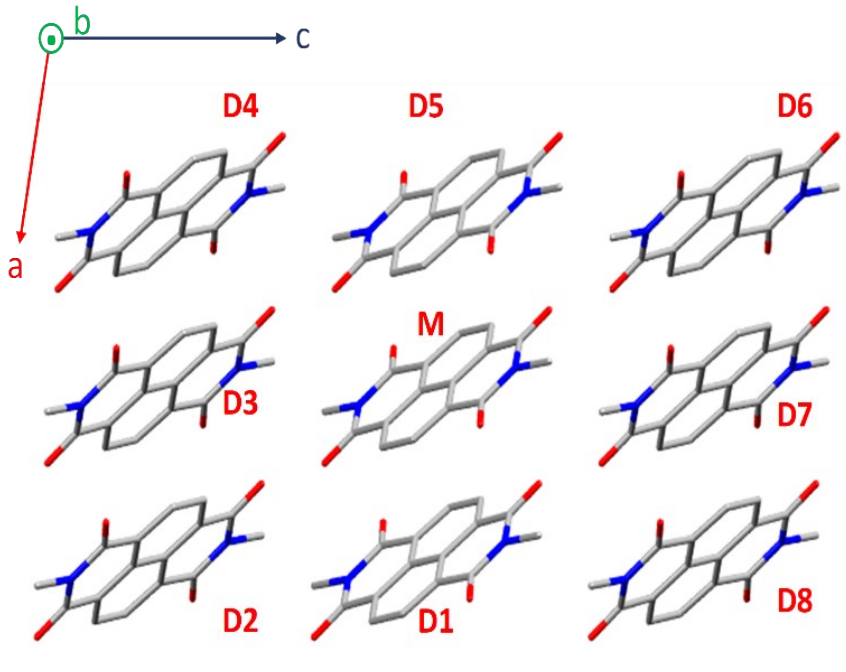


Pairs of IH	J_h (meV)	J_e (meV)	Distance (r_i) (A^0)	Theta(θ)	Gamma (γ)
M-D1	62.9	39.7	4.5	19	0
M-D2	5.6e-2	0.2	12	69	36
M-D3	0.8	1.9	10.2	90	44
M-D4	1.0	0.6	10.1	65	45
M-D5	62.9	39.7	4.5	19	0
M-D6	5.6e-2	0.2	12	69	36
M-D7	0.8	1.9	10.2	90	44
M-D8	1.0	0.6	10.1	65	45

Fig S8: Charge transfer integrals for **IH** along with geometrical parameters.

4.2. Charge transfer integral of I

For IH we considered *a* as the reference axis and *ac* as the reference plane.

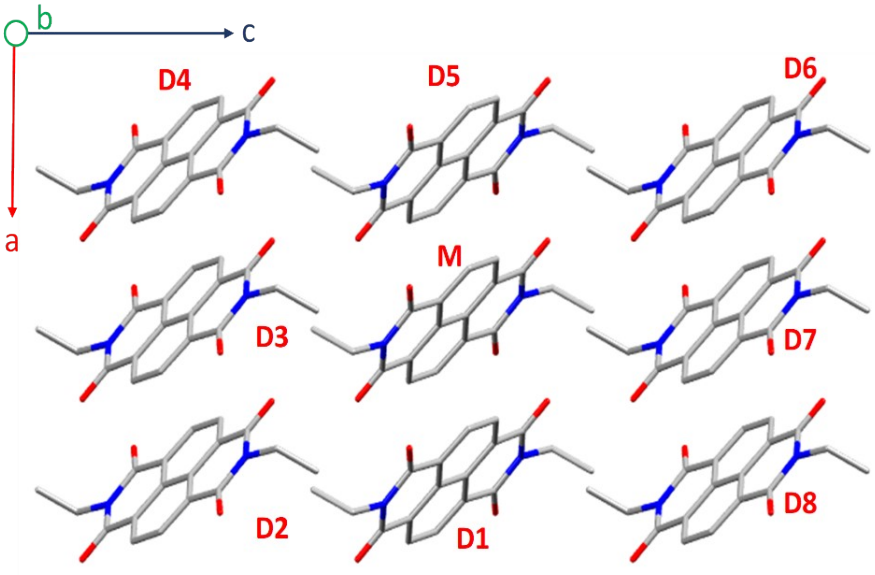


Pairs of I	J_h (meV)	J_e (meV)	Distance (r_i) (A^0)	Theta(θ)	Gamma (γ)
M-D1	76.6	0.5	4.6	4	0
M-D2	5.1e-5	5.4e-2	13.6	47	17
M-D3	6.6e-3	0.3	10.7	65	22
M-D4	1.0	1.5	9.4	90	25
M-D5	76.6	0.5	4.6	4	0
M-D6	5.1e-5	5.4e-2	13.6	47	17
M-D7	6.6e-3	0.3	10.7	65	22
M-D8	1.0	1.5	9.4	90	25

Fig S9: Charge transfer integrals for **I** along with geometrical parameters

4.3. Charge transfer integral of II

For **II** we considered *a* as the reference axis and *ac* as the reference plane.

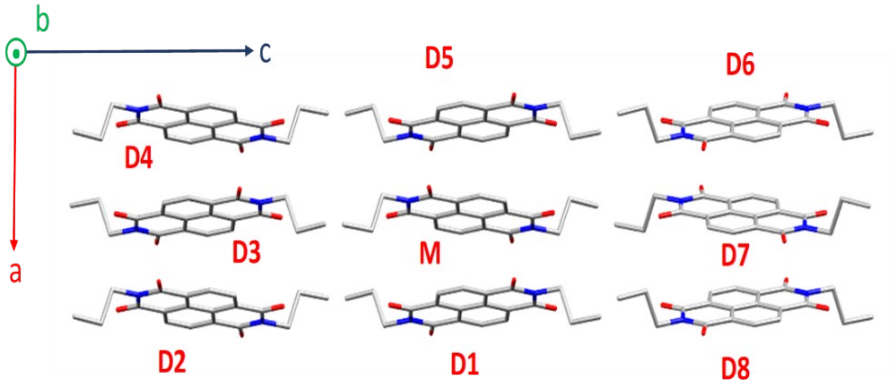


Pairs of II	J_h (meV)	J_e (meV)	Distance (r_i) (A^0)	Theta(θ)	Gamma (γ)
M-D1	64.4	91.4	4.8	0	0
M-D2	0.3	1.6	11.1	64	21
M-D3	2.9e-2	0.7	9.9	90	23
M-D4	1.1e-2	8.5e-4	11.0	64	21
M-D5	64.4	91.4	4.8	0	0
M-D6	0.3	1.6	11.1	64	21
M-D7	2.9e-2	0.7	9.9	90	23
M-D8	1.1e-2	8.5e-4	11.0	64	21

Fig S10: Charge transfer integrals for **I** along with geometrical parameters

4.4. Charge transfer integral of III

For **III** we considered *a* as the reference axis and *ac* as the reference plane.

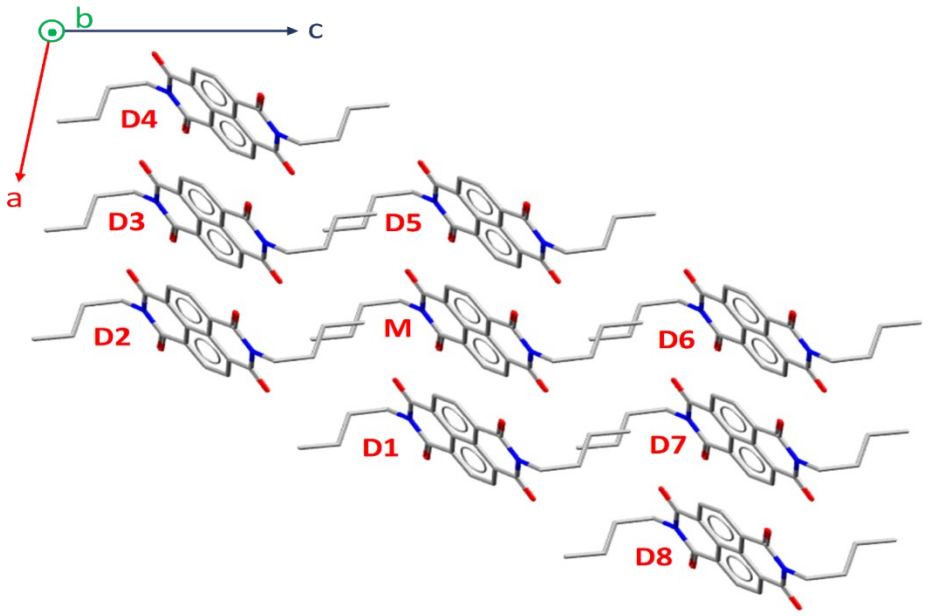


Pairs of III	J_h (meV)	J_e (meV)	Distance (r_i) (A^0)	Theta(θ)	Gamma (γ)
M-D1	105.5	84.0	3.5	2	0
M-D2	2.1e-3	5.4e-3	14.7	76	17
M-D3	3.2e-2	1.8e-5	14.4	90	17
M-D4	6.6e-3	3.3e-3	14.6	76	17
M-D5	105.5	84.0	3.5	2	0
M-D6	2.1e-3	5.4e-3	14.7	76	17
M-D7	3.2e-2	1.8e-5	14.4	90	17
M-D8	6.6e-3	3.3e-3	14.6	76	17

Fig S11: Charge transfer integrals for **I** along with geometrical parameters

4.5. Charge transfer integral of IV

For **IV** we considered *a* as the reference axis and *ac* as the reference plane.

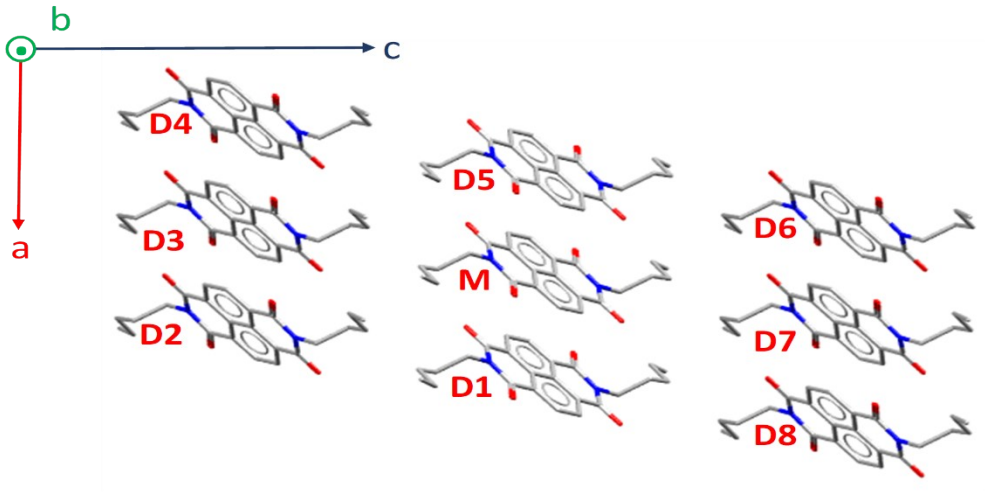


Pairs of IV	J_h (meV)	J_e (meV)	Distance (r_i) (A^0)	Theta(θ)	Gamma (γ)
M-D1	23.4	143.9	5.2	7	0
M-D2	2.1	0.6	11.1	90	0
M-D3	0.4	0.3	12.0	64	0
M-D4	6.2e-3	4.5e-2	14.7	45	0
M-D5	23.4	143.9	5.2	7	0
M-D6	2.1	0.6	11.1	90	0
M-D7	0.4	0.3	12.0	64	0
M-D8	6.2e-3	4.5e-2	14.7	45	0

Fig S12: Charge transfer integrals for **I** along with geometrical parameters

4.6. Charge transfer integral of V

For **V** we considered *a* as the reference axis and *ac* as the reference plane.

