Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.


# SUPPORTING INFORMATION

## Quantitative Prediction of Morphology and Electron-Transport in Crystal and Disordered Organic Semiconductors

Ilhan Yavuz[1], Steven A. Lopez[2], Janice B. Lin[2] and K. N. Houk[2]*

[1] Department of Physics, Marmara University, 34722, Ziverbey, Istanbul, Turkey.

[2]Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095, United States.

*Correspondence: houk@chem.ucla.edu

### TABLE OF CONTENTS

## B3LYP/6-311G(d,p) optimized Cartesian coordinates

**pMSB**

C 5.2820000 -0.2550000 -0.0010000
C 6.1600000 -1.3500000 0.0070000
C 7.5400000 -1.1770000 0.0080000
C 8.1070000 0.0990000 0.0010000
C 7.2340000 1.1970000 -0.0080000
C 5.8590000 1.0290000 -0.0080000
C 9.6010000 0.3010000 0.0040000
C 3.8400000 -0.5010000 -0.0010000
C 2.8570000 0.4200000 -0.0010000
C 1.4170000 0.1730000 -0.0010000
C 0.5360000 1.2720000 0.0050000
C -0.8380000 1.1080000 0.0060000
H 5.7500000 -2.3550000 0.0120000
H 8.1870000 -2.0480000 0.0140000
H 7.6450000 2.2020000 -0.0140000
H 5.2240000 1.9080000 -0.0160000
H 10.1320000 -0.6530000 -0.0160000
H 9.9260000 0.8450000 0.8960000
H 9.9260000 0.8830000 -0.8650000
H 3.5680000 -1.5530000 0.0000000
H 3.1290000 1.4720000 0.0000000
H 0.9500000 2.2750000 0.0110000
H -1.4700000 1.9890000 0.0110000
C -5.2820000 0.2550000 0.0010000
C -6.1600000 1.3500000 0.0010000
C -7.5400000 1.1770000 0.0010000
C -8.1070000 -0.0990000 0.0010000
C -7.2340000 -1.1970000 0.0010000
C -5.8590000 -1.0290000 0.0010000
C -9.6020000 -0.3010000 0.0000000
C -3.8400000 0.5010000 0.0020000
C -2.8570000 -0.4200000 -0.0010000
C -1.4170000 -0.1730000 -0.0010000
C -0.5360000 -1.2720000 -0.0080000
C 0.8380000 -1.1080000 -0.0080000
H -5.7490000 2.3550000 0.0010000
H -8.1870000 2.0490000 0.0010000
H -7.6450000 -2.2020000 0.0010000
H -5.2240000 -1.9080000 0.0020000
H -10.1320000 0.6540000 0.0050000
H -9.9260000 -0.8590000 -0.8840000
H -9.9260000 -0.8690000 0.8770000
H -3.5680000 1.5530000 0.0040000
H -3.1290000 -1.4720000 -0.0050000
H -0.9500000 -2.2750000 -0.0140000
H 1.4700000 -1.9890000 -0.0150000

**oMSB**

C -1.4190000 3.0740000 4.0550000
C -1.6950000 2.7970000 5.4160000
C -1.9020000 3.8640000 6.2940000
C -1.8500000 5.1860000 5.8640000
C -1.5910000 5.4620000 4.5230000
C -1.3850000 4.4150000 3.6350000
C -1.7460000 1.3820000 5.9420000
C -1.1890000 1.9790000 3.1050000

C -0.4850000 2.0640000 1.9600000
C -0.2640000 1.0010000 0.9810000
C 0.6640000 1.2100000 -0.0570000
C -0.9270000 -0.2380000 1.0080000
H -2.1060000 3.6500000 7.3380000
H -2.0190000 5.9930000 6.5680000
H -1.5630000 6.4860000 4.1690000
H -1.2220000 4.6350000 2.5860000
H -1.6150000 1.0190000 3.3780000
H 0.0070000 3.0040000 1.7240000
H 1.1950000 2.1560000 -0.1040000
H -1.6660000 -0.4410000 1.7750000
H -0.8090000 0.8470000 5.7610000
H -1.9310000 1.3780000 7.0170000
H -2.5460000 0.8000000 5.4700000
C 1.4190000 -3.0740000 -4.0550000
C 1.6950000 -2.7970000 -5.4160000
C 1.9020000 -3.8640000 -6.2940000
C 1.8500000 -5.1860000 -5.8640000
C 1.5910000 -5.4620000 -4.5230000
C 1.3850000 -4.4150000 -3.6350000
C 1.7460000 -1.3820000 -5.9420000
C 1.1890000 -1.9790000 -3.1050000
C 0.4850000 -2.0640000 -1.9600000
C 0.2640000 -1.0010000 -0.9810000
C -0.6640000 -1.2100000 0.0570000
C 0.9270000 0.2380000 -1.0080000
H 2.1060000 -3.6500000 -7.3380000
H 2.0190000 -5.9930000 -6.5680000
H 1.5630000 -6.4860000 -4.1690000
H 1.2220000 -4.6350000 -2.5860000
H 1.6150000 -1.0190000 -3.3780000
H -0.0070000 -3.0040000 -1.7240000
H -1.1950000 -2.1560000 0.1040000
H 1.6660000 0.4410000 -1.7750000
H 0.8090000 -0.8470000 -5.7610000
H 1.9310000 -1.3780000 -7.0170000
H 2.5460000 -0.8000000 -5.4700000

**ANTH**

C -1.5770000 0.1720000 3.3690000
C -0.7670000 0.9370000 2.5770000
C -0.3690000 0.4880000 1.2800000
C 0.4580000 1.2470000 0.4470000
C -0.8400000 -0.7960000 0.8200000
C -1.6850000 -1.5620000 1.6810000
C -2.0420000 -1.0950000 2.9140000
H -1.8700000 0.5260000 4.3500000
H -0.4120000 1.9020000 2.9220000
H 0.8120000 2.2130000 0.7930000
H -2.0390000 -2.5280000 1.3340000
H -2.6840000 -1.6880000 3.5570000
C 0.8400000 0.7960000 -0.8200000
C -0.4580000 -1.2470000 -0.4470000
C 0.3690000 -0.4880000 -1.2800000
C 1.6850000 1.5620000 -1.6810000
H -0.8120000 -2.2130000 -0.7930000
C 0.7670000 -0.9370000 -2.5770000
C 2.0420000 1.0950000 -2.9140000
H 2.0390000 2.5280000 -1.3340000

C 1.5770000 -0.1720000 -3.3690000
H 0.4120000 -1.9020000 -2.9220000
H 2.6840000 1.6880000 -3.5570000
H 1.8700000 -0.5260000 -4.3500000

**C60**

C 0.0000000 0.6960000 3.4750000
C -1.1740000 1.4220000 3.0260000
C -0.7260000 2.5960000 2.3000000
C 0.0000000 -0.6960000 3.4750000
C 1.1740000 -1.4220000 3.0260000
C 0.7260000 -2.5960000 2.3000000
C 1.1740000 1.4220000 3.0260000
C 0.7260000 2.5960000 2.3000000
C -1.1740000 -1.4220000 3.0260000
C -0.7260000 -2.5960000 2.3000000
C -0.6960000 3.4750000 0.0000000
C -1.4220000 3.0260000 1.1740000
C -2.5960000 2.3000000 0.7260000
C -3.4750000 0.0000000 0.6960000
C -3.0260000 1.1740000 1.4220000
C -2.3000000 0.7260000 2.5960000
C -1.4220000 3.0260000 -1.1740000
C -2.5960000 2.3000000 -0.7260000
C -3.4750000 0.0000000 -0.6960000
C -3.0260000 1.1740000 -1.4220000
C -2.3000000 0.7260000 -2.5960000
C 0.6960000 -3.4750000 0.0000000
C 1.4220000 -3.0260000 1.1740000
C 2.5960000 -2.3000000 0.7260000
C 3.4750000 0.0000000 0.6960000
C 3.0260000 -1.1740000 1.4220000
C 2.3000000 -0.7260000 2.5960000
C 0.6960000 3.4750000 0.0000000
C 1.4220000 3.0260000 1.1740000
C 2.5960000 2.3000000 0.7260000
C 3.0260000 1.1740000 1.4220000
C 2.3000000 0.7260000 2.5960000
C -0.6960000 -3.4750000 0.0000000
C -1.4220000 -3.0260000 -1.1740000
C -2.5960000 -2.3000000 -0.7260000
C -3.0260000 -1.1740000 -1.4220000
C -2.3000000 -0.7260000 -2.5960000
C -1.4220000 -3.0260000 1.1740000
C -2.5960000 -2.3000000 0.7260000
C -3.0260000 -1.1740000 1.4220000
C -2.3000000 -0.7260000 2.5960000
C 1.4220000 3.0260000 -1.1740000
C 2.5960000 2.3000000 -0.7260000
C 1.4220000 -3.0260000 -1.1740000
C 2.5960000 -2.3000000 -0.7260000
C 0.0000000 0.6960000 -3.4750000
C -1.1740000 1.4220000 -3.0260000
C -0.7260000 2.5960000 -2.3000000
C 0.0000000 -0.6960000 -3.4750000
C -1.1740000 -1.4220000 -3.0260000
C -0.7260000 -2.5960000 -2.3000000
C 3.4750000 0.0000000 -0.6960000
C 3.0260000 1.1740000 -1.4220000
C 2.3000000 0.7260000 -2.5960000

C 1.1740000 1.4220000 -3.0260000
C 0.7260000 2.5960000 -2.3000000
C 3.0260000 -1.1740000 -1.4220000
C 2.3000000 -0.7260000 -2.5960000
C 1.1740000 -1.4220000 -3.0260000
C 0.7260000 -2.5960000 -2.3000000

**DPA**

C -2.4710000 0.5310000 1.3160000
C -0.2640000 2.4040000 1.6430000
C -3.5220000 -0.3310000 1.1800000
C 0.0530000 2.3770000 3.0060000
C -3.3930000 -1.4990000 0.3830000
C -0.0740000 3.5220000 3.7900000
C -2.2170000 -1.7720000 -0.2570000
C -0.5210000 4.7130000 3.2210000
C -0.8390000 4.7520000 1.8650000
C -0.7120000 3.6060000 1.0830000
C -0.1290000 1.1730000 0.8020000
C -1.2180000 0.2890000 0.6660000
C -1.0870000 -0.8990000 -0.1450000
H -2.5750000 1.4190000 1.9260000
H -4.4610000 -0.1250000 1.6830000
H 0.4010000 1.4510000 3.4510000
H -4.2350000 -2.1760000 0.2820000
H 0.1770000 3.4830000 4.8440000
H -2.1250000 -2.6630000 -0.8640000
H -0.6200000 5.6050000 3.8310000
H -1.1870000 5.6750000 1.4150000
H -0.9600000 3.6390000 0.0280000
C 0.1290000 -1.1730000 -0.8020000
C 0.2640000 -2.4040000 -1.6430000
C -0.0530000 -2.3770000 -3.0060000
C 0.0740000 -3.5220000 -3.7900000
C 0.5210000 -4.7130000 -3.2210000
C 0.8390000 -4.7520000 -1.8650000
C 0.7120000 -3.6060000 -1.0830000
H 0.9600000 -3.6390000 -0.0280000
H 1.1870000 -5.6750000 -1.4150000
H 0.6200000 -5.6050000 -3.8310000
H -0.1770000 -3.4830000 -4.8440000
H -0.4010000 -1.4510000 -3.4510000
C 1.2180000 -0.2890000 -0.6660000
C 2.4710000 -0.5310000 -1.3160000
C 3.5220000 0.3310000 -1.1800000
C 3.3930000 1.4990000 -0.3830000
C 2.2170000 1.7720000 0.2570000
C 1.0870000 0.8990000 0.1450000
H 2.1250000 2.6630000 0.8640000
H 4.2350000 2.1760000 -0.2820000
H 4.4610000 0.1250000 -1.6830000
H 2.5750000 -1.4190000 -1.9260000

**FPTTF**

S -0.3490000 2.0370000 0.7970000
S -1.0100000 -0.7170000 1.8360000
F -3.4720000 4.9010000 6.9030000
F -4.0620000 2.4630000 7.8210000
N -1.4810000 3.0390000 3.0070000
N -2.1030000 0.4570000 3.9800000
C -0.2820000 0.2740000 0.5460000
C -1.1780000 1.9580000 2.3550000
C -2.1220000 2.8770000 4.2030000
C -2.4780000 4.0140000 4.9600000
C -3.1200000 3.8460000 6.1570000
C -3.4320000 2.5560000 6.6430000
C -3.1000000 1.4340000 5.9320000
C -2.4370000 1.5740000 4.6940000
C -1.4940000 0.6470000 2.8490000
H -2.2410000 5.0030000 4.5920000
H -3.3400000 0.4490000 6.3070000
S 0.3490000 -2.0370000 -0.7970000
S 1.0100000 0.7170000 -1.8360000
F 3.4720000 -4.9010000 -6.9030000
F 4.0620000 -2.4630000 -7.8210000
N 1.4810000 -3.0390000 -3.0070000
N 2.1030000 -0.4570000 -3.9800000
C 0.2820000 -0.2740000 -0.5460000
C 1.1780000 -1.9580000 -2.3550000
C 2.1220000 -2.8770000 -4.2030000
C 2.4780000 -4.0140000 -4.9600000
C 3.1200000 -3.8460000 -6.1570000
C 3.4320000 -2.5560000 -6.6430000
C 3.1000000 -1.4340000 -5.9320000
C 2.4370000 -1.5740000 -4.6940000
C 1.4940000 -0.6470000 -2.8490000
H 2.2410000 -5.0030000 -4.5920000
H 3.3400000 -0.4490000 -6.3070000

**FRUB**

C 1.3950000 -0.9630000 0.3870000
C 0.6950000 -2.1220000 0.7670000
C 1.3780000 -3.3150000 1.1940000
H 2.4500000 -3.2860000 1.3200000
C 0.7090000 -4.4740000 1.4490000
H 1.2530000 -5.3510000 1.7810000
C 0.4830000 4.9600000 -1.2850000
H 0.9740000 5.8480000 -1.6660000
C 1.1960000 3.8150000 -1.0970000
H 2.2530000 3.8020000 -1.3210000
C 0.5790000 2.6100000 -0.6100000
C 1.3400000 1.4680000 -0.3010000
C 0.6970000 0.2460000 0.0750000
C 2.8770000 -1.1580000 0.2380000
C 3.3610000 -1.7780000 -0.9200000
H 2.6690000 -2.0210000 -1.7180000
C 4.7060000 -2.0980000 -1.0550000
H 5.0640000 -2.5840000 -1.9540000
C 5.5920000 -1.8100000 -0.0180000
C 5.1230000 -1.2100000 1.1500000
H 5.8090000 -1.0030000 1.9620000
C 3.7750000 -0.8950000 1.2760000

