Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

Stereoisomers of an azine-linked donor-acceptor conjugated polymer: the impact of molecular conformation on electrical performance

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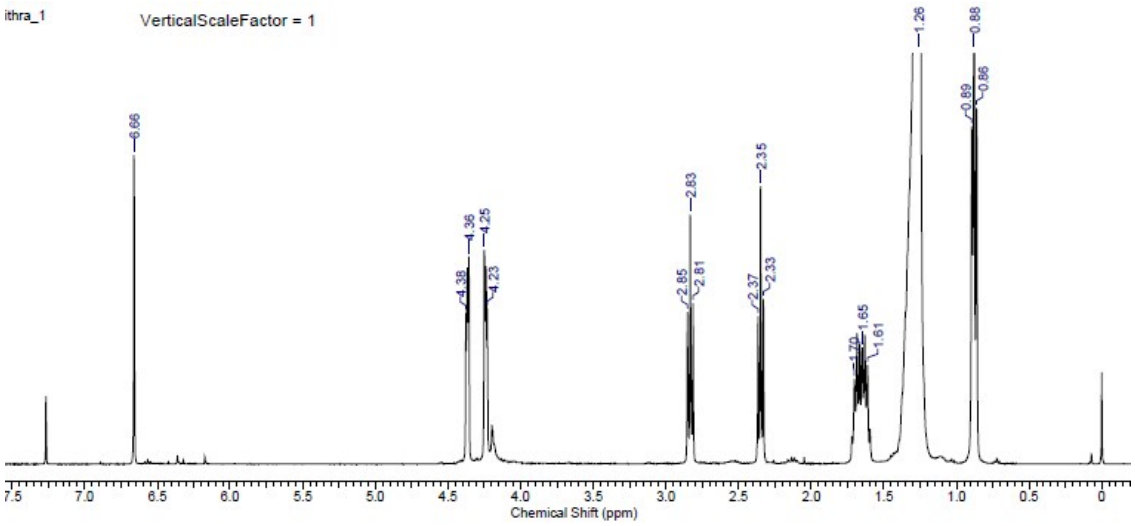


Figure S1.[1]H NMR spectrum of compound **1**

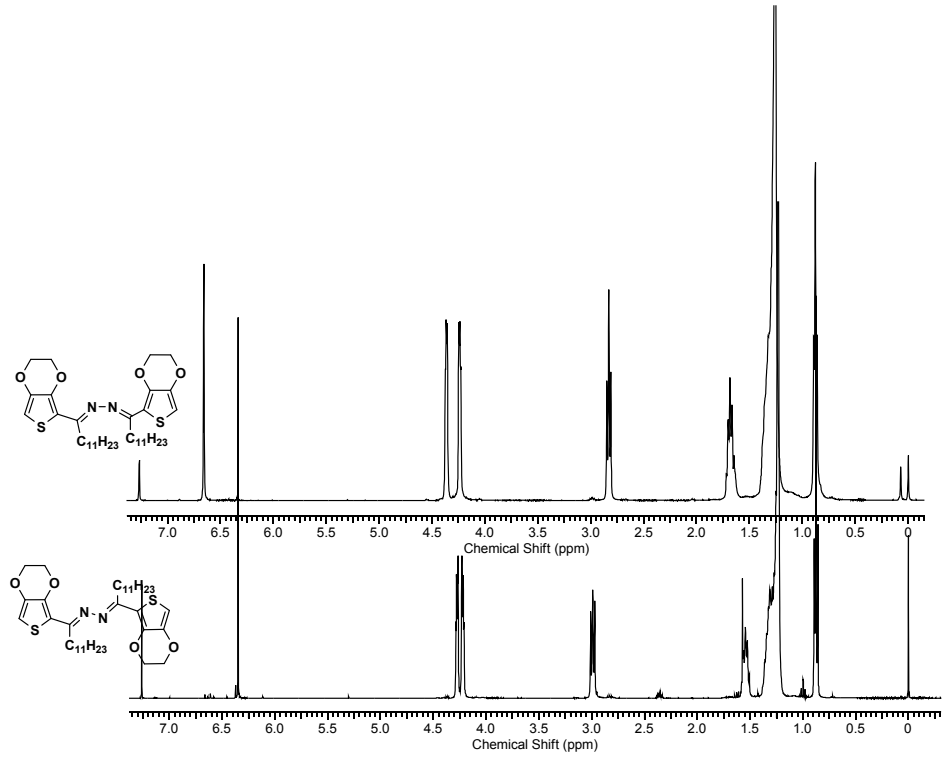


Figure S2. [1]H NMR spectra of the azine molecule **2a**(lower) and **2b** (upper)