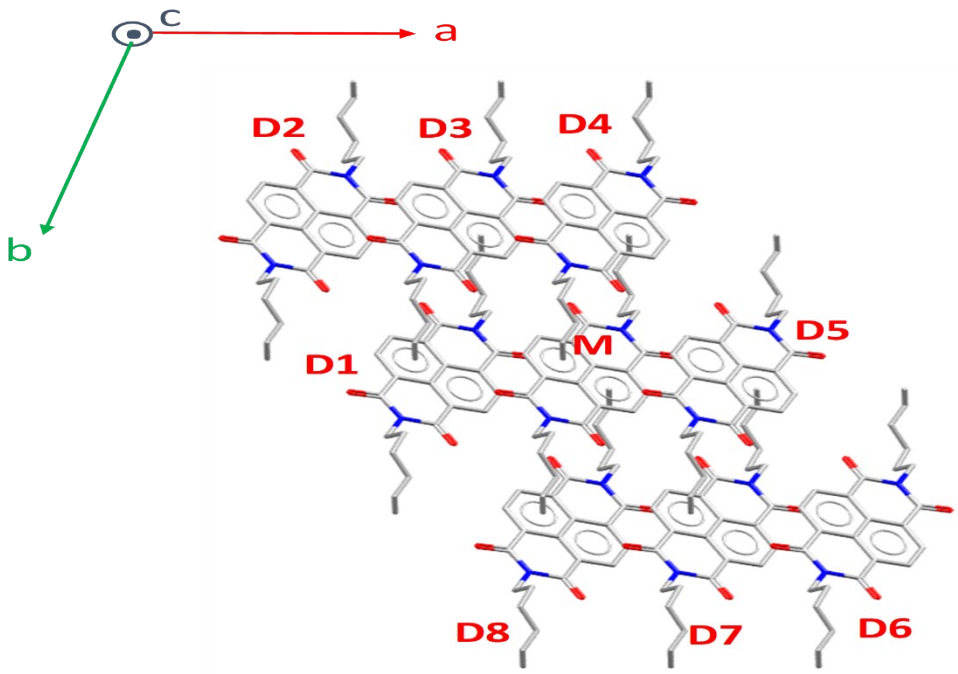


Pairs of V	J_h (meV)	J_e (meV)	Distance (r_i) (A^0)	Theta(θ)	Gamma (γ)
M-D1	92.8	103.9	5.0	1	0
M-D2	4.7e-4	2.1e-2	14.7	59	16
M-D3	0.1	6.8e-3	12.9	78	18
M-D4	5.0e-3	6.7e-3	13.0	79	18
M-D5	92.8	103.9	5.0	1	0
M-D6	4.7e-4	2.1e-2	14.7	59	16
M-D7	0.1	6.8e-3	12.9	78	18
M-D8	5.0e-3	6.7e-3	13.0	79	18

Fig S13: Charge transfer integrals for **V** along with geometrical parameters

4.7. Charge transfer integral of VI

For **VI** we considered *a* as the reference axis and *ab* as the reference plane.

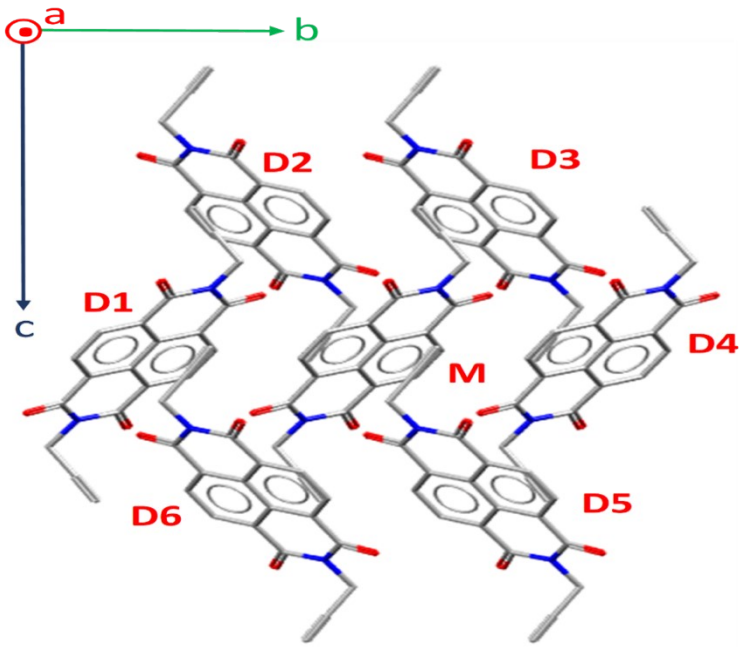


Pairs of VI	J_h (meV)	J_e (meV)	Distance (r_i) (A^0)	Theta(θ)	Gamma (γ)
M-D1	8.0	79.8	4.9	9	0
M-D2	2.1e-4	0.1	12.4	39	0
M-D3	1.1	26.8	9.4	59	0
M-D4	19.6	29.8	8.3	90	0
M-D5	8.0	79.8	4.9	9	0
M-D6	2.1e-4	0.1	12.4	39	0
M-D7	1.1	26.8	9.4	59	0
M-D8	19.6	29.8	8.3	90	0

Fig S14: Charge transfer integrals for **VI** along with geometrical parameters

4.8. Charge transfer integral of IIIp

For IIIp we considered *b* as the reference axis and *bc* as the reference plane.



Pairs of VI	J_h (meV)	J_e (meV)	Distance (r_i) (A^0)	Theta(θ)	Gamma (γ)
M-D1	62.6	60.0	6.3	0	0
M-D2	37.8	6.7	7.2	0	0
M-D3	37.8	6.7	7.2	0	0
M-D4	62.6	60.0	6.3	0	0
M-D5	37.8	6.7	7.2	0	0
M-D6	37.8	6.7	7.2	0	0

Fig S15: Charge transfer integrals for **IIIp** along with geometrical parameters

5. Energy splitting values the along the different hoping dimers

	Monomer		Dimers	E_{LUMO+1}	E_{LUMO}	E_{HOMO}	E_{HOMO-1}	$\Delta E_{(LUMO+1)-LUMO}$	$\Delta E_{HOMO-(HOMO-1)}$
	LUMO	HOMO							
IH	-3.97	-7.76	M-D1	-4.03	-4.125	-7.623	-7.74	0.095	0.117
			M-D2	-3.949	-3.955	-7.557	-7.592	0.006	0.035
			M-D3	-3.953	-3.954	-7.557	-7.559	0.001	0.002
			M-D4	-3.915	-3.98	-7.557	-7.588	0.065	0.031
I	-3.78	-7.35	M-D1	-3.719	-3.732	-7.309	-7.458	0.013	0.149
			M-D2	-3.66	-3.661	-7.313	-7.316	0.001	0.003
			M-D3	-3.639	-3.679	-7.294	-7.327	0.04	0.033
			M-D4	-3.677	-3.72	-7.333	-7.369	0.043	0.036
II	-3.74	-7.30	M-D1	-3.607	-3.778	-7.279	-7.414	0.171	0.135
			M-D2	-3.62	-3.689	-7.267	-7.355	0.069	0.088
			M-D3	-3.682	-3.688	-7.329	-7.332	0.006	0.003
			M-D4	-3.669	-3.683	-7.318	-7.33	0.014	0.012
III	-3.72	-7.28	M-D1	-3.625	-3.798	-7.251	-7.458	0.173	0.207
			M-D2	-3.643	-3.644	-7.279	-7.279	0.001	0
			M-D3	-3.602	-3.66	-7.238	-7.295	0.058	0.057
			M-D4	-3.642	-3.642	-7.277	-7.278	0	0.001
IV	-3.72	-7.28	M-D1	-3.544	-3.825	-7.273	-7.309	0.281	0.036
			M-D2	-3.663	-3.666	-7.276	-7.28	0.003	0.004
			M-D3	-3.654	-3.657	-7.273	-7.275	0.003	0.002
			M-D4	-3.633	-3.637	-7.253	-7.255	0.004	0.002
V	-3.71	-7.27	M-D1	-3.602	-3.803	-7.21	-7.401	0.201	0.191
			M-D2	-3.66	-3.669	-7.263	-7.267	0.009	0.004
			M-D3	-3.662	-3.695	-7.264	-7.292	0.033	0.028
			M-D4	-3.685	-3.692	-7.287	-7.29	0.007	0.003
VI	-3.70	-7.27	M-D1	-3.57	-3.721	-6.177	-6.178	0.151	0.001
			M-D2	-3.618	-3.619	-6.134	-6.136	0.001	0.002
			M-D3	-3.54	-3.593	-6.02	-6.026	0.053	0.006
			M-D4	-3.575	-3.636	-6.147	-6.151	0.061	0.004
IIIp	-3.87	-7.43	M-D1	-3.892	-4.014	-7.454	-7.573	0.122	0.119
			M-D2	-3.742	-3.96	-7.289	-7.541	0.218	0.252

Table S3: Energy splitting values along the different hoping dimers (all energies are in eV) Frontier molecular orbitals of the dimers are shown below

6. Interaction energy framework analysis of dimers along different hoping pathway

Interactions energies are calculated for different dimers at HF/6-31+G* level of theory using CrystalExplorer17.5 software.