H 3.4140000 -0.4420000 2.1920000
C 2.8260000 1.6880000 -0.2900000
C 3.6230000 1.4500000 -1.4120000
H 3.1770000 1.0070000 -2.2960000
C 4.9810000 1.7760000 -1.4170000
C 5.5300000 2.3670000 -0.2740000
H 6.5850000 2.6280000 -0.2710000
C 4.7560000 2.6360000 0.8550000
C 3.4020000 2.2960000 0.8290000
H 2.7770000 2.5190000 1.6880000
C 7.0560000 -2.0980000 -0.1820000
F 7.2820000 -3.1820000 -0.9560000
F 7.6740000 -2.3120000 1.0000000
F 7.7110000 -1.0630000 -0.7730000
C 5.8470000 1.4870000 -2.6190000
H 5.2460000 1.2090000 -3.4870000
H 6.5360000 0.6630000 -2.4070000
H 6.4540000 2.3560000 -2.8910000
C 5.3710000 3.2620000 2.0850000
H 6.2200000 3.8990000 1.8260000
H 5.7380000 2.4950000 2.7760000
H 4.6440000 3.8690000 2.6290000
C -1.4530000 -1.0140000 0.3090000
C -0.7440000 -2.1730000 0.6600000
C -1.3940000 -3.4380000 0.8730000
H -2.4620000 -3.5070000 0.7330000
C -0.6990000 -4.5430000 1.2630000
H -1.2200000 -5.4790000 1.4320000
C -0.9030000 5.0020000 -0.9640000
H -1.4550000 5.9280000 -1.0800000
C -1.5350000 3.8840000 -0.5100000
H -2.5860000 3.9280000 -0.2650000
C -0.8440000 2.6320000 -0.3650000
C -1.4950000 1.4610000 0.0530000
C -0.7740000 0.2320000 0.1470000
C -2.8920000 -1.1880000 -0.0760000
C -3.2180000 -1.2000000 -1.4360000
H -2.4430000 -1.0060000 -2.1690000
C -4.5140000 -1.4700000 -1.8630000
H -4.7480000 -1.4860000 -2.9190000
C -5.5090000 -1.7370000 -0.9250000
C -5.2000000 -1.7300000 0.4370000
H -5.9710000 -1.9410000 1.1670000
C -3.9030000 -1.4640000 0.8530000
H -3.6700000 -1.4590000 1.9100000
C -2.8960000 1.5970000 0.5690000
C -3.9890000 1.8660000 -0.2610000
H -3.8450000 1.8930000 -1.3350000
C -5.2630000 2.0890000 0.2670000
C -5.4270000 2.0500000 1.6540000
H -6.4120000 2.2270000 2.0750000
C -4.3540000 1.7980000 2.5120000
C -3.0940000 1.5710000 1.9540000
H -2.2460000 1.3840000 2.6050000
C -6.9200000 -2.0140000 -1.3550000
F -7.0260000 -2.2340000 -2.6810000
F -7.4370000 -3.0950000 -0.7270000
F -7.7520000 -0.9780000 -1.0640000
C -6.4420000 2.3410000 -0.6420000
H -6.1250000 2.7750000 -1.5940000
H -6.9690000 1.4080000 -0.8640000

H -7.1600000 3.0230000 -0.1820000
C -4.5450000 1.8110000 4.0110000
H -5.5130000 1.3900000 4.2930000
H -3.7640000 1.2400000 4.5180000
H -4.5080000 2.8340000 4.4020000

**NAPH**
C -0.8900000 0.1080000 2.3660000
C -0.1470000 0.9690000 1.5960000
C 0.2130000 0.6300000 0.2650000
C 0.9800000 1.4950000 -0.5580000
C -1.3110000 -1.1370000 1.8420000
H -1.1580000 0.3800000 3.3810000
H 0.1760000 1.9240000 1.9970000
H 1.3020000 2.4490000 -0.1540000
H -1.8980000 -1.8070000 2.4600000
C -0.2130000 -0.6300000 -0.2650000
C 1.3110000 1.1370000 -1.8420000
C -0.9800000 -1.4950000 0.5580000
C 0.1470000 -0.9690000 -1.5960000
C 0.8900000 -0.1080000 -2.3660000
H 1.8980000 1.8070000 -2.4600000
H -1.3020000 -2.4490000 0.1540000
H -0.1760000 -1.9240000 -1.9970000
H 1.1580000 -0.3800000 -3.3810000

**PERY**
C -0.9290000 -1.0140000 0.4580000
C 0.4660000 -1.0010000 0.9400000
C -1.3590000 -0.0130000 -0.4690000
C 0.9460000 -1.9430000 1.8400000
C -2.7140000 -0.0260000 -0.9370000
C -1.8460000 -1.9700000 0.8750000
C -3.6040000 -1.0270000 -0.4760000
C -3.1460000 0.9620000 -1.8550000
C -3.1730000 -1.9790000 0.4140000
C 2.2750000 -1.9270000 2.2950000
H 2.6040000 -2.6840000 2.9980000
H -1.5500000 -2.7400000 1.5750000
H 0.2940000 -2.7210000 2.2130000
H -4.1740000 0.9420000 -2.2010000
H -3.8530000 -2.7460000 0.7670000
H -4.6260000 -1.0260000 -0.8370000
C 0.9290000 1.0140000 -0.4580000
C -0.4660000 1.0010000 -0.9400000
C 1.3590000 0.0130000 0.4690000
C -0.9460000 1.9430000 -1.8400000
C 2.7140000 0.0260000 0.9370000
C 1.8460000 1.9700000 -0.8750000
C 3.6040000 1.0270000 0.4760000
C 3.1460000 -0.9620000 1.8550000
C 3.1730000 1.9790000 -0.4140000
C -2.2750000 1.9270000 -2.2950000
H -2.6040000 2.6840000 -2.9980000
H 1.5500000 2.7400000 -1.5750000
H -0.2940000 2.7210000 -2.2130000
H 4.1740000 -0.9420000 2.2010000
H 3.8530000 2.7460000 -0.7670000
H 4.6260000 1.0260000 0.8370000

**TCNQ**

C -0.4830000 0.5470000 1.2060000
C -1.3740000 0.1790000 0.2590000
C 0.9390000 0.3880000 0.9980000
C 1.8530000 0.7660000 1.9680000
C 1.4400000 1.3260000 3.2100000
C 3.2560000 0.6150000 1.7780000
H -0.8270000 0.9700000 2.1420000
H -2.4360000 0.3060000 0.4330000
N 1.0980000 1.7810000 4.2160000
N 4.3940000 0.4890000 1.6170000
C -0.9390000 -0.3880000 -0.9980000
C 1.3740000 -0.1790000 -0.2590000
C 0.4830000 -0.5470000 -1.2060000
C -1.8530000 -0.7660000 -1.9680000
H 2.4360000 -0.3060000 -0.4330000
H 0.8270000 -0.9700000 -2.1420000
C -1.4400000 -1.3260000 -3.2100000
C -3.2560000 -0.6150000 -1.7780000
N -1.0980000 -1.7810000 -4.2160000
N -4.3940000 -0.4890000 -1.6170000

**TFAPT**

S 2.1010000 0.6140000 -0.0040000
F 9.2270000 1.6980000 0.9510000
F 10.9480000 0.5710000 0.2580000
O 9.5010000 -1.5710000 0.5910000
C 0.9640000 -1.6450000 -0.4930000
C 4.5740000 -0.7110000 -0.0600000
C 6.7080000 -1.7810000 0.3820000
C 5.2600000 0.4970000 -0.2750000
C 7.3870000 -0.5700000 0.1670000
C 6.6400000 0.5710000 -0.1610000
C 2.3490000 -1.9130000 -0.4230000
C 9.6410000 0.7440000 0.0870000
C 3.1220000 -0.7990000 -0.1790000
C 0.6490000 -0.3170000 -0.2970000
C 8.8610000 -0.5850000 0.3100000
C 5.3320000 -1.8510000 0.2760000
H 0.2190000 -2.3990000 -0.7110000
H 7.2880000 -2.6570000 0.6440000
H 4.7080000 1.3870000 -0.5540000
H 7.1270000 1.5200000 -0.3370000
H 2.7700000 -2.8960000 -0.5890000
H 4.8310000 -2.7890000 0.4780000
F 9.4400000 1.2170000 -1.1650000
S -2.1010000 -0.6140000 -0.0040000
F -9.4400000 -1.2180000 -1.1650000
F -10.9480000 -0.5710000 0.2580000
O -9.5010000 1.5710000 0.5900000
C -0.9640000 1.6450000 -0.4920000
C -4.5750000 0.7110000 -0.0600000
C -6.7080000 1.7810000 0.3810000
C -5.2600000 -0.4970000 -0.2750000
C -7.3870000 0.5700000 0.1670000
C -6.6400000 -0.5710000 -0.1610000
C -2.3490000 1.9130000 -0.4230000
C -9.6410000 -0.7450000 0.0870000
C -3.1220000 0.8000000 -0.1790000

C -0.6490000 0.3170000 -0.2970000
C -8.8610000 0.5850000 0.3100000
C -5.3330000 1.8510000 0.2760000
H -0.2190000 2.3990000 -0.7110000
H -7.2880000 2.6570000 0.6440000
H -4.7080000 -1.3870000 -0.5540000
H -7.1270000 -1.5200000 -0.3370000
H -2.7700000 2.8960000 -0.5880000
H -4.8310000 2.7890000 0.4780000
F -9.2260000 -1.6980000 0.9520000

**TFPTP**

S -0.6450000 2.1260000 0.0130000
F -1.4370000 9.3680000 1.1540000
F -0.5710000 10.9690000 -0.0270000
O 1.6190000 9.5780000 -0.0930000
C 1.6670000 0.9590000 0.0080000
C 0.7260000 4.5760000 -0.0020000
C 1.8280000 6.7530000 -0.0640000
C -0.5150000 5.2670000 0.0400000
C 0.5850000 7.4350000 -0.0230000
C -0.5850000 6.6420000 0.0310000
C 1.9340000 2.3280000 0.0030000
C -0.7480000 9.6430000 0.0160000
C 0.8050000 3.1460000 0.0050000
C 0.3080000 0.6370000 0.0130000
C 0.6080000 8.8860000 -0.0410000
C 1.8980000 5.3830000 -0.0530000
H 2.4390000 0.2000000 0.0080000
H 2.7300000 7.3520000 -0.1060000
H -1.4370000 4.6980000 0.0840000
H -1.5600000 7.1100000 0.0650000
H 2.9400000 2.7260000 0.0010000
H 2.8710000 4.9080000 -0.0900000
F -1.5650000 9.3160000 -1.0200000
S 0.6450000 -2.1260000 0.0130000
F 1.5650000 -9.3160000 -1.0200000
F 0.5710000 -10.9690000 -0.0270000
O -1.6190000 -9.5780000 -0.0930000
C -1.6670000 -0.9590000 0.0080000
C -0.7260000 -4.5760000 -0.0020000
C -1.8280000 -6.7530000 -0.0640000
C 0.5150000 -5.2670000 0.0400000
C -0.5850000 -7.4350000 -0.0230000
C 0.5850000 -6.6420000 0.0310000
C -1.9340000 -2.3280000 0.0030000
C 0.7480000 -9.6430000 0.0160000
C -0.8050000 -3.1460000 0.0050000
C -0.3080000 -0.6370000 0.0130000
C -0.6080000 -8.8860000 -0.0410000
C -1.8980000 -5.3830000 -0.0530000
H -2.4390000 -0.2000000 0.0080000
H -2.7300000 -7.3520000 -0.1060000
H 1.4370000 -4.6980000 0.0840000
H 1.5600000 -7.1100000 0.0650000
H -2.9400000 -2.7260000 0.0010000
H -2.8710000 -4.9080000 -0.0900000
F 1.4370000 -9.3680000 1.1540000

**TFTT**

S 0.8310000 1.9010000 -0.0360000
S -0.8310000 -1.9010000 -0.0360000
S 4.7220000 -0.2390000 -0.0640000
S -4.7220000 0.2390000 -0.0640000
F 11.7600000 -1.9320000 -0.1140000
F 12.1260000 -0.2940000 1.2600000
F 12.3150000 0.0290000 -0.8770000
F -12.1260000 0.2940000 1.2610000
F -12.3150000 -0.0290000 -0.8770000
F -11.7600000 1.9320000 -0.1140000
N 1.6840000 -0.5870000 -0.0340000
N -1.6840000 0.5870000 -0.0340000
C -0.3360000 0.6060000 -0.0380000
C 0.3360000 -0.6060000 -0.0380000
C 2.1130000 0.6550000 -0.0310000
C -2.1130000 -0.6550000 -0.0310000
C 3.5070000 1.0150000 -0.0230000
C 4.0900000 2.2640000 0.0120000
C 5.5010000 2.2190000 0.0130000
C 6.0130000 0.9390000 -0.0200000
C 7.4190000 0.5300000 -0.0180000
C 8.4110000 1.3930000 -0.5140000
C 9.7490000 1.0260000 -0.5000000
C 10.1270000 -0.2210000 -0.0030000
C 9.1550000 -1.0960000 0.4820000
C 7.8190000 -0.7230000 0.4770000
C -3.5070000 -1.0150000 -0.0230000
C -4.0900000 -2.2640000 0.0110000
C -5.5010000 -2.2190000 0.0120000
C -6.0130000 -0.9390000 -0.0210000
C -7.4190000 -0.5300000 -0.0180000
C -7.8190000 0.7230000 0.4780000
C -9.1550000 1.0960000 0.4830000
C -10.1270000 0.2210000 -0.0030000
C -9.7490000 -1.0260000 -0.5010000
C -8.4110000 -1.3930000 -0.5150000
C 11.5790000 -0.6040000 0.0610000
C -11.5790000 0.6040000 0.0610000
H 3.5220000 3.1840000 0.0490000
H 6.1230000 3.1020000 0.0700000
H 8.1280000 2.3490000 -0.9370000
H 10.5000000 1.6990000 -0.8950000
H 9.4450000 -2.0670000 0.8640000
H 7.0790000 -1.4050000 0.8790000
H -3.5220000 -3.1840000 0.0480000
H -6.1230000 -3.1020000 0.0690000
H -7.0790000 1.4040000 0.8790000
H -9.4450000 2.0670000 0.8640000
H -10.5000000 -1.6990000 -0.8950000
H -8.1280000 -2.3490000 -0.9370000

**BPFT**

| | | | |
|---|---|---|---|
| S | -1.88250700 | 1.31848500 | -0.10446700 |
| O | 2.05322700 | 0.57024500 | -0.20534500 |
| C | -2.74944600 | -0.20740300 | -0.19945300 |
| C | -1.85296200 | -1.24017400 | -0.36444900 |
| C | -0.50130900 | -0.83296000 | -0.42528900 |
| C | -0.33632900 | 0.52936000 | -0.31334700 |
| C | 0.88804100 | 1.28125900 | -0.31751200 |
| C | 1.18029100 | 2.61969700 | -0.40154400 |
| C | 2.59395400 | 2.73364800 | -0.34115300 |

| | | | |
|---|---|---|---|
| C | 3.09505700 | 1.46170700 | -0.22599900 |
| C | -4.20724300 | -0.25929900 | -0.11017900 |
| C | -4.98922900 | 0.89697700 | 0.04097500 |
| C | -6.37109600 | 0.83371100 | 0.12913100 |
| C | -7.06618800 | -0.38552800 | 0.06681300 |
| C | -6.27682000 | -1.54103700 | -0.07387500 |
| C | -4.89586600 | -1.48371800 | -0.16252400 |
| C | -8.54893200 | -0.45451100 | 0.18136400 |
| C | -9.32123900 | 0.69038100 | 0.44571400 |
| C | -10.70733800 | 0.62968300 | 0.53581200 |
| C | -11.37430900 | -0.57963900 | 0.35843400 |
| C | -10.63125900 | -1.72546700 | 0.08724800 |
| C | -9.24522500 | -1.66208800 | -0.00298900 |
| C | 4.44005800 | 0.92518100 | -0.12492600 |
| C | 4.70808000 | -0.43227000 | -0.35586600 |
| C | 5.99751500 | -0.93191800 | -0.25705700 |
| C | 7.09149300 | -0.11545200 | 0.07918300 |
| C | 6.80604000 | 1.24133700 | 0.31892700 |
| C | 5.52032800 | 1.74861900 | 0.22820600 |
| C | 8.47695700 | -0.65541400 | 0.17395300 |
| C | 8.75968300 | -2.00823200 | -0.08561300 |
| C | 10.05195400 | -2.51367300 | 0.00209700 |
| C | 11.11262000 | -1.68363900 | 0.35497600 |
| C | 10.85732200 | -0.34058100 | 0.61843700 |
| C | 9.56409800 | 0.16241700 | 0.52979100 |
| H | -2.15572400 | -2.27487000 | -0.44806600 |
| H | 0.33151500 | -1.51011300 | -0.55312100 |
| H | 0.46661300 | 3.42068200 | -0.51120000 |
| H | 3.17170400 | 3.64177900 | -0.40141900 |
| H | -4.51216600 | 1.86957400 | 0.08796600 |
| H | -6.91084400 | 1.76558200 | 0.23210000 |
| H | -6.74106700 | -2.51781000 | -0.10363600 |
| H | -4.34552300 | -2.41064300 | -0.26712300 |
| H | -8.84164100 | 1.64751100 | 0.60255000 |
| H | -11.26742500 | 1.53394900 | 0.74680600 |
| H | -12.45492200 | -0.62778700 | 0.42791700 |
| H | -11.13185600 | -2.67595200 | -0.06084100 |
| H | -8.70731200 | -2.57237100 | -0.23248600 |
| H | 3.89531300 | -1.09644000 | -0.62098300 |
| H | 6.14251000 | -1.98632100 | -0.45009100 |
| H | 7.59764400 | 1.92550900 | 0.59309600 |
| H | 5.35016400 | 2.79694500 | 0.44479100 |
| H | 7.96594100 | -2.68790800 | -0.36516400 |
| H | 10.22854900 | -3.56291000 | -0.20729000 |
| H | 12.12047000 | -2.07654500 | 0.42371400 |
| H | 11.66879600 | 0.32310300 | 0.89591800 |
| H | 9.41132800 | 1.21148300 | 0.74507200 |

