Supplementary Information

Molecular Design, Synthesis and Characterization of Aromatic Polythioester and Polydithioester

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conformation								
	bond							
j – 1	j	<i>j</i> + 1	$l_j{}^b$	$\angle (j-1) \wedge j^c$	$\angle j \wedge (j+1)^d$	$\phi_j{}^e$		
bond $a(c)$								
t	t	t	1 803	98 5	1173	0.0		
σ+	t	ι	1.802	99.4	117.3	0.0		
5 σ ⁻			1.802	99.4	117.3	-0.4		
5 t	t	cis	1.802	98.7	118.5	0.1		
σ ⁺	t	015	1.803	99.3	118.7	-0.4		
5 σ ⁻			1.803	99.3	118.7	0.1		
5			1.005	bond b	110.7	0.1		
t	t	t	5 787	117.3	1173	-0.7		
ť	cis	t	5 786	118.5	118.5	178.7		
	015		2.700	bond d (f)	110.0	170.7		
t	t	t	1.835	98.6	108.6	-0.2		
·	σ ⁺	·	1.833	99.4	112.3	99.4		
	5 9 ⁻		1.833	99.4	112.3	-99.4		
	5 t	σ^+		_		_		
	σ^+	Б	1.829	99.3	115.0	99.1		
	в g-		1.830	100.6	114.0	-69.4		
	t	g ⁻	_	_	_	_		
	g^+	0	1.830	100.6	114.0	69.4		
	5 9 ⁻		1.830	99.3	115.0	-99.1		
	Ð		11000	bond e	11010	///1		
t	t	t	1.522	108.6	108.6	0.0		
	g ⁺		1.520	112.3	111.7	113.6		
	g_		1.520	112.3	111.7	-113.6		
g^+	t		_	_	_	_		
0	g ⁺		_	_	-	_		
	g ⁻		_	_	_	_		
g ⁻	t		_	_	-	_		
C	g^+		_	_	_	_		
	g ⁻		-	_	_	-		
t	t	g^+	_	_	-	_		
	g^+	-	_	_	-	_		
	g ⁻		-	_	-	-		
g^+	t		1.525	111.9	111.9	7.0		
	g^+		1.523	115.0	115.0	116.3		
	g ⁻		-	-	-	-		
g ⁻	t		1.523	112.3	112.3	0.0		
	g^+		1.525	114.0	115.0	113.1		
	g ⁻		1.525	115.0	114.0	-113.1		
t	t	g ⁻	-	-	-	-		
	g^+		—	-	-	-		
	g ⁻		-	—	-	-		
g ⁺	t		1.523	112.3	112.3	0.0		
	g^+		1.525	115.0	114.0	113.1		
	g ⁻		1.525	114.0	115.0	-113.1		
g ⁻	t		1.525	111.9	111.9	-7.0		
	g^+		_	_	-	_		
	g ⁻		1.523	115.0	115.0	-116.3		

Table S1.	Geometrical	parameters of	of PETS ₂ .	used in the	e refined RI	S calculations ^a
14010010	Geometrical	parameters	$n 1 \mathbf{D} 1 \mathbf{D} 2,$	abea m me		, carearanono

^{*a*}For bonds a, b, and c, obtained from S'^1, S^1 -ethane-1,2-diyl S', S^4 -dimethyl bis(benzene-1,4-bis(carbothioate)). For bonds d, e, and f, obtained from EDBS₂. The symbol *j* denotes the current bond. ^{*b*}Length of bond *j*. ^{*c*}Angle formed between bonds *j* – 1 and *j*. ^{*d*}Angle formed between bonds *j* and *j* + 1. ^{*e*}Dihedral angle of bond *j*.