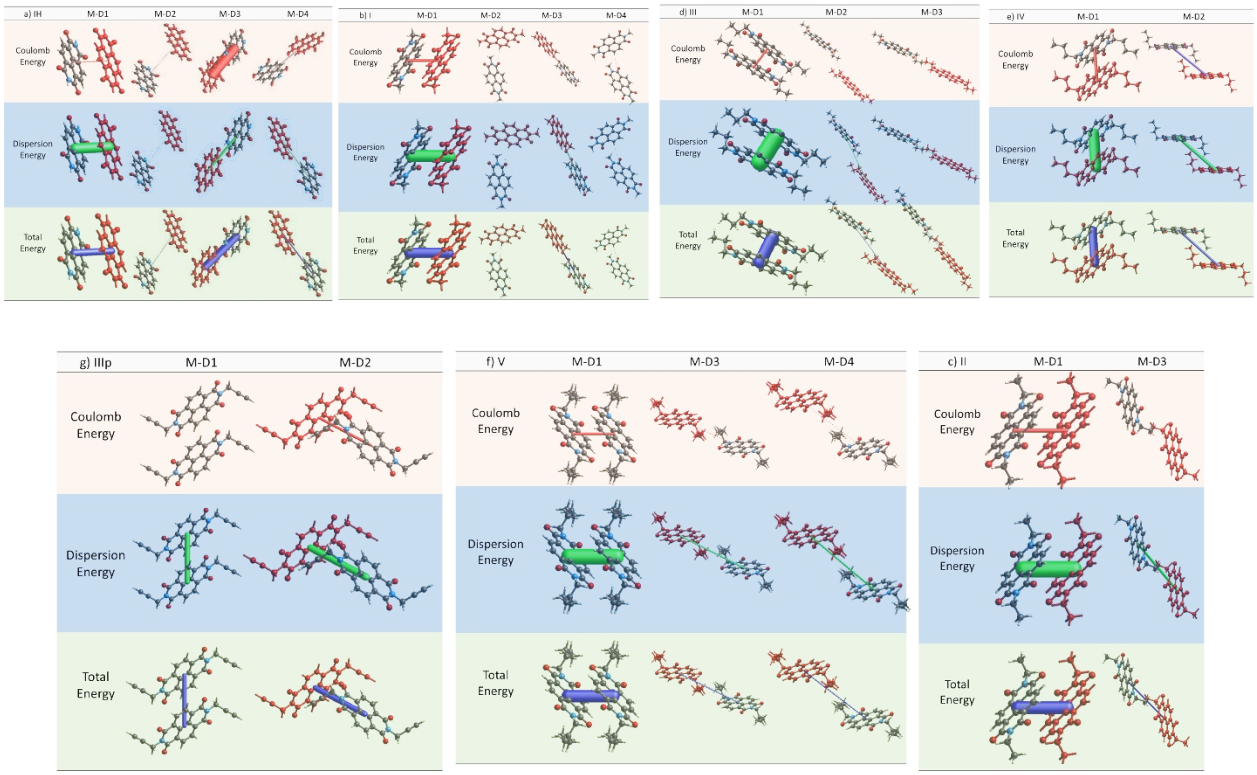


Fig S16: Crystal Explorer-based energy frameworks of different dimers of a) **IH** b) **I** c) **II** d) **III** e) **IV** f) **V** and g) **IIIp** with 100 energy scale factor and zero energy threshold.

IH	r (A^0)	$E_{Coulomb}$	$E_{polarization}$	$E_{dispersion}$	$E_{repulsion}$	E_{total}
M-D1	4.5	-5.3	-3.1	-74.8	40.8	-41.7
M-D2	12.0	-1.4	-0.1	-1.1	0	-2.5
M-D3	10.2	-69.2	-18.4	-14.2	58.1	-48.2
M-D4	10.1	-4.9	-0.6	-5	0.1	-9.8

I	r (A^0)	$E_{Coulomb}$	$E_{polarization}$	$E_{dispersion}$	$E_{repulsion}$	E_{total}
M-D1	4.6	-17.2	-3.6	-78.1	37.9	-59.5
M-D2	13.6	-0.5	0	-0.4	0	-0.8
M-D3	10.7	-8.14	-2.2	-8.2	4.2	-8.2
M-D4	9.4	2.2	-0.6	-12.7	4	-6.4

II	r (A^0)	$E_{Coulomb}$	$E_{polarization}$	$E_{dispersion}$	$E_{repulsion}$	E_{total}
M-D1	4.84	-19.5	-5.1	-86.1	47.4	-62.4
M-D3	9.94	-0.4	-0.6	-22.1	11.1	-11.7

III	r (A^0)	$E_{Coulomb}$	$E_{polarization}$	$E_{dispersion}$	$E_{repulsion}$	E_{total}
M-D1	3.48	-17.5	-4.0	-119.2	59.5	-79.6
M-D2	15.02	-0.5	-0.2	-8.9	3.4	-5.9
M-D3	14.51	0.2	-1.1	-7.4	2.1	-5.6

IV	r (A^0)	$E_{Coulomb}$	$E_{polarization}$	$E_{dispersion}$	$E_{repulsion}$	E_{total}
M-D1	5.2	-22.9	-6.3	-96.4	57.4	-68.7
M-D2	11.1	-4.3	-0.5	-40.9	20.1	-25.3

V	r (A^0)	$E_{Coulomb}$	$E_{polarization}$	$E_{dispersion}$	$E_{repulsion}$	E_{total}
M-D1	5.03	-16.2	-4.4	-93.6	46.6	-65.8
M-D3	12.98	-2.2	-0.5	-15.2	6.2	-11.2
M-D4	13.04	-1.0	0.0	-12.0	5.5	-7.4

IIIp	r (A^0)	$E_{Coulomb}$	$E_{polarization}$	$E_{dispersion}$	$E_{repulsion}$	E_{total}
M-D1	6.3	0.9	-1.8	-39.3	9.0	-28.4
M-D2	7.2	-16.0	-4.8	-44.5	29.5	-35.6

Table S4: Pairwise interaction energy for different dimers of **IH**, **I**, **II**, **III**, **IV**, **V** and **IIIp** (all energies are in kJ/mol)

7. Density Overlap Region Indicator (DORI) analysis: Non Covalent Interaction plot

As non-covalent interactions predominantly govern the molecular arrangement and thereby electronic coupling in the organic molecular system, we tried to address this aspect by qualitatively visualizing different non-covalent interaction present in the NDIs. For this purpose single point calculations for molecular aggregates were carried out at B3LYP-D3/6-31+G* level of theory. To visualize the Non Covalent Interaction (NCI) plot, we have done Density Overlap Region Indicator (DORI) analysis using open source code Multiwfn.[4] The NCI plots are generated using VMD software.[5]

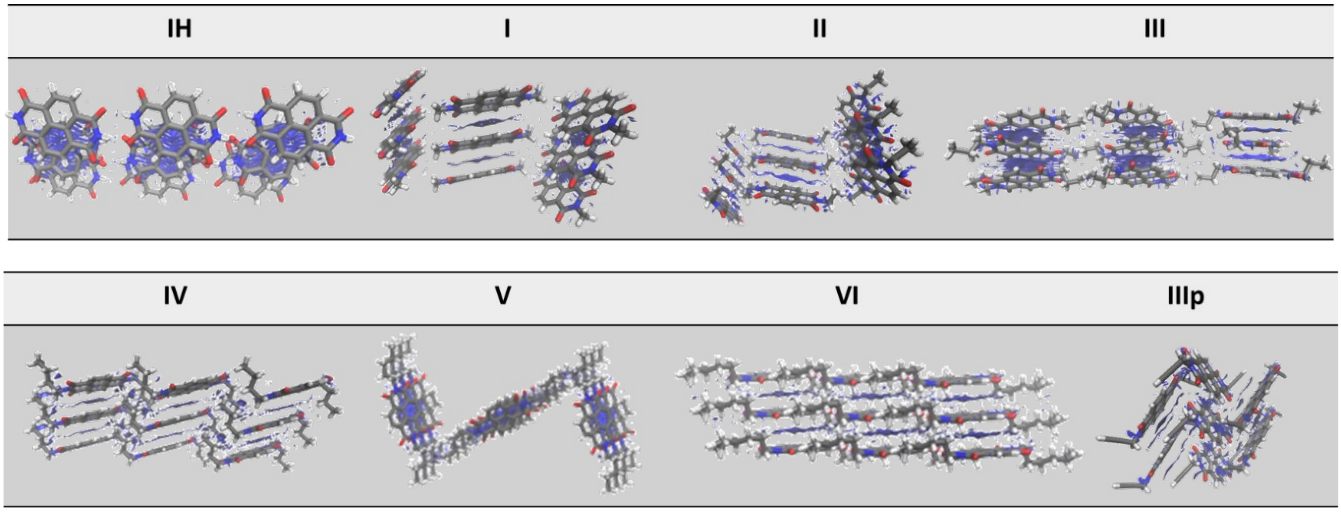


Fig S17: Non Covalent Interaction plot for **IH**, **I**, **II**, **III**, **IV**, **V**, **VI** and **IIIp** (all plots are generated at isosurface value of 0.6)

8. Rate of electron transfer and charge carrier mobility of NDIs

Rate of electron transfer and mobility is calculate using the following equations:

$$k = \frac{V^2}{\hbar}\left(\frac{\pi}{\lambda K_B T}\right)^{\frac{1}{2}} \exp\left(-\frac{\lambda}{4K_B T}\right)$$

$$\mu = \frac{er_i^2}{K_B T}k$$

Pairs of IH	Distance (r_i) (A^0)	k_h (s^{-1})	k_e (s^{-1})	μ_h ($cm^2V^{-1}s^{-1}$)	μ_e ($cm^2V^{-1}s^{-1}$)
M-D1	4.5	1.2e11	3.3e11	9.4e-3	2.5e-2
M-D2	12.0	5.2e7	4.0e5	2.9e-5	2.3e-7
M-D3	10.2	7.8e9	2.1e7	3.1e-3	8.4e-6
M-D4	10.1	1.3e9	5.3e7	5.3e-4	2.1e-5

Table S5: Hole and electron transfer rate of different dimers of **IH**

Pairs of I	Distance (r_i) (A^0)	k_h (s^{-1})	k_e (s^{-1})	μ_h ($cm^2V^{-1}s^{-1}$)	μ_e ($cm^2V^{-1}s^{-1}$)
M-D1	4.6	1.3e11	1.1e11	1.1e-2	9.3e-3
M-D2	13.6	2.9e4	6.7e-1	2.1e-08	4.8e-13
M-D3	10.7	2.4e7	3.6e7	1.1e-05	1.6e-5
M-D4	9.4	3.5e9	6.4e7	1.2e-3	2.2e-5

Table S6: Hole and electron transfer rate of different dimers of **I**

Pairs of II	Distance (r_i) (A^0)	k_h (s^{-1})	k_e (s^{-1})	μ_h ($cm^2V^{-1}s^{-1}$)	μ_e ($cm^2V^{-1}s^{-1}$)
M-D1	4.8	2.1e11	2.3e12	2.0e-2	2.1e-1
M-D2	11.1	2.7e9	3.1e8	1.3e-3	1.5e-4
M-D3	9.9	1.3e-3	5.6e6	1.0e-3	2.1e-6
M-D4	11.0	1.2e8	8.2e3	5.6e-5	3.9e-9