**TFDT**

| | | | |
|---|---|---|---|
| S | -2.06601 | -0.78413 | 0.02002 |
| C | -7.42332 | -0.00965 | 0.03552 |
| C | -6.56830 | -1.10991 | 0.05317 |
| C | -6.88552 | 1.27823 | 0.00881 |
| C | -5.19331 | -0.92343 | 0.04557 |
| C | -5.51188 | 1.46133 | 0.00054 |
| C | -4.63060 | 0.36404 | 0.01719 |
| C | -3.18167 | 0.57008 | 0.00978 |
| C | -2.47691 | 1.75296 | -0.00603 |
| C | -1.07451 | 1.58968 | -0.00983 |
| C | -0.66944 | 0.27246 | 0.00332 |
| H | -6.97803 | -2.11144 | 0.08149 |
| H | -7.54473 | 2.13729 | 0.00364 |
| H | -5.12143 | 2.47061 | -0.01712 |
| H | -4.54999 | -1.79522 | 0.06456 |
| H | -2.95066 | 2.72477 | -0.01414 |
| H | -0.37944 | 2.41900 | -0.02136 |

| | | | |
|---|---|---|---|
| C | -8.91145 | -0.20380 | -0.01138 |
| F | -9.37946 | -0.20355 | -1.28308 |
| F | -9.28995 | -1.37745 | 0.53986 |
| F | -9.57189 | 0.77862 | 0.64118 |
| S | 2.06591 | 0.78808 | -0.01557 |
| C | 7.42305 | 0.01063 | -0.03834 |
| C | 6.56942 | 1.11127 | 0.00041 |
| C | 6.88384 | -1.27676 | -0.06617 |
| C | 5.19417 | 0.92573 | 0.01147 |
| C | 5.51020 | -1.45888 | -0.05569 |
| C | 4.63020 | -0.36115 | -0.01341 |
| C | 3.18119 | -0.56642 | -0.00289 |
| C | 2.47616 | -1.74913 | 0.01272 |
| C | 1.07382 | -1.58548 | 0.01692 |
| C | 0.66908 | -0.26815 | 0.00376 |
| H | 6.98006 | 2.11269 | 0.01464 |
| H | 7.54205 | -2.13568 | -0.10712 |
| H | 5.11849 | -2.46737 | -0.08628 |
| H | 4.55178 | 1.79792 | 0.04080 |
| H | 2.94976 | -2.72096 | 0.02556 |
| H | 0.37854 | -2.41459 | 0.03059 |
| C | 8.91205 | 0.19888 | 0.00498 |
| F | 9.39338 | 0.11492 | 1.26884 |
| F | 9.28820 | 1.40464 | -0.47343 |
| F | 9.56277 | -0.74112 | -0.71660 |

**PYDIC8**

| | | | |
|---|---|---|---|
| C | 0.75345 | -0.32839 | -1.09682 |
| C | 0.08685 | 0.89081 | -1.13189 |
| H | 0.15171 | 1.55951 | -1.98103 |
| C | -0.66881 | 1.19600 | -0.00592 |
| C | -1.49067 | 2.38152 | 0.28589 |
| C | -2.89975 | 3.12791 | 2.23815 |
| H | -3.57381 | 2.54723 | 2.86869 |
| H | -3.48151 | 3.63567 | 1.46802 |
| C | -2.11072 | 4.13948 | 3.07618 |
| H | -1.42207 | 4.68337 | 2.42166 |
| H | -1.50302 | 3.59792 | 3.80829 |
| C | -3.03341 | 5.12804 | 3.79710 |
| H | -3.65576 | 5.65029 | 3.05959 |
| H | -3.72363 | 4.57484 | 4.44634 |
| C | -2.26792 | 6.15968 | 4.63385 |
| H | -1.58182 | 6.71477 | 3.98177 |
| H | -1.63793 | 5.63591 | 5.36379 |
| C | -3.17877 | 7.14881 | 5.36961 |
| H | -3.81291 | 7.66894 | 4.64022 |
| H | -3.86192 | 6.59333 | 6.02495 |
| C | -2.41143 | 8.18365 | 6.20021 |
| H | -1.72989 | 8.74088 | 5.54437 |
| H | -1.77445 | 7.66379 | 6.92754 |
| C | -3.31800 | 9.17280 | 6.94145 |
| H | -3.99810 | 8.61644 | 7.59791 |
| H | -3.95491 | 9.69203 | 6.21501 |
| C | -2.54218 | 10.20318 | 7.76697 |
| H | -1.92256 | 9.71616 | 8.52640 |
| H | -3.21686 | 10.89256 | 8.28189 |
| H | -1.87879 | 10.79965 | 7.13289 |
| C | -1.62936 | 0.95466 | 2.10014 |
| S | -1.73591 | 3.69503 | -0.67505 |
| S | -2.06002 | 0.35576 | 3.57142 |
| N | -2.03060 | 2.16810 | 1.55021 |
| C | -0.75345 | 0.32839 | 1.09682 |
| C | -0.08685 | -0.89081 | 1.13189 |
| H | -0.15171 | -1.55951 | 1.98103 |
| C | 0.66881 | -1.19600 | 0.00592 |
| C | 1.49067 | -2.38152 | -0.28589 |
| C | 2.89975 | -3.12791 | -2.23815 |

| | | | |
|---|---|---|---|
| H | 3.57381 | -2.54723 | -2.86869 |
| H | 3.48151 | -3.63567 | -1.46802 |
| C | 2.11072 | -4.13948 | -3.07618 |
| H | 1.42207 | -4.68337 | -2.42166 |
| H | 1.50302 | -3.59792 | -3.80829 |
| C | 3.03341 | -5.12804 | -3.79710 |
| H | 3.65576 | -5.65029 | -3.05959 |
| H | 3.72363 | -4.57484 | -4.44634 |
| C | 2.26792 | -6.15968 | -4.63385 |
| H | 1.58182 | -6.71477 | -3.98177 |
| H | 1.63793 | -5.63591 | -5.36379 |
| C | 3.17877 | -7.14881 | -5.36961 |
| H | 3.81291 | -7.66894 | -4.64022 |
| H | 3.86192 | -6.59333 | -6.02495 |
| C | 2.41143 | -8.18365 | -6.20021 |
| H | 1.72989 | -8.74088 | -5.54437 |
| H | 1.77445 | -7.66379 | -6.92754 |
| C | 3.31800 | -9.17280 | -6.94145 |
| H | 3.99810 | -8.61644 | -7.59791 |
| H | 3.95491 | -9.69203 | -6.21501 |
| C | 2.54218 | -10.20318 | -7.76697 |
| H | 1.92256 | -9.71616 | -8.52640 |
| H | 3.21686 | -10.89256 | -8.28189 |
| H | 1.87879 | -10.79965 | -7.13289 |
| C | 1.62936 | -0.95466 | -2.10014 |
| S | 1.73591 | -3.69503 | 0.67505 |
| S | 2.06002 | -0.35576 | -3.57142 |
| N | 2.03060 | -2.16810 | -1.55021 |

**HXNTCDI**

| | | | |
|---|---|---|---|
| O | 3.73574 | -1.90812 | -0.24339 |
| O | 3.25185 | 2.62632 | -0.42949 |
| N | 3.50026 | 0.35909 | -0.36314 |
| C | 2.99558 | -0.94380 | -0.23384 |
| C | 1.52098 | -1.07940 | -0.08724 |
| C | 0.95320 | -2.33481 | 0.03285 |
| H | 1.60251 | -3.20109 | 0.01785 |
| C | 0.70239 | 0.07220 | -0.07121 |
| C | 1.25936 | 1.36528 | -0.19025 |
| C | 0.43830 | 2.47803 | -0.17066 |
| H | 0.89029 | 3.45752 | -0.26334 |
| C | 2.73067 | 1.53188 | -0.33615 |
| C | 4.96385 | 0.51199 | -0.50688 |
| H | 5.13000 | 1.38878 | -1.13170 |
| H | 5.31924 | -0.37740 | -1.02186 |
| C | 5.66561 | 0.68364 | 0.84558 |
| H | 5.48625 | -0.20860 | 1.45492 |
| H | 5.20956 | 1.53151 | 1.36502 |
| C | 7.17649 | 0.92894 | 0.71633 |
| H | 7.34686 | 1.81882 | 0.09685 |
| H | 7.56750 | 1.17559 | 1.71019 |
| C | 7.97824 | -0.25045 | 0.14983 |
| H | 7.65594 | -0.46925 | -0.87516 |
| H | 7.75712 | -1.15183 | 0.73574 |
| C | 9.49182 | -0.00576 | 0.14904 |
| H | 9.71038 | 0.90301 | -0.42493 |
| H | 9.82387 | 0.19624 | 1.17466 |
| C | 10.29401 | -1.17678 | -0.42536 |
| H | 10.12064 | -2.09335 | 0.14702 |
| H | 11.36792 | -0.97213 | -0.40711 |
| H | 10.01221 | -1.37837 | -1.46356 |
| O | -3.73571 | 1.90838 | 0.24350 |
| O | -3.25182 | -2.62606 | 0.42971 |
| N | -3.50024 | -0.35884 | 0.36327 |
| C | -2.99556 | 0.94405 | 0.23398 |
| C | -1.52095 | 1.07965 | 0.08742 |
| C | -0.95317 | 2.33507 | -0.03266 |

| | | | |
|---|---|---|---|
| H | -1.60248 | 3.20134 | -0.01768 |
| C | -0.70236 | -0.07194 | 0.07140 |
| C | -1.25933 | -1.36503 | 0.19045 |
| C | -0.43827 | -2.47778 | 0.17086 |
| H | -0.89026 | -3.45727 | 0.26355 |
| C | -2.73064 | -1.53163 | 0.33634 |
| C | -4.96384 | -0.51176 | 0.50694 |
| H | -5.13000 | -1.38843 | 1.13195 |
| H | -5.31930 | 0.37772 | 1.02169 |
| C | -5.66547 | -0.68377 | -0.84555 |
| H | -5.48619 | 0.20838 | -1.45506 |
| H | -5.20927 | -1.53166 | -1.36479 |
| C | -7.17632 | -0.92927 | -0.71639 |
| H | -7.34659 | -1.81903 | -0.09673 |
| H | -7.56719 | -1.17622 | -1.71023 |
| C | -7.97832 | 0.25012 | -0.15024 |
| H | -7.65605 | 0.46932 | 0.87467 |
| H | -7.75741 | 1.15138 | -0.73643 |
| C | -9.49185 | 0.00508 | -0.14937 |
| H | -9.71015 | -0.90360 | 0.42485 |
| H | -9.82382 | -0.19731 | -1.17493 |
| C | -10.29440 | 1.17601 | 0.42471 |
| H | -10.12123 | 2.09253 | -0.14781 |
| H | -11.36825 | 0.97107 | 0.40642 |
| H | -10.01273 | 1.37783 | 1.46290 |

**CHNTCDI**

| | | | |
|---|---|---|---|
| O | 2.09652 | -3.63191 | 0.00000 |
| O | -2.47983 | -3.37974 | 0.00000 |
| N | -0.19106 | -3.54787 | 0.00000 |
| C | -1.40030 | -2.82077 | 0.00000 |
| C | -1.30240 | -1.33574 | 0.00000 |
| C | -2.45390 | -0.56863 | 0.00000 |
| H | -3.41217 | -1.07156 | 0.00000 |
| C | -0.03877 | -0.70834 | 0.00000 |
| C | 2.37684 | -0.83503 | 0.00000 |
| H | 3.27382 | -1.44047 | 0.00000 |
| C | 1.14810 | -1.47092 | 0.00000 |
| C | 1.08309 | -2.95919 | 0.00000 |
| C | -0.30639 | -5.03906 | 0.00000 |
| H | -1.38297 | -5.20819 | 0.00000 |
| C | 0.26382 | -5.67709 | 1.27672 |
| H | -0.20421 | -5.21707 | 2.15321 |
| H | 1.33757 | -5.48890 | 1.33816 |
| C | -0.00028 | -7.19141 | 1.26772 |
| H | 0.44156 | -7.64521 | 2.16026 |
| H | -1.08068 | -7.37438 | 1.32721 |
| C | 0.55656 | -7.85501 | 0.00000 |
| H | 0.32184 | -8.92428 | 0.00000 |
| H | 1.65054 | -7.77322 | 0.00000 |
| O | -2.09626 | 3.63178 | 0.00000 |
| O | 2.48009 | 3.37962 | 0.00000 |
| N | 0.19132 | 3.54775 | 0.00000 |
| C | 1.40056 | 2.82065 | 0.00000 |
| C | 1.30266 | 1.33561 | 0.00000 |
| C | 2.45417 | 0.56851 | 0.00000 |
| H | 3.41240 | 1.07142 | 0.00000 |
| C | 0.03903 | 0.70821 | 0.00000 |
| C | -2.37658 | 0.83491 | 0.00000 |
| H | -3.27357 | 1.44036 | 0.00000 |
| C | -1.14783 | 1.47080 | 0.00000 |
| C | -1.08283 | 2.95907 | 0.00000 |
| C | 0.30664 | 5.03894 | 0.00000 |
| H | 1.38323 | 5.20805 | 0.00000 |
| C | -0.26451 | 5.67738 | 1.27710 |
| H | 0.20284 | 5.21769 | 2.15413 |
| H | -1.33831 | 5.48924 | 1.33780 |

| | | | |
|---|---|---|---|
| C | -0.00028 | 7.19169 | 1.26763 |
| H | -0.44269 | 7.64588 | 2.15972 |
| H | 1.08007 | 7.37460 | 1.32776 |
| C | -0.55612 | 7.85484 | 0.00000 |
| H | -0.32140 | 8.92414 | 0.00000 |
| H | -1.65011 | 7.77307 | 0.00000 |
| C | -0.26451 | 5.67738 | -1.27710 |
| H | 0.20284 | 5.21769 | -2.15413 |
| H | -1.33831 | 5.48924 | -1.33780 |
| C | -0.00028 | 7.19169 | -1.26763 |
| H | -0.44269 | 7.64588 | -2.15972 |
| H | 1.08007 | 7.37460 | -1.32776 |
| C | 0.26382 | -5.67709 | -1.27672 |
| H | -0.20421 | -5.21707 | -2.15321 |
| H | 1.33757 | -5.48890 | -1.33816 |
| C | -0.00028 | -7.19141 | -1.26772 |
| H | 0.44156 | -7.64521 | -2.16026 |
| H | -1.08068 | -7.37438 | -1.32721 |