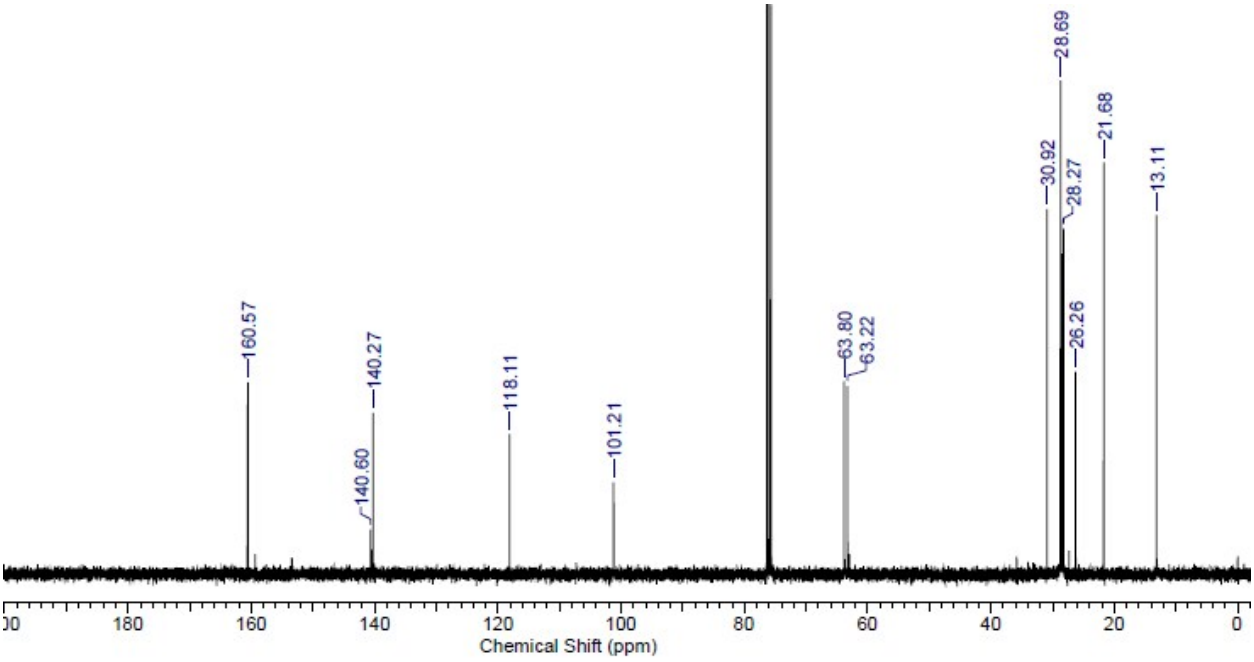


Figure S3. ^{13}C NMR spectrum of the azine molecule **2a**

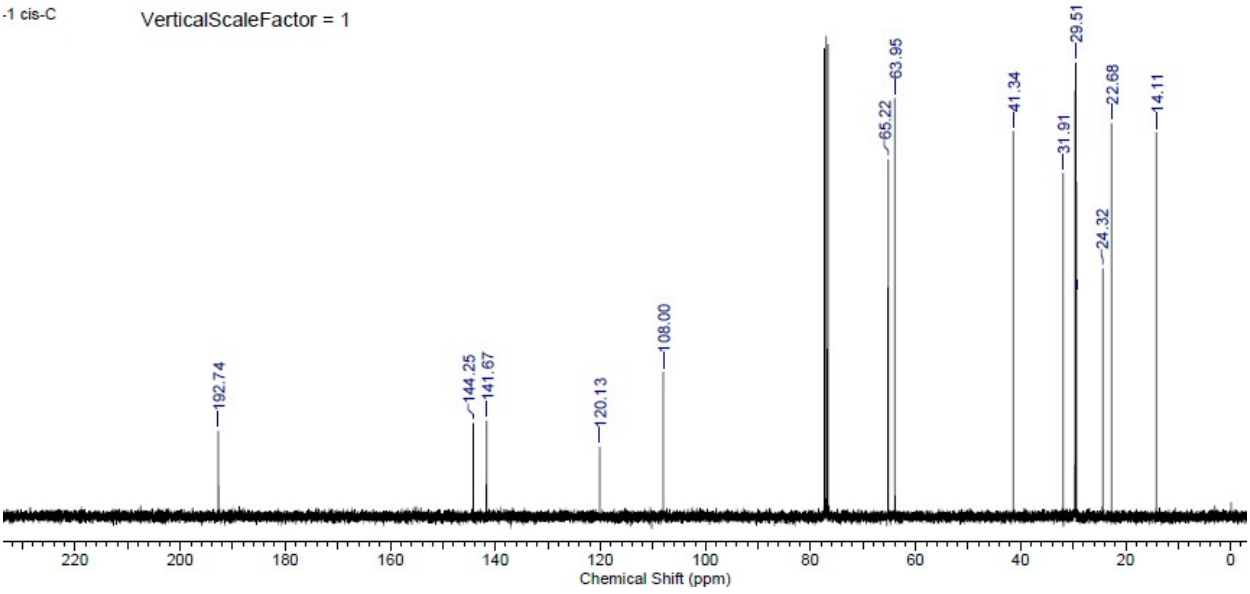


Figure S4. ^{13}C NMR spectrum of the azine molecule **2b**

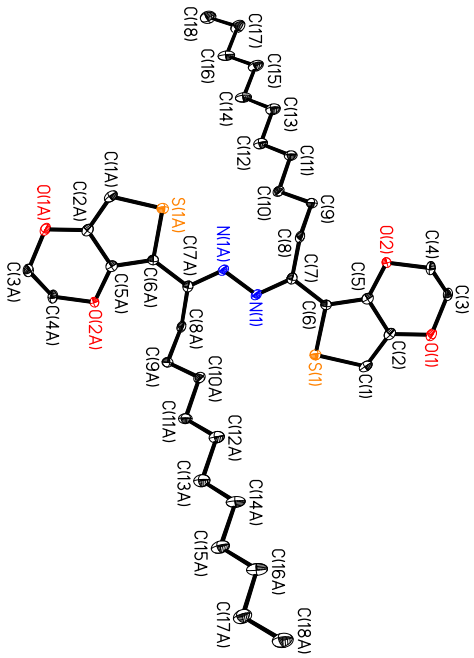


Figure S5. Single crystal structure of (*E,E*) isomer (**2a**) of azine molecule

Table S1. Crystal data and structure refinement for molecule **2a**

Identification code	p21c	
Empirical formula	C36 H56 N2 O4 S2	
Formula weight	644.95	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.9983(12) Å	α= 90°.
	b = 8.7827(6) Å	β= 111.777(3)°.
	c = 14.3552(12) Å	γ = 90°.
Volume	1756.0(2) Å^3	
Z	2	
Density (calculated)	1.220 Mg/m^3	
Absorption coefficient	0.192 mm^{-1}	
F(000)	700	
Crystal size	0.20 x 0.10 x 0.02 mm^3	

Theta range for data collection	2.74 to 24.71°.
Index ranges	-17<=h<=17, -9<=k<=10, -16<=l<=16
Reflections collected	29585
Independent reflections	3001 [R(int) = 0.1095]
Completeness to theta = 24.71°	100.0 %
Absorption correction	Empirical
Max. and min. transmission	0.9962 and 0.9627
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3001 / 0 / 199
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0420, wR2 = 0.0862
R indices (all data)	R1 = 0.0647, wR2 = 0.0951
Largest diff. peak and hole	0.271 and -0.354 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for molecule **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	3692(1)	6731(1)	104(1)	13(1)
O(1)	4741(1)	3191(2)	1762(1)	15(1)
O(2)	6181(1)	5549(2)	2066(1)	13(1)
N(1)	4799(1)	9298(2)	26(1)	13(1)
C(1)	3673(2)	4954(2)	595(2)	15(1)
C(2)	4551(2)	4552(2)	1259(2)	12(1)
C(3)	5760(2)	2914(2)	2218(2)	14(1)
C(4)	6267(2)	4312(2)	2762(2)	17(1)
C(5)	5259(2)	5711(2)	1401(2)	11(1)
C(6)	4911(1)	6971(2)	815(2)	11(1)
C(7)	5351(1)	8418(2)	741(2)	12(1)
C(8)	6332(2)	8809(2)	1499(2)	12(1)
C(9)	7186(2)	8121(2)	1291(2)	14(1)
C(10)	7328(2)	8730(2)	362(2)	15(1)
C(11)	8267(2)	8157(2)	294(2)	16(1)