Table S7: Hole and electron transfer rate of different dimers of **II**

Pairs of III	Distance (r_i) (A^0)	k_h (s^{-1})	k_e (s^{-1})	μ_h ($cm^2V^{-1}s^{-1}$)	μ_e ($cm^2V^{-1}s^{-1}$)
M-D1	3.5	2.1e12	2.1e12	1.0e-1	9.6e-2
M-D2	14.7	3.6e6	1.8e6	3.0e-6	1.5e-6
M-D3	14.4	2.5e7	2.7e2	2.0e-5	2.1e-10
M-D4	14.6	9.7e7	5.9e6	8.1e-5	5.0e-06

Table S8: Hole and electron transfer rate of different dimers of **III**

Pairs of IV	Distance (r_i) (A^0)	k_h (s^{-1})	k_e (s^{-1})	μ_h ($cm^2V^{-1}s^{-1}$)	μ_e ($cm^2V^{-1}s^{-1}$)
M-D1	5.2	3.1e10	4.7e12	3.1e-3	5.0e-1
M-D2	11.1	6.2e7	3.1e6	3.0e-05	1.5e-6
M-D3	12.0	2.4e9	8.1e7	1.3e-3	4.5e-5
M-D4	14.7	8.1e2	2.7e5	6.8e-10	2.3e-7

Table S9: Hole and electron transfer rate of different dimers of **IV**

Pairs of V	Distance (r_i) (A^0)	k_h (s^{-1})	k_e (s^{-1})	μ_h ($cm^2V^{-1}s^{-1}$)	μ_e ($cm^2V^{-1}s^{-1}$)
M-D1	5.0	4.5e11	2.6e12	4.4e-2	2.5e-1
M-D2	14.7	1.1e3	1.4e5	9.5e-10	1.2e-7
M-D3	12.9	2.5e7	3.9e7	1.6e-5	2.5e-5
M-D4	13.0	8.0e5	2.5e5	5.3e-7	1.6e-7

Table S10: Hole and electron transfer rate of different dimers of **V**

Pairs of VI	Distance (r_i) (A^0)	k_h (s^{-1})	k_e (s^{-1})	μ_h ($cm^2V^{-1}s^{-1}$)	μ_e ($cm^2V^{-1}s^{-1}$)
M-D1	4.9	2.3e11	1.8e12	2.2e-2	1.7e-1
M-D2	12.4	3.9e6	1.3e8	2.4e-6	7.8e-05
M-D3	9.4	3.5e9	5.0e9	1.2e-3	1.7e-3
M-D4	8.3	6.7e10	1.7e11	1.8e-2	4.6e-2

Table S11: Hole and electron transfer rate of different dimers of **VI**

Pairs of IIIp	Distance (r_i) (A^0)	k_h (s^{-1})	k_e (s^{-1})	μ_h ($cm^2V^{-1}s^{-1}$)	μ_e ($cm^2V^{-1}s^{-1}$)
M-D1	6.3	4.5e12	3.7e11	7.0e-1	5.8e-2
M-D2	7.2	1.3e12	4.2e9	2.7e-1	8.4e-4

Table S12: Hole and electron transfer rate of different dimers of **IIIp**

Anisotropic carrier mobility (μ_ϕ) is calculate by the method proposed by Deng et. al.[6]

$$\mu_\phi = \frac{e}{2K_BT}\sum_i k_i r_i^2 p_i \cos^2\gamma_i \cos^2(\theta_i - \phi)$$

Where *i* represents a specific hopping pathway with hopping distance r_i, k_i is the charge-hopping rate described by the Marcus-Hush equation. Theta (θ) is the angle between any dimer of our interest (vector connecting two centroids) and the reference axis (crystallographic axis such as a, b or c). Gamma (γ) is the projection angle of any dimer of our interest to the reference plane we considered for anisotropic mobility calculation and phi (φ) varies from 0˚ to 360˚.

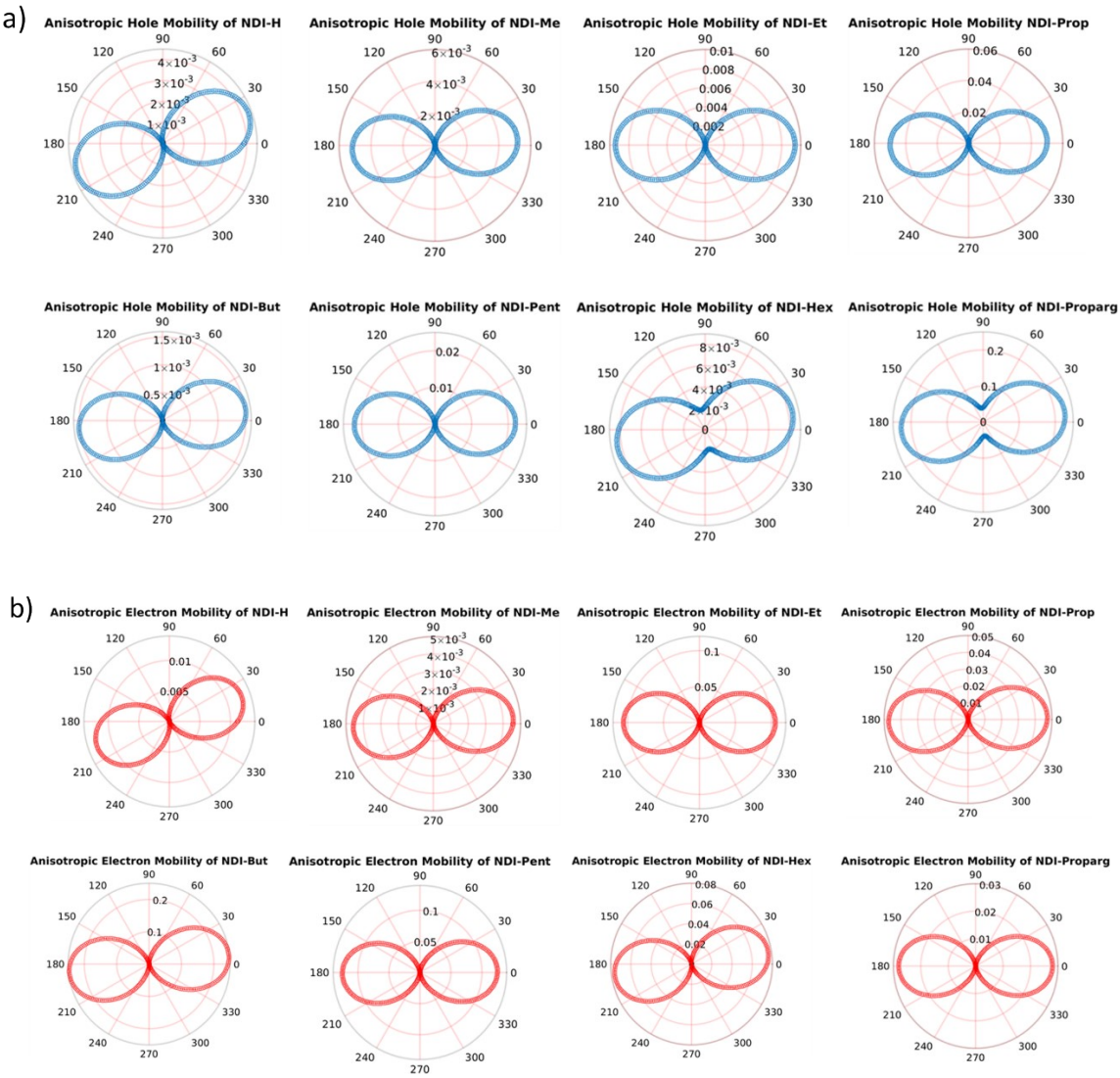


Fig S18: Angular hole and electron anisotropic mobility plot for the NDIs. (Radial values are in **$cm^2V^{-1}s^{-1}$**)

9. Coordinates of the optimized structures:

Optimization of all the neutral structures were carried out using B3LYP-D3/6-31+G* level of theory whereas optimization of all the charged species were done at uB3LYP-D3/6-31+G* level of theory.

A) NDI-H (lH)

a) Neutral

C	-0.64036	-1.06663	8.36741
C	-1.36019	-2.11166	7.72673
C	-0.71950	-3.44226	7.54209
O	-1.26462	-4.39337	7.00325

N	0.58141	-3.55051	8.03349
H	1.02703	-4.45618	7.91143
C	1.34996	-2.57599	8.66999
O	2.48512	-2.82370	9.04704
C	0.68624	-1.25504	8.84216
C	1.36488	-0.21883	9.46314
H	2.37672	-0.39308	9.81497
C	0.74768	1.03579	9.63198
H	1.27178	1.85297	10.11728
C	-1.26439	0.20197	8.53808
C	-0.54456	1.24701	9.17876
C	-1.18527	2.57759	9.36345
O	-0.64012	3.52872	9.90221
N	-2.48614	2.68588	8.87192
H	-2.93175	3.59156	8.99397
C	-3.25469	1.71135	8.23544
O	-4.38985	1.95907	7.85839
C	-2.59098	0.39039	8.06331
C	-3.26963	-0.64582	7.44233
H	-4.28146	-0.47156	7.09048
C	-2.65243	-1.90045	7.27351
H	-3.17653	-2.71762	6.78822

b) Cationic

C	-0.64087	-1.06564	8.36758
C	-1.35232	-2.10890	7.73100
C	-0.70886	-3.44915	7.54428
O	-1.28672	-4.37093	7.00158
N	0.58855	-3.56524	8.03165
H	1.03546	-4.47333	7.90910
C	1.34843	-2.58797	8.66555
O	2.48148	-2.79358	9.05549
C	0.67872	-1.25871	8.83793
C	1.37326	-0.20648	9.47054
H	2.38516	-0.38853	9.81976

C	0.76326	1.03353	9.63740
H	1.28100	1.85589	10.12185
C	-1.26389	0.20098	8.53791
C	-0.55244	1.24424	9.17450
C	-1.19594	2.58446	9.36131
O	-0.61804	3.50627	9.90394
N	-2.49328	2.70061	8.87377
H	-2.94018	3.60870	8.99631
C	-3.25313	1.72335	8.23982
O	-4.38621	1.92894	7.84993
C	-2.58346	0.39406	8.06753
C	-3.27800	-0.65817	7.43490
H	-4.28988	-0.47610	7.08566
C	-2.66801	-1.89819	7.26809
H	-3.18575	-2.72055	6.78366

c) Anionic

C	-0.63739	-1.07264	8.36659
C	-1.36098	-2.11807	7.72433
C	-0.73376	-3.42348	7.54274
O	-1.26018	-4.40692	7.00100
N	0.56915	-3.52544	8.03675
H	1.01394	-4.42945	7.91488
C	1.34399	-2.55372	8.67489
O	2.49314	-2.83563	9.04605
C	0.69196	-1.25870	8.84321
C	1.37856	-0.20033	9.47480
H	2.39023	-0.38342	9.82355
C	0.77180	1.03314	9.64074
H	1.28859	1.85604	10.12489
C	-1.26736	0.20799	8.53889
C	-0.54377	1.25341	9.18116
C	-1.17100	2.55883	9.36276
O	-0.64454	3.54228	9.90444
N	-2.47387	2.66081	8.86867

