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Supporting Information

Novel Periphery-Functionalized Solvatochromic Nitrostilbenes as Precursors for Class II Hybrid Materials

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Solvent Parameter Sets:

Table S1. KAMLET–TAFT [S1,2] parameter set.

solvent	KAMLET–TAFT parameter		
	α	β	π^*
cyclohexane	0.00	0.00	0.00
n-hexane	0.00	0.00	–0.04
triethylamine	0.00	0.71	0.14
tetrachloromethane	0.00	0.10	0.28
p-xylene	0.00	0.12	0.43
toluene	0.00	0.11	0.54
benzene	0.00	0.10	0.59
diethyl ether	0.00	0.47	0.27
1,4-dioxane	0.00	0.37	0.55
anisole	0.00	0.32	0.73
tetrahydrofurane	0.00	0.55	0.58
ethyl acetate	0.00	0.45	0.55
chloroform	0.20	0.10	0.53
1,1,2,2-tetrachloroethane	0.00	0.00	0.95
pyridine	0.00	0.64	0.87
dichloromethane	0.13	0.10	0.82
hexamethylphosphoramide	0.00	1.05	0.87
tetramethylurea	0.00	0.80	0.83
1,2-dichloroethane	0.00	0.10	0.81
benzonitrile	0.00	0.37	0.90
acetone	0.08	0.43	0.71
N,*N*-dimethylacetamide	0.00	0.76	0.88
N,*N*-dimethylformamide	0.00	0.69	0.88
dimethyl sulfoxide	0.00	0.76	1.00
acetonitrile	0.19	0.40	0.75
nitromethane	0.22	0.06	0.85
1-decanol	0.70	0.82	0.45
1-butanol	0.84	0.84	0.47
2-propanol	0.76	0.84	0.48
1-propanol	0.84	0.90	0.52
ethanol	0.86	0.75	0.54
methanol	0.98	0.66	0.60
ethane-1,2-diol	0.90	0.52	0.92
2,2,2-trifluoroethanol	1.51	0.00	0.73
1,1,1,3,3,3-hexafluoro-2-propanol	1.96	0.00	0.65

Single crystal X-ray structure analysis:

Crystal data was collected on a Oxford Gemini Diffractometer at low temperature (100 K) using Cu-K_α-radiation (λ = 1.54 Å). The structure was solved by direct methods using SHELXS-97[S4]. The structure was refined by full-matrix least squares procedures on F^2, using SHELXL-97[S5]. All non hydrogen atoms were refined anisotropically. All hydrogen atoms were added on calculated positions, except of OH and NH which were found in difference fourier synthesis.

Table S2: Crystallographic data and collection parameters for **1-M**

empirical formula	$C_{17}H_{17}N_3O_4$
formula weight	327.34
color	red
wavelength (Å)	1.54184
temperature (K)	150
crystal system	orthorhombic
space group	*Pbca*
a [Å]	14.0954(2)
b [Å]	13.6059(2)
c [Å]	16.2976(2)
α [°]	90
β [°]	90
γ [°]	90
volume (Å^3)	3125.56(7)
Z	8
calcd density (g*cm^{-3})	1.391
absorption coeffizient (mm^{-1})	0.838
F(000)	1376
crystal size (mm^3)	0.35 x 0.29 x 0.16
Θ range for data collection(°)	5.27–61.99
index ranges	−16≤h≤15, −15≤k≤10, −18≤l≤14
reflections collected	9226
independent reflections	2445
R_{int}	0.0202
data/restraints/parameter	2445/0/222
refinement method	full-matrix least-squares on F^2
goodness-of-fit on F^2	1.052
final *R* indicates [$I>2\sigma(I)$]	R1 = 0.0355, *w*R2 = 0.1025
R indicates all data	R1 = 0.0426, *w*R2 = 0.1056
largest diff. peak and hole (e* Å^3)	0.303, −0.201