C(12)	8451(2)	8699(3)	-624(2)	19(1)
C(13)	9399(2)	8129(3)	-665(2)	20(1)
C(14)	9600(2)	8726(3)	-1562(2)	22(1)
C(15)	10524(2)	8112(3)	-1645(2)	22(1)
C(16)	10704(2)	8754(3)	-2543(2)	23(1)
C(17)	11600(2)	8134(3)	-2675(2)	25(1)
C(18)	11766(2)	8849(3)	-3563(2)	27(1)

Table S3. Bond lengths [Å] and angles [°] for molecule 2a.

S(1)-C(1)	1.717(2)
S(1)-C(6)	1.745(2)
O(1)-C(2)	1.370(2)
O(1)-C(3)	1.443(2)
O(2)-C(5)	1.364(2)
O(2)-C(4)	1.449(2)
N(1)-C(7)	1.306(3)
N(1)-N(1)#1	1.387(3)
C(1)-C(2)	1.355(3)
C(2)-C(5)	1.431(3)
C(3)-C(4)	1.501(3)
C(5)-C(6)	1.371(3)
C(6)-C(7)	1.453(3)
C(7)-C(8)	1.510(3)
C(8)-C(9)	1.541(3)
C(9)-C(10)	1.524(3)
C(10)-C(11)	1.532(3)
C(11)-C(12)	1.520(3)
C(12)-C(13)	1.529(3)
C(13)-C(14)	1.521(3)
C(14)-C(15)	1.531(3)
C(15)-C(16)	1.520(3)
C(16)-C(17)	1.525(3)
C(17)-C(18)	1.522(3)

C(1)-S(1)-C(6)	92.48(10)
C(2)-O(1)-C(3)	111.40(15)
C(5)-O(2)-C(4)	111.61(15)
C(7)-N(1)-N(1)#1	114.0(2)
C(2)-C(1)-S(1)	111.48(16)
C(1)-C(2)-O(1)	123.78(18)
C(1)-C(2)-C(5)	113.05(19)
O(1)-C(2)-C(5)	123.16(19)
O(1)-C(3)-C(4)	110.18(17)
O(2)-C(4)-C(3)	110.89(17)
O(2)-C(5)-C(6)	124.73(18)
O(2)-C(5)-C(2)	122.12(18)
C(6)-C(5)-C(2)	113.15(19)
C(5)-C(6)-C(7)	132.09(19)
C(5)-C(6)-S(1)	109.82(15)
C(7)-C(6)-S(1)	117.97(15)
N(1)-C(7)-C(6)	113.69(18)
N(1)-C(7)-C(8)	126.57(18)
C(6)-C(7)-C(8)	119.62(18)
C(7)-C(8)-C(9)	115.41(17)
C(10)-C(9)-C(8)	115.34(17)
C(9)-C(10)-C(11)	111.77(18)
C(12)-C(11)-C(10)	114.74(18)
C(11)-C(12)-C(13)	113.63(19)
C(14)-C(13)-C(12)	113.51(19)
C(13)-C(14)-C(15)	114.5(2)
C(16)-C(15)-C(14)	112.7(2)
C(15)-C(16)-C(17)	114.5(2)
C(18)-C(17)-C(16)	112.4(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for molecule **2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	12(1)	15(1)	13(1)	0(1)	5(1)	-1(1)
O(1)	18(1)	11(1)	19(1)	1(1)	9(1)	-2(1)
O(2)	11(1)	12(1)	16(1)	5(1)	3(1)	1(1)
N(1)	14(1)	11(1)	19(1)	1(1)	10(1)	-1(1)
C(1)	17(1)	13(1)	18(1)	-4(1)	11(1)	-5(1)
C(2)	17(1)	11(1)	12(1)	-4(1)	10(1)	-2(1)
C(3)	18(1)	15(1)	13(1)	5(1)	9(1)	2(1)
C(4)	20(1)	15(1)	15(1)	6(1)	6(1)	0(1)
C(5)	14(1)	12(1)	9(1)	-4(1)	8(1)	-1(1)
C(6)	11(1)	12(1)	10(1)	-1(1)	5(1)	0(1)
C(7)	15(1)	11(1)	13(1)	0(1)	11(1)	2(1)
C(8)	15(1)	8(1)	15(1)	0(1)	7(1)	-1(1)
C(9)	10(1)	13(1)	18(1)	1(1)	5(1)	0(1)
C(10)	14(1)	11(1)	21(1)	-1(1)	8(1)	-2(1)
C(11)	11(1)	16(1)	22(1)	-2(1)	7(1)	-1(1)
C(12)	15(1)	21(1)	23(1)	-3(1)	9(1)	-3(1)
C(13)	16(1)	19(1)	28(1)	-6(1)	11(1)	-3(1)
C(14)	14(1)	29(1)	25(1)	-7(1)	10(1)	-5(1)
C(15)	19(1)	23(1)	30(1)	-7(1)	15(1)	-5(1)
C(16)	15(1)	31(1)	26(1)	-10(1)	10(1)	-6(1)
C(17)	24(1)	22(1)	37(2)	-3(1)	20(1)	-3(1)
C(18)	22(1)	31(1)	34(2)	-4(1)	18(1)	-2(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) formolecule **2a**.