**PTCDA**

| | | | |
|---|---|---|---|
| C | 0.15125600 | -0.46377100 | 1.35334500 |
| C | -0.02991700 | 1.41238300 | -0.27068500 |
| C | 0.12283800 | 0.95930600 | 1.09446400 |
| C | 0.30175600 | -0.71943200 | 2.70000200 |
| C | -0.03718200 | 2.78983900 | -0.33784200 |
| C | 0.24471300 | 1.91374100 | 2.18355400 |
| C | 0.40524500 | 0.11246700 | 3.61836700 |
| C | 0.06866700 | 3.59135500 | 0.60691100 |
| C | 0.39717100 | 1.48106700 | 3.54305800 |
| C | 0.21816400 | 3.32843900 | 1.94408600 |
| C | 0.52334300 | 2.43822100 | 4.65688200 |
| C | 0.34000600 | 4.30745400 | 3.03906800 |
| O | 0.48458200 | 3.78465500 | 4.31796000 |
| O | 0.65364600 | 2.13288900 | 5.80328400 |
| O | 0.32234900 | 5.49227000 | 2.89622400 |
| C | -0.15125600 | 0.46377100 | -1.35334500 |
| C | 0.02991700 | -1.41238300 | 0.27068500 |
| C | -0.12283800 | -0.95930600 | -1.09446400 |
| C | -0.30175600 | 0.71943200 | -2.70000200 |
| C | 0.03718200 | -2.78983900 | 0.33784200 |
| C | -0.24471300 | -1.91374100 | -2.18355400 |
| C | -0.40524500 | -0.11246700 | -3.61836700 |
| C | -0.06866700 | -3.59135500 | -0.60691100 |
| C | -0.39717100 | -1.48106700 | -3.54305800 |
| C | -0.21816400 | -3.32843900 | -1.94408600 |
| C | -0.52334300 | -2.43822100 | -4.65688200 |
| C | -0.34000600 | -4.30745400 | -3.03906800 |
| O | -0.48458200 | -3.78465500 | -4.31796000 |
| O | -0.65364600 | -2.13288900 | -5.80328400 |
| O | -0.32234900 | -5.49227000 | -2.89622400 |

**DFBDTT**

| | | | |
|---|---|---|---|
| S | -0.02527 | -1.54917 | -0.15649 |
| S | -1.94942 | 2.20538 | 0.09773 |
| S | 1.95011 | 2.18508 | -0.04422 |
| O | -4.85257 | 2.59432 | 0.09013 |
| O | 4.82547 | 2.56832 | -0.19481 |
| C | -0.71500 | 0.99460 | -0.00018 |
| C | -1.25340 | -0.29523 | -0.04562 |
| C | -2.65973 | -0.31985 | 0.00508 |
| H | -3.25859 | -1.21784 | -0.02184 |
| C | -3.18824 | 0.95184 | 0.08606 |
| C | -4.57792 | 1.41000 | 0.13159 |
| C | -5.69516 | 0.38701 | 0.14443 |
| C | -5.76486 | -0.66778 | 1.05384 |
| C | -6.82882 | -1.56041 | 1.06393 |
| C | -7.85221 | -1.41479 | 0.13554 |

| | | | |
|---|---|---|---|
| C | -7.80672 | -0.37844 | -0.79007 |
| C | -6.73984 | 0.51094 | -0.77683 |
| C | 0.69947 | 0.98794 | -0.05759 |
| C | 1.22007 | -0.30706 | -0.14103 |
| C | 2.62594 | -0.34730 | -0.19120 |
| H | 3.20789 | -1.25308 | -0.26238 |
| C | 3.17421 | 0.91779 | -0.13657 |
| C | 4.56325 | 1.38030 | -0.19345 |
| C | 5.69734 | 0.37530 | -0.15323 |
| C | 6.71513 | 0.55101 | 0.78995 |
| C | 7.79267 | -0.32205 | 0.86952 |
| C | 7.87695 | -1.39601 | -0.00895 |
| C | 6.88106 | -1.59420 | -0.95712 |
| C | 5.80647 | -0.71637 | -1.01320 |
| F | -4.81250 | -0.82862 | 1.98588 |
| F | -6.87733 | -2.54792 | 1.96126 |
| F | -8.87446 | -2.26716 | 0.13187 |
| F | -8.78306 | -0.25131 | -1.69039 |
| F | -6.72218 | 1.47211 | -1.70025 |
| F | 6.66010 | 1.54816 | 1.67296 |
| F | 8.74186 | -0.14283 | 1.78968 |
| F | 8.90962 | -2.23306 | 0.05817 |
| F | 6.96623 | -2.61708 | -1.81103 |
| F | 4.88474 | -0.92942 | -1.96706 |

**FBBDTT**

| | | | |
|---|---|---|---|
| S | 3.23164 | -1.74950 | -0.49482 |
| S | 1.04166 | 1.66963 | 0.67206 |
| S | -0.66402 | -1.93854 | -0.71677 |
| O | 6.07078 | -2.09551 | -0.12805 |
| O | -3.56250 | -2.45277 | -0.88811 |
| C | 4.38326 | -0.49389 | -0.04147 |
| C | 3.76104 | 0.66155 | 0.38363 |
| H | 4.29117 | 1.52001 | 0.76703 |
| C | 2.35622 | 0.56000 | 0.30346 |
| C | 1.91105 | -0.67708 | -0.16636 |
| C | 0.49845 | -0.74544 | -0.24259 |
| C | -0.11459 | 0.43975 | 0.17627 |
| C | -1.51925 | 0.39920 | 0.11483 |
| H | -2.17107 | 1.21040 | 0.40377 |
| C | -1.97435 | -0.81355 | -0.36204 |
| C | 5.80402 | -0.90620 | -0.02995 |
| C | 6.89858 | 0.10439 | 0.13191 |
| C | 8.13704 | -0.36518 | 0.59253 |
| H | 8.22438 | -1.41148 | 0.85657 |
| C | 9.21922 | 0.49658 | 0.70913 |
| H | 10.16674 | 0.12559 | 1.08243 |
| C | 9.09082 | 1.83475 | 0.33492 |
| H | 9.93762 | 2.50624 | 0.41921 |
| C | 7.87846 | 2.30142 | -0.16642 |
| H | 7.78410 | 3.33156 | -0.48992 |
| C | 6.78775 | 1.44190 | -0.27105 |
| H | 5.86883 | 1.80560 | -0.71099 |
| C | -3.33641 | -1.31429 | -0.52411 |
| C | -4.49911 | -0.40337 | -0.17522 |
| C | -5.51605 | -0.88142 | 0.65560 |
| C | -6.66116 | -0.13694 | 0.90614 |
| C | -6.82433 | 1.10227 | 0.29679 |
| C | -5.84001 | 1.59237 | -0.55192 |
| C | -4.69741 | 0.83630 | -0.78077 |
| F | -5.39250 | -2.05976 | 1.26830 |
| F | -7.60485 | -0.59982 | 1.72860 |
| F | -7.92219 | 1.81935 | 0.52844 |
| F | -6.00234 | 2.77566 | -1.14972 |
| F | -3.78658 | 1.33059 | -1.63408 |

**FPENQ**

| | | | |
|---|---|---|---|
| O | 0.00011 | -2.70938 | 0.00044 |
| C | 0.00002 | -1.49125 | 0.00021 |
| C | 1.27376 | -0.71273 | 0.00003 |
| C | 2.46636 | -1.40424 | 0.00000 |
| H | 2.44445 | -2.48592 | -0.00001 |
| C | 3.69838 | -0.71664 | -0.00009 |
| C | 4.93820 | -1.39584 | -0.00013 |
| C | 6.12347 | -0.70646 | -0.00003 |
| C | 6.12355 | 0.70640 | 0.00004 |
| C | 4.93826 | 1.39590 | 0.00003 |
| C | 3.69839 | 0.71678 | -0.00007 |
| C | 2.46635 | 1.40435 | -0.00012 |
| H | 2.44439 | 2.48601 | -0.00010 |
| C | 1.27377 | 0.71284 | -0.00011 |
| F | 4.95976 | -2.73540 | -0.00037 |
| F | 7.29365 | -1.34454 | 0.00017 |
| F | 7.29368 | 1.34439 | 0.00015 |
| F | 4.95994 | 2.73542 | 0.00016 |
| O | -0.00011 | 2.70939 | -0.00049 |
| C | -0.00002 | 1.49126 | -0.00025 |
| C | -1.27376 | 0.71274 | -0.00005 |
| C | -2.46637 | 1.40425 | -0.00002 |
| H | -2.44446 | 2.48593 | -0.00002 |
| C | -3.69838 | 0.71664 | 0.00008 |
| C | -4.93820 | 1.39584 | 0.00013 |
| C | -6.12348 | 0.70645 | 0.00004 |
| C | -6.12355 | -0.70640 | -0.00001 |
| C | -4.93825 | -1.39590 | -0.00002 |
| C | -3.69839 | -0.71677 | 0.00006 |
| C | -2.46634 | -1.40434 | 0.00011 |
| H | -2.44438 | -2.48601 | 0.00009 |
| C | -1.27377 | -0.71283 | 0.00009 |
| F | -4.95977 | 2.73539 | 0.00036 |
| F | -7.29365 | 1.34454 | -0.00014 |
| F | -7.29368 | -1.34440 | -0.00011 |
| F | -4.95993 | -2.73542 | -0.00014 |

**FPEN**

| | | | |
|---|---|---|---|
| F | 7.30521 | 1.33864 | 0.00002 |
| F | 7.30521 | -1.33865 | -0.00002 |
| F | 5.01831 | -2.74121 | -0.00005 |
| F | 2.48493 | -2.73086 | 0.00003 |
| F | 0.00001 | 2.73074 | -0.00010 |
| F | 2.48496 | 2.73085 | -0.00007 |
| F | 5.01827 | 2.74123 | 0.00011 |
| C | 4.96069 | 1.40643 | 0.00002 |
| C | 6.12964 | 0.71104 | -0.00005 |
| C | 6.12966 | -0.71104 | -0.00000 |
| C | 4.96070 | -1.40641 | -0.00001 |
| C | 3.69801 | -0.72792 | -0.00004 |
| C | 2.48062 | -1.39364 | 0.00000 |
| C | 1.23295 | -0.72650 | 0.00001 |
| C | 0.00000 | 1.39498 | -0.00005 |
| C | 1.23294 | 0.72650 | 0.00000 |
| C | 2.48062 | 1.39365 | -0.00003 |
| C | 3.69800 | 0.72793 | 0.00001 |
| F | -7.30520 | -1.33864 | -0.00005 |
| F | -7.30522 | 1.33865 | 0.00002 |
| F | -5.01831 | 2.74120 | 0.00009 |
| F | -2.48493 | 2.73086 | -0.00002 |
| F | -0.00001 | -2.73074 | 0.00011 |
| F | -2.48496 | -2.73085 | 0.00007 |
| F | -5.01826 | -2.74123 | -0.00013 |
| C | -4.96069 | -1.40643 | -0.00003 |
| C | -6.12964 | -0.71105 | 0.00003 |
| C | -6.12966 | 0.71104 | -0.00000 |

| | | | |
|---|---|---|---|
| C | -4.96070 | 1.40641 | 0.00003 |
| C | -3.69801 | 0.72792 | 0.00005 |
| C | -2.48062 | 1.39364 | 0.00001 |
| C | -1.23295 | 0.72650 | -0.00001 |
| C | 0.00000 | -1.39498 | 0.00006 |
| C | -1.23294 | -0.72650 | 0.00000 |
| C | -2.48062 | -1.39365 | 0.00003 |
| C | -3.69800 | -0.72793 | -0.00001 |

**FPTT**

| | | | |
|---|---|---|---|
| S | -3.91071 | 0.72578 | -0.04227 |
| S | -0.00164 | -1.31988 | 0.06832 |
| S | 3.91020 | 0.72678 | -0.01400 |
| F | -7.31280 | -2.41680 | -0.13321 |
| F | -9.87683 | -1.76473 | -0.21749 |
| F | -10.66967 | 0.84558 | -0.13753 |
| F | -8.77864 | 2.81342 | 0.03661 |
| F | -6.19452 | 2.20886 | 0.13792 |
| F | 6.18464 | 2.20690 | 0.00605 |
| F | 8.76653 | 2.81930 | -0.03990 |
| F | 10.67032 | 0.85586 | -0.08474 |
| F | 9.88935 | -1.75949 | -0.08507 |
| F | 7.32970 | -2.42128 | -0.04407 |
| C | -7.61664 | -1.10970 | -0.07631 |
| C | -8.96571 | -0.79198 | -0.12625 |
| C | -9.37418 | 0.53455 | -0.08847 |
| C | -8.41153 | 1.52977 | -0.00011 |
| C | -7.06777 | 1.19062 | 0.05331 |
| C | -6.60305 | -0.13640 | 0.02309 |
| C | -5.18358 | -0.48670 | 0.07817 |
| C | -4.61696 | -1.73942 | 0.22048 |
| H | -5.19732 | -2.64114 | 0.32262 |
| C | -3.20847 | -1.73491 | 0.23180 |
| H | -2.61664 | -2.63334 | 0.34700 |
| C | -2.65553 | -0.47945 | 0.09641 |
| C | -1.26309 | -0.10109 | 0.07407 |
| C | -0.70513 | 1.15964 | 0.05799 |
| H | -1.29810 | 2.06479 | 0.06443 |
| C | 0.70549 | 1.15848 | 0.04526 |
| H | 1.29968 | 2.06283 | 0.03744 |
| C | 1.26184 | -0.10310 | 0.05225 |
| C | 2.65384 | -0.48343 | 0.04767 |
| C | 3.20551 | -1.74592 | 0.09133 |
| H | 2.61314 | -2.65018 | 0.13806 |
| C | 4.61373 | -1.75170 | 0.07403 |
| H | 5.19148 | -2.65994 | 0.10591 |
| C | 5.18295 | -0.49291 | 0.01739 |
| C | 6.60263 | -0.13991 | -0.01344 |
| C | 7.06286 | 1.18945 | -0.01557 |
| C | 8.40624 | 1.53322 | -0.03980 |
| C | 9.37515 | 0.54060 | -0.06224 |
| C | 8.97249 | -0.78814 | -0.06178 |
| C | 7.62382 | -1.11062 | -0.03854 |

**TFPT_DTBQ**

| | | | |
|---|---|---|---|
| S | 6.05096 | 0.37664 | 0.08618 |
| S | 2.35506 | -2.05578 | 0.12539 |
| F | 13.74505 | -0.41689 | 0.36705 |
| F | 13.22620 | 1.64143 | 0.84553 |
| F | 13.34661 | 1.00477 | -1.22447 |
| O | -0.72229 | -2.61566 | 0.22158 |
| N | 6.94605 | -2.03208 | -0.14837 |
| C | 12.95224 | 0.61508 | 0.01051 |
| C | 11.49424 | 0.24626 | 0.03566 |
| C | 10.53181 | 1.25062 | 0.14331 |
| C | 9.18387 | 0.92318 | 0.12247 |
| C | 8.77530 | -0.41195 | -0.00765 |

| | | | |
|---|---|---|---|
| C | 9.75261 | -1.41342 | -0.11441 |
| C | 11.10033 | -1.08592 | -0.09327 |
| C | 7.36155 | -0.79819 | -0.03508 |
| C | 5.59109 | -2.11562 | -0.15151 |
| C | 4.89736 | -0.93196 | -0.03531 |
| C | 3.47021 | -0.70764 | -0.01352 |
| C | 2.79280 | 0.49278 | -0.09266 |
| C | 1.39059 | 0.33422 | -0.04938 |
| C | 0.99619 | -0.98613 | 0.06095 |
| C | -0.39750 | -1.44470 | 0.12349 |
| H | 10.83806 | 2.28338 | 0.25237 |
| H | 8.44933 | 1.71534 | 0.21072 |
| H | 9.43408 | -2.44280 | -0.21128 |
| H | 11.84886 | -1.86399 | -0.16940 |
| H | 5.12442 | -3.08712 | -0.25272 |
| H | 3.27119 | 1.45764 | -0.18924 |
| S | -6.05077 | -0.37874 | -0.08229 |
| S | -2.35458 | 2.05315 | -0.12145 |
| F | -13.73900 | 0.40637 | -0.43156 |
| F | -13.22097 | -1.67372 | -0.80710 |
| F | -13.36258 | -0.93992 | 1.22912 |
| O | 0.72271 | 2.61306 | -0.21659 |
| N | -6.94536 | 2.03047 | 0.14921 |
| C | -12.95329 | -0.60991 | -0.01833 |
| C | -11.49423 | -0.24551 | -0.04392 |
| C | -10.53223 | -1.25228 | -0.12825 |
| C | -9.18399 | -0.92562 | -0.10353 |
| C | -8.77499 | 0.41084 | 0.00904 |
| C | -9.75207 | 1.41493 | 0.09257 |
| C | -11.09975 | 1.08831 | 0.06725 |
| C | -7.36111 | 0.79654 | 0.03724 |
| C | -5.59039 | 2.11362 | 0.15350 |
| C | -4.89690 | 0.92962 | 0.03938 |
| C | -3.46977 | 0.70513 | 0.01836 |
| C | -2.79239 | -0.49529 | 0.09805 |
| C | -1.39017 | -0.33680 | 0.05451 |
| C | -0.99576 | 0.98350 | -0.05635 |
| C | 0.39792 | 1.44209 | -0.11854 |
| H | -10.83878 | -2.28636 | -0.22254 |
| H | -8.44970 | -1.71984 | -0.17323 |
| H | -9.43312 | 2.44544 | 0.17522 |
| H | -11.84805 | 1.86821 | 0.12540 |
| H | -5.12353 | 3.08509 | 0.25405 |
| H | -3.27083 | -1.46009 | 0.19500 |

