

Supporting electronic information

Effect of N-substituents on redox, optical and electronic properties of naphthalene bisimides used for field-effect transistors fabrication

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Synthesis of semiconducting molecules

Reagents

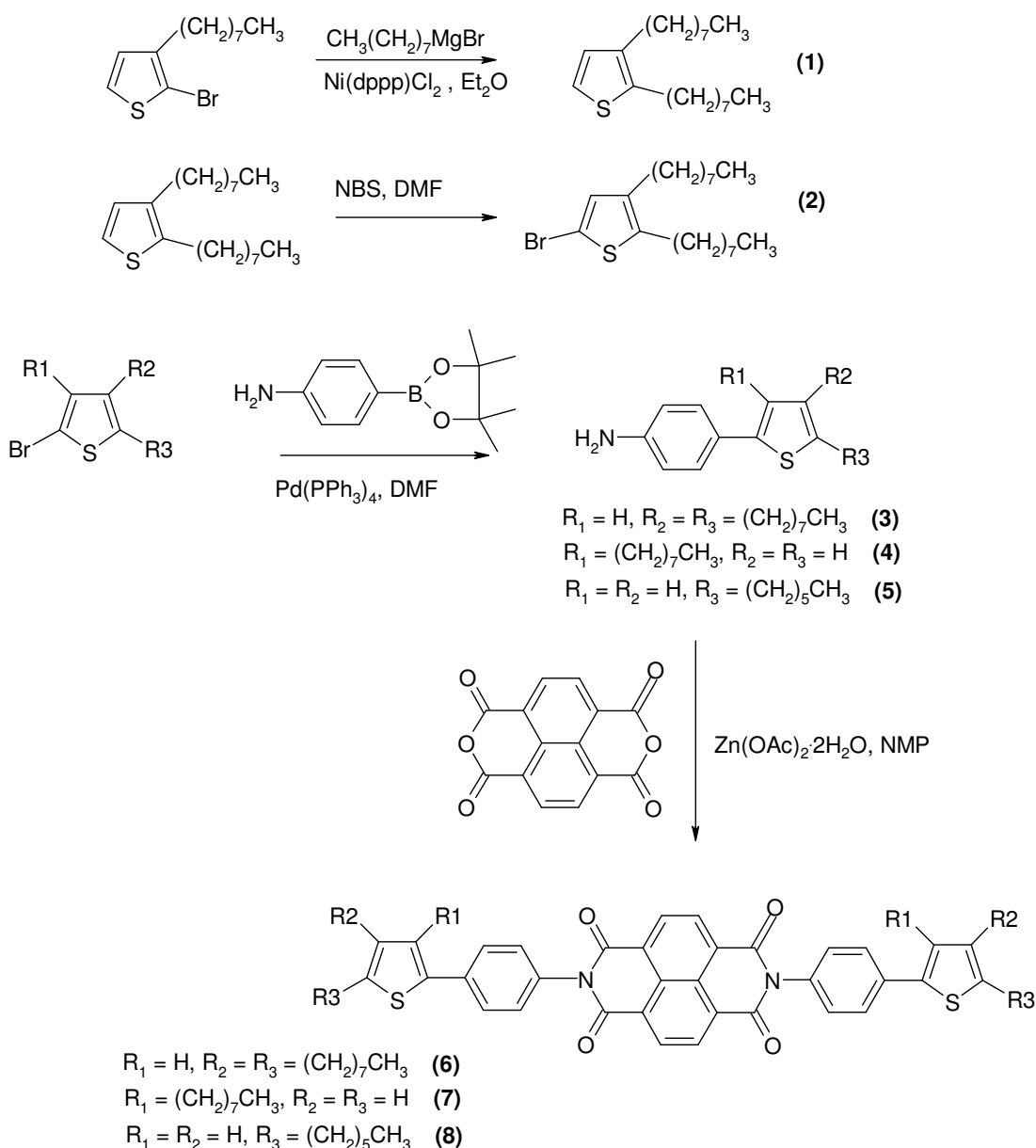
NMP, 2-thienylmethylamine, 1-bromooctane, 4-aminophenylboronic acid pinacol ester, 1,4,5,8-naphthalenetetracarboxylic acid bisanhydride tetrakis(triphenylphosphine)palladium, [1,3-bis(diphenylphosphino)propane]dichloronickel(II) were purchased from Sigma Aldrich Co. and used as received. Diethyl ether was dried and stored over sodium. Dry DMF, zinc acetate dihydrate and potassium phosphate were purchased from Fluka and used as received. N-bromosuccinimide (Fluka) was crystallized from water before use. 2-bromo-3-octylthiophene, 2-bromo-5-dodecylthiophene and 2-bromo-5-hexylthiophene were prepared according to methods already described¹. 5-hexyl-2-thienylboronic acid neopentyl glycol ester was prepared according to modified method already described².

Preparation of alkylthienylphenyl naphthalenebisimides

Alkylthienylphenyl bisimides were prepared using the reaction sequence depicted in **Scheme 1**:

¹ (a) P. Bauerle; F. Wurthner, G. Gotz, F. Effenberger, *Synthesis*, 1993, 1099-1103.; (b) C. Xia, X. Fan, J. Locklin, R. C. Advincula *Org. Lett.*, 2002, **4**, 2067–2070.

² D. Didier, S. Sergeyev, Y. H. Geerts, *Tetrahedron* 2007, **63**, 941–946.



Scheme 1

Synthesis of 2,3-dioctylthiophene via Kumada coupling³ (1)

To a stirred mixture of 0.38 g (15.9 mmol) of magnesium turnings and 7 mL of dry diethyl ether a solution of n-octyl bromide (3.07 g; 15.9 mmol) in 8 mL of dry diethyl ether was added dropwise, under argon atmosphere and then stirred for 1 hour at RT. The resulting solution of the Grignard reagent formed was then slowly added, at RT, to a solution of 2-bromo-3-octylthiophene (3.98 g; 14.5 mmol) and 30 mg of [1,3-bis(diphenylphosphino)propane]dichloronickel(II) in 8 mL of dry diethyl ether. The obtained mixture was stirred for 12 hours at RT, and then it was cooled to 0°C with an ice bath. In the next step 25 mL of 1M HCl were carefully added, the obtained biphasic mixture was shaken with diethyl ether and finally its organic phase was separated, washed with water and dried over anhydrous magnesium sulphate. The solvent was removed in a rotary

³ K. Tamao, K. Sumitani, Y. Kiso, M. Zembayashi, A. Fujioka, S.-I. Kodama, I. Nakajima, A. Minato, M. Kumada, *Bull. Chem. Soc. Jpn.* 1976, **49**, 1958-1969.

evaporator and the crude product was purified using a chromatographic column (silica gel, hexane). Further purification was carried out by distillation in Kugelrohr vacuum oven, yielding 2 g (45%) of colorless oil.

¹H NMR (CDCl₃, 400 MHz, ppm): 7.02 (d, 2H, J=5.2 Hz), 6.81 (d, 2H, J=5.2 Hz), 2.71 (t, 2H, J=7.8 Hz), 2.47 (t, 2H, J=7.8 Hz), 1.50-1.68 (m, 4H), 1.22-1.40 (m, 20H), 0.88 (apparent triplet, 6H, J=6.8 Hz).

Synthesis of 2-bromo-4,5-dioctylthiophene (2)

To a stirred solution of 2,3-dioctylthiophene (1.03 g; 3.35 mmol) in 10 mL of dry DMF a solution of N-bromosuccinimide (0.61 g (3.35 mmol) in 10 mL of dry DMF was added dropwise, under argon atmosphere and stirred for 1 hour at RT. Then, the reaction mixture was poured onto ice water. The resulting biphasic mixture was shaken with diethyl ether and the resulting organic phase was washed with brine and water, and then dried over anhydrous magnesium sulphate. The solvent was then removed using a rotary evaporator. In the final step the crude product was purified using a chromatographic column (silica gel, hexane) yielding 0.97 g (75%) of colorless oil.

¹H NMR (CDCl₃, 400 MHz, ppm): 6.74 (s, 1H), 2.64 (t, 2H, J=7.6 Hz), 2.43 (t, 2H, J=7.8 Hz), 1.46-1.62 (m, 4H), 1.22-1.38 (m, 20H), 0.88 (apparent triplet, 6H, J=6.8 Hz).

General procedure for the synthesis of alkylthienylanilines via Suzuki coupling⁴

To a solution of 10 mmol of appropriate bromoalkylthiophene in 30 mL of dry DMF 0.29g (0.5 mmol) of tetrakis(triphenylphosphine)palladium was added under argon atmosphere and then stirred for 10 minutes at RT. Next, 2.31 g (8.23 mmol) of potassium phosphate were added, followed by immediate addition of 4-aminophenylboronic acid pinacol ester (2.4 g; 10.97 mmol). The resulting mixture was heated at 110°C for 18 hours. After cooling to RT it was poured onto 100 mL of chloroform. DMF was then removed by several extractions with water. The organic phase was dried with anhydrous magnesium sulphate which was followed by evaporation of chloroform in a rotary evaporator. The crude product was then purified using a chromatographic column (silica gel, methylene chloride + 1 % vol. triethylamine).

4-(4,5-dioctyl-2-thienyl)aniline (41 %). (3)

¹H NMR (CDCl₃, 400 MHz, ppm): 7.35-7.40 (m, 2H), 6.89 (s, 1H), 6.70-6.74 (m, 2H), 4.2 (broad, 2H), 2.70 (t, 2H, J=7.8 Hz), 2.47 (t, 2H, J=7.6 Hz), 1.52-1.68 (m, 4H), 1.22-1.42 (m, 20H), 0.88 (apparent triplet, 6H, J=6.8 Hz).

4-(3-octyl-2-thienyl)aniline (57 %) (4)

¹H NMR (CDCl₃, 400 MHz, ppm): 7.22-7.25 (m, 2H), 7.15 (d, 1H, J=5.2 Hz), 6.95 (d, 1H, J=5.2 Hz), 6.74-6.79 (m, 2H), 4.10 (broad, 2H), 2.61 (t, 2H, J=7.8 Hz), 1.54-1.64 (m, 2H), 1.20-1.34 (m, 10H), 0.88 (t, 3H, J=6.8 Hz).

4-(5-hexyl-2-thienyl)aniline (35 %) (5)

¹H NMR (CDCl₃, 400 MHz, ppm): 7.34-7.39 (m, 2H), 6.95 (d, 1H, J=3.6 Hz), 6.65-6.70 (m, 1H+2H), 3.70 (broad, 2H), 2.79 (t, 2H, J=7.6 Hz), 1.64-1.72 (m, 2H), 1.28-1.42 (m, 6H), 0.88 (t, 3H, J=7.0 Hz).