	x	y	z	U(eq)
H(1)	3117	4330	422	18
H(3A)	6013	2634	1694	17
H(3B)	5882	2054	2696	17
H(4A)	5986	4626	3257	20
H(4B)	6954	4077	3130	20
H(8A)	6368	8461	2168	15
H(8B)	6402	9931	1528	15
H(9A)	7780	8312	1882	17
H(9B)	7096	7005	1221	17
H(10A)	7335	9857	381	18
H(10B)	6782	8407	-244	18
H(11A)	8808	8492	902	19
H(11B)	8260	7030	295	19
H(12A)	8452	9827	-631	23
H(12B)	7917	8351	-1234	23
H(13A)	9930	8440	-42	24
H(13B)	9387	7002	-688	24
H(14A)	9640	9850	-1521	26
H(14B)	9052	8458	-2182	26
H(15A)	11074	8370	-1025	27
H(15B)	10483	6989	-1701	27
H(16A)	10761	9875	-2474	28
H(16B)	10139	8529	-3158	28
H(17A)	12165	8331	-2056	30
H(17B)	11536	7018	-2772	30
H(18A)	12347	8417	-3617	41
H(18B)	11843	9952	-3463	41
H(18C)	11214	8639	-4180	41

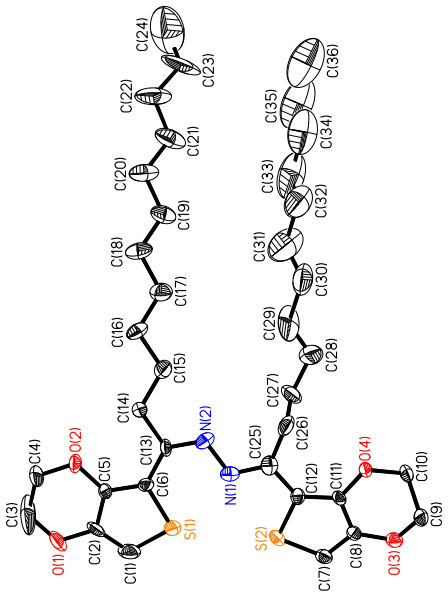


Figure S6. Single crystal structure of (*E,Z*) isomer (**2b**) of azine molecule

Table S6. Crystal data and structure refinement for molecule **2b**.

Identification code	p21c	
Empirical formula	C36 H56 N2 O4 S2	
Formula weight	644.95	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 25.7143(12) Å	α= 90°.
	b = 7.7086(3) Å	β= 107.4390(10)°.
	c = 18.8672(8) Å	γ = 90°.
Volume	3568.0(3) $Å^3$	
Z	4	
Density (calculated)	1.201 Mg/m^3	
Absorption coefficient	0.189 mm^{-1}	
F(000)	1400	

Crystal size	0.40 x 0.30 x 0.02 mm^3
Theta range for data collection	1.66 to 20.81°.
Index ranges	-25<=h<=25, -7<=k<=7, -18<=l<=18
Reflections collected	25257
Independent reflections	3739 [R(int) = 0.0635]
Completeness to theta = 20.81°	100.0 %
Absorption correction	Empirical
Max. and min. transmission	0.9962 and 0.9284
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3739 / 127 / 397
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0916, wR2 = 0.2062
R indices (all data)	R1 = 0.1091, wR2 = 0.2208
Largest diff. peak and hole	0.692 and -0.806 $e.Å^{-3}$

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for molecule **2b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	880(1)	753(3)	-4436(1)	40(1)
C(1)	734(3)	-832(11)	-5091(4)	54(2)
C(2)	1088(3)	-2164(10)	-4922(3)	37(2)
O(1)	1071(2)	-3597(7)	-5355(3)	52(2)
C(3)	1507(4)	-4685(16)	-5093(7)	136(7)
C(4)	1852(5)	-4574(11)	-4395(4)	80(4)
O(2)	1903(2)	-3080(5)	-3956(2)	33(1)

C(5)	1494(2)	-1907(8)	-4230(3)	26(2)
C(6)	1445(2)	-382(8)	-3880(3)	26(2)
C(13)	1782(3)	234(8)	-3159(3)	28(2)
C(14)	2249(3)	-906(9)	-2704(3)	37(2)
C(15)	2464(3)	-448(10)	-1891(4)	41(2)
C(16)	2935(3)	-1555(10)	-1438(4)	43(2)
C(17)	3119(3)	-1112(11)	-639(4)	50(2)
C(18)	3577(3)	-2143(12)	-118(4)	55(2)
C(19)	3699(3)	-1764(11)	671(4)	51(2)
C(20)	4140(3)	-2726(12)	1220(4)	63(3)
C(21)	4222(4)	-2321(13)	2019(4)	74(3)
C(22)	4647(5)	-3245(14)	2601(5)	108(5)
C(23)	4684(7)	-2826(18)	3397(6)	169(8)
C(24)	4976(9)	-3750(20)	3947(9)	189(9)
S(2)	351(1)	4626(2)	-3956(1)	31(1)
C(7)	-24(3)	6459(9)	-3978(3)	30(2)
C(8)	212(3)	7551(8)	-3417(3)	25(2)
O(3)	-14(2)	9081(6)	-3282(2)	31(1)
C(9)	383(3)	10174(9)	-2791(3)	32(2)
C(10)	719(3)	9208(8)	-2137(3)	31(2)
O(4)	1024(2)	7835(5)	-2348(2)	28(1)
C(11)	723(2)	6915(8)	-2944(3)	22(2)
C(12)	854(2)	5346(8)	-3162(3)	25(2)
C(25)	1318(3)	4213(9)	-2840(4)	32(2)
C(26)	1723(3)	4704(9)	-2119(4)	43(2)
C(27)	1569(4)	4044(11)	-1461(4)	75(3)
C(28)	1909(6)	4567(13)	-708(5)	123(5)
C(29)	2370(4)	3680(14)	-368(7)	129(5)
C(30)	2735(4)	3929(13)	416(6)	101(4)

C(31)	2993(7)	2869(17)	924(9)	237(9)
C(32)	3388(5)	3146(15)	1661(7)	128(5)
C(33)	3310(6)	2061(18)	2260(9)	152(5)
C(34)	3754(6)	2357(17)	2975(8)	133(4)
C(35)	3746(8)	1380(30)	3649(11)	181(7)
C(36)	4168(8)	1570(20)	4286(10)	179(7)
N(1)	1328(2)	2756(8)	-3206(3)	32(2)
N(2)	1756(2)	1687(8)	-2820(3)	34(2)

Table S8. Bond lengths [Å] and angles [°] for molecule **2b**.

