

HOMO-LUMO Energies (eV) of *cis* and *trans* oligomers of size n = 1-6. Orbital energies calculated at the B3LYP/6-31G(d) level, using geometries calculated at the MPWB1K/6-31G(d) level.

(2FSO)<sub>n</sub>

|   | cis   |       |      | trans |       |      |
|---|-------|-------|------|-------|-------|------|
|   | HOMO  | LUMO  | Gap  | HOMO  | LUMO  | Gap  |
| 1 | -5.60 | -1.06 | 4.54 | -5.60 | -1.06 | 4.54 |
| 2 | -5.08 | -1.76 | 3.32 | -5.09 | -1.71 | 3.38 |
| 3 | -4.90 | -2.02 | 2.88 | -4.92 | -1.95 | 2.97 |
| 4 | -4.88 | -2.16 | 2.72 | -4.84 | -2.06 | 2.78 |
| 5 | -4.80 | -2.23 | 2.57 | -4.79 | -2.12 | 2.67 |
| 6 | -4.84 | -2.21 | 2.63 | -4.76 | -2.15 | 2.61 |

(2FOS)<sub>n</sub>

|   | cis   |       |      | trans |       |      |
|---|-------|-------|------|-------|-------|------|
|   | HOMO  | LUMO  | Gap  | HOMO  | LUMO  | Gap  |
| 1 | -5.59 | -1.05 | 4.55 | -5.60 | -1.03 | 4.57 |
| 2 | -5.05 | -1.77 | 3.29 | -5.09 | -1.74 | 3.34 |
| 3 | -4.87 | -2.03 | 2.84 | -4.93 | -2.01 | 2.92 |
| 4 | -4.81 | -2.17 | 2.64 | -4.86 | -2.15 | 2.71 |
| 5 | -4.79 | -2.22 | 2.57 | -4.82 | -2.23 | 2.60 |
| 6 | -4.68 | -2.29 | 2.39 | -4.81 | -2.28 | 2.53 |

(FSFO)<sub>n</sub>

|   | cis   |       |      | trans |       |      |
|---|-------|-------|------|-------|-------|------|
|   | HOMO  | LUMO  | Gap  | HOMO  | LUMO  | Gap  |
| 1 | -5.57 | -1.10 | 4.48 | -5.57 | -1.10 | 4.47 |
| 2 | -5.05 | -1.77 | 3.24 | -5.05 | -1.77 | 3.28 |
| 3 | -4.84 | -2.06 | 2.78 | -4.86 | -2.03 | 2.83 |
| 4 | -4.81 | -2.20 | 2.62 | -4.78 | -2.17 | 2.61 |
| 5 | -4.78 | -2.23 | 2.54 | -4.73 | -2.24 | 2.49 |
| 6 | -4.70 | -2.29 | 2.56 | -4.70 | -2.29 | 2.41 |

(FOFS)<sub>n</sub>

|   | cis   |       |      | trans |       |      |
|---|-------|-------|------|-------|-------|------|
|   | HOMO  | LUMO  | Gap  | HOMO  | LUMO  | Gap  |
| 1 | -5.56 | -1.06 | 4.50 | -5.56 | -1.04 | 4.52 |
| 2 | -5.03 | -1.79 | 3.25 | -5.05 | -1.77 | 3.28 |
| 3 | -4.85 | -2.06 | 2.79 | -4.87 | -2.03 | 2.84 |
| 4 | -4.79 | -2.20 | 2.59 | -4.78 | -2.17 | 2.62 |
| 5 | -4.78 | -2.24 | 2.54 | -4.73 | -2.24 | 2.49 |
| 6 | -4.67 | -2.30 | 2.37 | -4.70 | -2.29 | 2.41 |