Table S3. Bond lengths [A] and angles [deg] for **1-M**

C(1)-C(6)	1.381(2)
C(1)-C(2)	1.376(2)
C(1)-N(1)	1.4628(19)
C(2)-C(3)	1.376(2)
C(2)-H(2)	0.9300
C(3)-C(4)	1.395(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.400(2)
C(4)-C(7)	1.459(2)
C(5)-C(6)	1.376(2)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.330(2)
C(7)-H(7)	0.9300
C(8)-C(9)	1.457(2)
C(8)-H(8)	0.9300
C(9)-C(14)	1.380(2)
C(9)-C(10)	1.413(2)
C(10)-C(11)	1.357(2)
C(10)-H(10)	0.9300
C(11)-C(12)	1.416(2)
C(11)-H(11)	0.9300
C(12)-N(2)	1.3427(19)
C(12)-C(13)	1.424(2)
C(13)-C(14)	1.394(2)
C(13)-N(3)	1.4366(19)
C(14)-H(14)	0.9300
C(15)-N(2)	1.4522(18)
C(15)-C(16)	1.513(2)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(17)	1.515(2)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
N(1)-O(2)	1.2137(18)
N(1)-O(1)	1.22275(19)
N(2)-H(2N)	0.81(2)
N(3)-O(4)	1.2290(15)
N(3)-O(3)	1.2411(15)

C(2)-C(1)-C(6)	121.82(13)
C(2)-C(1)-N(1)	119.04(14)
C(6)-C(1)-N(1)	119.14(13)
C(1)-C(2)-C(3)	118.59(14)
C(1)-C(2)-H(2)	120.7
C(3)-C(2)-H(2)	120.7
C(2)-C(3)-C(4)	121.69(14)
C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(3)-C(4)-C(5)	117.83(13)
C(3)-C(4)-C(7)	118.82(13)
C(5)-C(4)-C(7)	123.33(13)
C(6)-C(5)-C(4)	121.11(14)
C(4)-C(5)-H(5)	119.4

C(6)-C(5)-H(5)	119.4
C(5)-C(6)-C(1)	118.93(14)
C(1)-C(6)-H(6)	120.5
C(5)-C(6)-H(6)	120.5
C(8)-C(7)-C(4)	126.66(14)
C(8)-C(7)-H(7)	116.7
C(4)-C(7)-H(7)	116.7
C(7)-C(8)-C(9)	126.55(13)
C(7)-C(8)-H(8)	116.7
C(9)-C(8)-H(8)	116.7
C(14)-C(9)-C(10)	116.69(13)
C(14)-C(9)-C(8)	120.24(13)
C(10)-C(9)-C(8)	123.06(13)
C(11)-C(10)-C(9)	122.62(13)
C(11)-C(10)-H(10)	118.7
C(9)-C(10)-H(10)	118.7
C(10)-C(11)-C(12)	121.98(13)
C(10)-C(11)-H(11)	119.0
C(12)-C(11)-H(11)	119.0
N(2)-C(12)-C(11)	120.28(13)
N(2)-C(12)-C(13)	124.45(13)
C(11)-C(12)-C(13)	115.28(12)
C(14)-C(13)-C(12)	121.87(13)
C(14)-C(13)-N(3)	116.88(12)
C(12)-C(13)-N(3)	121.25(12)
C(9)-C(14)-C(13)	121.56(13)
C(9)-C(14)-H(14)	119.2
C(13)-C(14)-H(14)	119.2
N(2)-C(15)-C(16)	108.94(12)
N(2)-C(15)-H(15A)	109.9
C(16)-C(15)-H(15A)	109.9
N(2)-C(15)-H(15B)	109.9
C(16)-C(15)-H(15B)	109.9
H(15A)-C(15)-H(15B)	108.3
C(15)-C(16)-C(17)	112.60(13)
C(15)-C(16)-H(16A)	109.1
C(17)-C(16)-H(16A)	109.1
C(15)-C(16)-H(16B)	109.1
C(17)-C(16)-H(16B)	109.1
H(16A)-C(16)-H(16B)	107.8
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(2)-N(1)-O(1)	123.16(14)
O(2)-N(1)-C(1)	118.98(13)
O(1)-N(1)-C(1)	117.85(14)
C(12)-N(2)-C(15)	125.01(13)
C(12)-N(2)-H(2N)	118.80(12)
C(15)-N(2)-H(2N)	116.10(12)
O(4)-N(3)-O(3)	121.33(12)
O(4)-N(3)-C(13)	119.14(12)
O(3)-N(3)-C(13)	119.52(12)