⁴ D. Aldakov, C. Querner, Y. Kervella, B. Jousselme, R. Demadrille, E. Rositto, P. Reiss, A. Pron, *Microchimica Acta* 2008, **160**, 335-344.

Condensing of alkylthienylanilines and naphthalene bisanhydride⁵

In this step a modification of the methods already described in the literature was used. In a typical preparation 1.96 mmol of amine and 0.20 g (1.86 mmol) of zinc acetate dihydrate were added to a stirred suspension of 0.25 g (1.86 mmol) of 1,4,5,8-naphthalenetetracarboxylic acid bisanhydride in 30 mL of dry NMP. The resulting mixture was stirred at the temperature of 180°C for 3 hours, and then was poured onto 100 ml of water. The obtained precipitate was filtered off, washed with water and dried in air. In the next step the crude product was vigorously stirred with 50 mL of acetone for 2 hours to remove the excess of the primary amine and remaining zinc acetate. The obtained bisimides were next purified using a chromatographic column (silica gel, chloroform) (twice), which was followed by drying in vacuum at 65°C for 12 hours.

***N, N'*- bis[(4,5-dioctyl-2-thienyl)phenyl]-1,4,5,8-naphthalenetetracarboxylic-1,4:5,8-bisimide (NBI-8)(42 %) (6).**

Orange solid.

¹H NMR (CDCl₃, 400 MHz, ppm): 8.86 (s, 4H), 7.72-7.76 (m, 4H), 7.30-7.34 (m, 4H), 7.12 (s, 2H), 2.75 (t, 4H, J=7.6 Hz), 2.53 (t, 4H, J=7.6Hz), 1.54-1.72 (m, 8H), 1.24-1.46 (m, 40H), 0.89 (apparent triplet, 12H, J=6.8 Hz).

¹³C NMR (CDCl₃, 100 MHz, ppm): 163.0; 139.9, 139.1; 138.2; 135.9; 132.7; 131.5; 128.7; 127.2; 127.0; 126.4; 125.8; 31.9 (2C); 31.8; 30.8; 29.5; 29.4 (2C); 29.3; 29.2; 28.3; 28.0; 22.7; 14.1.

FTIR (KBr, cm⁻¹): 3073, 2954, 2920, 2851, 1713, 1675, 1580, 1511, 1467, 1445, 1345, 1250, 1193, 1137, 1118, 1106, 980, 854, 830, 768, 751.

UV-vis (CHCl₃) λ_{max} = 237 nm, 314 nm, 340nm, 381 nm.

Elemental analysis: Calcd for C₆₈H₈₂N₂O₄S₂: C, 76.85, H, 8.01, N, 2.72, S, 6.22. Found: C, 76.85, H, 8.09, N, 2.75, S, 5.95.

Melting point: 171°C.

***N, N'*- bis[(3-octyl-2-thienyl)phenyl]-1,4,5,8-naphthalenetetracarboxylic-1,4:5,8-bisimide (NBI-9)(52 %) (7).**

Orange fluorescent solid.

¹H NMR (CDCl₃, 400 MHz, ppm): 8.89 (s, 4H), 7.62-7.65 (m, 4H), 7.37-7.41 (m, 4H), 7.29 (d, 2H, J=4.8 Hz), 7.03 (d, 2H, J=5.6 Hz), 2.73 (t, 4H, J=8.0 Hz), 1.62-1.72 (m, 4H), 1.22-1.40 (m, 20H), 0.88 (t, 6H, J=7.8 Hz).

¹³C NMR (CDCl₃, 100 MHz, ppm): 163.0; 139.4, 136.5; 135.9; 133.3; 131.5; 130.4; 129.6; 128.5; 127.2; 127.0; 124.3; 31.8 ; 31.1; 29.5; 29.3; 28.8 ; 22.7; 14.1.

FTIR (KBr, cm⁻¹): 3079, 3062, 3039, 2954, 2921, 2850, 1708, 1669, 1580, 1529, 1448, 1347, 1248, 1191, 1142, 1121, 983, 923, 886, 856, 845, 835, 771, 764, 751, 721, 709.

UV-vis (CHCl₃) λ_{max} = 237 nm, 282 nm, 343 nm, 360nm, 380 nm.

Elemental analysis: Calcd for C₅₀H₅₀N₂O₄S₂: C, 74.41, H, 6.24, N, 3.47, S, 7.95. Found: C, 74.26, H, 6.30, N, 3.52, S, 7.64.

Melting point: 217°C.

⁵ (a) A. Rademacher, S. Markle, H. Langhals, *Chem. Ber.* 1982, **115**, 2927-2934. (b) H. Langhals, *Chem. Ber.* 1985, **118**, 4641-4645. (c) S. Demmig, H. Langhals, *Chem. Ber.* 1988, **121**, 225-230. (d) H. Langhals, H. Jaschke, *Chem. Eur. J.* 2006, **12**, 2815-2824.

***N, N'*- bis[(5-hexyl-2-thienyl)phenyl]-1,4,5,8-naphthalenetetracarboxylic-1,4:5,8-bisimide (NBI-10)(52 %) (8)**

Pink-red solid.

¹H NMR (CDCl₃+CF₃COOD, 400 MHz, ppm): 8.95 (s, 4H), 7.74-7.80 (m, 4H), 7.30-7.35 (m, 4H), 7.22 (d, 2H, J=3.6 Hz), 6.80 (d, 2H, J=3.6 Hz), 2.86 (t, 4H, J=7.6 Hz), 1.59-1.88 (m, 4H), 1.30-1.46 (m, 12H), 0.91 (t, 6H, J=7.2 Hz).

¹³C NMR (CDCl₃, 100 MHz, ppm): 164.3; 147.4; 139.7; 137.0; 132.7 (2C); 131.5; 128.6; 127.2; 126.9; 125.3; 124.1; 31.6 (2C); 30.3; 28.8; 22.6; 14.0.

FTIR (KBr, cm⁻¹): 3068, 2947, 2922, 2848, 1719, 1676, 1583, 1512, 1467, 1449, 1349, 1251, 1196, 1139, 1118, 980, 951, 882, 855, 834, 814, 767, 749.

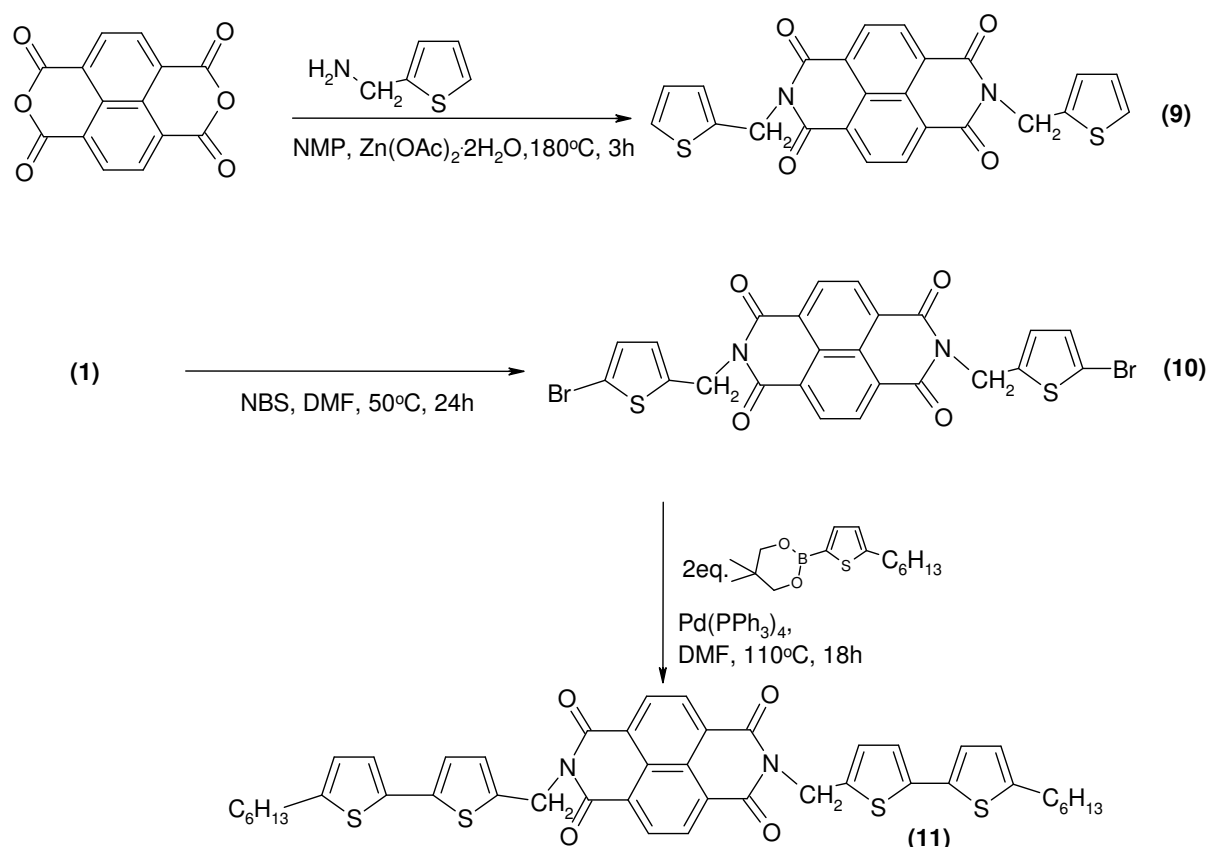
UV-vis (CHCl₃) λ_{max} = 237 nm, 311 nm, 340 nm, 360nm, 381 nm.

Elemental analysis: Calcd for C₄₆H₄₂N₂O₄S₂: C, 73.57, H, 5.64, N, 3.73, S, 8.54. Found: C, 72.00, H, 5.12, N, 3.84, S, 8.41.

Melting point: >340 °C, gradually darkens upon heating.

Preparation of alkylbithiophenemethyl naphthalenenebisimide

NBI-7 was synthesized using the reaction sequence presented in *Scheme 2*:



Scheme 2

Synthesis of *N, N'*- bis[(2-thienyl)methyl]-1,4,5,8-naphthalenetetracarboxylic-1,4:5,8-bisimide (9)

1.266 g (11.19 mmol) of 2-thienylmethylamine and 0.81g (3.73 mmol) of zinc acetate dihydrate were added to a stirred suspension of 1g (3.73 mmol) of 1,4,5,8-naphthalenetetracarboxylic acid bisanhydride in 40 mL of dry NMP. The resulting mixture was

stirred at the temperature of 180°C for 3 hours and then cooled to RT. Upon this cooling the obtained bisimide precipitated. The precipitate was filtered off and washed with acetone. As prepared bisimide is pure enough to be used for the next step. Yellow solid. 1.34 g (73%).