H	-2.91866	3.56482	8.99053
C	-3.24873	1.68907	8.23058
O	-4.39787	1.97100	7.85938
C	-2.59671	0.39405	8.06227
C	-3.28331	-0.66432	7.43067
H	-4.29498	-0.48123	7.08192
C	-2.67655	-1.89780	7.26474
H	-3.19334	-2.72070	6.78059

B) NDI-Me (I)

a) Neutral

C	3.25773	2.67038	2.50176
C	4.94170	1.19982	1.39921
C	5.19999	2.27545	0.40251
C	6.13521	2.07460	-0.60186
H	6.66508	1.12850	-0.64166
C	4.49276	3.50056	0.47944
C	3.53311	3.72936	1.49548
C	2.85235	4.93600	1.55224
H	2.12156	5.08829	2.33992
C	3.68726	0.44560	3.39691
H	4.31223	-0.42043	3.19097
H	2.62932	0.17728	3.34646
H	3.89614	0.84244	4.39327
N	3.98108	1.47439	2.38759
O	5.53288	0.12899	1.36446
O	2.43938	2.81248	3.40105
C	5.98527	5.34862	-2.50176
C	4.30130	6.81918	-1.39921
C	4.04301	5.74355	-0.40251
C	3.10779	5.94440	0.60186
H	2.57792	6.89051	0.64166
C	4.75024	4.51844	-0.47944
C	5.70989	4.28964	-1.49548
C	6.39065	3.08300	-1.55224

H	7.12143	2.93071	-2.33992
C	5.55574	7.57340	-3.39691
H	4.93077	8.43943	-3.19097
H	6.61368	7.84172	-3.34646
H	5.34686	7.17657	-4.39327
N	5.26192	6.54462	-2.38759
O	3.71012	7.89001	-1.36446
O	6.80362	5.20652	-3.40105

b) Cationic

C	3.26187	2.65741	2.50529
C	4.93225	1.19905	1.41104
C	5.19326	2.28093	0.40723
C	6.14630	2.07254	-0.61388
H	6.67229	1.12357	-0.64710
C	4.49303	3.50171	0.47841
C	3.53895	3.72310	1.49246
C	2.84411	4.95000	1.55330
H	2.11457	5.09533	2.34395
C	3.68290	0.42950	3.41225
H	4.30720	-0.43706	3.20773
H	2.62555	0.16360	3.35491
H	3.89604	0.83108	4.40486
N	3.97831	1.46432	2.39691
O	5.54177	0.14512	1.34372
O	2.43921	2.83534	3.38743
C	5.98113	5.36159	-2.50529
C	4.31075	6.81996	-1.41104
C	4.04974	5.73808	-0.40723
C	3.09670	5.94646	0.61388
H	2.57071	6.89543	0.64710
C	4.74997	4.51729	-0.47841
C	5.70406	4.29591	-1.49246
C	6.39889	3.06900	-1.55330
H	7.12843	2.92367	-2.34395

C	5.56010	7.58950	-3.41225
H	4.93580	8.45606	-3.20773
H	6.61745	7.85540	-3.35491
H	5.34696	7.18792	-4.40486
N	5.26469	6.55468	-2.39690
O	3.70123	7.87388	-1.34372
O	6.80379	5.18366	-3.38744

c) Anionic

C	3.25686	2.69184	2.48988
C	4.95159	1.21220	1.38006
C	5.20147	2.26909	0.40508
C	6.15274	2.06962	-0.61974
H	6.67828	1.12048	-0.65215
C	4.49150	3.49577	0.48416
C	3.52969	3.72770	1.50097
C	2.83924	4.95808	1.55417
H	2.11002	5.10222	2.34526
C	3.69373	0.46947	3.37361
H	4.32125	-0.39493	3.16402
H	2.63434	0.19864	3.33003
H	3.89746	0.86238	4.37444
N	3.98535	1.49328	2.37030
O	5.53622	0.11714	1.36773
O	2.43321	2.80907	3.41161
C	5.98613	5.32716	-2.48989
C	4.29140	6.80679	-1.38006
C	4.04152	5.74991	-0.40509
C	3.09025	5.94938	0.61974
H	2.56471	6.89852	0.65214
C	4.75148	4.52323	-0.48417
C	5.71330	4.29129	-1.50098
C	6.40375	3.06091	-1.55417
H	7.13298	2.91678	-2.34526
C	5.54928	7.54954	-3.37360

H	4.92176	8.41394	-3.16400
H	6.60867	7.82036	-3.33000
H	5.34556	7.15664	-4.37444
N	5.25765	6.52572	-2.37030
O	3.70679	7.90187	-1.36772
O	6.80980	5.20993	-3.41160

C) NDI-Et (II)

a) Neutral

C	0.91989	1.35394	2.41718
C	1.22765	0.30495	1.40783
C	2.27774	0.50534	0.47881
C	3.04714	1.69438	0.48957
C	2.75655	2.75694	1.48977
C	0.48868	-0.86827	1.38000
H	-0.31016	-1.00072	2.10248
C	4.07216	1.86803	-0.42829
H	4.64951	2.78647	-0.40030
C	1.38826	3.57969	3.36749
H	0.31723	3.53313	3.56784
H	1.62828	4.53682	2.90301
C	2.19380	3.37800	4.65132
H	1.95317	2.41372	5.11079
H	1.95142	4.16995	5.36930
H	3.26803	3.42064	4.44388
N	1.68295	2.53102	2.36538
O	0.04119	1.21083	3.25778
O	3.41408	3.78782	1.55435
C	3.92411	-1.35394	-2.41718
C	3.61635	-0.30495	-1.40783
C	2.56626	-0.50534	-0.47881
C	1.79686	-1.69438	-0.48957
C	2.08745	-2.75694	-1.48977
C	4.35532	0.86827	-1.38000
H	5.15416	1.00072	-2.10248

C	0.77184	-1.86803	0.42829
H	0.19449	-2.78647	0.40030
C	3.45574	-3.57969	-3.36749
H	4.52677	-3.53313	-3.56784
H	3.21572	-4.53682	-2.90301
C	2.65020	-3.37800	-4.65132
H	2.89083	-2.41372	-5.11079
H	2.89258	-4.16995	-5.36930
H	1.57597	-3.42064	-4.44388
N	3.16105	-2.53102	-2.36538
O	4.80281	-1.21083	-3.25778
O	1.42992	-3.78782	-1.55435

b) Cationic

C	0.92643	1.36706	2.42092
C	1.23323	0.31181	1.40350
C	2.27818	0.50425	0.47804
C	3.03858	1.69044	0.49236
C	2.74716	2.75791	1.50151
C	0.47905	-0.88175	1.37884
H	-0.31870	-1.00561	2.10459
C	4.08356	1.87061	-0.44011
H	4.65551	2.79265	-0.40553
C	1.38439	3.59659	3.38548
H	0.31224	3.54895	3.57860
H	1.62127	4.55127	2.91477
C	2.19316	3.38701	4.66378
H	1.95172	2.42537	5.12784
H	1.94925	4.17949	5.37879
H	3.26781	3.43275	4.46026
N	1.67819	2.54161	2.37190
O	0.04713	1.18562	3.24720
O	3.42873	3.76927	1.53922
C	3.91757	-1.36706	-2.42092
C	3.61077	-0.31181	-1.40350

C	2.56582	-0.50425	-0.47804
C	1.80542	-1.69044	-0.49236
C	2.09684	-2.75791	-1.50151
C	4.36495	0.88175	-1.37884
H	5.16270	1.00561	-2.10459
C	0.76044	-1.87061	0.44011
H	0.18849	-2.79265	0.40553
C	3.45961	-3.59659	-3.38548
H	4.53176	-3.54895	-3.57860
H	3.22273	-4.55127	-2.91477
C	2.65084	-3.38701	-4.66378
H	2.89228	-2.42537	-5.12784
H	2.89475	-4.17949	-5.37879
H	1.57619	-3.43275	-4.46026
N	3.16581	-2.54161	-2.37190
O	4.79687	-1.18562	-3.24720
O	1.41527	-3.76927	-1.53922

c) Anionic

C	0.91680	1.33294	2.40291
C	1.22251	0.30745	1.41182
C	2.27538	0.51082	0.48247
C	3.04767	1.70124	0.49072
C	2.76649	2.74574	1.46913
C	0.47400	-0.88958	1.38033
H	-0.32327	-1.01386	2.10638
C	4.09129	1.87263	-0.44502
H	4.66371	2.79423	-0.41007
C	1.39411	3.55478	3.34173
H	0.32359	3.50595	3.54817
H	1.63894	4.51335	2.88098
C	2.19626	3.36162	4.63119
H	1.95499	2.39522	5.08678
H	1.95483	4.15471	5.35151
H	3.27010	3.40178	4.41926

N	1.69189	2.51002	2.35148
O	0.02810	1.21652	3.26243
O	3.41328	3.80248	1.55327
C	3.92720	-1.33294	-2.40291
C	3.62149	-0.30745	-1.41182
C	2.56862	-0.51082	-0.48247
C	1.79633	-1.70124	-0.49072
C	2.07751	-2.74574	-1.46913
C	4.37000	0.88958	-1.38033
H	5.16727	1.01386	-2.10638
C	0.75271	-1.87263	0.44502
H	0.18029	-2.79423	0.41007
C	3.44989	-3.55478	-3.34173
H	4.52041	-3.50595	-3.54817
H	3.20506	-4.51335	-2.88098
C	2.64774	-3.36162	-4.63119
H	2.88901	-2.39522	-5.08678
H	2.88917	-4.15471	-5.35151
H	1.57390	-3.40178	-4.41926
N	3.15211	-2.51002	-2.35148
O	4.81590	-1.21652	-3.26243
O	1.43072	-3.80248	-1.55327

D) NDI-Prop (III)

a) Neutral

C	2.18891	3.72708	7.54780
C	1.81540	2.36279	7.47604
C	1.61880	1.75779	6.20436
C	1.80312	2.52860	5.03055
C	1.60478	1.90453	3.69455
C	1.04151	-0.25106	4.80715
C	1.24531	0.39349	6.13258
C	1.07265	-0.34253	7.29525
H	0.78790	-1.38665	7.21594
C	1.26312	0.25818	8.55550