S(1)-C(1)	1.698(8)
S(1)-C(6)	1.749(6)
C(1)-C(2)	1.346(9)
C(2)-O(1)	1.367(8)
C(2)-C(5)	1.420(9)
O(1)-C(3)	1.370(10)
C(3)-C(4)	1.352(11)
C(4)-O(2)	1.401(9)
O(2)-C(5)	1.366(7)
C(5)-C(6)	1.371(8)
C(6)-C(13)	1.457(8)
C(13)-N(2)	1.301(8)
C(13)-C(14)	1.528(9)
C(14)-C(15)	1.508(9)
C(15)-C(16)	1.517(9)
C(16)-C(17)	1.478(9)
C(17)-C(18)	1.513(10)

C(18)-C(19)	1.456(10)
C(19)-C(20)	1.485(10)
C(20)-C(21)	1.492(11)
C(21)-C(22)	1.481(11)
C(22)-C(23)	1.510(15)
C(23)-C(24)	1.300(16)
S(2)-C(7)	1.704(7)
S(2)-C(12)	1.750(6)
C(7)-C(8)	1.346(8)
C(8)-O(3)	1.372(7)
C(8)-C(11)	1.434(8)
O(3)-C(9)	1.428(7)
C(9)-C(10)	1.478(8)
C(10)-O(4)	1.443(7)
O(4)-C(11)	1.358(7)
C(11)-C(12)	1.353(8)
C(12)-C(25)	1.457(9)
C(25)-N(1)	1.323(9)
C(25)-C(26)	1.493(9)
C(26)-C(27)	1.500(10)
C(27)-C(28)	1.483(11)
C(28)-C(29)	1.352(12)
C(29)-C(30)	1.508(12)
C(30)-C(31)	1.283(13)
C(31)-C(32)	1.471(13)
C(32)-C(33)	1.469(15)
C(33)-C(34)	1.500(15)
C(34)-C(35)	1.485(16)
C(35)-C(36)	1.364(18)

N(1)-N(2)	1.392(8)

C(1)-S(1)-C(6)	92.2(3)
C(2)-C(1)-S(1)	112.9(5)
C(1)-C(2)-O(1)	125.1(6)
C(1)-C(2)-C(5)	111.7(6)
O(1)-C(2)-C(5)	123.2(6)
C(2)-O(1)-C(3)	113.7(6)
C(4)-C(3)-O(1)	122.7(8)
C(3)-C(4)-O(2)	123.1(8)
C(5)-O(2)-C(4)	113.4(6)
O(2)-C(5)-C(6)	123.9(5)
O(2)-C(5)-C(2)	121.6(6)
C(6)-C(5)-C(2)	114.5(6)
C(5)-C(6)-C(13)	127.8(6)
C(5)-C(6)-S(1)	108.6(4)
C(13)-C(6)-S(1)	123.5(5)
N(2)-C(13)-C(6)	129.5(6)
N(2)-C(13)-C(14)	111.5(5)
C(6)-C(13)-C(14)	119.0(5)
C(15)-C(14)-C(13)	115.1(5)
C(14)-C(15)-C(16)	115.4(6)
C(17)-C(16)-C(15)	113.7(6)
C(16)-C(17)-C(18)	119.3(7)
C(19)-C(18)-C(17)	116.5(7)
C(18)-C(19)-C(20)	119.9(7)
C(19)-C(20)-C(21)	116.6(8)
C(22)-C(21)-C(20)	119.9(9)
C(21)-C(22)-C(23)	116.5(11)

C(24)-C(23)-C(22)	121.7(14)
C(7)-S(2)-C(12)	91.5(3)
C(8)-C(7)-S(2)	112.4(5)
C(7)-C(8)-O(3)	124.6(6)
C(7)-C(8)-C(11)	112.9(5)
O(3)-C(8)-C(11)	122.5(5)
C(8)-O(3)-C(9)	111.5(5)
O(3)-C(9)-C(10)	111.7(5)
O(4)-C(10)-C(9)	111.7(5)
C(11)-O(4)-C(10)	112.9(4)
C(12)-C(11)-O(4)	125.9(5)
C(12)-C(11)-C(8)	112.4(5)
O(4)-C(11)-C(8)	121.7(5)
C(11)-C(12)-C(25)	131.1(6)
C(11)-C(12)-S(2)	110.9(5)
C(25)-C(12)-S(2)	118.0(5)
N(1)-C(25)-C(12)	115.7(6)
N(1)-C(25)-C(26)	125.0(6)
C(12)-C(25)-C(26)	119.2(6)
C(25)-C(26)-C(27)	112.5(6)
C(28)-C(27)-C(26)	118.3(9)
C(29)-C(28)-C(27)	119.9(10)
C(28)-C(29)-C(30)	127.0(10)
C(31)-C(30)-C(29)	133.0(10)
C(30)-C(31)-C(32)	132.0(12)
C(33)-C(32)-C(31)	115.4(12)
C(32)-C(33)-C(34)	111.2(10)
C(35)-C(34)-C(33)	119.4(13)
C(36)-C(35)-C(34)	119.2(17)

C(25)-N(1)-N(2)	111.4(5)
C(13)-N(2)-N(1)	113.7(5)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for molecule **2b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	45(1)	49(1)	27(1)	5(1)	11(1)	21(1)
C(1)	41(5)	87(7)	26(4)	4(4)	0(4)	24(5)
C(2)	42(5)	55(5)	15(4)	-8(4)	9(4)	3(4)
O(1)	59(4)	62(4)	30(3)	-23(3)	9(3)	7(3)
C(3)	59(7)	143(12)	161(13)	-128(10)	-37(7)	47(8)
C(4)	153(10)	44(6)	43(5)	-4(5)	27(6)	49(6)
O(2)	36(3)	22(3)	39(3)	-10(2)	7(2)	6(2)
C(5)	28(4)	30(4)	23(4)	1(3)	15(3)	8(3)
C(6)	31(4)	30(4)	21(4)	8(3)	11(3)	8(3)
C(13)	44(4)	15(4)	28(4)	-3(3)	17(4)	4(3)
C(14)	53(5)	30(4)	24(4)	-1(3)	5(4)	14(4)
C(15)	38(4)	35(5)	43(5)	-3(4)	3(4)	7(4)
C(16)	29(4)	46(5)	46(5)	10(4)	-1(4)	11(4)
C(17)	44(5)	52(5)	44(5)	0(4)	-2(4)	1(4)
C(18)	30(4)	75(6)	49(5)	12(5)	-5(4)	4(4)
C(19)	49(5)	59(6)	38(5)	-4(4)	1(4)	-17(4)
C(20)	52(5)	71(7)	50(6)	17(5)	-11(4)	-9(5)
C(21)	92(7)	70(7)	43(6)	-3(5)	-6(5)	-37(6)
C(22)	127(10)	69(7)	74(8)	31(6)	-51(7)	-21(7)