Table S3. torsion angles [deg] for **1-M**

C(6)-C(1)-C(2)-C(3)	-1.2(2)
N(1)-C(1)-C(2)-C(3)	178.68(14)
C(1)-C(2)-C(3)-C(4)	2.0(2)
C(2)-C(3)-C(4)-C(5)	-1.3(2)
C(2)-C(3)-C(4)-C(7)	177.13(15)
C(3)-C(4)-C(5)-C(6)	-0.2(2)
C(7)-C(4)-C(5)-C(6)	-178.59(14)
C(4)-C(5)-C(6)-C(1)	1.0(2)
C(2)-C(1)-C(6)-C(5)	-0.3(2)
N(1)-C(1)-C(6)-C(5)	179.83(14)
C(3)-C(4)-C(7)-C(8)	-175.08(16)
C(5)-C(4)-C(7)-C(8)	3.3(3)
C(4)-C(7)-C(8)-C(9)	177.26(14)
C(7)-C(8)-C(9)-C(14)	171.82(15)
C(7)-C(8)-C(9)-C(10)	-9.7(2)
C(14)-C(9)-C(10)-C(11)	-0.5(2)
C(8)-C(9)-C(10)-C(11)	-179.05(14)
C(9)-C(10)-C(11)-C(12)	1.1(2)
C(10)-C(11)-C(12)-N(2)	178.83(14)
C(10)-C(11)-C(12)-C(13)	-1.2(2)
N(2)-C(12)-C(13)-C(14)	-179.27(14)
C(11)-C(12)-C(13)-C(14)	0.7(2)
N(2)-C(12)-C(13)-N(3)	1.3(2)
C(11)-C(12)-C(13)-N(3)	-178.73(13)
C(10)-C(9)-C(14)-C(13)	0.1(2)
C(8)-C(9)-C(14)-C(13)	178.64(14)
C(12)-C(13)-C(14)-C(9)	-0.2(2)
N(3)-C(13)-C(14)-C(9)	179.26(13)
N2(3)-C(15)-C(16)-C(17)	-179.95(14)
C(2)-C(1)-N(1)-O(2)	-170.48(15)
C(6)-C(1)-N(1)-O(2)	-9.4(2)
C(2)-C(1)-N(1)-O(1)	10.2(2)
C(6)-C(1)-N(1)-O(1)	-169.98(16)
C(11)-C(12)-N(2)-C(15)	2.7(2)
C(13)-C(12)-N(2)-C(15)	-177.30(14)
C(16)-C(15)-N(2)-C(12)	-177.12(14)
C(14)-C(13)-N(3)-O(4)	-5.5(2)
C(12)-C(13)-N(3)-O(4)	173.93(14)
C(14)-C(13)-N(3)-O(3)	174.82(13)
C(12)-C(13)-N(3)-O(3)	-5.7(2)

Table S4: Crystallographic data and collection parameters for **3**

empirical formula	$C_{17}H_{17}N_3O_6$
formula weight	359.34
color	red
wavelength (Å)	1.54184
temperature (K)	100 (0)
crystal system	monclinic
space group	*P2(1)/n*
a [Å]	6.6544 (3)
b [Å]	14.0082 (5)
c [Å]	17.2852 (7)
α [°]	95.732 (8)
β [°]	90
γ [°]	98.891 (4)
volume ($Å^3$)	90
Z	4
calcd density (g^*cm^{-3})	1.499
absorption coeffizient (mm^{-1})	0.976
F(000)	752
crystal size (mm^3)	0.4 x 0.08 x 0.08
Θ range for data collection(°)	4.08–61.99
index ranges	$-7\leq h\leq 6$, $-14\leq k\leq 16$, $-15\leq l\leq 19$
reflections collected	4972
independent reflections	2454
R_{int}	0.0441
data/restraints/parameter	2454/0/248
refinement method	full-matrix least-squares on F^2
goodness-of-fit on F^2	1.001
final *R* indicates [$I>2\sigma(I)$]	R1 = 0.0821, *w*R2 = 0.2173
R indicates all data	R1 = 0.1008, *w*R2 = 0.2268
largest diff. peak and hole (e^* $Å^3$)	0.463, −0.471