**CBTZ**

| | | | |
|---|---|---|---|
| S | -1.94745 | -1.35404 | 0.12299 |
| C | -0.69583 | -0.19271 | -0.00022 |
| C | -1.23247 | 1.06794 | -0.18558 |
| N | -2.57536 | 1.15738 | -0.23653 |
| C | -3.13183 | -0.01913 | -0.09929 |
| C | -4.57252 | -0.25941 | -0.09819 |
| C | -5.44393 | 0.84236 | -0.11930 |
| H | -5.02406 | 1.83929 | -0.13827 |
| C | -6.81658 | 0.65399 | -0.11709 |
| H | -7.46381 | 1.52012 | -0.13479 |
| C | -7.35569 | -0.64163 | -0.09637 |
| C | -6.48532 | -1.74201 | -0.09789 |
| H | -6.90897 | -2.73832 | -0.10685 |
| C | -5.11540 | -1.55553 | -0.09234 |
| H | -4.46518 | -2.42310 | -0.09267 |
| C | -8.81128 | -0.93141 | -0.13624 |
| O | -9.27162 | -2.02295 | -0.36716 |
| C | -9.80253 | 0.22357 | 0.19462 |
| F | -9.48414 | 0.80560 | 1.36985 |
| F | -9.75981 | 1.18245 | -0.76000 |
| F | -11.05152 | -0.22360 | 0.27432 |

| | | | |
|---|---|---|---|
| C | -0.11396 | 2.08464 | -0.29145 |
| O | -0.19005 | 3.27214 | -0.45197 |
| C | 1.12463 | 1.22495 | -0.14195 |
| C | 0.75349 | -0.09604 | 0.02733 |
| S | 2.14299 | -1.08120 | 0.20070 |
| C | 3.14688 | 0.39890 | 0.01368 |
| N | 2.44494 | 1.49179 | -0.14479 |
| C | 4.60565 | 0.35450 | 0.07503 |
| C | 5.31853 | 1.56537 | 0.15372 |
| H | 4.76671 | 2.49580 | 0.17633 |
| C | 6.69941 | 1.55703 | 0.20746 |
| H | 7.25380 | 2.48363 | 0.28892 |
| C | 7.41302 | 0.34869 | 0.15871 |
| C | 6.70494 | -0.85872 | 0.08223 |
| H | 7.22763 | -1.80476 | 0.05460 |
| C | 5.31905 | -0.85250 | 0.03885 |
| H | 4.79349 | -1.79807 | -0.03075 |
| C | 8.89108 | 0.42444 | 0.27614 |
| O | 9.48254 | 1.39185 | 0.68798 |
| C | 9.72800 | -0.82181 | -0.13999 |
| F | 9.36296 | -1.27029 | -1.35948 |
| F | 9.53634 | -1.83477 | 0.73883 |
| F | 11.02660 | -0.54117 | -0.16889 |

**FPQT**

| | | | |
|---|---|---|---|
| S | 2.17424 | -0.37056 | -0.16745 |
| S | 5.48333 | -0.11749 | 0.08727 |
| F | 9.34759 | 2.40175 | 0.11791 |
| F | 11.77222 | 1.33814 | 0.22354 |
| F | 12.12575 | -1.36789 | 0.13733 |
| F | 9.94124 | -2.99738 | -0.06456 |
| F | 7.48915 | -1.97533 | -0.18966 |
| C | 0.60421 | 0.39267 | 0.00358 |
| C | 0.75399 | 1.75844 | 0.13073 |
| H | -0.08463 | 2.43162 | 0.25000 |
| C | 2.09603 | 2.19087 | 0.10494 |
| H | 2.39073 | 3.22499 | 0.21909 |
| C | 3.00736 | 1.16769 | -0.05184 |
| C | 4.44702 | 1.27003 | -0.11835 |
| C | 5.19997 | 2.40294 | -0.34836 |
| H | 4.76316 | 3.37395 | -0.53597 |
| C | 6.58837 | 2.16872 | -0.34783 |
| H | 7.31237 | 2.94848 | -0.51922 |
| C | 6.93842 | 0.84928 | -0.12916 |
| C | 8.27924 | 0.26888 | -0.06157 |
| C | 9.43651 | 1.06307 | 0.05402 |
| C | 10.71474 | 0.52842 | 0.11607 |
| C | 10.89967 | -0.84720 | 0.07649 |
| C | 9.78776 | -1.67107 | -0.02561 |
| C | 8.51823 | -1.11633 | -0.09228 |
| S | -2.17426 | 0.37042 | 0.16694 |
| S | -5.48334 | 0.11750 | -0.08715 |
| F | -9.34751 | -2.40155 | -0.11996 |
| F | -11.77216 | -1.33787 | -0.22500 |
| F | -12.12570 | 1.36809 | -0.13637 |
| F | -9.94125 | 2.99740 | 0.06736 |
| F | -7.48915 | 1.97524 | 0.19193 |
| C | -0.60423 | -0.39282 | -0.00409 |
| C | -0.75402 | -1.75859 | -0.13126 |
| H | 0.08457 | -2.43175 | -0.25054 |
| C | -2.09607 | -2.19100 | -0.10548 |
| H | -2.39078 | -3.22515 | -0.21963 |
| C | -3.00739 | -1.16782 | 0.05132 |
| C | -4.44705 | -1.27015 | 0.11784 |
| C | -5.20004 | -2.40312 | 0.34744 |
| H | -4.76324 | -3.37428 | 0.53464 |
| C | -6.58843 | -2.16884 | 0.34709 |

| | | | |
|---|---|---|---|
| H | -7.31247 | -2.94864 | 0.51820 |
| C | -6.93843 | -0.84931 | 0.12898 |
| C | -8.27924 | -0.26884 | 0.06166 |
| C | -9.43647 | -1.06294 | -0.05485 |
| C | -10.71469 | -0.52824 | -0.11661 |
| C | -10.89963 | 0.84734 | -0.07581 |
| C | -9.78774 | 1.67113 | 0.02721 |
| C | -8.51823 | 1.11634 | 0.09359 |

**DFPTT**

| | | | |
|---|---|---|---|
| S | -1.07218 | -1.78229 | -0.23460 |
| S | -4.86520 | 0.48791 | 0.01893 |
| F | -7.07975 | 2.08036 | -0.26388 |
| F | -9.63258 | 2.80868 | -0.12801 |
| F | -11.60682 | 0.93748 | 0.14918 |
| F | -10.93365 | -1.70311 | 0.30078 |
| F | -8.40207 | -2.47553 | 0.18752 |
| C | 0.24086 | -0.64670 | -0.08893 |
| C | -1.65000 | 0.75107 | 0.07024 |
| H | -2.19951 | 1.67598 | 0.17843 |
| C | -2.26060 | -0.47583 | -0.08285 |
| C | -3.67109 | -0.77759 | -0.12757 |
| C | -4.28631 | -2.00029 | -0.29342 |
| H | -3.74029 | -2.92634 | -0.41473 |
| C | -5.69344 | -1.93291 | -0.29436 |
| H | -6.31926 | -2.80184 | -0.41463 |
| C | -6.19606 | -0.65575 | -0.13579 |
| C | -7.59571 | -0.23706 | -0.06122 |
| C | -7.99810 | 1.10854 | -0.12681 |
| C | -9.32333 | 1.51134 | -0.05607 |
| C | -10.32834 | 0.56488 | 0.08418 |
| C | -9.98100 | -0.77758 | 0.15759 |
| C | -8.64927 | -1.15907 | 0.09114 |
| S | 1.07137 | 1.78404 | 0.21193 |
| S | 4.86417 | -0.48648 | -0.04120 |
| F | 7.07441 | -2.08090 | 0.24218 |
| F | 9.62834 | -2.81073 | 0.15010 |
| F | 11.60876 | -0.94067 | -0.08814 |
| F | 10.94043 | 1.70096 | -0.24454 |
| F | 8.40809 | 2.47524 | -0.17430 |
| C | -0.24169 | 0.64848 | 0.06613 |
| C | 1.64915 | -0.74930 | -0.09315 |
| H | 2.19865 | -1.67420 | -0.20149 |
| C | 2.25977 | 0.47758 | 0.06001 |
| C | 3.67028 | 0.77914 | 0.10547 |
| C | 4.28570 | 2.00166 | 0.27192 |
| H | 3.73985 | 2.92773 | 0.39383 |
| C | 5.69280 | 1.93409 | 0.27297 |
| H | 6.31854 | 2.80280 | 0.39483 |
| C | 6.19531 | 0.65732 | 0.11032 |
| C | 7.59508 | 0.23659 | 0.05046 |
| C | 7.99550 | -1.10928 | 0.12316 |
| C | 9.32148 | -1.51300 | 0.07505 |
| C | 10.32964 | -0.56713 | -0.04485 |
| C | 9.98464 | 0.77576 | -0.12161 |
| C | 8.65226 | 1.15818 | -0.07791 |

**HPT**

| | | | |
|---|---|---|---|
| S | 1.89075 | 1.08208 | 0.40399 |
| O | 8.37300 | -1.31293 | -1.73775 |
| O | 9.34900 | 2.76858 | 0.12710 |
| N | 9.20525 | 0.67180 | -0.86310 |
| C | 15.89104 | -1.90974 | 1.75205 |
| H | 16.70953 | -2.50330 | 1.33949 |
| H | 15.21860 | -2.58356 | 2.29137 |
| H | 16.31950 | -1.24148 | 2.50427 |
| C | 15.13657 | -1.11793 | 0.66409 |

| | | | |
|---|---|---|---|
| H | 15.36820 | -1.52533 | -0.32647 |
| H | 15.51349 | -0.08883 | 0.63782 |
| C | 13.61838 | -1.08156 | 0.86912 |
| H | 13.23368 | -2.10909 | 0.88187 |
| H | 13.39828 | -0.66109 | 1.85892 |
| C | 12.87474 | -0.27547 | -0.20025 |
| H | 13.06529 | -0.71556 | -1.18784 |
| H | 13.28482 | 0.74154 | -0.23952 |
| C | 11.36209 | -0.19863 | 0.04017 |
| H | 10.96443 | -1.20742 | 0.19484 |
| H | 11.16310 | 0.37185 | 0.95320 |
| C | 10.62452 | 0.45901 | -1.13151 |
| H | 11.05924 | 1.43464 | -1.35866 |
| H | 10.68017 | -0.17469 | -2.01895 |
| C | 8.69115 | 1.82566 | -0.24550 |
| C | 8.20175 | -0.24749 | -1.19316 |
| C | 7.21807 | 1.61635 | -0.17261 |
| C | 6.92145 | 0.37807 | -0.73829 |
| C | 6.21049 | 2.41883 | 0.33494 |
| H | 6.43270 | 3.38431 | 0.77336 |
| C | 5.63284 | -0.10325 | -0.81609 |
| H | 5.44745 | -1.07702 | -1.25080 |
| C | 4.90114 | 1.94719 | 0.25903 |
| H | 4.10281 | 2.57157 | 0.64306 |
| C | 4.58328 | 0.69426 | -0.30706 |
| C | 3.20175 | 0.22065 | -0.38096 |
| C | 2.70772 | -0.88829 | -1.03246 |
| H | 3.32961 | -1.56778 | -1.59874 |
| C | 1.31167 | -1.05349 | -0.91076 |
| H | 0.76804 | -1.87147 | -1.36509 |
| C | 0.69983 | -0.07043 | -0.16231 |
| S | -1.88715 | -1.06924 | -0.39760 |
| O | -8.37033 | 1.33254 | 1.73225 |
| O | -9.34499 | -2.75680 | -0.11706 |
| N | -9.20184 | -0.65759 | 0.86857 |
| C | -15.90259 | 1.88212 | -1.73996 |
| H | -16.72690 | 2.44811 | -1.30072 |
| H | -15.22690 | 2.58900 | -2.23039 |
| H | -16.32302 | 1.26004 | -2.53500 |
| C | -15.15695 | 1.02651 | -0.69380 |
| H | -15.38683 | 1.37551 | 0.31814 |
| H | -15.50150 | -0.01095 | -0.76102 |
| C | -13.63403 | 1.02933 | -0.88995 |
| H | -13.26892 | 2.06372 | -0.88205 |
| H | -13.39936 | 0.62370 | -1.88250 |
| C | -12.88136 | 0.21617 | 0.16990 |
| H | -13.11394 | 0.61728 | 1.16476 |
| H | -13.24944 | -0.81705 | 0.15369 |
| C | -11.36215 | 0.21151 | -0.04231 |
| H | -11.01024 | 1.24137 | -0.16502 |
| H | -11.12247 | -0.32707 | -0.96474 |
| C | -10.61995 | -0.44157 | 1.12955 |
| H | -11.06511 | -1.40952 | 1.37007 |
| H | -10.68501 | 0.19204 | 2.01675 |
| C | -8.68744 | -1.81313 | 0.25383 |
| C | -8.19869 | 0.26425 | 1.19362 |
| C | -7.21442 | -1.60362 | 0.18081 |
| C | -6.91823 | -0.36317 | 0.74191 |
| C | -6.20659 | -2.40747 | -0.32410 |
| H | -6.42851 | -3.37455 | -0.75915 |
| C | -5.62972 | 0.11872 | 0.81823 |
| H | -5.44464 | 1.09416 | 1.24930 |
| C | -4.89741 | -1.93510 | -0.25002 |
| H | -4.09888 | -2.56056 | -0.63185 |
| C | -4.57995 | -0.68017 | 0.31186 |
| C | -3.19848 | -0.20630 | 0.38511 |
| C | -2.70452 | 0.90301 | 1.03605 |

| | | | |
|---|---|---|---|
| H | -3.32661 | 1.58320 | 1.60126 |
| C | -1.30827 | 1.06737 | 0.91554 |
| H | -0.76470 | 1.88570 | 1.36933 |
| C | -0.69620 | 0.08325 | 0.16868 |