C(23)	270(20)	103(11)	47(7)	-3(7)	-81(10)	-20(12)
C(24)	330(30)	135(15)	141(15)	13(13)	127(18)	17(17)
S(2)	37(1)	34(1)	22(1)	-7(1)	9(1)	-2(1)
C(7)	30(4)	39(4)	21(4)	0(4)	8(3)	5(3)
C(8)	33(4)	27(4)	20(4)	1(3)	17(3)	5(4)
O(3)	29(3)	40(3)	24(3)	0(2)	8(2)	10(2)
C(9)	42(4)	28(4)	30(4)	-3(4)	17(4)	8(4)
C(10)	40(4)	27(4)	27(4)	-8(3)	12(3)	1(3)
O(4)	31(3)	23(3)	25(3)	-7(2)	0(2)	6(2)
C(11)	28(4)	25(4)	18(4)	-3(3)	13(3)	0(3)
C(12)	22(4)	24(4)	29(4)	-3(3)	10(3)	1(3)
C(25)	31(4)	28(4)	39(4)	-2(4)	14(4)	-7(4)
C(26)	34(4)	28(4)	56(5)	-2(4)	0(4)	12(4)
C(27)	148(9)	40(5)	24(4)	-6(4)	6(4)	1(6)
C(28)	205(12)	50(6)	62(5)	-2(5)	-39(7)	29(7)
C(29)	52(6)	79(8)	197(10)	-91(8)	-51(7)	2(5)
C(30)	81(7)	56(7)	142(9)	-36(6)	-5(6)	16(6)
C(31)	203(15)	63(8)	291(13)	-43(9)	-158(12)	0(10)
C(32)	76(8)	56(7)	199(10)	-22(7)	-36(7)	-11(6)
C(33)	98(10)	66(9)	301(13)	-12(10)	74(9)	-16(8)
C(34)	144(11)	78(9)	216(11)	9(9)	112(8)	-18(9)
C(35)	191(18)	105(12)	303(16)	62(15)	160(12)	19(14)
C(36)	210(20)	107(13)	266(16)	86(17)	147(13)	19(15)
N(1)	30(3)	37(4)	26(3)	4(3)	3(3)	-1(3)
N(2)	28(3)	32(4)	38(4)	9(3)	3(3)	5(3)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3)for molecule **2b**.

	x	y	z	U(eq)
H(1)	434	-784	-5531	64
H(3A)	1361	-5882	-5153	164
H(3B)	1732	-4571	-5433	164
H(4A)	2220	-4837	-4429	97
H(4B)	1755	-5532	-4109	97
H(14A)	2123	-2126	-2747	45
H(14B)	2553	-831	-2924	45
H(15A)	2162	-542	-1670	49
H(15B)	2584	778	-1849	49
H(16A)	2822	-2788	-1492	52
H(16B)	3245	-1423	-1641	52
H(17A)	2799	-1200	-452	60
H(17B)	3232	122	-597	60
H(18A)	3485	-3390	-194	66
H(18B)	3911	-1945	-263	66
H(19A)	3359	-1944	806	62
H(19B)	3788	-513	738	62
H(20A)	4486	-2496	1110	76
H(20B)	4063	-3983	1145	76
H(21A)	4300	-1064	2088	89
H(21B)	3870	-2524	2119	89
H(22A)	5005	-2988	2528	129
H(22B)	4583	-4508	2526	129
H(23A)	4817	-1617	3489	202

H(23B)	4307	-2831	3429	202
H(24A)	4936	-3309	4414	283
H(24B)	5360	-3692	3963	283
H(24C)	4854	-4964	3880	283
H(7)	-361	6685	-4345	36
H(9A)	196	11141	-2623	38
H(9B)	623	10676	-3063	38
H(10A)	975	10019	-1799	37
H(10B)	479	8708	-1866	37
H(26A)	1754	5984	-2089	51
H(26B)	2084	4232	-2102	51
H(27A)	1190	4419	-1519	90
H(27B)	1567	2761	-1482	90
H(28A)	2013	5796	-737	148
H(28B)	1675	4527	-378	148
H(29A)	2609	3822	-689	154
H(29B)	2263	2442	-403	154
H(30A)	3022	4730	361	122
H(30B)	2511	4621	657	122
H(31A)	3184	2084	669	284
H(31B)	2702	2159	1025	284
H(32A)	3759	2930	1624	153
H(32B)	3371	4379	1799	153
H(33A)	3307	824	2118	183
H(33B)	2953	2333	2332	183
H(34A)	4106	2107	2881	159
H(34B)	3754	3608	3094	159
H(35A)	3407	1692	3763	217
H(35B)	3721	129	3521	217