H	1.12610	-0.31250	9.46826
C	1.63107	1.59199	8.64984
C	1.82936	2.21607	9.98586
C	2.39276	4.37162	8.87323
C	2.36158	4.46310	6.38514
H	2.64636	5.50722	6.46445
C	2.17107	3.86241	5.12489
H	2.30807	4.43309	4.21213
C	1.00335	-0.07033	2.35094
H	0.63729	0.70558	1.67637
H	0.23436	-0.83526	2.47179
C	2.29825	-0.68711	1.81210
H	2.65912	-1.43383	2.53012
H	3.06001	0.09885	1.73910
C	2.07881	-1.33685	0.44191
H	1.73209	-0.60080	-0.29444
H	1.32934	-2.13646	0.49827
H	3.00814	-1.77643	0.06260
C	2.43089	4.19093	11.32945
H	3.20041	4.95537	11.20876
H	2.79626	3.41484	12.00417
C	1.13623	4.80855	11.86787
H	0.37404	4.02299	11.94096
H	0.77586	5.55523	11.14957
C	1.35576	5.45860	13.23790
H	2.10555	6.25786	13.18137
H	1.70209	4.72263	13.97452
H	0.42656	5.89866	13.61697
N	1.19796	0.56127	3.67313
N	2.23625	3.55931	10.00726
O	1.65269	1.59617	11.02693
O	2.68759	5.55494	8.98347
O	0.74683	-1.43441	4.69690
O	1.78138	2.52447	2.65349

b) Cationic

C	2.19138	3.71803	7.55278
C	1.81644	2.36198	7.47466
C	1.61786	1.75888	6.20559
C	1.79642	2.52130	5.03411
C	1.59689	1.89199	3.69015
C	1.03845	-0.24466	4.79290
C	1.24293	0.40283	6.12747
C	1.06819	-0.35038	7.30898
H	0.78154	-1.39365	7.22048
C	1.26121	0.24181	8.55409
H	1.12804	-0.32212	9.47207
C	1.63787	1.59956	8.64614
C	1.83739	2.22888	9.99010
C	2.39587	4.36551	8.88735
C	2.36611	4.47123	6.37127
H	2.65277	5.51450	6.45977
C	2.17309	3.87905	5.12616
H	2.30625	4.44298	4.20819
C	0.99759	-0.07994	2.32888
H	0.62811	0.69804	1.65896
H	0.22520	-0.84053	2.45334
C	2.29800	-0.69300	1.80100
H	2.65824	-1.43922	2.52027
H	3.05956	0.09362	1.72866
C	2.08168	-1.34415	0.43057
H	1.73864	-0.61033	-0.30847
H	1.33635	-2.14657	0.48502
H	3.01493	-1.77999	0.05990
C	2.43672	4.20081	11.35136
H	3.20919	4.96132	11.22691
H	2.80610	3.42281	12.02132
C	1.13635	4.81401	11.87918
H	0.37472	4.02746	11.95151
H	0.77620	5.56025	11.15988

C	1.35268	5.46517	13.24961
H	2.09808	6.26751	13.19517
H	1.69562	4.73133	13.98867
H	0.41945	5.90110	13.62023
N	1.18707	0.55857	3.66175
N	2.24723	3.56229	10.01851
O	1.64682	1.57990	11.00587
O	2.68451	5.54918	8.95728
O	0.74985	-1.42834	4.72297
O	1.78743	2.54097	2.67438

c) Anionic

C	2.19060	3.73292	7.55092
C	1.81695	2.36566	7.48208
C	1.61736	1.75520	6.19818
C	1.80329	2.52992	5.02387
C	1.61159	1.92234	3.71198
C	1.04429	-0.24865	4.83242
C	1.24372	0.38794	6.12934
C	1.06980	-0.35749	7.31602
H	0.78562	-1.40135	7.22759
C	1.25573	0.23336	8.55501
H	1.12020	-0.33002	9.47286
C	1.63103	1.59094	8.65639
C	1.82272	2.19852	9.96828
C	2.39003	4.36951	8.84783
C	2.36452	4.47835	6.36423
H	2.64870	5.52221	6.45266
C	2.17859	3.88750	5.12525
H	2.31412	4.45087	4.20739
C	1.00857	-0.05450	2.38357
H	0.64796	0.72200	1.70537
H	0.24283	-0.82405	2.50354
C	2.29857	-0.67537	1.83570
H	2.65810	-1.42226	2.55416

H	3.05981	0.11104	1.76235
C	2.07678	-1.32487	0.46551
H	1.72632	-0.58707	-0.26882
H	1.32388	-2.12244	0.52419
H	3.00302	-1.76780	0.07798
C	2.42574	4.17537	11.29668
H	3.19154	4.94485	11.17674
H	2.78624	3.39886	11.97491
C	1.13576	4.79636	11.84448
H	0.37445	4.01001	11.91782
H	0.77631	5.54325	11.12597
C	1.35755	5.44590	13.21465
H	2.11050	6.24341	13.15597
H	1.70794	4.70810	13.94903
H	0.43132	5.88890	13.60214
N	1.20992	0.57056	3.69649
N	2.22439	3.55030	9.98377
O	1.65419	1.59306	11.03932
O	2.69240	5.56565	8.98909
O	0.74192	-1.44479	4.69116
O	1.78010	2.52780	2.64093

E) NDI-But (IV)

a) Neutral

O	2.59023	6.47699	3.98498
O	-0.83966	3.84205	2.48346
N	0.86969	5.16460	3.22720
C	1.99658	5.40753	4.03040
C	2.43240	4.30555	4.93118
C	1.71868	3.08272	4.95172
C	0.58643	2.88370	4.12535
C	0.13303	3.97031	3.21637
C	3.53944	4.47758	5.74889
C	-0.09791	1.67803	4.16166
C	0.42121	6.23551	2.30683

C	0.87748	6.00266	0.86101
C	2.39955	5.95195	0.67716
C	2.80092	5.76707	-0.79078
H	2.81387	5.12648	1.27249
H	4.07164	5.42268	5.71653
H	3.89062	5.72375	-0.90443
H	0.82598	7.16970	2.69701
H	2.38352	4.83837	-1.20118
H	0.46270	6.82292	0.25757
H	0.42070	5.07807	0.48684
H	-0.96300	1.54789	3.51952
H	-0.66911	6.26443	2.35914
H	2.84865	6.86972	1.07848
H	2.43315	6.59668	-1.40843
O	1.27463	-1.35699	6.78217
O	4.70452	1.27796	8.28369
N	2.99516	-0.04459	7.53997
C	1.86822	-0.28750	6.73681
C	1.43244	0.81447	5.83600
C	2.14616	2.03729	5.81546
C	3.27842	2.23631	6.64182
C	3.73184	1.14968	7.55076
C	0.32540	0.64244	5.01828
C	3.96276	3.44198	6.60550
C	3.44365	-1.11550	8.46031
C	2.98749	-0.88262	9.90616
C	1.46543	-0.83186	10.09013
C	1.06417	-0.64695	11.55809
H	1.05110	-0.00637	9.49482
H	-0.20681	-0.30266	5.05065
H	-0.02551	-0.60359	11.67181
H	3.03882	-2.04969	8.07017
H	1.48164	0.28174	11.96845
H	3.40228	-1.70289	10.50958
H	3.44433	0.04195	10.28030

H	4.82786	3.57211	7.24763
H	4.53396	-1.14447	8.40793
H	1.01627	-1.74962	9.68884
H	1.43196	-1.47657	12.17572

b) Cationic

O	2.59951	6.46246	4.00725
O	-0.83533	3.81998	2.49521
N	0.85967	5.17798	3.22794
C	1.98152	5.41052	4.02545
C	2.42225	4.30216	4.93176
C	1.71873	3.08201	4.95329
C	0.59360	2.88956	4.12669
C	0.13663	3.98482	3.21449
C	3.54818	4.48190	5.76470
C	-0.10343	1.66268	4.15821
C	0.41149	6.25449	2.29513
C	0.87450	6.00768	0.85496
C	2.39730	5.94325	0.67786
C	2.80114	5.76083	-0.78970
H	2.80436	5.10879	1.26935
H	4.07267	5.43159	5.72899
H	3.89002	5.70785	-0.89759
H	0.81662	7.18693	2.68848
H	2.37607	4.83947	-1.20721
H	0.46890	6.83198	0.25325
H	0.40741	5.09047	0.47529
H	-0.96712	1.54033	3.51212
H	-0.67812	6.28305	2.35571
H	2.85288	6.85648	1.08225
H	2.44564	6.59825	-1.40194
O	1.26541	-1.34242	6.75996
O	4.70026	1.30005	8.27200
N	3.00527	-0.05796	7.53926
C	1.88342	-0.29050	6.74174

C	1.44269	0.81787	5.83544
C	2.14621	2.03801	5.81391
C	3.27134	2.23047	6.64050
C	3.72831	1.13521	7.55270
C	0.31676	0.63812	5.00250
C	3.96836	3.45735	6.60898
C	3.45343	-1.13446	8.47209
C	2.99041	-0.88763	9.91226
C	1.46761	-0.82320	10.08933
C	1.06375	-0.64076	11.55688
H	1.06055	0.01126	9.49783
H	-0.20773	-0.31156	5.03821
H	-0.02513	-0.58778	11.66476
H	3.04830	-2.06690	8.07874
H	1.48881	0.28060	11.97439
H	3.39600	-1.71193	10.51397
H	3.45750	0.02958	10.29192
H	4.83206	3.57970	7.25508
H	4.54305	-1.16302	8.41152
H	1.01203	-1.73643	9.68495
H	1.41924	-1.47818	12.16914

b) Anionic

O	2.59885	6.48504	3.97310
O	-0.84792	3.84423	2.47404
N	0.88026	5.14292	3.23925
C	2.01360	5.39261	4.04357
C	2.43542	4.31072	4.92666
C	1.71694	3.08742	4.94706
C	0.58156	2.88516	4.12121
C	0.13422	3.94650	3.22702
C	3.56273	4.48090	5.76025
C	-0.11302	1.65646	4.16345
C	0.42960	6.21059	2.33266
C	0.87919	5.99012	0.88126

C	2.40059	5.94867	0.69333
C	2.80197	5.75750	-0.77424
H	2.81769	5.13159	1.29556
H	4.09035	5.42856	5.71995
H	3.89271	5.72013	-0.89170
H	0.83619	7.14538	2.72166
H	2.38969	4.82247	-1.17710
H	0.45764	6.80807	0.27553
H	0.42904	5.05943	0.51371
H	-0.97756	1.53478	3.51849
H	-0.66197	6.23680	2.37758
H	2.84565	6.86980	1.09151
H	2.42609	6.57980	-1.39922
O	1.26609	-1.36497	6.79412
O	4.71287	1.27583	8.29317
N	2.98469	-0.02285	7.52797
C	1.85136	-0.27255	6.72363
C	1.42953	0.80934	5.84055
C	2.14800	2.03265	5.82016
C	3.28338	2.23491	6.64602
C	3.73071	1.17358	7.54021
C	0.30222	0.63916	5.00697
C	3.97797	3.46361	6.60378
C	3.43535	-1.09052	8.43456
C	2.98571	-0.87008	9.88594
C	1.46431	-0.82867	10.07383
C	1.06288	-0.63753	11.54140
H	1.04721	-0.01159	9.47160
H	-0.22540	-0.30850	5.04726
H	-0.02786	-0.60018	11.65883
H	3.02879	-2.02532	8.04554
H	1.47512	0.29751	11.94428
H	3.40726	-1.68803	10.49168
H	3.43583	0.06062	10.25352
H	4.84250	3.58529	7.24874