**FBOQT**

| | | | |
|---|---|---|---|
| S | -5.66150 | -1.62200 | -0.87688 |
| S | -2.08206 | 0.66899 | 0.31702 |
| F | -8.95227 | 1.41315 | -1.61256 |
| F | -11.20405 | 2.76078 | -0.98916 |
| F | -13.05010 | 1.64335 | 0.67095 |
| F | -12.63026 | -0.83274 | 1.71426 |
| F | -10.38234 | -2.19556 | 1.10429 |
| O | -8.54493 | -2.33790 | -1.20264 |
| C | -9.59794 | -0.43368 | -0.27112 |
| C | -9.83609 | 0.83945 | -0.78211 |
| C | -10.99314 | 1.54533 | -0.47648 |
| C | -11.93872 | 0.97448 | 0.36657 |
| C | -11.72454 | -0.29407 | 0.89451 |
| C | -10.56558 | -0.98619 | 0.56797 |
| C | -8.38452 | -1.25840 | -0.66479 |
| C | -7.06624 | -0.72062 | -0.35821 |
| C | -6.69986 | 0.42330 | 0.32089 |
| H | -7.41617 | 1.11813 | 0.73702 |
| C | -5.30809 | 0.58309 | 0.43200 |
| H | -4.83930 | 1.41487 | 0.94075 |
| C | -4.58999 | -0.44075 | -0.16675 |
| C | -3.15861 | -0.59808 | -0.24151 |
| C | -2.42853 | -1.66763 | -0.71712 |
| H | -2.88929 | -2.56562 | -1.10720 |
| C | -1.03401 | -1.48523 | -0.63663 |
| H | -0.31805 | -2.22762 | -0.96367 |
| C | -0.66163 | -0.27073 | -0.09553 |
| S | 5.66180 | 1.60588 | 0.90926 |
| S | 2.08268 | -0.68915 | -0.27791 |
| F | 8.99418 | -1.41721 | 1.61068 |
| F | 11.24524 | -2.74416 | 0.93869 |
| F | 13.04850 | -1.60517 | -0.75390 |
| F | 12.58718 | 0.87079 | -1.77938 |
| F | 10.34080 | 2.21264 | -1.12004 |
| O | 8.54472 | 2.33270 | 1.21644 |
| C | 9.59837 | 0.43905 | 0.26386 |
| C | 9.85746 | -0.83359 | 0.76556 |
| C | 11.01403 | -1.52876 | 0.43472 |
| C | 11.93780 | -0.94690 | -0.42487 |
| C | 11.70245 | 0.32161 | -0.94383 |
| C | 10.54453 | 1.00302 | -0.59188 |
| C | 8.38493 | 1.25110 | 0.68272 |
| C | 7.06670 | 0.70920 | 0.38291 |
| C | 6.70046 | -0.43466 | -0.29641 |
| H | 7.41681 | -1.12702 | -0.71656 |
| C | 5.30863 | -0.59752 | -0.40254 |
| H | 4.83987 | -1.42916 | -0.91155 |
| C | 4.59040 | 0.42367 | 0.20056 |
| C | 3.15898 | 0.57878 | 0.27914 |
| C | 2.42871 | 1.64740 | 0.75654 |
| H | 2.88929 | 2.54576 | 1.14597 |
| C | 1.03424 | 1.46380 | 0.67817 |
| H | 0.31815 | 2.20551 | 1.00646 |
| C | 0.66207 | 0.24926 | 0.13706 |

**TFPA**

| | | | |
|---|---|---|---|
| F | -9.90164 | -0.74996 | -1.11539 |
| F | -10.12346 | 0.81799 | 0.37633 |
| F | -9.73111 | -1.22865 | 0.99105 |
| C | 0.49792 | 1.28664 | -0.23477 |
| C | -0.88334 | 1.08246 | -0.20614 |

| | | | |
|---|---|---|---|
| C | -1.82183 | 2.14083 | -0.40064 |
| C | -3.16561 | 1.91041 | -0.36499 |
| C | -3.69347 | 0.59537 | -0.14044 |
| C | -2.80794 | -0.43974 | 0.05471 |
| C | -1.39719 | -0.24367 | 0.02773 |
| C | -5.15939 | 0.37578 | -0.08671 |
| C | -6.02544 | 1.37314 | 0.38392 |
| C | -7.40031 | 1.17035 | 0.43403 |
| C | -7.94207 | -0.03719 | 0.00251 |
| C | -7.09850 | -1.03913 | -0.48184 |
| C | -5.72843 | -0.83101 | -0.52879 |
| C | -9.42135 | -0.29129 | 0.06418 |
| H | 0.88189 | 2.28631 | -0.41319 |
| H | -1.44580 | 3.14119 | -0.58744 |
| H | -3.85126 | 2.72970 | -0.54400 |
| H | -3.17618 | -1.43750 | 0.26664 |
| H | -5.62139 | 2.31038 | 0.74644 |
| H | -8.05070 | 1.94930 | 0.81016 |
| H | -7.51723 | -1.97254 | -0.83882 |
| H | -5.09155 | -1.60369 | -0.94166 |
| F | 9.91339 | 0.62804 | 1.16345 |
| F | 10.11696 | -0.76378 | -0.49539 |
| F | 9.71885 | 1.33903 | -0.87417 |
| C | -0.49589 | -1.29615 | 0.22736 |
| C | 0.88543 | -1.09208 | 0.19845 |
| C | 1.82360 | -2.15026 | 0.39560 |
| C | 3.16738 | -1.92021 | 0.35730 |
| C | 3.69496 | -0.60712 | 0.12098 |
| C | 2.81009 | 0.43036 | -0.06274 |
| C | 1.39929 | 0.23394 | -0.03641 |
| C | 5.16146 | -0.38691 | 0.09442 |
| C | 6.02948 | -1.36810 | -0.40530 |
| C | 7.40337 | -1.15824 | -0.45595 |
| C | 7.94047 | 0.04402 | -0.00471 |
| C | 7.09345 | 1.03455 | 0.49723 |
| C | 5.72451 | 0.81939 | 0.54491 |
| C | 9.41929 | 0.30379 | -0.05470 |
| H | -0.87987 | -2.29575 | 0.40615 |
| H | 1.44736 | -3.14933 | 0.58871 |
| H | 3.85409 | -2.73823 | 0.53871 |
| H | 3.17861 | 1.42912 | -0.26946 |
| H | 5.62722 | -2.29880 | -0.78651 |
| H | 8.05585 | -1.92527 | -0.85223 |
| H | 7.50800 | 1.96705 | 0.86168 |
| H | 5.08432 | 1.58436 | 0.96694 |

**PCBM**

| | | | |
|---|---|---|---|
| O | -7.29652 | -3.60600 | 0.13800 |
| O | -8.08805 | -1.49870 | 0.21345 |
| C | -2.13960 | 0.17072 | 0.25853 |
| C | -1.82898 | 0.84041 | -1.18090 |
| C | -0.96012 | 2.05407 | -1.14524 |
| C | -0.56460 | 2.67305 | 0.02600 |
| C | -0.84426 | 2.06022 | 1.33684 |
| C | -1.50932 | 0.85188 | 1.42736 |
| C | -1.02664 | -0.15431 | 2.33832 |
| C | -1.16235 | -1.45029 | 1.70497 |
| C | -1.73441 | -1.26093 | 0.39449 |
| C | -1.26858 | -2.02454 | -0.66151 |
| C | -0.98579 | -1.41189 | -1.97351 |
| C | -1.17986 | -0.05796 | -2.18058 |
| C | -0.17641 | 0.69658 | -2.88939 |
| C | -0.04282 | 1.99213 | -2.25523 |
| C | 1.20454 | 2.61310 | -2.19676 |
| C | 1.60474 | 3.28604 | -0.98664 |
| C | 0.73801 | 3.29952 | 0.10704 |
| C | 1.26453 | 3.09102 | 1.44194 |

| | | | |
|---|---|---|---|
| C | 0.29090 | 2.32447 | 2.19465 |
| C | 0.72536 | 1.36969 | 3.11547 |
| C | 0.05036 | 0.09824 | 3.18744 |
| C | 1.04259 | -0.93364 | 3.42821 |
| C | 0.91367 | -2.17752 | 2.81948 |
| C | -0.21311 | -2.44319 | 1.94312 |
| C | 0.24611 | -3.26152 | 0.84867 |
| C | -0.26505 | -3.04305 | -0.43129 |
| C | 0.62663 | -3.07408 | -1.57449 |
| C | 0.18372 | -2.06774 | -2.51960 |
| C | 1.12634 | -1.34552 | -3.25228 |
| C | 0.94177 | 0.07190 | -3.44048 |
| C | 2.24160 | 0.71477 | -3.37195 |
| C | 2.36999 | 1.95872 | -2.76322 |
| C | 3.49713 | 2.22898 | -1.89107 |
| C | 3.02297 | 3.05043 | -0.79111 |
| C | 3.52443 | 2.84851 | 0.49197 |
| C | 2.62642 | 2.87509 | 1.63311 |
| C | 3.07588 | 1.87188 | 2.58236 |
| C | 2.14390 | 1.13493 | 3.30778 |
| C | 2.34073 | -0.29079 | 3.50253 |
| C | 3.45875 | -0.92024 | 2.96051 |
| C | 3.32451 | -2.21963 | 2.32537 |
| C | 2.07703 | -2.83548 | 2.25641 |
| C | 1.66363 | -3.50646 | 1.03650 |
| C | 2.51660 | -3.53370 | -0.06333 |
| C | 1.98577 | -3.31890 | -1.39752 |
| C | 2.96507 | -2.55826 | -2.15315 |
| C | 2.54317 | -1.59207 | -3.06257 |
| C | 3.23399 | -0.31661 | -3.13651 |
| C | 4.31537 | -0.05991 | -2.29725 |
| C | 4.45003 | 1.23937 | -1.66175 |
| C | 4.97196 | 1.03173 | -0.32442 |
| C | 4.51949 | 1.82182 | 0.73007 |
| C | 4.24189 | 1.21786 | 2.02252 |
| C | 4.42913 | -0.15045 | 2.20579 |
| C | 4.89659 | -0.97313 | 1.10516 |
| C | 5.16200 | -0.39465 | -0.13291 |
| C | 4.75445 | -1.06870 | -1.35219 |
| C | 4.09367 | -2.29325 | -1.28351 |
| C | 3.81639 | -2.89693 | 0.00906 |
| C | 4.21161 | -2.25089 | 1.17819 |
| C | -3.23743 | 0.72214 | -0.62800 |
| C | -3.93017 | 2.00005 | -0.21293 |
| C | -4.13911 | 3.01099 | -1.15711 |
| C | -4.84733 | 4.16126 | -0.82190 |
| C | -5.35814 | 4.31724 | 0.46524 |
| C | -5.15660 | 3.31648 | 1.41196 |
| C | -4.44738 | 2.16537 | 1.07464 |
| C | -4.17772 | -0.28168 | -1.30678 |
| C | -5.25551 | -0.84699 | -0.37470 |
| C | -6.15447 | -1.86473 | -1.09886 |
| C | -7.21797 | -2.45078 | -0.19539 |
| C | -9.13243 | -1.94621 | 1.09661 |
| H | -3.73937 | 2.89907 | -2.15924 |
| H | -4.99641 | 4.93697 | -1.56446 |
| H | -5.90667 | 5.21437 | 0.72868 |
| H | -5.54866 | 3.43036 | 2.41626 |
| H | -4.29206 | 1.39434 | 1.82013 |
| H | -3.60247 | -1.10673 | -1.73094 |
| H | -4.65189 | 0.23148 | -2.15077 |
| H | -4.77627 | -1.33644 | 0.48036 |
| H | -5.87622 | -0.04136 | 0.02164 |
| H | -6.65240 | -1.37538 | -1.94257 |
| H | -5.56724 | -2.70013 | -1.48346 |
| H | -8.70768 | -2.36980 | 2.00797 |
| H | -9.72176 | -1.06053 | 1.32334 |

H -9.74789 -2.70290 0.60776

**RUBR**

| | | | |
|---|---|---|---|
| C | -1.406000 | 1.233000 | -0.250000 |
| C | -0.698000 | 2.444000 | -0.194000 |
| C | -1.317000 | 3.709000 | -0.476000 |
| H | -2.330000 | 3.720000 | -0.852000 |
| C | -0.663000 | 4.886000 | -0.259000 |
| H | -1.157000 | 5.828000 | -0.471000 |
| C | 0.663000 | 4.886000 | 0.260000 |
| H | 1.157000 | 5.828000 | 0.471000 |
| C | 1.317000 | 3.709000 | 0.476000 |
| H | 2.330000 | 3.720000 | 0.852000 |
| C | 0.698000 | 2.444000 | 0.194000 |
| C | 1.406000 | 1.233000 | 0.250000 |
| C | 0.727000 | 0.000000 | -0.000000 |
| C | 1.406000 | -1.233000 | -0.250000 |
| C | 0.698000 | -2.444000 | -0.194000 |
| C | 1.317000 | -3.709000 | -0.476000 |
| H | 2.330000 | -3.720000 | -0.852000 |
| C | 0.663000 | -4.886000 | -0.260000 |
| H | 1.157000 | -5.828000 | -0.471000 |
| C | -0.663000 | -4.886000 | 0.259000 |
| H | -1.157000 | -5.828000 | 0.471000 |
| C | -1.317000 | -3.709000 | 0.476000 |
| H | -2.330000 | -3.720000 | 0.852000 |
| C | -0.698000 | -2.444000 | 0.194000 |
| C | -1.406000 | -1.233000 | 0.250000 |
| C | -0.727000 | 0.000000 | 0.000000 |
| C | 2.821000 | -1.260000 | -0.737000 |
| C | 3.870000 | -1.811000 | 0.009000 |
| C | 3.094000 | -0.801000 | -2.032000 |
| C | 5.155000 | -1.888000 | -0.519000 |
| H | 3.677000 | -2.168000 | 1.014000 |
| C | 4.377000 | -0.885000 | -2.565000 |
| H | 2.287000 | -0.386000 | -2.626000 |
| C | 5.414000 | -1.427000 | -1.809000 |
| H | 5.957000 | -2.307000 | 0.079000 |
| H | 4.565000 | -0.531000 | -3.573000 |
| H | 6.415000 | -1.492000 | -2.221000 |
| C | -2.821000 | -1.260000 | 0.737000 |
| C | -3.094000 | -0.802000 | 2.032000 |
| C | -3.870000 | -1.811000 | -0.009000 |
| C | -4.377000 | -0.885000 | 2.565000 |
| H | -2.287000 | -0.386000 | 2.626000 |
| C | -5.155000 | -1.888000 | 0.519000 |
| H | -3.677000 | -2.168000 | -1.014000 |
| C | -5.414000 | -1.427000 | 1.809000 |
| H | -4.565000 | -0.531000 | 3.573000 |
| H | -5.957000 | -2.307000 | -0.079000 |
| H | -6.415000 | -1.492000 | 2.221000 |
| C | -2.821000 | 1.260000 | -0.737000 |
| C | -3.870000 | 1.811000 | 0.009000 |
| C | -3.094000 | 0.802000 | -2.032000 |
| C | -5.155000 | 1.888000 | -0.519000 |

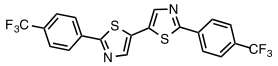
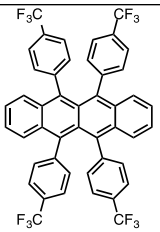
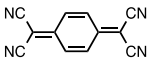
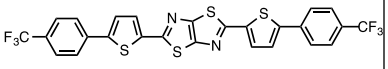
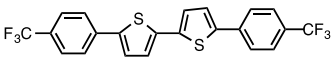
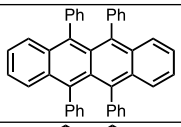
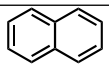
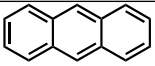
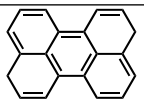
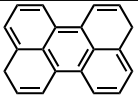
| | | | |
|---|---|---|---|
| H | -3.677000 | 2.168000 | 1.014000 |
| C | -4.377000 | 0.885000 | -2.565000 |
| H | -2.287000 | 0.386000 | -2.626000 |
| C | -5.414000 | 1.427000 | -1.809000 |
| H | -5.957000 | 2.307000 | 0.079000 |
| H | -4.566000 | 0.531000 | -3.573000 |
| H | -6.415000 | 1.492000 | -2.221000 |
| C | 2.821000 | 1.260000 | 0.737000 |
| C | 3.094000 | 0.801000 | 2.032000 |
| C | 3.870000 | 1.811000 | -0.009000 |
| C | 4.377000 | 0.885000 | 2.565000 |
| H | 2.287000 | 0.386000 | 2.626000 |
| C | 5.155000 | 1.888000 | 0.519000 |
| H | 3.677000 | 2.168000 | -1.014000 |
| C | 5.414000 | 1.427000 | 1.809000 |
| H | 4.566000 | 0.531000 | 3.573000 |
| H | 5.957000 | 2.307000 | -0.079000 |
| H | 6.415000 | 1.492000 | 2.221000 |