H(36A)	4102	858	4680	269
H(36B)	4196	2795	4438	269
H(36C)	4509	1212	4198	269

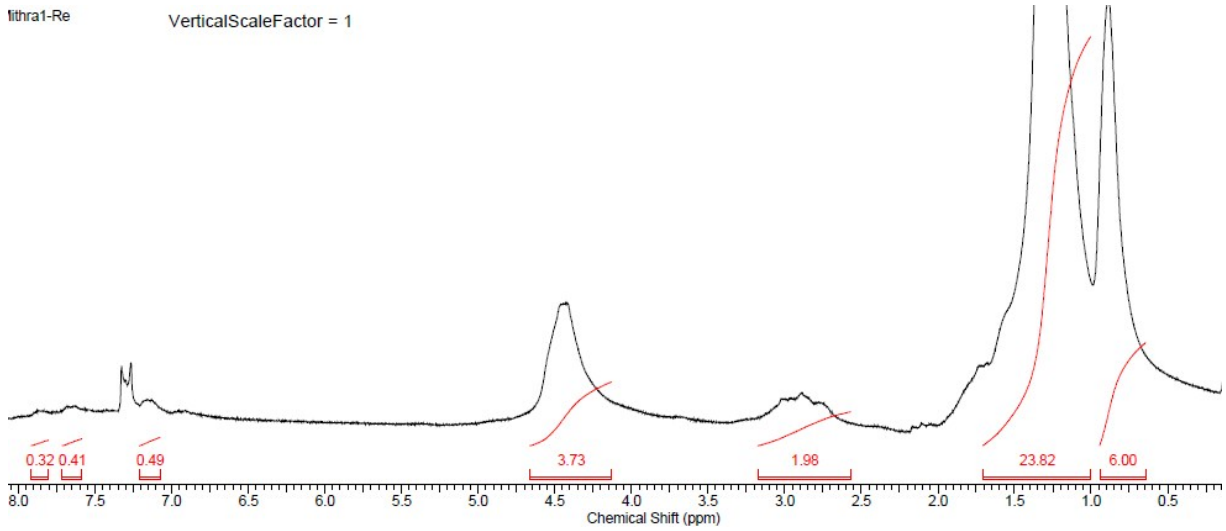


Figure S7. [1]H NMR spectrum of the **PAZ-I**

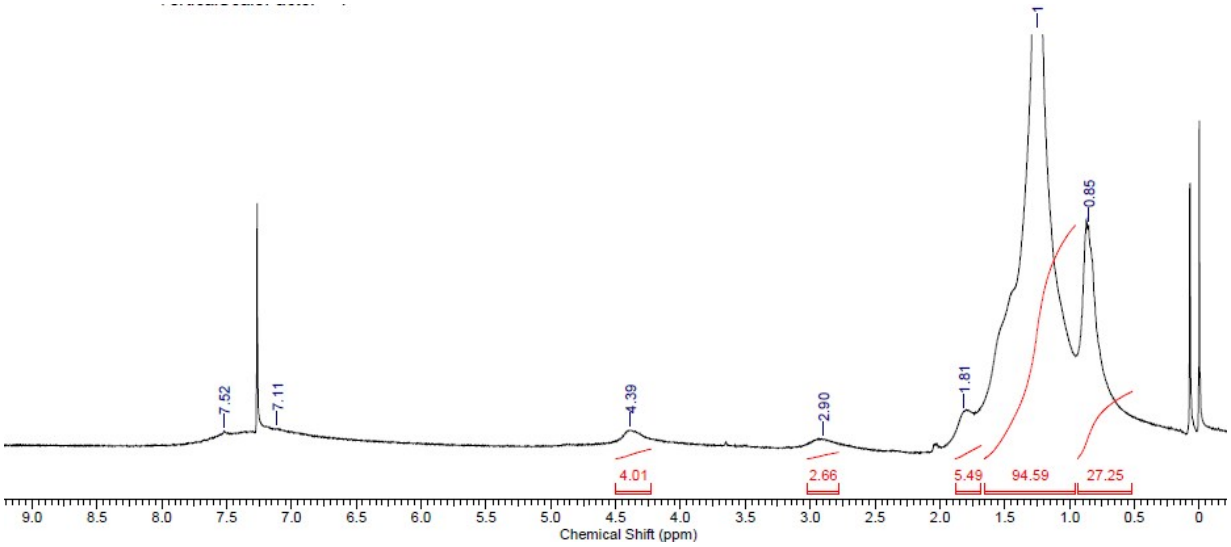


Figure S8. [1]H NMR spectrum of the **PAZ-II**

Table S11. Molecular weights and TGA data of polyazines

	M_w (D)	T_d (°C)
PAz-I	17165	335
PAz-II	16364	335

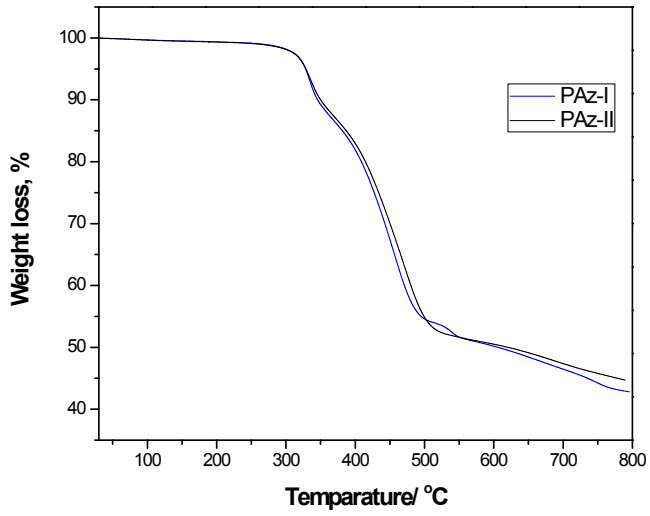


Figure S9. TGA diagram of the polymers **PAz-I** and **PAz-II**

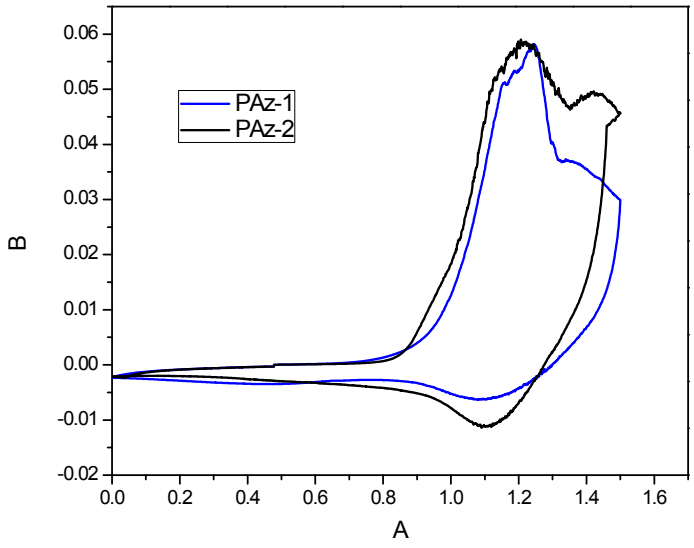


Figure S10. Cyclic voltagram of polymers **PAz-I** and **PAz-II**

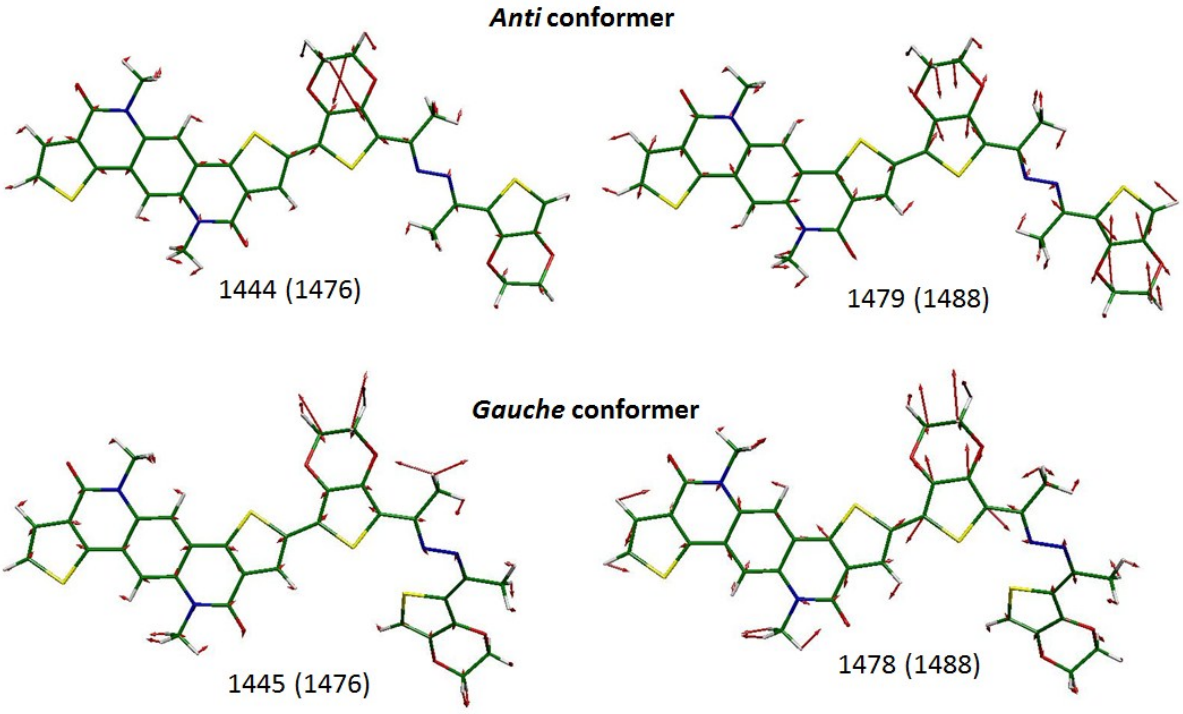


Figure S11. DFT/B3LYP/6-31G** theoretical eigenvectors for the most intense Raman bands of **PAz-I** (*anti* conformation) and **PAz-II** (*gauche* conformation).

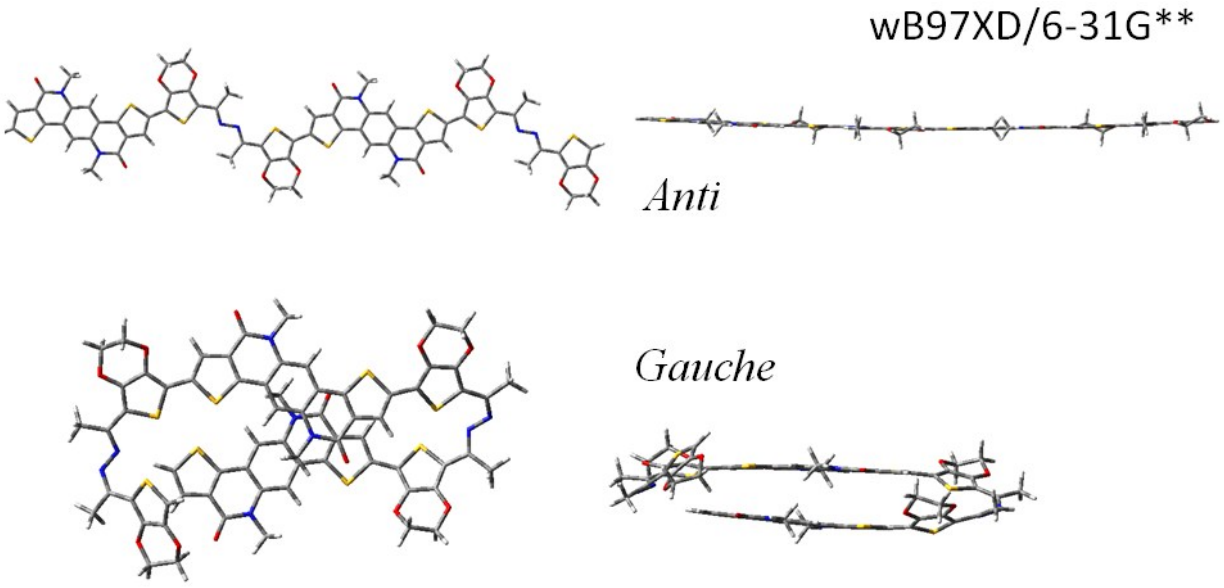


Figure S12. DFT/wB97XD/6-31G** optimized geometries for a dimeric model of the *anti* and *gauche* conformers.