¹H NMR (CDCl₃+CF₃COOD, 400 MHz, ppm): 8.86 (s, 4H), 7.27-7.29 (m, 2H), 7.24-7.27 (m, 2H), 6.95-6.98 (m, 2H), 5.58 (s, 4H).

¹³C NMR (CDCl₃+CF₃COOD, 100 MHz, ppm): 163.4, 136.7, 132.1, 129.1, 126.8, 126.7, 126.6, 126.5, 39.0.

FTIR (KBr, cm⁻¹): 3080, 2963, 1703, 1669, 1581, 1450, 1419, 1357, 1320, 1253, 1158, 1104, 995, 884, 857, 770, 714.

UV-vis (CHCl₃) λ_{max} = 237 nm, 340 nm, 361 nm, 381 nm.

Elemental analysis: Calcd for C₂₄H₁₄N₂O₄S₂: C, 62.87, H, 3.08, N, 6.11, S, 13.95. Found: C, 62.75, H, 3.00, N, 6.21, S, 13.80.

Melting point: 329-331 °C, partial decomposition.

Synthesis of *N, N'*- bis[(5-bromo-2-thienyl)methyl]-1,4,5,8-naphthalenetetracarboxylic-1,4:5,8-bisimide (10)

0.3 g (0.65 mmol) of **(1)** and 0.25 g (0.133 mmol) of NBS were suspended in 40 mL of dry DMF and stirred at 50°C for 24 hours. After cooling, the reaction mixture was poured onto 100 mL of water. The obtained yellow precipitate was filtered off and washed with water and finally dried. The crude product was purified with a chromatography column (silica gel, methylene chloride). Pale yellow solid. 0.3 g (74%).

¹H NMR (CDCl₃+CF₃COOD, 400 MHz, ppm): 8.78 (s, 4H), 7.05 (d, 2H, J=3.6 Hz), 6.95 (d, 2H, J=4.0 Hz), 5.44 (s, 4H).

¹³C NMR (CDCl₃+CF₃COOD, 100 MHz, ppm): 162.8, 138.7, 131.7, 129.5, 129.4, 126.7, 126.5, 113.2 (C-Br), 38.8.

FTIR (KBr, cm⁻¹): 3079, 2961, 1706, 1668, 1581, 1453, 1441, 1372, 1329, 1247, 1222, 1161, 1107, 998, 962, 890, 797, 771.

UV-vis (CHCl₃) λ_{max} = 238 nm, 340 nm, 361 nm, 381 nm.

Melting point: 272-273 °C, partial decomposition.

Synthesis of *N, N'*- bis[(5'-hexyl-2,2'-bithiophen-5-yl)methyl]-1,4,5,8-naphthalenetetracarboxylic -1,4:5,8-bisimide (NBI-7)(11).

To a suspension of 0.24 g (0.39 mmol) of **(2)** in 30 mL of dry DMF at 40°C, 10 mg of tetrakis(triphenylphosphine)palladium was added under argon atmosphere and then stirred for 5 minutes. In the next step 0.282 g (1.33 mmol) of potassium phosphate and 0.282 g (1 mmol) of 5-hexyl-2-thienylboronic acid neopentyl glycol ester were consecutively added. The resulting mixture was heated at 110°C for 18 hours. After cooling to RT the reaction mixture was poured onto 100 mL of chloroform. DMF was then removed by repeated extractions with water. The organic phase was dried with anhydrous magnesium sulphate which was followed by evaporation of chloroform. The crude product was then purified using a chromatographic column (silica gel, methylene chloride) to yield 0.13 g of pink powder. Careful rinsing of the product with 50 mL of acetone/methylene chloride (1:1 v/v), followed by drying, yielded 0.122 g of light grey solid (40%).

¹H NMR (CDCl₃, 400 MHz, ppm): 8.78 (s, 4H), 7.15 (d, 2H, J=3.6 Hz), 6.89 (apparent doublet, 4H, J=3.6 Hz), 6.61 (d, 2H, J=3.6 Hz), 5.47 (s, 4H), 2.73 (t, 4H, J=7.4 Hz), 1.58-1.66 (m, 4H), 1.24-1.38 (m, 12H), 0.86 (t, 6H, J=6.8 Hz).

¹³C NMR (CDCl₃, 100 MHz, ppm): 162.4, 145.5, 138.7, 135.9, 134.4, 131.2, 130.0, 126.7, 126.6, 124.6, 123.4, 122.2, 38.6, 31.5, 31.4, 30.1, 28.7, 22.5, 14.1.

FTIR (KBr, cm⁻¹): 3071, 2958, 2927, 2855, 1705, 1668, 1581, 1451, 1411, 1368, 1325, 1245, 1190, 1102, 1044, 884, 838, 796, 771, 697.

UV-vis (CHCl₃) λ_{max} = 237 nm, 326 nm, 339 nm, 361 nm, 381 nm.

Elemental analysis: Calcd for C₄₄H₄₂N₂O₄S₄: C, 66.81, H, 5.35, N, 3.54, S, 16.21. Found: C, 66.54, H, 5.48, N, 3.53, S, 16.44.

Melting point: 252-253 °C, partial decomposition.

Test transistors fabrication and testing

Gold source and drain electrodes (30 nm thick) were deposited on the substrate by evaporation in vacuum and then, patterned by photolithography giving a channel width W of 0.5 mm and a channel length L of 20 μm. In the next step naphthalene bisimide-based semiconductor layer was spin coated from 1,2-dichlorobenzene and dried at 110°C until the complete removal of the solvent. An insulating layer, consisting of Cytop from Asahi Glass (Japan), was then spin coated onto the organic semiconductor one and also dried at 100°C. The thickness of the dielectric layer was determined using a surface step profiler. The films were typically 1.2 μm thick, which corresponds to the gate capacitance of $C_i = 1.4$ nF/cm². In the final step, the Ag (100 nm) gate electrode was deposited by ink-jet using Dimatix. The electrical characteristics of the fabricated devices were taken at ambient atmosphere conditions, using a HP4155A semiconductor parameter analyzer. In the calculations of the key device parameters, such as charge carriers mobility (μ), threshold voltage (V_T), on/off current ratio equation (1) was used:

$$I_D = \frac{1}{2} \frac{W}{L} C_{ox} \mu_{SAT} (V_G - V_T)^2 \quad (1)$$

where W is the channel width, L is the channel length, C_{ox} is the dielectric capacity, μ_{SAT} is the saturation field mobility and V_G and V_T are the gate voltage and the threshold voltage, respectively. The saturation mobilities were taken at the drain voltage of 100 V.

The optimal B3LYP/6-31G* geometries (x, y, z coordinates in Ångstroms) and total energies in parentheses in Hartree of studied systems.

NBI-1 (-1262.1071821)

6	-1.767252	-1.741933	0.462747
6	-0.544087	-2.434876	0.382944
6	0.636663	-1.751736	0.134937
6	0.616954	-0.349388	-0.039986
6	-0.616954	0.349388	0.039986
6	-1.808856	-0.366579	0.293815
6	-0.636663	1.751736	-0.134937

6	0.544087	2.434876	-0.382944
6	1.767252	1.741933	-0.462747
6	1.808856	0.366579	-0.293815
6	1.922367	-2.496412	0.054166
7	3.090067	-1.745695	-0.197280
6	3.109503	-0.354123	-0.381785
8	4.151122	0.247201	-0.605582
8	1.960909	-3.709646	0.201616
6	-3.109503	0.354123	0.381785
7	-3.090067	1.745695	0.197280
6	-1.922367	2.496412	-0.054166
8	-4.151122	-0.247201	0.605582
8	-1.960909	3.709646	-0.201616
6	4.379407	-2.507357	-0.270174
6	4.984304	-2.445060	-1.685991
6	6.107760	-3.467636	-1.895393
6	5.333389	-2.090163	0.856092
6	-4.379407	2.507357	0.270174
6	-4.984304	2.445060	1.685991
6	-6.107760	3.467636	1.895393
1	-4.068836	3.536583	0.087113
1	-2.694488	-2.270193	0.656839
1	-0.504860	-3.510888	0.513654
1	0.504860	3.510888	-0.513654
1	2.694488	2.270193	-0.656839
1	4.068836	-3.536583	-0.087113
1	4.180363	-2.646345	-2.406158
1	5.350955	-1.435269	-1.889116
1	6.452734	-3.447906	-2.934896
1	6.975381	-3.259645	-1.259785
1	5.767957	-4.487655	-1.676978
1	6.181204	-2.781765	0.893411
1	5.714425	-1.077496	0.711053
1	4.825730	-2.141347	1.825574
6	-5.333389	2.090163	-0.856092
1	-5.350955	1.435269	1.889116
1	-4.180363	2.646345	2.406158
1	-6.452734	3.447906	2.934896
1	-5.767957	4.487655	1.676978
1	-6.975381	3.259645	1.259785
1	-5.714425	1.077496	-0.711053
1	-4.825730	2.141347	-1.825574
1	-6.181204	2.781765	-0.893411

NBI-2 (-1576.6110183)

6	-0.659582	2.725799	0.290452
6	0.708337	2.741783	-0.042260
6	-1.350462	1.526743	0.368594
6	-0.681805	0.306361	0.111390

6	0.699374	0.322372	-0.220807
6	1.384594	1.558215	-0.293849
6	-1.366852	-0.929954	0.180995
6	-0.691655	-2.113275	-0.073826
6	0.677523	-2.097375	-0.401821
6	1.368646	-0.898178	-0.474501
6	2.832556	1.590603	-0.636775
7	3.463970	0.351987	-0.845085
6	2.814996	-0.893417	-0.820568
8	3.425110	-1.922389	-1.073869
8	3.448796	2.642930	-0.725951
6	-2.794805	1.525844	0.727150
7	-3.437078	0.275815	0.768662
6	-2.812317	-0.958818	0.531116
8	-3.439777	-2.005034	0.614870
8	-3.398267	2.559489	0.974499
6	4.898219	0.343630	-1.211905
6	5.838031	-0.112060	-0.075077
6	7.237455	-0.333419	-0.690420
6	8.307050	-0.882008	0.263259
6	9.644239	-1.161342	-0.436721
6	10.719406	-1.700213	0.512566
6	5.839635	0.878298	1.118893
6	5.887147	0.205923	2.497582
6	-4.863967	0.238718	1.154726
6	-5.850932	0.047943	-0.017630
6	-7.286674	-0.029756	0.569468
6	-8.171516	-1.126347	-0.042772
6	-9.580531	-1.172172	0.562103
6	10.454842	-2.283806	-0.027252
6	-5.688264	1.150261	-1.082997
6	-6.584807	0.995309	-2.316882
1	-1.194326	3.647800	0.491857
1	1.254887	3.676618	-0.105417
1	-1.239154	-3.047831	-0.013615
1	1.213099	-3.019214	-0.602052
1	4.997911	-0.332566	-2.063958
1	5.138658	1.358865	-1.529344
1	5.469244	-1.085436	0.273656
1	7.139385	-1.027817	-1.537451
1	7.592829	0.618385	-1.115312
1	8.477695	-0.172140	1.083548
1	7.942206	-1.809585	0.728426
1	9.482578	-1.879181	-1.253335
1	10.004511	-0.237411	-0.911229
1	11.660549	-1.891224	-0.015559
1	10.929023	-0.987272	1.319540
1	10.401583	-2.641445	0.977828
1	6.687403	1.570027	1.014189
1	4.947129	1.511781	1.077373