**TFPT**

| | | | |
|---|---|---|---|
| S | -2.01431300 | 0.91213400 | -0.00681600 |
| F | -9.52911300 | -0.76119400 | -0.58405100 |
| F | -9.29008100 | -0.06747800 | 1.45683900 |
| N | -2.56442200 | -1.59022500 | -0.31088800 |
| C | -3.14891800 | -0.43460300 | -0.14688500 |
| C | -1.21029100 | -1.47901100 | -0.34549300 |
| C | -0.68948600 | -0.21283200 | -0.20539700 |
| C | -4.60187800 | -0.25426200 | -0.07573700 |
| C | -5.19318000 | 1.00933500 | 0.05502200 |
| C | -6.57368900 | 1.14154700 | 0.12330800 |
| C | -7.38481000 | 0.01001700 | 0.05752500 |
| C | -6.80776800 | -1.25476700 | -0.07706100 |
| C | -5.42979500 | -1.38680000 | -0.14387200 |
| C | -8.87760400 | 0.13902800 | 0.18395400 |
| H | -0.61164100 | -2.36884500 | -0.49043000 |
| H | -4.57747700 | 1.90036600 | 0.10043000 |
| H | -7.02163700 | 2.12204700 | 0.21843300 |
| H | -7.43970500 | -2.13202000 | -0.13740600 |
| H | -4.97042300 | -2.36044500 | -0.25075700 |
| F | -9.31521000 | 1.36533400 | -0.17361900 |
| S | 2.01431300 | -0.91206100 | -0.00678100 |
| F | 9.52915800 | 0.76168800 | -0.58334100 |
| F | 9.31517300 | -1.36515000 | -0.17459400 |
| N | 2.56443600 | 1.59028800 | -0.31090500 |
| C | 3.14892500 | 0.43466800 | -0.14687300 |
| C | 1.21030400 | 1.47908000 | -0.34551700 |
| C | 0.68949200 | 0.21290600 | -0.20539700 |
| C | 4.60188400 | 0.25431800 | -0.07571400 |
| C | 5.19317200 | -1.00929400 | 0.05500600 |
| C | 6.57367500 | -1.14152000 | 0.12329800 |
| C | 7.38481000 | -0.00999200 | 0.05756300 |
| C | 6.80778600 | 1.25480000 | -0.07697700 |
| C | 5.42981000 | 1.38684700 | -0.14379600 |
| C | 8.87759800 | -0.13910900 | 0.18393500 |

| | | | |
|---|---|---|---|
| H | 0.61165900 | 2.36891300 | -0.49048000 |
| H | 4.57745900 | -1.90032000 | 0.10037500 |
| H | 7.02161600 | -2.12202900 | 0.21839100 |
| H | 7.43973100 | 2.13204900 | -0.13727100 |
| H | 4.97044900 | 2.36050100 | -0.25064700 |
| F | 9.29003500 | 0.06636000 | 1.45700200 |

**Table S2(a).** Single crystal electron mobility test set (SCEM20).

| | MOLECULAR STRUCTURE | ACRONYM | NAME | Reference of the crystal structure | Experimental $\mu_e$ ($cm^2/Vs$) | Reference of exp. $\mu_e$ | Theoretical $\mu_e$ ($cm^2/Vs$) |
|---|---|---|---|---|---|---|---|
| **1** |  | **TFPT** | 2,2'-bis[4-(trifluoromethyl) phenyl]-5,5'-bithiazole | [1] | 1.83 | [1] | 1.23 |
| **2** |  | **FRUB** | Tetra(trifluoromethyl)rubrene | [2] | 4.2 | [2] | 5.23 |
| **3** |  | **TCNQ** | 7,7',8,8'-tetracyanoquinodimethane | [3] | 1.6 | [4] | 0.75 |
| **4** |  | **TFTT** | 2,5-bis[5-[4-(trifluoromethyl) phenyl]-2-thienyl]-thiazolo[5,4-d] thiazole | [5] | 0.3-1.2 | [5] | 0.22 |
| **5** |  | **TFDT** | 5,5'-bis(4-(trifluoromethyl)phenyl)-2,2'-dithiophene | [5] | 0.18 | [5] | 0.14 |
| **6** |  | **RUB** | Rubrene | [6] | 0.81 | [7] | 1.03 |
| **7** |  | **NAPH** | Naphthalene | [8] | ~0.6 | [9] | 0.26 |
| **8** |  | **ANTH** | Anthracene | [10] | 1.7 | [11] | 0.9 |
| **9** |  | **PERY-α** | Perylene (α-phase) | [12] | 5.5 | [13] | 0.95 |
| **10** |  | **PERY-β** | Perylene (β-phase) | [14] | 0.4 | [15] | 0.4 |
| | | | 2-(6,7-difluoro-1,3-dithiolo[4,5-b] | | | | |

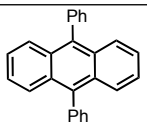
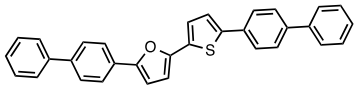
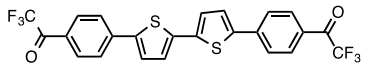
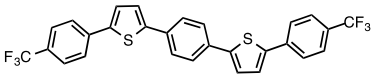
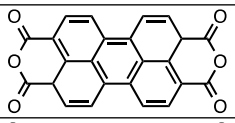
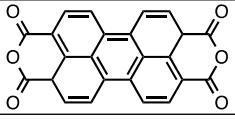
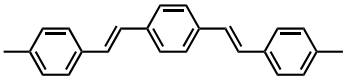
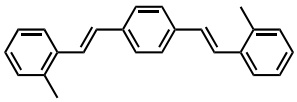
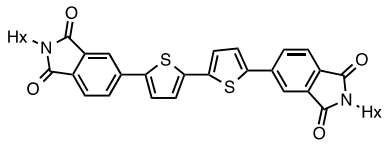
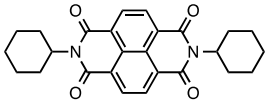
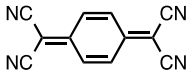
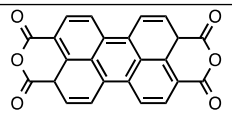
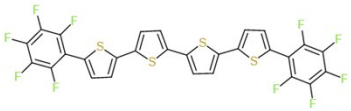
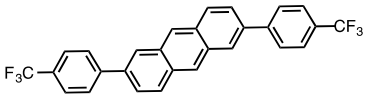
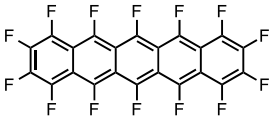
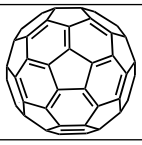
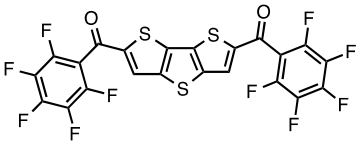
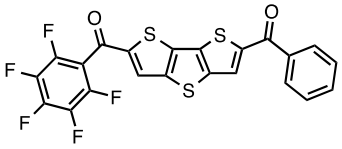
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | quinoxalin-2-ylidene)-6,7-difluoro-1,3-dithiolo[4,5-b] quinoxaline | | | | |
| **12** |  | **DPA** | Diphenyl anthracene | [17] | 13 | [18] | 11.6 |
| **13** |  | **C60** | Fullerene | [19] | 11 | [20] | 5.1 |
| **14** |  | **BPFT** | 2-(4-biphenyl)-5-[5-(4-biphenyl)-2-thienyl] furan | [21] | 0.013 | [21] | 0.15 |
| **15** |  | **TFAPT** | 1,1'-([2,2'-bithiophene]-5,5'-diyldi-4,1-phenylene)bis[2,2,2-trifluoro-ethanone | [22] | 2.4 | [22] | 0.68 |
| **16** |  | **TFPTP** | 1,4-bis(5-(4-(trifluoromethyl)phenyl)thiophen-2-yl) benzene | [23] | 3.1 | [23] | 5.66 |
| **17** |  | **PTCDA-α** | Perylenetetracarboxylic dianhydride (α phase) | [24] | 0.005 | [25] | 0.017 |
| **18** |  | **PTCDA-β** | Perylenetetracarboxylic dianhydride (β phase) | [24] | 0.005 | [25] | 0.005 |
| **19** |  | **pMSB** | *p*-bis(*p*-methylstyryl) benzene | [26] | 0.1 | [26] | 0.124 |
| **20** |  | **oMSB** | *p*-bis(*o*-methylstyryl) benzene | [26] | 0.009 | [26] | 0.0066 |

**Table S2(b).** Thin-film electron mobility test set (TFEM21).

| | MOLECULAR STRUCTURE | ACRONYM | NAME | Reference of the crystal structure | Experimental $\mu_e$ ($cm^2/Vs$) | Reference of exp. $\mu_e$ | Theoretical $\mu_e$ ($cm^2/Vs$) |
|---|---|---|---|---|---|---|---|
| **1** |  | **HPT** | 5,5'-[2,2'-bithiophene]-5,5'-diylbis[2-hexyl-1H-isoindole-1,3(2H)-dione | [27] | **0.21** | [27] | **8.45E-03** |
| **2** |  | **CHNTCDI** | N,N'-Dicyclohexylnaphthalene-1,4,5,8-tetracarboxylic acid diimide | [28] | **0.11-0.52** | [29] | **4.25E-02** |
| **3** |  | **TCNQ** | 7,7',8,8'-tetracyanoquinodimethane | [3] | **3.0E-05** | [30] | **1.09E-05** |
| **4** |  | **PTCDA** | Perylenetetracarboxylic dianhydride | [24] | **1.0E-4** | [31] | **4.93E-05** |
| **5** |  | **FPQT** | 5,5'''-Diperfluorophenyl-2,2':5',2'': 5'',2'''-quaterthiophene | [32] | **0.43** | [33] | **0.395** |
| **6** |  | **TFPA** | 2,6-bis[4-(trifluoromethyl) phenyl]-anthracene | [34] | **3.4E-03** | [34] | **2.80E-03** |
| **7** |  | **FPEN** | 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoropentacene | [35] | **0.22** | [36] | **0.332** |
| **8** |  | **C60** | Fullerene | [19] | **5.3** | [37] | **3.12** |
| **9** |  | **DFBDTT** | 1,1'-dithieno[3,2-b:2',3'-d] thiophene-2,6-diylbis[1-(2,3,4,5,6-pentafluorophenyl) -methanone | [38] | **2.0E-03** | [38] | **1.71E-04** |
| **10** |  | **FBBDTT** | (6-benzoyldithieno[3,2-b:2',3'-d]thien-2-yl)(2,3,4,5,6-pentafluorophenyl) -methanone | [38] | **3.0E-02** | [38] | **3.29E-04** |

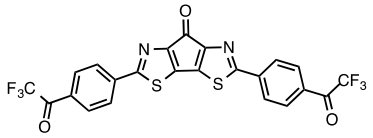
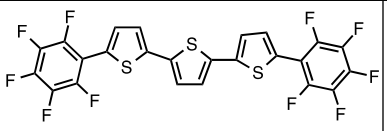
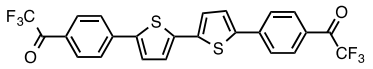
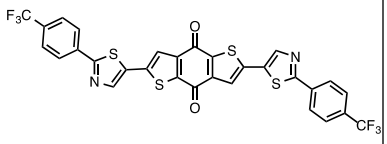
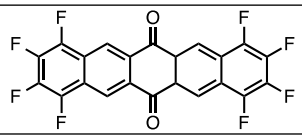
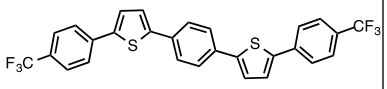
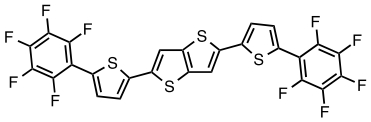
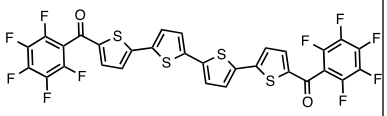
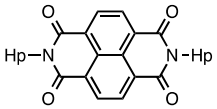
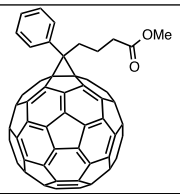
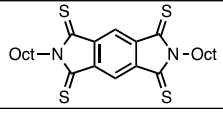
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **11** |  | **CBTZ** | 2,5-bis[4-(2,2,2-trifluoroacetyl) phenyl]- 7*H*-cyclopenta[1,2-*d*:4,3-*d*']bisthiazol-7-one | [39] | **6.0E-02** | [39] | **2.79E-03** |
| **12** |  | **FPTT** | 5,5''-bis(2,3,4,5,6-pentafluorophenyl) -2,2':5',2''-terthiophene | [33] | **3.0E-03** | [33] | **8.39E-03** |
| **13** |  | **TFAPT** | 1,1'-([2,2'-bithiophene]-5,5'-diyldi-4,1-phenylene)bis[2,2,2-trifluoroethanone | [22] | **8.0E-02** | [22] | **3.05E-02** |
| **14** |  | **TFPT-DTBQ** | 2,6-bis[2-[4-(trifluoromethyl) phenyl]-5-thiazolyl] -benzo[1,2-b:4,5-b']dithiophene-4,8-dione | [40] | **0.15** | [40] | **0.136** |
| **15** |  | **FPENQ** | 1,2,3,4,8,9,10,11-octafluoropentacene[6,13]quinine | [41] | **0.18** | [41] | **1.35E-02** |
| **16** |  | **TFPTP** | 1,4-bis(5-(4-(trifluoromethyl)phenyl)thiophen-2-yl)benzene | [23] | **0.6** | [23] | **2.1E-02** |
| **17** |  | **DFPTT** | 5,5'-perfluorophenyl-2,5-dithiophenylthieno [3,2-*b*]thiophene | [42] | **0.33** | [42] | **0.145** |
| **18** |  | **FBOQT** | 1,1'-[2,2':5',2'':5'', 2'''-quaterthiophene]-5,5'''-diylbis[1-(2,3,4,5,6-pentafluorophenyl) -methanone | [43] | **0.45** | [43] | **1.92E-02** |
| **19** |  | **HXNTDCI** | 2,7-diheptyl-benzo[lmn][3,8] phenanthroline-1, 3,6,8(2H,7H)-tetrone | [44] | **0.7** | [44] | **1.66E-02** |
| **20** |  | **PCBM** | Phenyl-C61-butyric acid methyl ester | [45] | **2.85E-02** | [46] | **3.1E-02** |
| **21** |  | **PYDIC8** | (*N*-octyl) pyromellitic diimide | [47] | **5.80E-03** | [47] | **1.80E-02** |

**Table S3.** B3LYP/6-311G(d,p) calculated reorganization energies of SCEM20 and TFEM21.

| SCEM20 set | | | TFEM21 set | |
|---|---|---|---|---|
| | $\lambda_e$ (meV) | | | $\lambda_e$ (meV) |
| ANTH | 204 | | C60 | 135 |
| BPFT | 229 | | CBTZ | 366 |
| C60 | 135 | | CHNTCDI | 375 |
| DPA | 213 | | DFBDTT | 333 |
| FPTTF | 233 | | DFPTT | 283 |
| FRUB | 130 | | FBBDTT | 321 |
| NAPH | 266 | | FBOQT | 301 |
| *o*MSB | 369 | | FPENQ | 323 |
| PERY | 177 | | FPEN | 241 |
| PERY | 177 | | FPQT | 280 |
| *p*MSB | 272 | | FPTT | 306 |
| PTCDA-$\alpha$ | 241 | | HPT | 275 |
| PTCDA-$\beta$ | 241 | | HXNTDCI | 363 |
| RUBR | 204 | | PCBM | 150 |
| TCNQ | 264 | | PTCDA | 241 |
| TFAPT | 307 | | PYDIC8 | 260 |
| TFDT | 351 | | TCNQ | 264 |
| TFPT | 349 | | TFAPT | 307 |
| TFPTP | 285 | | TFPA | 262 |
| TFTT | 352 | | TFPT_DTBQ | 257 |

| | |
|---|---|
| TFPTP | 285 |

**Table S4.** Paracrystalline order parameter, g, and energetic disorder, σ, for TFEM21 set.

| **TFEM21 set** | | |
|---|---|---|
| | g[%] | σ (meV) |
| CBTZ | 3.8 | 102 |
| C60 | 1.0 | **4** |
| CHNTCDI | 2.3 | 88 |
| DFBDTT | 2.7 | 88 |
| DFPTT | 3.5 | 63 |
| FBBDTT | 4.1 | 131 |
| FBOQT | 1.9 | 81 |
| FPENQ | 3.6 | 143 |
| FPEN | 3.0 | **65** |
| FPQT | 1.5 | 82 |
| FPTT | 4.7 | 89 |
| HPT | 2.4 | 61 |
| HXNTDCI | 2.4 | 88 |
| PCBM | 1.8 | 69 |
| PTCDA | 6.2 | 165 |
| PYDIC8 | 3.0 | 48 |
| TCNQ | 3.4 | 149 |
| TFAPT | 3.4 | 76 |
| TFPA | 2.3 | 87 |
| TFPT_DTBQ | 2.3 | 68 |

| | | |
|---|---|---|
| TFPTP | 7.2 | 111 |
| **average** | **3.0** | **90** |

## Details of the kinetic Monte Carlo (kMC) Simulations:

### Transfer Rates

We employ the charge-transport simulations procedure implemented in **VOTCA** package developed by Andrienko and co-workers.[48,49] On the basis of the assumption that charges are localized on a single molecule and charge-transfer reactions take place via an intersite hopping mechanism, the charge-hopping rate is evaluated by the nonadiabatic, high-temperature limit of the Marcus rate[50,51]

$$k_{ij} = \frac{J_{ij}^2}{\hbar}\sqrt{\frac{\pi}{\lambda k_b T}} exp\left[-\frac{\left(\Delta E_{ij} - \lambda_e\right)^2}{4\lambda k_b T}\right]$$

where $T$ is the temperature, $J_{ij}$ is the transfer integral between the initial and final states. $\lambda_e$ is the electron-transfer reorganization energy and $\Delta E_{ij} = \varepsilon_i - \varepsilon_j$ is called the site-energy difference of the transfer reaction. $\varepsilon_i$ is the energy difference of the entire system when molecule *i* is charged or neutral. Thus, for reactions involving identical molecules, $\Delta E_{ij}=0$.