Table S5. Bond lengths [A] and angles [deg] for **3**

C(1)-C(6)	1.379(5)
C(1)-C(2)	1.380(5)
C(1)-N(1)	1.458(5)
C(2)-C(3)	1.386(5)
C(2)-H(2)	0.9300
C(3)-C(4)	1.398(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.400(5)
C(4)-C(7)	1.467(5)
C(5)-C(6)	1.401(5)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.324(5)
C(7)-H(7)	0.9300
C(8)-C(9)	1.462(5)
C(8)-H(8)	0.9300
C(9)-C(14)	1.379(5)
C(9)-C(10)	1.424(5)
C(10)-C(11)	1.364(5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.418(5)
C(11)-H(11)	0.9300
C(12)-N(2)	1.349(5)
C(12)-C(13)	1.427(5)
C(13)-C(14)	1.392(5)
C(13)-N(3)	1.430(5)
C(14)-H(14)	0.9300
C(15)-O(3)	1.426(4)
C(15)-C(17)	1.513(5)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-O(4)	1.417(5)
C(16)-C(17)	1.517(5)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-N(2)	1.464(5)
C(17)-H(17)	0.9800
N(1)-O(1)	1.226(4)
N(1)-O(2)	1.232(4)
N(2)-H(2N)	0.85(5)
N(3)-O(6)	1.237(4)
N(3)-O(5)	1.251(4)
O(3)-H(3O)	0.94(4)
O(4)-H(4O)	0.80(4)

C(6)-C(1)-C(2)	121.4(3)
C(6)-C(1)-N(1)	119.1(3)
C(2)-C(1)-N(1)	119.5(3)
C(1)-C(2)-C(3)	119.5(3)
C(1)-C(2)-H(2)	120.2
C(3)-C(2)-H(2)	120.2
C(2)-C(3)-C(4)	121.1(4)
C(2)-C(3)-H(3)	119.5
C(4)-C(3)-H(3)	119.5
C(3)-C(4)-C(5)	118.1(4)
C(3)-C(4)-C(7)	118.6(3)

C(5)-C(4)-C(7)	123.3(3)
C(4)-C(5)-C(6)	121.1(3)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(1)-C(6)-C(5)	118.8(3)
C(1)-C(6)-H(6)	120.6
C(5)-C(6)-H(6)	120.6
C(8)-C(7)-C(4)	124.6(3)
C(8)-C(7)-H(7)	117.7
C(4)-C(7)-H(7)	117.7
C(7)-C(8)-C(9)	127.7(3)
C(7)-C(8)-H(8)	116.2
C(9)-C(8)-H(8)	116.2
C(14)-C(9)-C(10)	116.8(3)
C(14)-C(9)-C(8)	118.8(3)
C(10)-C(9)-C(8)	124.3(3)
C(11)-C(10)-C(9)	122.0(3)
C(11)-C(10)-H(10)	119.0
C(9)-C(10)-H(10)	119.0
C(10)-C(11)-C(12)	122.2(3)
C(10)-C(11)-H(11)	118.9
C(12)-C(11)-H(11)	118.9
N(2)-C(12)-C(11)	121.0(3)
N(2)-C(12)-C(13)	123.9(3)
C(11)-C(12)-C(13)	115.2(3)
C(14)-C(13)-C(12)	122.1(3)
C(14)-C(13)-N(3)	116.0(3)
C(12)-C(13)-N(3)	121.9(3)
C(9)-C(14)-C(13)	121.7(3)
C(9)-C(14)-H(14)	119.2
C(13)-C(14)-H(14)	119.2
O(3)-C(15)-C(17)	111.3(3)
O(3)-C(15)-H(15A)	109.4
C(17)-C(15)-H(15A)	109.4
O(3)-C(15)-H(15B)	109.4
C(17)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
O(4)-C(16)-C(17)	112.0(3)
O(4)-C(16)-H(16A)	109.2
C(17)-C(16)-H(16A)	109.2
O(4)-C(16)-H(16B)	109.2
C(17)-C(16)-H(16B)	109.2
H(16A)-C(16)-H(16B)	107.9
N(2)-C(17)-C(15)	110.0(3)
N(2)-C(17)-C(16)	108.1(3)
C(15)-C(17)-C(16)	113.1(3)
N(2)-C(17)-H(17)	108.5
C(15)-C(17)-H(17)	108.5
C(16)-C(17)-H(17)	108.5
O(1)-N(1)-O(2)	124.0(4)
O(1)-N(1)-C(1)	118.2(4)
O(2)-N(1)-C(1)	117.8(3)
C(12)-N(2)-C(17)	125.8(3)
C(12)-N(2)-H(2N)	126(3)
C(17)-N(2)-H(2N)	108(3)
O(6)-N(3)-O(5)	121.5(3)
O(6)-N(3)-C(13)	119.0(3)
O(5)-N(3)-C(13)	119.6(3)
C(15)-O(3)-H(3O)	112(2)
C(16)-O(4)-H(4O)	107(3)