1	5.894196	0.954290	3.298759
1	5.009479	-0.434562	2.649902
1	6.775230	-0.422288	2.621859
1	-4.975250	-0.590667	1.856344
1	-5.064242	1.177412	1.673019
1	-5.616080	-0.919545	-0.481377
1	-7.231109	-0.211547	1.652733
1	-7.779474	0.947260	0.461505
1	-8.248592	-0.986676	-1.129244
1	-7.682101	-2.100500	0.102998
1	-9.502901	-1.305893	1.650664
1	10.072271	-0.200448	0.410722
1	11.454094	-2.288095	0.422957
1	10.578099	-2.159657	-1.110245
1	10.008441	-3.271274	0.142951
1	-5.870456	2.127871	-0.616459
1	-4.642930	1.166674	-1.417754
1	-6.363243	1.775282	-3.054316
1	-6.431358	0.024369	-2.804037
1	-7.647785	1.077100	-2.064948

NBI-3 (-2205.6440543)

6	-0.601816	1.896412	-1.557879
6	0.681669	1.464491	-1.943052
6	1.301642	0.420602	-1.274962
6	0.646783	-0.218791	-0.195141
6	-0.646885	0.219459	0.195816
6	-1.261075	1.286671	-0.502308
6	-1.301741	-0.419934	1.275639
6	-0.681768	-1.463820	1.943733
6	0.601704	-1.895761	1.558540
6	1.260961	-1.286022	0.502966
6	2.657619	-0.026336	-1.692183
7	3.213081	-1.106400	-0.988494
6	2.616173	-1.752764	0.105348
8	3.192238	-2.656483	0.693788
8	3.268621	0.511982	-2.604150
6	-2.616301	1.753395	-0.104708
7	-3.213207	1.107027	0.989134
6	-2.657738	0.026972	1.692828
8	-3.192432	2.657003	-0.693252
8	-3.268660	-0.511216	2.604926
1	-1.094398	2.711050	-2.077908
1	1.205085	1.938673	-2.766374
1	-1.205184	-1.938001	2.767054
1	1.094274	-2.710419	2.078548
6	4.556532	-1.564653	-1.398049
6	5.681466	-0.825351	-0.665839
6	7.067941	-1.303511	-1.115149

6	8.216553	-0.576430	-0.403786
6	9.606205	-1.039558	-0.859558
6	10.756893	-0.308258	-0.156149
6	12.146423	-0.764501	-0.619458
6	13.298242	-0.027701	0.076341
6	14.687271	-0.480620	-0.391750
6	15.839792	0.261502	0.297215
6	17.228413	-0.190475	-0.173001
6	18.381296	0.556107	0.510507
6	19.769734	0.103634	0.040243
6	20.922800	0.853212	0.719767
6	22.311422	0.400061	0.250939
6	23.456588	1.155650	0.932873
6	-4.556687	1.565218	1.398664
6	-5.681549	0.825776	0.666486
6	-7.068084	1.303755	1.115800
6	-8.216581	0.576640	0.404285
6	-9.606317	1.039565	0.860005
6	-10.756857	0.308144	0.156480
6	-12.146490	0.764277	0.619589
6	-13.298139	0.027288	-0.076286
6	-14.687283	0.480180	0.391489
6	-15.839623	-0.262151	-0.297550
6	-17.228365	0.189855	0.172277
6	-18.381064	-0.556897	-0.511352
6	-19.769627	-0.104386	-0.041496
6	-20.922507	-0.854087	-0.721192
6	-22.311255	-0.400905	-0.252768
6	-23.456234	-1.156613	-0.934883
1	4.600849	-2.634348	-1.188233
1	4.628834	-1.401921	-2.474432
1	5.581529	0.251065	-0.854083
1	5.566350	-0.981613	0.414208
1	7.156639	-2.385157	-0.936309
1	7.167343	-1.162630	-2.201474
1	8.120188	0.506037	-0.573659
1	8.121666	-0.723896	0.682114
1	9.703238	-2.121581	-0.685809
1	9.697170	-0.897611	-1.946756
1	10.655500	0.774256	-0.324429
1	10.670035	-0.455253	0.930751
1	12.249664	-1.846025	-0.445792
1	12.230496	-0.623288	-1.707379
1	13.192644	1.054083	-0.094266
1	13.216851	-0.171830	1.164090
1	14.794675	-1.561370	-0.215717
1	14.766342	-0.342111	-1.480416
1	15.731438	1.342348	0.122393
1	15.762003	0.121870	1.385826
1	17.338260	-1.270408	0.006515

1	17.304450	-0.055638	-1.262352
1	18.271436	1.636013	0.330897
1	18.305450	0.421422	1.599878
1	19.880662	-0.975612	0.223332
1	19.844445	0.234830	-1.049674
1	20.813382	1.932607	0.536033
1	20.848715	0.723099	1.809959
1	22.421981	-0.677860	0.436766
1	22.385504	0.529021	-0.838381
1	24.433822	0.808499	0.578047
1	23.393931	2.232877	0.734832
1	23.429346	1.018518	2.021022
1	-4.629012	1.402496	2.475049
1	-4.601055	2.634906	1.188830
1	-5.566486	0.981975	-0.413576
1	-5.581456	-0.250611	0.854804
1	-7.167536	1.162663	2.202092
1	-7.156870	2.385427	0.937154
1	-8.121655	0.724172	-0.681601
1	-8.120095	-0.505825	0.574107
1	-9.697344	0.897493	1.947181
1	-9.703469	2.121595	0.686360
1	-10.669892	0.455049	-0.930422
1	-10.655371	-0.774346	0.324869
1	-12.230686	0.623104	1.707506
1	-12.249818	1.845784	0.445862
1	-13.216587	0.171202	-1.164051
1	-13.192478	-1.054454	0.094557
1	-14.766539	0.341823	1.480160
1	-14.794732	1.560899	0.215282
1	-15.761628	-0.122787	-1.386180
1	-15.731237	-1.342948	-0.122436
1	-17.304644	0.055197	1.261633
1	-17.338211	1.269757	-0.007442
1	-18.304981	-0.422438	-1.600733
1	-18.271200	-1.636763	-0.331491
1	-19.844605	-0.235430	1.048421
1	-19.880530	0.974835	-0.224762
1	-20.848165	-0.724141	-1.811384
1	-20.813105	-1.933454	-0.537266
1	-22.385605	-0.529719	0.836550
1	-22.421791	0.676989	-0.438768
1	-24.433564	-0.809461	-0.580325
1	-23.428745	-1.019609	-2.023041
1	-23.393576	-2.233816	-0.736701

NBI-4 (-2038.7057221)

6	-2.427567	0.000000	0.703775
6	-2.427567	0.000000	-0.703775

6	-1.233308	0.000001	1.406772
6	0.000000	0.000000	0.711066
6	0.000000	0.000000	-0.711066
6	-1.233308	-0.000001	-1.406772
6	1.233308	-0.000001	1.406772
6	2.427567	0.000000	0.703775
6	2.427567	0.000000	-0.703775
6	1.233308	0.000001	-1.406772
6	-1.254238	-0.000004	-2.895062
7	0.000000	0.000000	-3.540422
6	1.254238	0.000004	-2.895062
8	2.292083	-0.000003	-3.534126
8	-2.292083	0.000003	-3.534126
6	-1.254238	0.000004	2.895062
7	0.000000	0.000000	3.540422
6	1.254238	-0.000004	2.895062
8	2.292083	0.000003	3.534126
8	-2.292083	-0.000003	3.534126
6	0.000000	0.000000	-4.991321
6	0.000000	0.000000	4.991321
1	-3.358122	0.000001	1.261330
1	-3.358122	-0.000001	-1.261330
1	3.358122	-0.000001	1.261330
1	3.358122	0.000001	-1.261330
6	0.000026	-1.211636	-5.672209
6	0.000029	-1.232057	-7.072396
6	-0.000026	1.211636	-5.672209
6	-0.000029	1.232057	-7.072396
6	0.000000	0.000000	-7.742874
6	0.000026	1.211636	5.672209
6	0.000029	1.232057	7.072396
6	0.000000	0.000000	7.742874
6	-0.000029	-1.232057	7.072396
6	-0.000026	-1.211636	5.672209
1	0.000000	0.000000	-8.823794
1	0.000000	0.000000	8.823794
1	0.000043	-2.133655	-5.099634
6	0.000051	-2.582983	-7.814152
1	-0.000043	2.133655	-5.099634
6	-0.000051	2.582983	-7.814152
1	0.000043	2.133655	5.099634
6	0.000051	2.582983	7.814152
6	-0.000051	-2.582983	7.814152
1	-0.000043	-2.133655	5.099634
6	-1.262402	-3.385527	-7.418830
6	1.262695	-3.385353	-7.419084
6	-0.000113	-2.414319	-9.345134
6	1.262402	3.385527	-7.418830
6	-1.262695	3.385353	-7.419084
6	0.000113	2.414319	-9.345134

6	-1.262402	3.385527	7.418830
6	1.262695	3.385353	7.419084
6	-0.000113	2.414319	9.345134
6	0.000113	-2.414319	9.345134
6	1.262402	-3.385527	7.418830
6	-1.262695	-3.385353	7.419084
1	-2.174164	-2.843732	-7.694566
1	-1.303182	-3.578532	-6.341802
1	-1.273065	-4.354906	-7.932042
1	1.303709	-3.578377	-6.342070
1	2.174327	-2.843420	-7.694982
1	1.273401	-4.354718	-7.932321
1	0.887893	-1.877286	-9.697456
1	-0.888303	-1.877479	-9.697287
1	-0.000053	-3.400170	-9.823517
1	2.174164	2.843732	-7.694566
1	1.303182	3.578532	-6.341802
1	1.273065	4.354906	-7.932042
1	-1.303709	3.578377	-6.342070
1	-2.174327	2.843420	-7.694982
1	-1.273401	4.354718	-7.932321
1	-0.887893	1.877286	-9.697456
1	0.888303	1.877479	-9.697287
1	0.000053	3.400170	-9.823517
1	-2.174164	2.843732	7.694566
1	-1.303182	3.578532	6.341802
1	-1.273065	4.354906	7.932042
1	1.303709	3.578377	6.342070
1	2.174327	2.843420	7.694982
1	1.273401	4.354718	7.932321
1	0.887893	1.877286	9.697456
1	-0.888303	1.877479	9.697287
1	-0.000053	3.400170	9.823517
1	-0.887893	-1.877286	9.697456
1	0.888303	-1.877479	9.697287
1	0.000053	-3.400170	9.823517
1	2.174164	-2.843732	7.694566
1	1.303182	-3.578532	6.341802
1	1.273065	-4.354906	7.932042
1	-1.303709	-3.578377	6.342070
1	-2.174327	-2.843420	7.694982
1	-1.273401	-4.354718	7.932321