H	4.52692	-1.11671	8.38967
H	1.01928	-1.74980	9.67563
H	1.43876	-1.45982	12.16637

F) NDI-Pent (V)

a) Neutral

C	4.48639	-0.49087	1.50495
H	5.28314	-0.44627	2.24038
C	3.66529	0.61467	1.34109
C	2.61574	0.58531	0.39055
C	1.76315	1.70138	0.20749
C	0.74046	1.64930	-0.72777
H	0.09863	2.51580	-0.84979
C	3.88396	1.83269	2.16709
C	1.96352	2.92966	1.02291
C	3.24059	4.13830	2.74778
H	2.93013	4.98616	2.13788
H	4.31016	4.21221	2.95317
C	2.44500	4.07136	4.05699
H	2.72868	3.15226	4.58442
H	1.37601	3.99856	3.81696
C	2.69324	5.28140	4.97065
H	2.18784	5.09940	5.92978
H	3.76726	5.34976	5.20148
C	2.20552	6.62280	4.40269
H	1.14761	6.52964	4.11782
H	2.75035	6.86205	3.47944
C	2.37374	7.77765	5.39718
H	1.80530	7.59148	6.31767
H	2.02346	8.72641	4.97338
H	3.42714	7.90534	5.67868
N	3.03881	2.92664	1.92501
O	1.23289	3.90677	0.91857
O	4.76056	1.89244	3.02004
C	0.54187	0.49090	-1.50496

H	-0.25490	0.44628	-2.24037
C	1.36297	-0.61465	-1.34111
C	2.41254	-0.58528	-0.39058
C	3.26514	-1.70133	-0.20753
C	4.28782	-1.64927	0.72774
H	4.92965	-2.51577	0.84974
C	1.14425	-1.83269	-2.16705
C	3.06482	-2.92959	-1.02302
C	1.78763	-4.13830	-2.74775
H	2.09819	-4.98613	-2.13785
H	0.71805	-4.21226	-2.95302
C	2.58309	-4.07137	-4.05703
H	2.29931	-3.15229	-4.58446
H	3.65210	-3.99851	-3.81711
C	2.33480	-5.28144	-4.97063
H	2.84010	-5.09944	-5.92982
H	1.26076	-5.34984	-5.20136
C	2.82263	-6.62280	-4.40270
H	3.88057	-6.52960	-4.11793
H	2.27790	-6.86206	-3.47938
C	2.65436	-7.77769	-5.39714
H	3.22269	-7.59152	-6.31769
H	3.00472	-8.72642	-4.97335
H	1.60093	-7.90542	-5.67852
N	1.98945	-2.92662	-1.92502
O	3.79534	-3.90677	-0.91854
O	0.26766	-1.89244	-3.02001

b) Cationic

C	4.49947	-0.50289	1.50269
H	5.29610	-0.44943	2.23814
C	3.66276	0.62108	1.33251
C	2.61678	0.58455	0.38867
C	1.77346	1.69967	0.20972
C	0.72899	1.64958	-0.73832

H	0.09250	2.52117	-0.85484
C	3.88271	1.84766	2.16205
C	1.97741	2.93496	1.03056
C	3.24886	4.15876	2.75843
H	2.93893	5.00497	2.14616
H	4.31967	4.23190	2.95595
C	2.45100	4.07901	4.06458
H	2.73775	3.16014	4.59201
H	1.38203	4.00339	3.82412
C	2.69479	5.29125	4.97790
H	2.18004	5.10484	5.92986
H	3.76590	5.35673	5.21955
C	2.21132	6.63265	4.40520
H	1.15690	6.53855	4.10753
H	2.76942	6.87823	3.49077
C	2.36481	7.78322	5.40669
H	1.78267	7.59378	6.31707
H	2.01900	8.73107	4.97946
H	3.41347	7.91217	5.70263
N	3.04939	2.94078	1.92374
O	1.22521	3.88772	0.90425
O	4.76472	1.86896	3.00555
C	0.52870	0.50284	-1.50263
H	-0.26794	0.44938	-2.23806
C	1.36542	-0.62113	-1.33244
C	2.41141	-0.58459	-0.38862
C	3.25474	-1.69970	-0.20969
C	4.29920	-1.64962	0.73836
H	4.93571	-2.52120	0.85486
C	1.14541	-1.84774	-2.16194
C	3.05084	-2.93496	-1.03058
C	1.77934	-4.15880	-2.75839
H	2.08937	-5.00500	-2.14615
H	0.70851	-4.23201	-2.95582
C	2.57709	-4.07898	-4.06460

H	2.29024	-3.16012	-4.59200
H	3.64607	-4.00329	-3.82422
C	2.33331	-5.29122	-4.97792
H	2.84796	-5.10477	-5.92991
H	1.26218	-5.35677	-5.21948
C	2.81691	-6.63260	-4.40528
H	3.87135	-6.53843	-4.10769
H	2.25890	-6.87822	-3.49081
C	2.66341	-7.78317	-5.40678
H	3.24547	-7.59367	-6.31719
H	3.00933	-8.73099	-4.97959
H	1.61474	-7.91218	-5.70263
N	1.97880	-2.94082	-1.92369
O	3.80298	-3.88776	-0.90421
O	0.26347	-1.86900	-3.00550

c) Anionic

C	4.49716	-0.51563	1.51448
H	5.28947	-0.46453	2.25463
C	3.66716	0.61468	1.34868
C	2.61742	0.59096	0.39410
C	1.76426	1.70934	0.20647
C	0.72616	1.65363	-0.74918
H	0.09082	2.52592	-0.86596
C	3.88513	1.80520	2.16229
C	1.95647	2.91455	1.00481
C	3.23840	4.10654	2.72838
H	2.92211	4.95507	2.12115
H	4.30802	4.17963	2.93857
C	2.44848	4.04790	4.04256
H	2.73740	3.13015	4.56899
H	1.37925	3.97138	3.80433
C	2.69600	5.25854	4.95498
H	2.20218	5.07962	5.92243
H	3.77295	5.33614	5.17282

C	2.19534	6.59634	4.38985
H	1.13412	6.49744	4.11994
H	2.72417	6.82953	3.45653
C	2.37352	7.75868	5.37444
H	1.82158	7.57484	6.30635
H	2.01253	8.70552	4.95259
H	3.43130	7.89182	5.63910
N	3.03164	2.90038	1.91717
O	1.23659	3.92254	0.91571
O	4.76510	1.89314	3.03411
C	0.53104	0.51570	-1.51457
H	-0.26126	0.46462	-2.25474
C	1.36104	-0.61460	-1.34879
C	2.41076	-0.59089	-0.39417
C	3.26390	-1.70929	-0.20653
C	4.30200	-1.65357	0.74913
H	4.93732	-2.52588	0.86592
C	1.14316	-1.80507	-2.16248
C	3.07162	-2.91454	-1.00477
C	1.78975	-4.10647	-2.72844
H	2.10589	-4.95502	-2.12115
H	0.72015	-4.17947	-2.93875
C	2.57982	-4.04795	-4.04253
H	2.29105	-3.13019	-4.56902
H	3.64904	-3.97153	-3.80419
C	2.33228	-5.25860	-4.95495
H	2.82624	-5.07974	-5.92235
H	1.25535	-5.33609	-5.17291
C	2.83275	-6.59642	-4.38973
H	3.89395	-6.49762	-4.11970
H	2.30379	-6.82954	-3.45647
C	2.65456	-7.75878	-5.37431
H	3.20663	-7.57502	-6.30616
H	3.01542	-8.70564	-4.95239
H	1.59679	-7.89181	-5.63908

N	1.99654	-2.90032	-1.91724
O	3.79159	-3.92247	-0.91578
O	0.26305	-1.89309	-3.03416

G) NDI-Hex (VI)

a) Neutral

O	-1.31921	4.32165	1.23922
O	1.83179	6.96228	3.24334
N	0.30328	5.61693	2.20084
C	-0.72603	5.39236	1.27339
C	-1.05116	6.50688	0.34286
C	-2.03420	6.34076	-0.62118
H	-2.55324	5.38959	-0.68040
C	-0.35800	7.73770	0.44570
C	0.64806	7.93114	1.42365
C	1.31218	9.14573	1.50745
H	2.07820	9.27180	2.26569
C	0.98942	6.83017	2.36442
C	0.62686	4.51962	3.13733
H	1.68776	4.60651	3.37930
H	0.45375	3.58784	2.59973
C	-0.22328	4.59482	4.41127
H	-1.28193	4.50347	4.13472
H	-0.08295	5.58607	4.85980
C	0.14246	3.51304	5.43918
H	1.20426	3.61296	5.71073
H	-0.42604	3.70621	6.35991
C	-0.13559	2.07474	4.97812
H	0.48358	1.83084	4.10301
H	-1.18086	1.99737	4.64248
C	0.12610	1.03231	6.07302
H	1.16803	1.12006	6.41445
H	-0.50244	1.26020	6.94637
C	-0.14253	-0.40378	5.60810
H	-1.18545	-0.52558	5.28806

H	0.04882	-1.12817	6.40898
H	0.49780	-0.66903	4.75682
O	0.28159	12.21384	-1.23916
O	-2.86939	9.57321	-3.24328
N	-1.34102	10.91863	-2.20067
C	-0.31178	11.14325	-1.27314
C	0.01336	10.02872	-0.34262
C	0.99643	10.19482	0.62139
H	1.51548	11.14598	0.68060
C	-0.67981	8.79790	-0.44545
C	-1.68586	8.60445	-1.42342
C	-2.34995	7.38985	-1.50724
H	-3.11595	7.26377	-2.26550
C	-2.02721	9.70542	-2.36419
C	-1.66444	12.01586	-3.13730
H	-2.72532	11.92901	-3.37938
H	-1.49133	12.94769	-2.59978
C	-0.81417	11.94048	-4.41115
H	0.24446	12.03178	-4.13450
H	-0.95453	10.94921	-4.85961
C	-1.17971	13.02220	-5.43919
H	-2.24149	12.92232	-5.71086
H	-0.61113	12.82891	-6.35985
C	-0.90162	14.46052	-4.97823
H	-1.52090	14.70455	-4.10324
H	0.14361	14.53784	-4.64244
C	-1.16306	15.50288	-6.07329
H	-2.20495	15.41517	-6.41487
H	-0.53440	15.27485	-6.94651
C	-0.89441	16.93897	-5.60847
H	0.14847	17.06072	-5.28825
H	-1.08555	17.66330	-6.40945
H	-1.53487	17.20436	-4.75733

a) Cationic

O	-1.32500	4.33674	1.22033
O	1.83315	6.98529	3.22772
N	0.31739	5.60402	2.20020
C	-0.70913	5.38881	1.28008
C	-1.03917	6.50929	0.34369
C	-2.04217	6.33656	-0.63420
H	-2.55434	5.38099	-0.68815
C	-0.35641	7.73822	0.44344
C	0.64644	7.92421	1.41625
C	1.32180	9.16025	1.50614
H	2.08820	9.27811	2.26582
C	0.99091	6.81520	2.36082
C	0.63968	4.50139	3.14897
H	1.70248	4.58776	3.38145
H	0.46538	3.57097	2.60963
C	-0.21218	4.58990	4.41986
H	-1.27174	4.50349	4.14399
H	-0.06638	5.58097	4.86865
C	0.14887	3.50439	5.44664
H	1.20751	3.60545	5.72713
H	-0.42742	3.70074	6.36045
C	-0.12820	2.06703	4.98061
H	0.50379	1.81784	4.11543
H	-1.16962	1.99203	4.63246
C	0.11595	1.02622	6.08170
H	1.15269	1.11284	6.43750
H	-0.52523	1.25728	6.94427
C	-0.14944	-0.40885	5.61292
H	-1.18802	-0.53009	5.27964
H	0.02884	-1.13010	6.41845
H	0.50384	-0.67824	4.77307
O	0.28759	12.19863	-1.22034
O	-2.87056	9.55008	-3.22773
N	-1.35479	10.93135	-2.20022
C	-0.32827	11.14656	-1.28010

