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Conformational Disorder and Ultrafast Exciton Relaxation Dynamics in PPV-family Conjugated Polymers

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Additional Supporting Information

The three archives contain information on the structure and calculations for the three PPV polymer chains described in the paper. There are 4 files for each of the three chains.

Detailed description of the data:

coords.dat

Column one : Atom number

Column two: Atom type (C or H).

Column three: Chromophore number (which atoms belong to oligomer 1, 2, and so forth). All the atoms for every chromophore are listed contiguously, that is, once the number changes from *n* to *n*+1 (from 1 to 2, for example), there will be no other atom in the list that will belong to chromophore *n*.

Column four: Monomer number. One phenyl group is considered one monomer and one vinyl group is also considered as one monomer

Columns five, six, seven: xyz-coordinates of the atom.

Structure of other data files:

Chromophores in PPV chain with size smaller or equal to 2 units (one vinylene or phenylene group being considered as one unit)-- isolated phenylene, isolated vinylene , phenylenevinylene group -- were not included in the calculations. The excitations energies, transition dipole moments, and coupling factors that are given in the different data files only concern the so-called "effective" chromophores with size larger than 2 (phenylene or vinylene) units.

res.dat files:

Line 1: total number of chromophores; number of effective chromophores (Neff) with size larger than two units, the number of excited states computed for all chromophores=30

Following lines:
Column two: Index of the chromophores,
Column three: number of atoms for this chromophore
Column four: the number excited states with energy lower than 4 eV.

The rest of the files deal with only the Neff effective chromophores.

coup.dat

Columns one and two: labels of chromophores of interest
Columns three and four: the index of the excited states considered for the two chromophores
Column five: the electronic coupling in cm-1.

Note: coupling is given between the first excited state of chromophore in column 1 with each of the n=30 excited states of chromophore in column 2. There are Neff blocks of 30 lines in this file, Neff being the number of effective chromophores

ene.dat

Columns one and two: For each effective chromophore the excitation energy of the first 30 singlet excited states (in eV and cm-1)
Columns three, four, five: xyz components of the corresponding transition dipole moments (in Debye).
There are thus Neff blocks of 30 lines in this file.