NBI-5 (-1724.2019298)

6	0.703756	2.672057	0.036288
6	-0.703760	2.672057	0.036280
6	1.406692	1.478408	-0.003856
6	0.711097	0.245673	-0.044626
6	-0.711100	0.245673	-0.044633

6	-1.406696	1.478408	-0.003873
6	1.406637	-0.987069	-0.085685
6	0.703739	-2.180764	-0.125052
6	-0.703740	-2.180764	-0.125060
6	-1.406639	-0.987069	-0.085698
6	-2.894712	1.499720	-0.004401
7	-3.540592	0.245683	-0.047743
6	-2.894612	-1.008362	-0.088191
8	-3.534220	-2.045124	-0.123295
8	-3.534442	2.536406	0.029463
6	2.894708	1.499719	-0.004341
7	3.540590	0.245683	-0.047697
6	2.894610	-1.008361	-0.088187
8	3.534218	-2.045126	-0.123198
8	3.534438	2.536407	0.029478
6	-4.989174	0.245102	-0.052446
6	4.989172	0.245103	-0.052358
1	1.261198	3.602139	0.067507
1	-1.261202	3.602139	0.067490
1	1.261234	-3.110807	-0.156345
1	-1.261235	-3.110807	-0.156356
6	-5.686584	0.189553	1.151980
6	-7.079904	0.191360	1.140917
6	-5.677987	0.304498	-1.261802
6	-7.071175	0.306446	-1.260679
6	-7.795596	0.248096	-0.062468
6	5.678021	0.304880	-1.261675
6	7.071209	0.306841	-1.260508
6	7.795594	0.248123	-0.062293
6	7.079865	0.191000	1.141051
6	5.686545	0.189180	1.152071
6	-9.308366	0.207150	-0.070071
6	-9.864283	-1.229399	-0.174288
6	9.308365	0.207209	-0.069857
6	9.864319	-1.229287	-0.174605
1	-5.140802	0.149109	2.089826
1	-7.620580	0.152084	2.083690
1	-5.125430	0.353858	-2.195251
1	-7.604948	0.358565	-2.206765
1	5.125492	0.354529	-2.195125
1	7.605011	0.359264	-2.206562
1	7.620513	0.151429	2.083829
1	5.140735	0.148438	2.089888
6	-11.397847	-1.308838	-0.241405
1	-9.439428	-1.702913	-1.069338
1	-9.501767	-1.816845	0.681117
6	11.397889	-1.308666	-0.241669
1	9.501770	-1.817072	0.680552
1	9.439524	-1.702463	-1.069864
6	12.116685	-0.849289	1.032568

6	-12.116725	-0.848996	1.032618
1	-9.689001	0.796423	-0.915325
1	-9.688783	0.685217	0.840493
1	9.688734	0.684931	0.840907
1	9.689022	0.796818	-0.914867
1	-11.680787	-2.348587	-0.453409
1	-11.753693	-0.717165	-1.097199
1	11.753769	-0.716662	-1.097220
1	11.680863	-2.348328	-0.454051
1	11.780152	-1.424940	1.904060
1	11.938586	0.210692	1.246340
1	13.200324	-0.986240	0.942913
1	-11.938664	0.211070	1.245998
1	-11.780227	-1.424308	1.904347
1	-13.200356	-0.986007	0.942955

NBI-6 (-1724.1838801)

6	2.407709	0.705604	0.012641
6	2.407707	-0.705605	0.012713
6	1.228677	1.393347	0.012981
6	0.000001	0.699947	0.013232
6	-0.000001	-0.699947	0.013232
6	1.228676	-1.393348	0.013073
6	-1.228676	1.393348	0.013073
6	-2.407707	0.705605	0.012713
6	-2.407709	-0.705604	0.012641
6	-1.228677	-1.393347	0.012981
6	1.238859	-2.883712	0.013266
7	0.000000	-3.522919	0.015848
6	-1.238859	-2.883712	0.012948
8	-2.256026	-3.503409	0.010730
8	2.256032	-3.503404	0.011403
6	1.238859	2.883712	0.012948
7	0.000000	3.522919	0.015848
6	-1.238859	2.883712	0.013266
8	-2.256032	3.503404	0.011403
8	2.256026	3.503409	0.010730
6	0.000001	-4.965260	0.017152
6	-0.000001	4.965260	0.017152
1	3.332982	1.248173	0.012308
1	3.332980	-1.248175	0.012489
1	-3.332980	1.248175	0.012489
1	-3.332982	-1.248173	0.012308
6	0.000026	-5.658681	-1.178962
6	0.000018	-7.038567	-1.172475
6	-0.000026	-5.656043	1.207077
6	-0.000026	-7.043520	1.204918
6	-0.000006	-7.767467	0.018995
6	0.000026	5.656043	1.207077

6	0.000026	7.043520	1.204918
6	0.000006	7.767467	0.018995
6	-0.000018	7.038567	-1.172475
6	-0.000026	5.658681	-1.178962
6	0.000012	-9.305039	-0.023809
6	-1.258520	-9.799805	-0.762994
6	1.258671	-9.799766	-0.762806
6	-0.000088	-9.928353	1.380353
6	-0.000012	9.305039	-0.023809
6	0.000088	9.928353	1.380353
6	1.258520	9.799805	-0.762994
6	-1.258671	9.799766	-0.762806
1	0.000038	-5.121466	-2.109944
1	0.000038	-7.550464	-2.116683
1	-0.000044	-5.119907	2.138713
1	-0.000041	-7.546084	2.151692
1	0.000044	5.119907	2.138713
1	0.000041	7.546084	2.151692
1	-0.000038	7.550464	-2.116683
1	-0.000038	5.121466	-2.109944
1	-1.276187	-10.885492	-0.791536
1	-2.160139	-9.461074	-0.262907
1	-1.294394	-9.444310	-1.786537
1	1.276373	-10.885452	-0.791358
1	1.294688	-9.444255	-1.786338
1	2.160204	-9.461014	-0.262578
1	-0.000079	-11.010219	1.297003
1	0.879691	-9.645220	1.948998
1	-0.879952	-9.645223	1.948867
1	0.000079	11.010219	1.297003
1	-0.879691	9.645220	1.948998
1	0.879952	9.645223	1.948867
1	1.276187	10.885492	-0.791536
1	2.160139	9.461074	-0.262907
1	1.294394	9.444310	-1.786537
1	-1.276373	10.885452	-0.791358
1	-1.294688	9.444255	-1.786338
1	-2.160204	9.461014	-0.262578

NBI-7 (-3705.2421057)

6	0.802204	-0.922457	2.214171
6	-0.320495	-1.690811	1.852406
6	1.242966	0.104953	1.395226
6	0.566203	0.389609	0.184512
6	-0.565502	-0.387635	-0.181681
6	-0.998260	-1.431248	0.671809
6	0.998958	1.433224	-0.668975
6	0.321180	1.692799	-1.849562
6	-0.801507	0.924430	-2.211338

6	-1.242254	-0.102993	-1.392404
6	-2.180629	-2.253093	0.300349
7	-2.808091	-1.939706	-0.915486
6	-2.431111	-0.904841	-1.784328
6	2.431900	0.906715	1.787090
7	2.808885	1.941578	0.918248
6	2.181356	2.255039	-0.297538
8	-2.591177	-3.164419	1.003945
8	-3.057734	-0.687807	-2.811709
8	2.591858	3.166420	-1.001085
8	3.058559	0.689626	2.814440
1	1.339281	-1.120693	3.135543
1	-0.672672	-2.495884	2.488389
1	0.673348	2.497880	-2.485540
1	-1.338570	1.122649	-3.132722
6	-4.000215	-2.741801	-1.287990
6	4.001218	2.743462	1.290552
6	-5.281023	-2.212476	-0.712500
6	-5.912575	-2.627274	0.431735
6	-7.107004	-1.910543	0.712919
6	-7.395668	-0.935729	-0.218580
6	-6.169581	-0.912018	-1.474701
6	5.281781	2.213981	0.714659
6	5.913153	2.628857	-0.429642
6	7.107247	1.911775	-0.711357
6	7.395867	0.936641	0.219825
6	6.170111	0.913014	1.476287
1	-4.026349	-2.764424	-2.377376
1	-3.827950	-3.748165	-0.906687
1	3.829026	3.749894	0.909405
1	4.027636	2.765960	2.379933
1	-5.514721	-3.416555	1.060369
1	-7.727253	-2.095273	1.583667
6	-8.514691	-0.015396	-0.257835
1	5.515357	3.418395	-1.057989
1	7.727307	2.096558	-1.582229
6	8.514541	0.015873	0.258482
6	8.670903	-1.132127	1.002080
6	9.911035	-1.792792	0.776062
6	10.717451	-1.167523	-0.139060
6	9.940656	0.285387	-0.734502
6	-8.670794	1.132954	-1.000940
6	-9.911491	1.792892	-0.775868
6	-10.718589	1.166697	0.138023
6	-9.941755	-0.286200	0.733420
1	7.908650	-1.502811	1.679673
1	10.196680	-2.716124	1.270558
6	12.084474	-1.574834	-0.610937
1	-7.907956	1.504389	-1.677462
1	-10.197056	2.716374	-1.270130

6	-12.086315	1.573101	0.608653
1	12.270910	-2.593142	-0.245734
6	13.225002	-0.649375	-0.139039
1	12.104069	-1.634623	-1.708470
1	-12.106959	1.632883	1.706171
6	-13.225774	0.646874	0.135701
1	-12.273102	2.591279	0.243269
1	-13.042460	-0.371934	0.503674
1	-13.202829	0.585235	-0.960562
6	-14.607108	1.121575	0.603209
1	-14.783986	2.143283	0.235225
1	-14.616038	1.189070	1.701409
6	-15.753144	0.212153	0.141920
1	-15.577991	-0.809504	0.510360
1	-15.744007	0.143957	-0.956063
6	-17.135772	0.687342	0.607378
1	-17.309946	1.708541	0.239398
1	-17.144549	0.754577	1.704641
6	-18.276064	-0.224163	0.142537
1	-18.147702	-1.245089	0.522776
1	-18.315799	-0.282531	-0.952199
1	-19.248528	0.141238	0.491803
1	13.203225	-0.587853	0.957255
1	13.041950	0.369591	-0.506707
6	14.605542	-1.124919	-0.608035
1	14.613250	-1.192367	-1.706247
1	14.782168	-2.146758	-0.240295
6	15.752651	-0.216244	-0.147947
1	15.744720	-0.148038	0.950045
1	15.577777	0.805526	-0.516205
6	17.134474	-0.692341	-0.614868
1	17.142036	-0.759608	-1.712139
1	17.308377	-1.713647	-0.247053
6	18.275857	0.218427	-0.151267
1	18.316735	0.276874	0.943423
1	18.147823	1.239405	-0.531477
1	19.247715	-0.147682	-0.501475