Table S5. torsion angles [deg] for **3**

C(6)-C(1)-C(2)-C(3)	0.8(5)
N(1)-C(1)-C(2)-C(3)	179.3(3)
C(1)-C(2)-C(3)-C(4)	0.4(5)
C(2)-C(3)-C(4)-C(5)	-0.7(5)
C(2)-C(3)-C(4)-C(7)	178.1(3)
C(3)-C(4)-C(5)-C(6)	-0.1(5)
C(7)-C(4)-C(5)-C(6)	-178.9(3)
C(2)-C(1)-C(6)-C(5)	-1.6(5)
N(1)-C(1)-C(6)-C(5)	179.9(3)
C(4)-C(5)-C(6)-C(1)	1.3(5)
C(3)-C(4)-C(7)-C(8)	-170.5(3)
C(5)-C(4)-C(7)-C(8)	8.2(6)
C(4)-C(7)-C(8)-C(9)	176.9(3)
C(7)-C(8)-C(9)-C(14)	178.6(3)
C(7)-C(8)-C(9)-C(10)	-1.8(6)
C(14)-C(9)-C(10)-C(11)	0.3(5)
C(8)-C(9)-C(10)-C(11)	-179.4(3)
C(9)-C(10)-C(11)-C(12)	0.6(5)
C(10)-C(11)-C(12)-N(2)	178.2(3)
C(10)-C(11)-C(12)-C(13)	-1.8(5)
N(2)-C(12)-C(13)-C(14)	-177.8(3)
C(11)-C(12)-C(13)-C(14)	2.3(5)
N(2)-C(12)-C(13)-N(3)	4.2(5)
C(11)-C(12)-C(13)-N(3)	-175.8(3)
C(10)-C(9)-C(14)-C(13)	0.2(5)
C(8)-C(9)-C(14)-C(13)	179.8(3)
C(12)-C(13)-C(14)-C(9)	-1.5(5)
N(3)-C(13)-C(14)-C(9)	176.7(3)
O(3)-C(15)-C(17)-N(2)	-175.9(3)
O(3)-C(15)-C(17)-C(16)	63.1(4)
O(4)-C(16)-C(17)-N(2)	-52.8(4)
O(4)-C(16)-C(17)-C(15)	69.2(4)
C(6)-C(1)-N(1)-O(1)	-170.3(3)
C(2)-C(1)-N(1)-O(1)	11.2(5)
C(6)-C(1)-N(1)-O(2)	10.3(5)
C(2)-C(1)-N(1)-O(2)	-168.2(3)
C(11)-C(12)-N(2)-C(17)	3.4(5)
C(13)-C(12)-N(2)-C(17)	-176.5(3)
C(15)-C(17)-N(2)-C(12)	80.8(4)
C(16)-C(17)-N(2)-C(12)	-155.3(3)
C(14)-C(13)-N(3)-O(6)	-0.5(5)
C(12)-C(13)-N(3)-O(6)	177.7(3)
C(14)-C(13)-N(3)-O(5)	179.8(3)
C(12)-C(13)-N(3)-O(5)	-2.1(5)

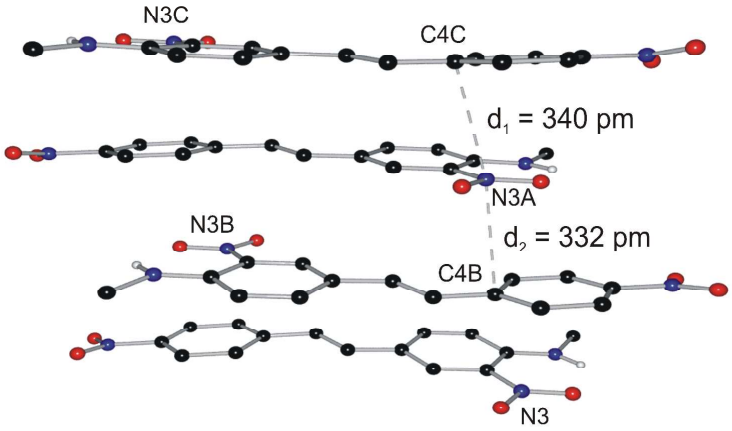

Figure S1. Selected part of the 3D-network of **3** caused by π-π-interactions between the nitro-groups and the aromatic ring superimposed 2D-layer.

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