### Reorganization Energy:

The reorganization energy λ is calculated from adiabatic potential energy surfaces of neutral and cationic states of compounds, using the following expression:

$$\lambda = \left(E_{q_c}^{\,n} - E_{q_n}^{\,n}\right) + \left(E_{q_n}^{\,c} - E_{q_c}^{\,c}\right)$$

where $E_{q_n}^{\,n}$ ($E_{q_n}^{\,c}$) is the energy of the neutral *n* (charged *c*) state of the molecule in its optimized *neutral* geometry and $E_{q_c}^{\,n}$ ($E_{q_c}^{\,c}$) is the energy of the neutral *n* (charged *c*) state of the molecule in its optimized *charged* geometry. We used in Gaussian09,[52] to calculate λ for an isolated molecule. We employ the B3LYP hybrid density functional with the 6- 31G(d) basis set.

### Site-energies:

A charge-transfer reaction from molecule *i* and *j* is driven by site-energy. Here, we calculate site-energies of the electron transfer from polarizable force-fields with the help of *ab initio* methods. Site-energies include contributions from electrostatic Coulombic interactions (with polarization effects) between atoms and the contributions from the external electric field. Thus, site energy difference is defined as follows:

$$\Delta E_{ij} = \Delta E_{elec.} + \Delta E_{ext.}$$

External electric field contributions are calculated using the expression $\Delta E_{ext.} = q\vec{F}.\vec{d}_{ij}$. Here $\vec{F}$ is the field-vector and $\vec{d}_{ij}$ is the position-vector between molecules *i* and *j*. Polarized Coulombic contributions to site energies are calculated self-consistently using Thole Model.[49,53–54] Partial charges of neutral and charged states are generated via Merz−Singh− Kollman scheme,16,17 using HF/6-31G(d) method based on B3LYP/6-31G(d,p) optimized geometries, as implemented in Gaussian09.[52] Isotropic atomic polarizabilities of the neutral and charged states are reparameterized for each species as to reproduce the molecular polarizabilities obtained from B3LYP/ 6-31G(d,p) method.[52]

## Energetic disorder

Energetic disorder σ is calculated by fitting the histogram of $\Delta E_{ij}$ site-energy differences to a Gaussian-distribution function

$$f(\varepsilon,\sigma) = \frac{1}{2\pi} exp[-\frac{\varepsilon^2}{2\sigma^2}]$$

## kMC simulations and electron-mobility:

Charge dynamics is simulated using the kinetic Monte Carlo (kMC) technique using the VOTCA package. In this stochastic procedure, a charge-carrier is initially chosen randomly within the system with periodic-boundaries and propagated by hopping between sites, where hopping probabilities (thus the hopping times) are defined by the Marcus rate. The simulations are performed until the results are converged. Charge-carrier mobility is calculated by

$$\mu_e = \frac{v}{|F|},$$

where $v$ is the charge-carrier velocity and F is applied electric field. The reported mobilities are the averages over 10-100 stochastic realizations.

**Table S5.** A test site-energy calculation for **CBTZ** with different RESP methodologies and the resulting energetic disorder and electron mobility.

| RESP method | Energetic disorder σ (meV) | Theoretical $\mu_e$ (cm²/Vs) |
|---|---|---|
| **MK** | 102 | 2.8E-3 |
| **MKUFF** | 119 | 1.1E-3 |
| **CHelp** | 131 | 3.1E-4 |

| | | |
|---|---|---|
| **CHelpG** | 123 | 5.0E-4 |
| **HLYGAt** | 117 | 1.2E-3 |

## REFERENCES


(1) Ando, S.; Murakami, R.; Nishida, J.-I. Tada, H.; Inoue, Y.; Tokito, S.; Yamashita, Y. *J. Am. Chem. Soc.* **2005**, *127*, 14996-14997.

(2) Xie, W.; Prabhumirashi, P. L.; Nakayama, Y.; McGarry, K. A.; Geier, M. L.; Uragami, Y.; Masei, K.; Douglas, C. J.; Ishii, H.; Hersam, M. C.; Frisbie, C. D. *ACS Nano* **2013**, *7*, 10245-10256.

(3) Long, R. E.; Sparks, R. A.; Trueblood, K. N. *Acta Cryst.* **1965**, *18*, 932-939.

(4) Menard, E.; Podzorov, V.; Hur, S.-H.; Gaur, A.; Gershenson, M. E.; Rogers, J. A. *Adv. Mater.* **2004**, *16*, 2097-2101.

(5) Ando, S.; Nishida, J.; Tada, H.; Inoue, Y.; Tokito, S.; Yamashita, Y. *J. Am. Chem. Soc.* **2005**, *12*, 5336–5337.

(6) Jurchescu, O. D.; Meetsma, A.; Palstra, T. T. M. *Acta Cryst.* **2006**, *62*, 330-334.

(7) Bisri, S. Z.; Takenobu, T.; Takahashi, T.; Iwasa, Y. *Appl. Phys. Lett.* **2010,** *96*, 183304.

(8) Alt, H. C.; Kalus, J. *Acta Crystallogr.* **1982**, *1*, 2595−2600.

(9) (a) Warta, W.; Stehle, R.; Karl, N. *Appl. Phys. A* **1985,** *36*, 163-170. (b) Karl, N. *Synthetic Metals* **2003***,* 133, 649-657.

(10) Brock, C. P.; Dunitz, J. D. *Acta Cryst.* **1990**, *46*, 795-806.

(11) Karl N.; Marktanner, J. *Mol. Cryst. Liq. C. A* **2001,** *335*, 149-173.

(12) Ranganathan, A.; Kulkarni, G. U. *Proc. Indian Acad. Sci.* **2003**, *115*, 637-647.

(13) Kim, S. H.; Yang, Y. S.; Lee, J. H.; Lee, J.-I.; Chu, H. Y.; Lee, H.; Oh, J.; Do, L.-M.; Zyung, T. *Opt. Mater.* **2002,** *21*, 439–443.

(14) Nather, C.; Bock, H.; Havlas, Z.; Hauck, T. *Organometallics* **1998**, *17*, 4707-4715.

(15) Kotania, M.; Kakinuma, K.; Yoshimura, M.; Ishii, K.; Yamazaki, S.; Kobori, T.; Okuyama, H.; Kobayashi, H.; Tada, H. *Chem. Phys.* **2006**, *325*, 160–169.

(16) Nishida, J.-I.; Kumaki, D.; Tokito, S.; Yamashita, Y. *J. Am. Chem. Soc.* **2006**, *128*, 9598-9599.

(17) Langer, V.; Becker, H.-D. *Z. Kristallogr*. **1992**, *199*, 313−315.

(18) Tripathi, A. K.; Heinrich, M.; Siegrist, T.; Pflaum, J. *Adv. Mater.* **2007**, *19*, 2097−2101.

(19) Dorset, D. L.; McCourt, M. P. *Acta Cryst.* **1994**, *50*, 344-351.

(20) Li, H.; Tee, B. C-K.; Cha, J. J.; Cui, Y.; Chung, J. W.; Lee, S. Y.; Bao, Z. *J. Am. Chem. Soc.* **2012**, *134*, 2760-2765.

(21) Oniwa, K.; Kanagasekaran, T.; Jin, T.; Akhtaruzzaman, M.; Yamamoto, Y.; Tamura, H.; Hamada, I.; Shimotani, H.; Asao, N.; Ikeda, S.; Tanigaki, K. *J. Mater. Chem. C* **2013**, *1*, 4163-4170.

(22) Ie, Y.; Nitani, M.; Uemura, T.; Tominari, Y.; Takeya, J.; Honsho, Y.; Saeki, A.; Seki, S.; Aso, Y. *J. Phys. Chem. C* **2009**, *113*, 17189–17193.

(23) Ichikawa, M.; Kato, T.; Uchino, T.; Tsuzuki, T.; Inoue, M.; Jeon, H.-G.; Koyama, T.; Taniguchi, Y. *Org. Electron.* **2010**, *11*, 1549-1554.

(24) Ogawa, T.; Kuwamoto, K.; Isoda, S.; Kobayashi, T.; Karl, N. *Acta Crystallogr. Sect. B-Struct. Sci.* **1999**, *55*, 123-130.

(25) Yamada, K.; Takeya, J.; Takenobu,T.; Iwasa, Y. *Appl. Phys. Lett.* **2008**, *92*, 253311.

(26) Kabe, R.; Nakanotani, H.; Sakanoue, T.; Yahiro, M.; Adachi, C. *Adv. Mater.* **2009**, *21*, 4034-4038.

(27) Sun, J.-P.; Hendsbee, A. D.; Eftaiha, A. F.; Macaulay, C.; Rutledge, L. R.; Welch, G. C.; Hill, I. G. *J. Mater. Chem. C* **2014**, *2*, 2612-2621.

(28) Shukla, D.; Rajeswaran, M. *Acta Crystallogr. Sect. E: Struct. Rep. Online* **2008**, 64, 1735.

(29) Kakinuma, T.; Kojima, H.; Ashizawa, M.; Matsumotoa, H.; Mori, T. *J. Mater. Chem. C* **2013**, *1*, 5395-5401.

(30) Brown, A. R.; de Leeuw, D. M.; Lous, E. J.; Havinga, E. E. *Synthetic Metals* **1994**, *66*, 257-261.

(31) Ostrick, J. R.; Dodabalapur, A.; Torsi, L.; Lovinger, A, J.; Kwock, E. W.; Miller, T. M.; Galvin, M.; Berggren, M.; Katz, H. E. *J. App. Phys.* **1997**, *81*, 6804-6808.

(32) Facchetti, A.; Yoon, M.-H.; Stern, C. L.; Katz, H. E.; Marks, T. J. *Angew. Chem. Int. Ed.* **2003**, *42*, 3900 -3903.

(33) Yoon, M.-H.; Facchetti, A.; Stern, C. E.; Marks, T. J. *J. Am. Chem. Soc*. **2006**, *128*, 5792-5801.

(34) Ando, S.; Nishida, J.; Fujiwara, E.; Tada, H.; Inoue, Y.; Tokito, S.; Yamashita, Y. *Chem. Mater.* **2005**, *17*, 1261-1264.

(35) Sakamoto, Y.; Suzuki, T.; Kobayashi, M.; Gao, Y.; Fukai, Y.; Inoue, Y.; Sato, F.; Tokito, S. *J. Am. Chem. Soc.* **2004**, *126*, 8138-8140.

(36) Sakamoto, Y.; Suzuki, T.; Kobayashi, M.; Gao, Y.; Inoue, Y.; Tokito, S. *Mol. Cryst. Liq. Crys.* **2006**, *444*, 225-232.

(37) Ito, Y.; Virkar, A. A.; Mannsfeld, S.; Oh, J. H.; Toney, M.; Locklin, J.; Bao, Z. *J. Am. Chem. Soc.* **2009**,

*131*, 9396-9404.

(38) Chen, M.-C.; Chiang, Y.-J.; Kim, C.; Guo, Y.-J.; Chen, S.-Y.; Liang, Y.-J.; Huang, Y.-W.; Hu, T.-S.; Lee, G.-H.; Facchetti, A.; Marks, T. J. *Chem. Commun.*, **2009**, 1846-1848.

(39) Ie, Y.; Nitani, M.; Karakawa, M.; Tada, H.; Aso, Y. *Adv. Funct. Mater.* **2010**, *20*, 907-913.

(40) Mamada, M.; Kumaki, D.; Nishida, J.; Tokito, S.; Yamashita, Y. *ACS Appl. Mater. Interfaces* **2010**, *2*, 1303-1307.

(41) Liang, Z.; Tang, Q.; Liu, J.; Li, J.; Yan, F.; Miao, Q. *Chem. Mater.* **2010**, *22*, 6438–6443.

(42) J. Youn, et. al, *Adv. Electron. Mater.* **2015**, *1*, 1500098.

(43) Letizia, J. A; Facchetti, A.; Stern, C. L.; Ratner, M. A.; Marks, T. J. *J. Am. Chem. Soc.* **2005**, *127*, 13476-13477.

(44) Shukla, D.; Nelson, S. F.; Freeman, D. C.; Rajeswaran, M.; Ahearn, W. G.; Meyer, D. M.; Carey, J. T. *Chem. Mater.* **2008**, *20*, 7486–7491.

(45) Rispens, M. T.; Meetsma, A.; Rittberger, R.; Brabec, C. J.; Sariciftci, N. S.; Hummelen, J. C. *Chem. Commun.* **2003**, 2116-2118.

(46) Yang, C.; Kim, J. Y.; Cho, S.; Lee, J. K.; Heeger, A. J.; Wudl, F. *J. Am. Chem. Soc.,* **2008**, *130*, 6444–6450.

(47) Yang, T.-F.; Huang, S.-H.; Chiu, Y.-P.; Chen, B.-H.; Shih, Y.-W.; Chang, Y.-C.; Yao, J.-Y.; Lee, Y.-J.; Kuo, M.-Y. *Chem. Commun.* **2015**, *51*, 13772-13775.

(48) Ruehle, V.; Junghans, C.; Lukyanov, A.; Kremer, K.; Andrienko, D. *J. Chem. Theory. Comput.* **2009**, 5, 3211−3223.

(49) Ruehle, V.; Lukyanov, A.; May, F.; Schrader, M.; Vehoff, T.; Kirkpatrick, J.; Baumeier, B.; Andrienko, D. *J. Chem. Theory. Comput.* **2011**, 7, 3335−3345.

(50) Marcus, R. A. *J. Chem. Phys.* **1956**, 24, 966−978.

(51) Marcus, R. A. *Rev. Mod. Phys.* **1993**, 65, 599−610.

(52) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, P. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.;

Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian09, revision D.01; Gaussian Inc.: Wallingford, CT, 2009.

(53) Thole, B. T. *Chem. Phys.* **1981**, 59, 341−350.

(54) Van Duijnen, P. T.; Swart, *J. Phys. Chem. A* **1998**, 102, 2399−2407.