NBI-8 (-3771.3679516)

6	-10.128189	-0.559874	0.595662
6	-9.278821	0.063346	-0.285505
16	-10.214048	0.940473	-1.480787
6	-11.732714	0.440584	-0.768805
6	-11.519890	-0.352965	0.336636
6	-7.812240	0.056924	-0.299722
6	-7.091816	-0.164225	0.889239
6	-5.702072	-0.194220	0.891179
6	-5.000489	0.016744	-0.295067
6	-5.691048	0.250822	-1.482326

6	-7.082164	0.263766	-1.484092
7	-3.553315	-0.001884	-0.289378
6	-2.916977	-1.149303	-0.812233
6	-1.429063	-1.152571	-0.785632
6	-0.722433	-0.044333	-0.259335
6	-1.406540	1.086111	0.249073
6	-2.893843	1.127665	0.243670
6	-0.693035	2.159978	0.757397
6	0.714082	2.137676	0.775002
6	1.405775	1.041126	0.285085
6	0.699171	-0.067496	-0.239859
6	1.383840	-1.199099	-0.744682
6	2.871143	-1.245452	-0.728492
7	3.531525	-0.117586	-0.191338
6	2.893182	1.035396	0.318615
6	-0.736860	-2.248350	-1.276469
6	0.670362	-2.271861	-1.255586
6	4.977614	-0.145999	-0.154017
6	5.634330	-0.983680	0.745545
6	7.024313	-0.999232	0.790773
6	7.788773	-0.181537	-0.061108
6	7.103142	0.645164	-0.970957
6	5.713826	0.667588	-1.014552
6	9.254191	-0.168585	-0.005058
16	10.171631	-1.543326	0.579402
6	11.697697	-0.719421	0.345162
6	11.500983	0.543419	-0.168377
6	10.114913	0.841841	-0.358488
8	3.538061	1.969816	0.761398
8	3.497855	-2.201203	-1.151081
8	-3.564103	-2.080885	-1.257470
8	-3.521862	2.078416	0.675536
1	-9.771690	-1.182855	1.410489
1	9.769138	1.804137	-0.723807
1	1.219163	-3.126496	-1.636511
1	-1.302328	-3.084285	-1.674184
1	1.279920	2.973708	1.171902
1	-1.241941	3.013586	1.140483
1	-5.159316	-0.362689	1.816081
1	-7.627852	-0.293443	1.824120
1	-7.609248	0.419307	-2.420921
1	-5.140975	0.408936	-2.404620
1	5.058575	-1.616441	1.413410
1	7.523039	-1.638195	1.513685
1	7.666597	1.262633	-1.663361
1	5.199117	1.312467	-1.719704
6	12.592930	1.548825	-0.453559
6	12.986085	-1.429145	0.663611
6	-12.601868	-0.988788	1.178793
6	-13.028789	0.935301	-1.352661

6	-12.807734	-2.487291	0.878759
1	-12.344794	-0.871762	2.240973
1	-13.552591	-0.460292	1.040364
6	-13.871375	-3.140146	1.770050
1	-13.083943	-2.605908	-0.178204
1	-11.851193	-3.014136	1.001711
6	-14.073290	-4.633953	1.484281
1	-13.591555	-3.007184	2.825917
1	-14.828479	-2.612515	1.642203
6	-15.129050	-5.292789	2.381558
1	-14.357876	-4.766769	0.429978
1	-13.114306	-5.158800	1.607074
6	-15.325922	-6.787887	2.100300
1	-14.844987	-5.156555	3.435789
1	-16.089259	-4.770212	2.257001
6	-16.376696	-7.449625	3.001095
1	-15.613534	-6.925255	1.047125
1	-14.365043	-7.310095	2.221725
6	-16.564413	-8.943048	2.714984
1	-16.089300	-7.311988	4.053325
1	-17.337612	-6.929638	2.878850
1	-17.319291	-9.385967	3.374761
1	-16.886917	-9.111062	1.679950
1	-15.628034	-9.495363	2.862121
6	-13.431730	2.345826	-0.871566
1	-12.967673	0.935416	-2.449161
1	-13.825794	0.226013	-1.097000
6	-14.759652	2.826182	-1.469711
1	-13.496587	2.343484	0.225029
1	-12.632295	3.054010	-1.128123
6	-15.162960	4.230280	-1.000464
1	-14.689893	2.815849	-2.567676
1	-15.556215	2.112959	-1.209707
6	-16.493240	4.715742	-1.590789
1	-15.227512	4.240865	0.097641
1	-14.367128	4.942463	-1.263849
6	-16.892974	6.121229	-1.123469
1	-16.429739	4.702860	-2.689089
1	-17.289553	4.004523	-1.325032
6	-18.224348	6.608170	-1.709836
1	-16.954440	6.135349	-0.024944
1	-16.097742	6.833041	-1.390997
6	-18.614295	8.012954	-1.238640
1	-18.163320	6.593835	-2.807415
1	-19.019374	5.898015	-1.441041
1	-19.568574	8.331356	-1.673688
1	-18.716760	8.050495	-0.147024
1	-17.855151	8.751741	-1.523993
6	13.475769	-2.379901	-0.449747
1	13.761722	-0.679157	0.862471

1	12.875066	-1.999577	1.595618
6	14.789039	-3.086161	-0.091648
1	12.696662	-3.126957	-0.653198
1	13.600542	-1.807905	-1.379261
6	15.286647	-4.041666	-1.184249
1	15.564559	-2.332709	0.112572
1	14.656228	-3.645781	0.846327
6	16.598361	-4.750766	-0.823341
1	14.510668	-4.794039	-1.388485
1	15.421108	-3.482667	-2.122080
6	17.096533	-5.711584	-1.910649
1	17.374707	-3.997757	-0.621181
1	16.463397	-5.306179	0.116782
6	18.407195	-6.421463	-1.547859
1	16.320663	-6.465006	-2.113231
1	17.233027	-5.157450	-2.851421
6	18.895988	-7.382467	-2.636510
1	19.183377	-5.668884	-1.348254
1	18.270974	-6.973429	-0.606903
1	19.832434	-7.873110	-2.347314
1	18.155441	-8.167537	-2.833299
1	19.074799	-6.853811	-3.581014
6	12.744644	2.609071	0.655871
1	13.552567	1.037995	-0.596967
1	12.376727	2.055785	-1.404237
6	13.839210	3.642755	0.362950
1	11.782872	3.121335	0.798233
1	12.959644	2.101976	1.606773
6	13.985141	4.699389	1.465639
1	14.800873	3.126181	0.224514
1	13.623324	4.141907	-0.593571
6	15.085803	5.731479	1.187550
1	13.024749	5.219194	1.598156
1	14.191852	4.197876	2.422727
6	15.225817	6.787790	2.291018
1	16.046937	5.211719	1.058447
1	14.881301	6.232072	0.229345
6	16.329309	7.818468	2.019539
1	14.265730	7.310095	2.417971
1	15.426463	6.287148	3.250128
6	16.460783	8.868965	3.126997
1	17.288847	7.296721	1.893994
1	16.129070	8.319402	1.061582
1	17.255992	9.589450	2.903794
1	15.527270	9.431342	3.252488
1	16.695904	8.401258	4.091104

NBI-9 (-3142.3337727)

6	9.813795	-2.692973	-0.033999
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6	8.715726	-3.054386	-0.790364
16	9.132263	-4.315109	-1.941645
6	10.774296	-4.346568	-1.395287
6	10.982102	-3.444943	-0.392338
6	7.328962	-2.552912	-0.753408
6	6.623542	-2.455150	0.459188
6	5.315589	-1.979597	0.492184
6	4.679805	-1.617319	-0.694002
6	5.351302	-1.727332	-1.910555
6	6.665255	-2.184449	-1.936971
7	3.316773	-1.131610	-0.666144
6	3.108272	0.233139	-0.967621
6	1.698727	0.709096	-0.952490
6	0.646522	-0.185091	-0.640813
6	0.906127	-1.542984	-0.336537
6	2.301155	-2.060307	-0.343827
6	-0.140348	-2.399876	-0.033866
6	-1.467370	-1.930867	-0.026871
6	-1.746200	-0.605918	-0.322717
6	-0.694139	0.288815	-0.633941
6	-0.953384	1.646823	-0.938670
6	-2.349215	2.162189	-0.938516
7	-3.364184	1.231158	-0.622867
6	-3.156065	-0.130724	-0.310880
6	1.420374	2.034551	-1.246711
6	0.093373	2.503707	-1.240185
6	-4.729385	1.711482	-0.616725
6	-5.171585	2.536563	0.415761
6	-6.487759	2.988958	0.423768
6	-7.385070	2.625764	-0.595770
6	-6.911397	1.806558	-1.635803
6	-5.597203	1.347992	-1.644880
6	-8.778690	3.110030	-0.586500
16	-9.085165	4.825372	-0.362528
6	-10.796245	4.588734	-0.476232
6	-11.104890	3.274190	-0.673597
6	-9.960565	2.410816	-0.736452
8	-4.090832	-0.867198	-0.048363
8	-2.616656	3.322935	-1.194560
8	4.042294	0.971276	-1.228071
8	2.566542	-3.221652	-0.087900
6	9.856266	-1.589595	0.998205
6	-10.090874	0.910181	-0.862458
1	-0.132655	3.539399	-1.470361
1	2.245102	2.698739	-1.481902
1	-2.291953	-2.595152	0.208599
1	0.085794	-3.435757	0.195264
1	4.781103	-1.912209	1.434175
1	7.097737	-2.777992	1.380342
1	7.191904	-2.244462	-2.884684