Energy difference between *gauche* and *trans* conformation

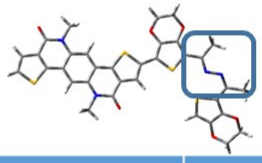
B3LYP/6-31G**

Molecule	*trans*	*gauche*
Monomer	0	+2.48 kcal/mol
Dimer	0	+5.73 Kcal/mol

wB97XD/6-31G**

Molecule	*trans*	*gauche*
Dimer	0	+19.67 kcal/mol

Dihedral Angles (°) in the C-C-N-N-N-CC region



B3LYP/6-31G**

Molecule	$\theta_{C\text{-}C\text{-}N\text{-}N}$	$\theta_{C\text{-}N\text{-}N\text{-}C}$	$\theta_{N\text{-}N\text{-}C\text{-}C}$
Monomer-gauche	-174°	-159°	6°
Dimer-gauche	-173.5°	-158°	6.5°
Monomer-trans	-180°	-179°	180°
Dimer-trans	-180°	-180°	180°

wB97XD/6-31G**

Molecule	$\theta_{C\text{-}C\text{-}N\text{-}N}$	$\theta_{C\text{-}N\text{-}N\text{-}C}$	$\theta_{N\text{-}N\text{-}C\text{-}C}$
Dimer-gauche	-176°	-150°/-141°	8°/6°
Dimer-trans	-180°	-180°	180°

Figure S13. Comparison between the theoretical data (energies and dihedral angles) obtained at B3LYP/6-31G** and wB97XD/6-31G** levels of calculations.