C	0.00177	10.02608	-0.34371
C	1.00477	10.19881	0.63418
H	1.51694	11.15438	0.68814
C	-0.68098	8.79715	-0.44346
C	-1.68383	8.61116	-1.41627
C	-2.35920	7.37512	-1.50616
H	-3.12559	7.25726	-2.26584
C	-2.02830	9.72017	-2.36085
C	-1.67709	12.03399	-3.14897
H	-2.73989	11.94760	-3.38146
H	-1.50280	12.96440	-2.60963
C	-0.82523	11.94549	-4.41987
H	0.23433	12.03191	-4.14400
H	-0.97102	10.95443	-4.86867
C	-1.18629	13.03101	-5.44664
H	-2.24493	12.92995	-5.72713
H	-0.61000	12.83468	-6.36045
C	-0.90924	14.46837	-4.98060
H	-1.54123	14.71755	-4.11542
H	0.13218	14.54338	-4.63245
C	-1.15340	15.50919	-6.08168
H	-2.19014	15.42256	-6.43747
H	-0.51221	15.27814	-6.94425
C	-0.88802	16.94425	-5.61288
H	0.15056	17.06550	-5.27960
H	-1.06631	17.66551	-6.41841
H	-1.54130	17.21363	-4.77303

a) Anionic

O	-1.31099	4.30583	1.23803
O	1.83485	6.96554	3.25923
N	0.29396	5.64205	2.19111
C	-0.73252	5.40462	1.25377
C	-1.04763	6.49862	0.34239
C	-2.04486	6.33141	-0.64332

H	-2.55614	5.37542	-0.69688
C	-0.35543	7.73280	0.44990
C	0.64913	7.93309	1.43202
C	1.31775	9.17402	1.51598
H	2.07945	9.29421	2.27989
C	0.98691	6.85851	2.35827
C	0.62246	4.55028	3.11609
H	1.68279	4.63954	3.36378
H	0.44501	3.61707	2.58090
C	-0.22256	4.61780	4.39503
H	-1.28160	4.52844	4.11897
H	-0.07885	5.60874	4.84253
C	0.14334	3.53649	5.42285
H	1.20938	3.62861	5.68352
H	-0.41510	3.72845	6.35171
C	-0.14502	2.09936	4.96423
H	0.45904	1.85963	4.07824
H	-1.19484	2.02661	4.64231
C	0.12950	1.05178	6.05079
H	1.17743	1.13404	6.37647
H	-0.48389	1.27820	6.93606
C	-0.15120	-0.38298	5.58716
H	-1.19940	-0.49888	5.28162
H	0.05004	-1.11306	6.38188
H	0.47348	-0.64599	4.72344
O	0.27352	12.22961	-1.23799
O	-2.87232	9.56990	-3.25920
N	-1.33148	10.89341	-2.19104
C	-0.30501	11.13085	-1.25368
C	0.01009	10.03684	-0.34230
C	1.00733	10.20406	0.64340
H	1.51862	11.16004	0.69696
C	-0.68212	8.80267	-0.44981
C	-1.68668	8.60238	-1.43192
C	-2.35528	7.36144	-1.51589

H	-3.11699	7.24125	-2.27980
C	-2.02446	9.67696	-2.35817
C	-1.65992	11.98516	-3.11607
H	-2.72025	11.89592	-3.36377
H	-1.48245	12.91837	-2.58091
C	-0.81488	11.91755	-4.39499
H	0.24416	12.00689	-4.11891
H	-0.95861	10.92661	-4.84245
C	-1.18072	12.99884	-5.42286
H	-2.24676	12.90674	-5.68355
H	-0.62227	12.80682	-6.35170
C	-0.89233	14.43598	-4.96429
H	-1.49640	14.67576	-4.07831
H	0.15749	14.50870	-4.64234
C	-1.16678	15.48352	-6.05089
H	-2.21471	15.40128	-6.37660
H	-0.55339	15.25705	-6.93614
C	-0.88605	16.91829	-5.58731
H	0.16214	17.03416	-5.28176
H	-1.08725	17.64834	-6.38207
H	-1.51074	17.18136	-4.72361

H) NDI-Proparg (IIIp)

a) Neutral

O	-10.44661	-2.66420	-8.80046
N	-8.60797	-1.30553	-8.71778
C	-8.26028	-1.60368	-12.20446
H	-7.92311	-2.01794	-13.12891
C	-8.64043	-1.13672	-11.15733
O	-6.75383	0.03356	-8.66272
C	-9.10795	-0.56129	-9.89452
H	-8.76115	0.46959	-9.79682
H	-10.19889	-0.58130	-9.85041
C	-9.38496	-2.38535	-8.26271
C	-8.85031	-3.14988	-7.10471

C	-9.56813	-4.22152	-6.59560
H	-10.51533	-4.48330	-7.05585
C	-7.60950	-2.78392	-6.52690
C	-6.85781	-1.69331	-7.02980
C	-9.07233	-4.95604	-5.50058
H	-9.63029	-5.79467	-5.09693
C	-7.36714	-0.91078	-8.18718
C	-7.86027	-4.61657	-4.91873
C	-7.10858	-3.52597	-5.42164
C	-5.86775	-3.16005	-4.84386
C	-5.33304	-3.92465	-3.68594
O	-4.27127	-3.64599	-3.14834
N	-6.11008	-5.00441	-3.23078
C	-5.60994	-5.74883	-2.05418
C	-6.07680	-5.17332	-0.79122
C	-6.45647	-4.70624	0.25602
H	-6.79355	-4.29191	1.18046
H	-5.95709	-6.77961	-2.15176
H	-4.51900	-5.72927	-2.09867
C	-7.35101	-5.39902	-3.76126
O	-7.96405	-6.34369	-3.28604
C	-5.14992	-2.08843	-5.35300
H	-4.20268	-1.82668	-4.89278
C	-5.64573	-1.35387	-6.44799
H	-5.08778	-0.51524	-6.85164

a) Cationic

O	-10.40938	-2.71349	-8.83141
N	-8.61101	-1.30124	-8.71915
C	-8.27205	-1.58834	-12.20461
H	-7.94236	-1.99224	-13.13861
C	-8.65219	-1.12140	-11.15259
O	-6.71730	-0.01500	-8.69303
C	-9.11682	-0.54900	-9.89434
H	-8.77351	0.48431	-9.79287

H	-10.20922	-0.56413	-9.84609
C	-9.36745	-2.39625	-8.28376
C	-8.84051	-3.15392	-7.11105
C	-9.57339	-4.23496	-6.59435
H	-10.51830	-4.49484	-7.06098
C	-7.60602	-2.78849	-6.53008
C	-6.85667	-1.70355	-7.03639
C	-9.08646	-4.95716	-5.50263
H	-9.64220	-5.79444	-5.09243
C	-7.36123	-0.92973	-8.20845
C	-7.86124	-4.60651	-4.91221
C	-7.11188	-3.52158	-5.41852
C	-5.87739	-3.15616	-4.83756
C	-5.35042	-3.91386	-3.66488
O	-4.30851	-3.59660	-3.11721
N	-6.10690	-5.00883	-3.22945
C	-5.60107	-5.76106	-2.05428
C	-6.06551	-5.18851	-0.79605
C	-6.44541	-4.72136	0.25597
H	-6.77477	-4.31714	1.18996
H	-5.94454	-6.79433	-2.15567
H	-4.50868	-5.74608	-2.10264
C	-7.35671	-5.38030	-3.74011
O	-8.00062	-6.29506	-3.25557
C	-5.14451	-2.07511	-5.35426
H	-4.19960	-1.81523	-4.88763
C	-5.63145	-1.35289	-6.44596
H	-5.07572	-0.51560	-6.85614

c) Anionic

O	-10.44695	-2.67433	-8.82034
N	-8.57875	-1.34517	-8.72265
C	-8.28965	-1.56234	-12.23893
H	-7.96382	-1.96107	-13.17305
C	-8.64265	-1.13361	-11.16460

O	-6.74376	0.03236	-8.68150
C	-9.08707	-0.59062	-9.87506
H	-8.73374	0.43829	-9.77265
H	-10.17837	-0.61672	-9.82632
C	-9.37216	-2.41813	-8.25901
C	-8.84923	-3.15731	-7.11685
C	-9.57964	-4.24512	-6.59064
H	-10.52383	-4.50277	-7.05979
C	-7.60860	-2.78459	-6.53646
C	-6.85041	-1.69616	-7.04175
C	-9.09801	-4.95967	-5.50678
H	-9.65157	-5.79697	-5.09389
C	-7.34011	-0.93281	-8.18277
C	-7.86746	-4.61388	-4.90686
C	-7.10926	-3.52545	-5.41216
C	-5.86864	-3.15273	-4.83177
C	-5.34570	-3.89192	-3.68962
O	-4.27091	-3.63571	-3.12827
N	-6.13912	-4.96487	-3.22596
C	-5.63080	-5.71940	-2.07354
C	-6.07507	-5.17631	-0.78400
C	-6.42799	-4.74745	0.29031
H	-6.75372	-4.34863	1.22443
H	-5.98424	-6.74828	-2.17587
H	-4.53949	-5.69343	-2.12236
C	-7.37777	-5.37721	-3.76583
O	-7.97411	-6.34240	-3.26711
C	-5.13822	-2.06492	-5.35798
H	-4.19404	-1.80728	-4.88883
C	-5.61985	-1.35036	-6.44184
H	-5.06629	-0.51307	-6.85472

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