1	4.852657	-1.440479	-2.830750
1	-4.489544	2.818705	1.211490
1	-6.833180	3.617915	1.238799
1	-7.574709	1.547845	-2.454858
1	-5.242390	0.715721	-2.452624
1	-12.123887	2.912639	-0.770661
1	-11.470131	5.431750	-0.400897
1	11.944956	-3.305616	0.089352
1	11.484090	-5.032708	-1.837875
6	-10.771295	0.256792	0.357704
1	-10.671677	0.668358	-1.764724
1	-9.104603	0.456150	-0.999239
6	-10.915575	-1.263624	0.216130
1	-10.186614	0.491198	1.257601
1	-11.762173	0.706140	0.512226
6	-11.585704	-1.926946	1.426393
1	-11.495508	-1.491622	-0.690894
1	-9.922039	-1.709467	0.061277
6	-11.729821	-3.448250	1.288772
1	-11.005450	-1.697655	2.332347
1	-12.579247	-1.480609	1.581920
6	-12.397724	-4.112665	2.499404
1	-12.310458	-3.677698	0.382722
1	-10.736161	-3.893786	1.132409
6	-12.542006	-5.633965	2.362963
1	-11.817172	-3.883963	3.405719
1	-13.391688	-3.667542	2.656768
6	-13.208734	-6.289429	3.576716
1	-13.123163	-5.862627	1.458128
1	-11.548969	-6.078615	2.205614
1	-13.297191	-7.374399	3.448682
1	-12.631623	-6.108046	4.491908
1	-14.217527	-5.889754	3.738525
6	10.754194	-0.405183	0.586174
1	8.847116	-1.213458	1.191175
1	10.222737	-1.998019	1.951651
6	10.831573	0.685239	1.662016
1	11.766371	-0.769788	0.362713
1	10.370443	0.022381	-0.349975
6	11.706300	1.879374	1.258416
1	9.816970	1.041241	1.894125
1	11.220510	0.247986	2.593963
6	11.807825	2.958010	2.344793
1	12.715806	1.521358	1.007035
1	11.305432	2.327246	0.337266
6	12.671893	4.158676	1.938503
1	10.797970	3.309585	2.603610
1	12.217092	2.510204	3.262743
6	12.784322	5.231465	3.029446
1	13.679763	3.807482	1.670733

1	12.257426	4.612600	1.025929
6	13.642170	6.430525	2.612468
1	11.777169	5.579073	3.300422
1	13.204100	4.779478	3.939454
1	13.704773	7.176612	3.412936
1	14.664978	6.119632	2.365914
1	13.225890	6.926334	1.726811

NBI-10 (-3024.4004339)

6	10.144889	2.401089	1.223462
6	9.478902	1.532143	0.390936
16	10.619486	0.767820	-0.705095
6	11.974172	1.644762	-0.029126
6	11.546979	2.462250	0.985130
6	8.043813	1.232049	0.346597
6	7.245511	1.415288	1.491481
6	5.878057	1.166936	1.459676
6	5.281373	0.714490	0.283862
6	6.053263	0.510047	-0.857615
6	7.419601	0.769935	-0.826113
7	3.856852	0.460529	0.248476
6	3.012121	1.565091	0.004366
6	1.551139	1.285705	-0.032043
6	1.071347	-0.029825	0.177689
6	1.960404	-1.104494	0.422331
6	3.429256	-0.867828	0.461893
6	1.465731	-2.382840	0.626526
6	0.079763	-2.626077	0.591859
6	-0.809878	-1.590620	0.352454
6	-0.328732	-0.276098	0.141679
6	-1.217994	0.797486	-0.104305
6	-2.686285	0.561144	-0.147994
7	-3.118838	-0.766876	0.069186
6	-2.271079	-1.869750	0.318590
6	0.661217	2.320696	-0.271462
6	-0.724345	2.076377	-0.308321
6	-4.543239	-1.016972	0.030091
6	-5.364060	-0.532563	1.046911
6	-6.733619	-0.771918	1.006020
6	-7.313439	-1.496780	-0.050661
6	-6.465291	-1.969776	-1.069524
6	-5.095343	-1.737395	-1.028669
6	-8.754505	-1.764537	-0.103751
16	-9.918696	-0.702760	0.672984
6	-11.272411	-1.685477	0.160136
6	-10.826523	-2.756467	-0.570466
6	-9.411411	-2.803323	-0.720809
8	-2.724713	-2.987098	0.494081

8	-3.483869	1.458027	-0.358339
8	3.469640	2.681525	-0.165740
8	4.231485	-1.761831	0.666194
1	9.639349	3.008966	1.966166
1	-8.892398	-3.600672	-1.241991
1	-1.427461	2.880866	-0.495629
1	1.055763	3.318853	-0.428754
1	-0.315099	-3.623858	0.750521
1	2.168399	-3.188144	0.812319
1	5.273307	1.313895	2.349317
1	7.706223	1.738906	2.419401
1	8.005600	0.633462	-1.730317
1	5.583020	0.159263	-1.771091
1	-4.931617	0.027523	1.869693
1	-7.358743	-0.407798	1.816121
1	-6.888499	-2.505306	-1.913475
1	-4.454196	-2.107414	-1.822290
1	-11.498731	-3.503052	-0.982251
6	-12.687448	-1.311505	0.500943
1	12.222595	3.105625	1.540445
6	13.373321	1.449330	-0.541166
6	-13.199004	-0.041674	-0.210364
1	-13.329412	-2.160546	0.232283
1	-12.792608	-1.179589	1.587184
6	-14.654272	0.291056	0.140224
1	-12.553843	0.807147	0.054794
1	-13.096982	-0.175745	-1.295640
6	-15.174212	1.555104	-0.556893
1	-15.297545	-0.561097	-0.125550
1	-14.746728	0.412483	1.229856
6	-16.627527	1.895570	-0.203357
1	-14.527655	2.405458	-0.294258
1	-15.084771	1.431821	-1.646341
6	-17.148312	3.159290	-0.900154
1	-17.275105	1.045302	-0.465127
1	-16.716917	2.019721	0.886293
6	-18.599598	3.493959	-0.540881
1	-16.501276	4.008870	-0.639269
1	-17.060438	3.034461	-1.988870
6	13.988128	0.071330	-0.219517
1	13.403455	1.608577	-1.628346
1	13.999496	2.235657	-0.099703
6	15.434696	-0.057572	-0.711425
1	13.946126	-0.093578	0.865475
1	13.372159	-0.716998	-0.673500
6	16.064065	-1.424038	-0.410359
1	15.468038	0.126672	-1.795675
1	16.046049	0.732901	-0.250896
6	17.515159	-1.546945	-0.892451
1	16.024974	-1.612314	0.672852

1	15.458339	-2.214775	-0.877352
6	18.138590	-2.913686	-0.590940
1	17.554325	-1.357245	-1.974638
1	18.119798	-0.757272	-0.424041
1	19.172944	-2.969658	-0.948951
1	18.148027	-3.116232	0.487150
1	17.574934	-3.721759	-1.073373
1	-18.940121	4.400671	-1.053825
1	-19.276421	2.677876	-0.822828
1	-18.713253	3.658779	0.537737

Table 1S: B3LYP/6-31G* normal modes for the optimal **NBI-1** molecule in C_i symmetry.

Number	1	2	3
Symmetry	AU	AU	AG
Frequency/ cm^{-1}	22.5162	32.4318	40.8545
Intensity / km mol^{-1}	0.248	0.1978	0
Number	4	5	6
Symmetry	AG	AU	AG
Frequency/ cm^{-1}	50.6393	59.9403	67.214
Intensity / km mol^{-1}	0	0.1496	0
Number	7	8	9
Symmetry	AU	AG	AU
Frequency/ cm^{-1}	67.6168	97.3589	106.2135
Intensity / km mol^{-1}	1.0885	0	7.3558
Number	10	11	12
Symmetry	AU	AG	AU
Frequency/ cm^{-1}	127.1669	152.0828	165.731
Intensity / km mol^{-1}	1.9559	0	1.9836
Number	13	14	15
Symmetry	AG	AU	AG
Frequency/ cm^{-1}	191.583	192.6003	205.8833
Intensity / km mol^{-1}	0	3.5412	0
Number	16	17	18
Symmetry	AU	AG	AU
Frequency/ cm^{-1}	215.7177	223.2312	243.6581
Intensity / km mol^{-1}	1.5991	0	3.2606
Number	19	20	21
Symmetry	AG	AU	AG
Frequency/ cm^{-1}	246.454	258.8611	260.1288
Intensity / km mol^{-1}	0	6.1389	0
Number	22	23	24
Symmetry	AG	AU	AU
Frequency/ cm^{-1}	286.563	293.9834	300.2765

Intensity / km mol ⁻¹	0	15.4862	15.5423
Number	25	26	27
Symmetry	AU	AG	AG
Frequency/ cm ⁻¹	303.8945	354.9218	362.4504
Intensity / km mol ⁻¹	0.0762	0	0
Number	28	29	30
Symmetry	AG	AU	AU
Frequency/ cm ⁻¹	411.9978	427.5871	431.6215
Intensity / km mol ⁻¹	0	0.5675	71.0297
Number	31	32	33
Symmetry	AU	AG	AG
Frequency/ cm ⁻¹	443.1621	447.8699	454.1003
Intensity / km mol ⁻¹	7.2181	0	0
Number	34	35	36
Symmetry	AU	AG	AG
Frequency/ cm ⁻¹	463.8932	468.4725	481.7462
Intensity / km mol ⁻¹	20.5742	0	0
Number	37	38	39
Symmetry	AU	AG	AG
Frequency/ cm ⁻¹	489.3182	498.6011	554.879
Intensity / km mol ⁻¹	0.0249	0	0
Number	40	41	42
Symmetry	AU	AU	AU
Frequency/ cm ⁻¹	586.6518	595.8215	614.4261
Intensity / km mol ⁻¹	14.2459	29.0031	0.0289
Number	43	44	45
Symmetry	AG	AG	AG
Frequency/ cm ⁻¹	617.9576	643.4021	718.6088
Intensity / km mol ⁻¹	0	0	0
Number	46	47	48
Symmetry	AG	AU	AU
Frequency/ cm ⁻¹	739.4004	746.188	749.2539
Intensity / km mol ⁻¹	0	15.5548	44.9916
Number	49	50	51
Symmetry	AU	AU	AG
Frequency/ cm ⁻¹	754.4335	769.393	769.9087
Intensity / km mol ⁻¹	7.136	0.2084	0
Number	52	53	54
Symmetry	AG	AU	AU
Frequency/ cm ⁻¹	788.038	788.9547	819.7918
Intensity / km mol ⁻¹	0	11.6319	0.6581
Number	55	56	57
Symmetry	AG	AU	AG
Frequency/ cm ⁻¹	825.7619	848.1577	882.7822

Intensity / km mol ⁻¹	0	26.3925	0
Number	58	59	60
Symmetry	AU	AG	AG
Frequency/ cm ⁻¹	901.328	904.2669	906.372
Intensity / km mol ⁻¹	30.5941	0	0
Number	61	62	63
Symmetry	AU	AG	AU
Frequency/ cm ⁻¹	925.7388	982.2847	984.0599
Intensity / km mol ⁻¹	22.2257	0	9.8527
Number	64	65	66
Symmetry	AU	AG	AU
Frequency/ cm ⁻¹	991.6293	1004.082	1005.184
Intensity / km mol ⁻¹	14.8653	0	0.0038
Number	67	68	69
Symmetry	AU	AG	AG
Frequency/ cm ⁻¹	1010.2428	1010.439	1040.4322
Intensity / km mol ⁻¹	3.8024	0	0
Number	70	71	72
Symmetry	AU	AG	AU
Frequency/ cm ⁻¹	1045.3696	1075.222	1100.916
Intensity / km mol ⁻¹	7.799	0	142.0493
Number	73	74	75
Symmetry	AG	AG	AU
Frequency/ cm ⁻¹	1103.1368	1156.341	1160.4249
Intensity / km mol ⁻¹	0	0	34.3545
Number	76	77	78
Symmetry	AG	AU	AG
Frequency/ cm ⁻¹	1168.8408	1170.572	1172.1054
Intensity / km mol ⁻¹	0	7.2607	0
Number	79	80	81
Symmetry	AG	AU	AG
Frequency/ cm ⁻¹	1202.0526	1206.217	1231.0804
Intensity / km mol ⁻¹	0	30.6678	0
Number	82	83	84
Symmetry	AU	AU	AG
Frequency/ cm ⁻¹	1235.3384	1241.692	1250.7156
Intensity / km mol ⁻¹	83.2971	47.2854	0
Number	85	86	87
Symmetry	AU	AG	AU
Frequency/ cm ⁻¹	1281.5625	1314.284	1314.7674
Intensity / km mol ⁻¹	250.2309	0	5.9978
Number	88	89	90
Symmetry	AG	AU	AU
Frequency/ cm ⁻¹	1348.5639	1357.66	1368.2847

Intensity / km mol ⁻¹	0	874.6626	16.2737
Number	91	92	93
Symmetry	AG	AU	AG
Frequency/ cm ⁻¹	1368.5672	1401.994	1405.8438
Intensity / km mol ⁻¹	0	2.7915	0
Number	94	95	96
Symmetry	AG	AU	AG
Frequency/ cm ⁻¹	1410.8271	1411.242	1433.3576
Intensity / km mol ⁻¹	0	4.2667	0
Number	97	98	99
Symmetry	AU	AU	AG
Frequency/ cm ⁻¹	1433.3975	1441.501	1442.332
Intensity / km mol ⁻¹	32.9674	22.0337	0
Number	100	101	102
Symmetry	AU	AG	AG
Frequency/ cm ⁻¹	1445.9679	1447.221	1454.0535
Intensity / km mol ⁻¹	27.0889	0	0
Number	103	104	105
Symmetry	AU	AG	AU
Frequency/ cm ⁻¹	1479.6788	1513.517	1520.4561
Intensity / km mol ⁻¹	133.1685	0	20.6926
Number	106	107	108
Symmetry	AG	AG	AU
Frequency/ cm ⁻¹	1520.4609	1524.807	1524.8122
Intensity / km mol ⁻¹	0	0	13.0827
Number	109	110	111
Symmetry	AU	AG	AU
Frequency/ cm ⁻¹	1534.4484	1534.458	1540.3669
Intensity / km mol ⁻¹	8.2529	0	10.5267
Number	112	113	114
Symmetry	AG	AG	AU
Frequency/ cm ⁻¹	1540.372	1542.935	1542.9421
Intensity / km mol ⁻¹	0	0	10.2478
Number	115	116	117
Symmetry	AU	AU	AG
Frequency/ cm ⁻¹	1564.6807	1626.64	1646.4379
Intensity / km mol ⁻¹	10.411	129.5785	0
Number	118	119	120
Symmetry	AG	AU	AG
Frequency/ cm ⁻¹	1667.6487	1736.783	1741.5026
Intensity / km mol ⁻¹	0	669.8841	0
Number	121	122	123
Symmetry	AU	AG	AU
Frequency/ cm ⁻¹	1773.5857	1776.787	3048.3149

Intensity / km mol ⁻¹	376.546	0	58.5938
Number	124	125	126
Symmetry	AG	AG	AU
Frequency/ cm ⁻¹	3048.3521	3050.011	3050.025
Intensity / km mol ⁻¹	0	0	54.4509
Number	127	128	129
Symmetry	AU	AG	AG
Frequency/ cm ⁻¹	3066.0368	3066.07	3105.3835
Intensity / km mol ⁻¹	40.9456	0	0
Number	130	131	132
Symmetry	AU	AU	AG
Frequency/ cm ⁻¹	3105.3843	3119.407	3119.4119
Intensity / km mol ⁻¹	15.8067	91.2198	0
Number	133	134	135
Symmetry	AG	AU	AU
Frequency/ cm ⁻¹	3123.1401	3123.153	3127.8792
Intensity / km mol ⁻¹	0	29.3718	79.821
Number	136	137	138
Symmetry	AG	AU	AG
Frequency/ cm ⁻¹	3127.9251	3139.48	3139.4898
Intensity / km mol ⁻¹	0	13.4089	0
Number	139	140	141
Symmetry	AU	AG	AU
Frequency/ cm ⁻¹	3167.1482	3167.159	3228.183
Intensity / km mol ⁻¹	21.6402	0	0.0257
Number	142	143	144
Symmetry	AG	AU	AG
Frequency/ cm ⁻¹	3228.4201	3238.882	3238.9702
Intensity / km mol ⁻¹	0	0.0077	0

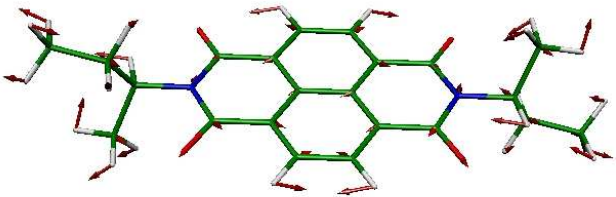
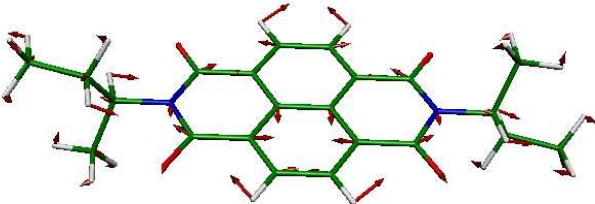
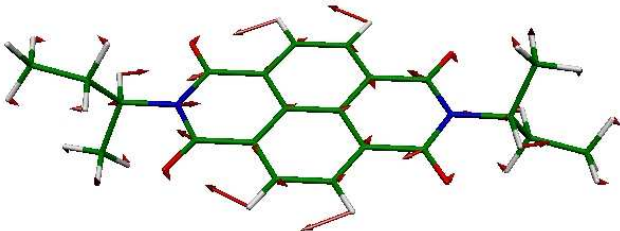
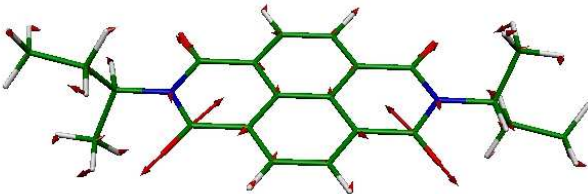
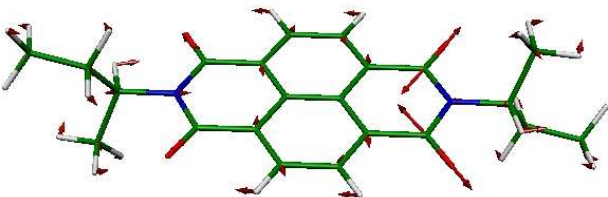
<p>1100.9 cm⁻¹ (142 km mol⁻¹)</p>	
<p>1281.6 cm⁻¹ (250 km mol⁻¹)</p>	
<p>1357.7 cm⁻¹ (875 km mol⁻¹)</p>	
<p>1736.8 cm⁻¹ (770 km mol⁻¹)</p>	
<p>1773.6 cm⁻¹ (377 km mol⁻¹)</p>	

Figure 1S. The visualization of the most intensive B3LYP normal modes observed contributed to the vibronic structure of optical spectrum for the smallest **NBI-1** molecule. See also Table 2S.

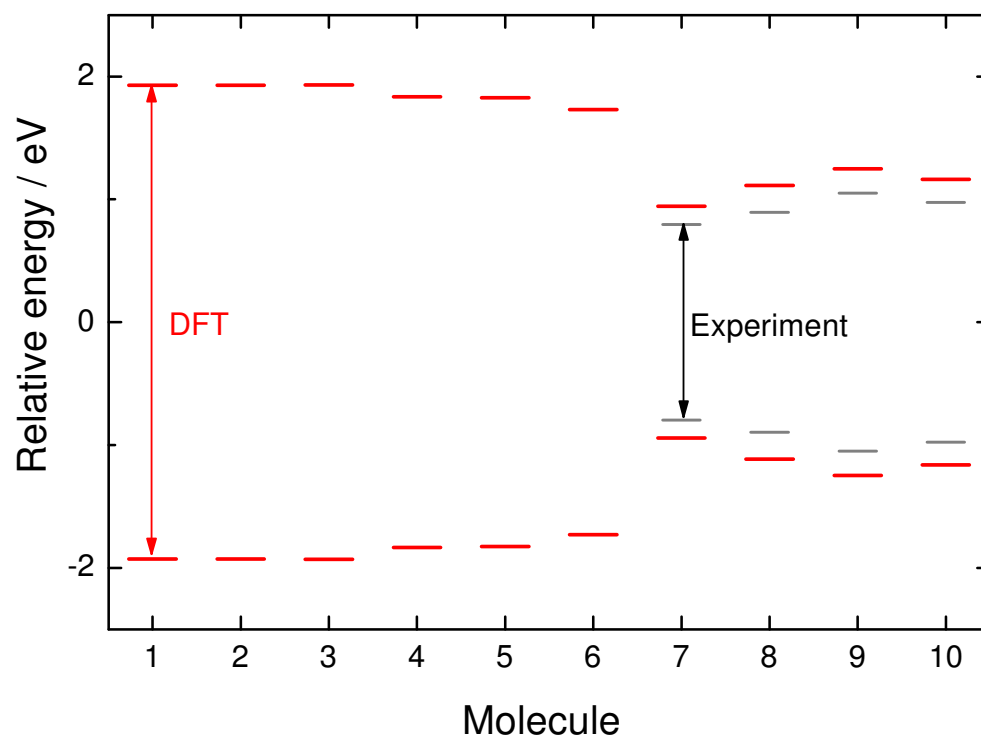


Figure 2S. Schematic representation of the relative energy between HOMOs and LUMOs for studied molecules. Grey lines stand for the experimentally determined values and the red lines indicate the B3LYP/6-31G* results. The order of molecules on x-axis is consistent with the order of molecules presented in Table 2.