$\begin{array}{c c c c c c c c c c c c c c c c c c c $	conformation							
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	bond							
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	j – 1	j	<i>j</i> + 1	l_i^{b}	$\angle (j-1) \wedge j^c$	$\angle j \wedge (j+1)^d$	ϕ_i^{e}	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		•		5	bond a (c) f		, ,	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	t	t	t-t	1.760	103.5	112.7	3.1	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	g^+			1.762	104.4	112.7	-3.7	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ ⁻			1.762	104.4	112.7	3.7	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	ð t	t	t-c	1.761	103.5	112.9	-4.3	
	σ^+	·		1 762	104.5	112.6	-3.6	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5 σ ⁻			1.762	104.5	112.0	3.6	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5 t	t	c-t	1.760	103.4	112.0	2.9	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	α ⁺	ι	υı	1.763	104.5	112.1	_2.9	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	g g ⁻			1.703	104.5	112.0	-2.9	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	g t	t	0.0	1.703	104.5	112.0	2.9	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	ι α ⁺	ι	U-U	1.701	103.3	113.2	2.9	
	g			1.705	104.4	115.0	-3.8	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	g			1./03	104.4	115.0	3.8	
t t t t 5.788 113.0 113.0 -0.5 t-c 5.788 113.1 113.1 -71.5 c-t 5.786 113.4 113.4 -106.3 c-c 5.788 113.4 113.4 -106.3 c-c 5.788 113.4 113.4 -177.8 bond d (f) t t t t 1.829 103.6 108.1 1.9 g ⁺ 1.827 104.6 112.4 96.7 g ⁻ 1.827 104.6 112.4 96.7 t g ⁺ 1.829 103.4 111.0 4.6 g ⁺ 1.824 104.1 114.8 93.4 g ⁻ 1.828 105.6 113.4 -64.8 t g ⁻ 1.828 105.6 113.4 -64.8 g ⁻ 1.828 105.6 113.4 64.8 g ⁻ 1.828 105.6 113.4 64.8 g ⁻ 1.823 104.1 114.8 -93.4 bond e t t t 1.526 108.1 108.1 0.0 g ⁺ 1.523 111.0 111.0 111.3 g ⁺ 1.525 111.9 108.3 1.3 g ⁺ 1.525 111.9 108.3 1.3 g ⁺ 1.525 111.9 108.3 -1.3 g ⁺ 1.524 115.6 111.0 -117.4 t g ⁻ g ⁻ t 1.524 115.6 111.0 -117.4 t g ⁻ g ⁻ t 1.524 115.6 111.0 117.4 g ⁻					bond b ⁻	112.0	0.5	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	t	t-t	t	5.788	113.0	113.0	-0.5	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		t-c		5.788	113.1	113.1	-/1.5	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		c-t		5.786	113.4	113.4	-106.3	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		c-c		5.788	113.4	113.4	177.8	
t t t 1.829 103.6 108.1 1.9 g^+ 1.827 104.6 112.4 96.7 g^- 1.827 104.6 112.4 96.7 t g^+ 1.829 103.4 111.0 4.6 g^+ 1.828 105.6 113.4 -64.8 t g^- 1.828 105.6 113.4 -64.8 t g^- 1.828 105.6 113.4 64.8 g^- 1.823 111.0 111.0 111.3 g^+ 1.523 111.0 111.0 111.3 g^- 1.523 111.0 111.0 111.3 g^+ 1.525 111.9 108.3 1.3 g^+ 1.524 115.6 111.0 117.4 g^- g^- t 1.524 115.6 111.0 117.4 g^- g^- t 1.524 115.6 111.0 -117.4 t g^+ 1.525 108.3 111.9 108.3 -1.3 g^+ 1.524 115.6 111.0 -117.4 t g^- g^- t 1.524 115.6 111.0 117.4 g^- 1.524 115.6 111.0 -117.4 t g^- 1.524 115.6 111.0 -117.4 t g^- 1.524 115.6 111.0 -117.4 t g^- 1.524 115.6 111.0 115.6 117.4 g^- 1.524 111.0 115.6 117.4 g^- 1.524 111.0 115.6 117.4 g^- 1.526 113.4 114.9 117.0 g^- 1.526 113.4 114.8 110.9 g^- 1.526 113.4 114.8 113.4 110.9 g^- 1.528 114.0 115.6 -117.4 g^- 1.528 114.0 115.4 114.9 113.4 114.8 -110.9					bond d (f)			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	t	t	t	1.829	103.6	108.1	1.9	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g^+		1.827	104.6	112.4	96.7	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		g ⁻		1.827	104.6	112.4	-96.7	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		t	g^+	1.829	103.4	111.0	4.6	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g^+		1.824	104.1	114.8	93.4	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		g ⁻		1.828	105.6	113.4	-64.8	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		t	g^{-}	1.829	103.4	111.0	-4.6	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g^+	•	1.828	105.6	113.4	64.8	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g ⁻		1.824	104.1	114.8	-93.4	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		U			bond e			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	t	t	t	1.526	108.1	108.1	0.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g^+		1.523	111.0	111.0	111.3	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		σ_		1.523	111.0	111.0	-111.3	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	σ^+	t		1.525	111.9	108.3	1.3	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Б	σ^+		1.525	115.6	111.0	117.4	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		5 σ ⁻		-				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	α ⁻	5 t		1 525	111.0	108.3	_13	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8	α ⁺		1.525	-	100.5	1.5	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		8 σ ⁻		1 524	1156	111.0	_117 /	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	t	g t	a^{+}	1.524	109.2	111.0	-117.4	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	ι	ι α ⁺	g	1.525	108.3	111.9	1.5	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g ·		1.324	111.0	115.0	11/.4	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$. +	g		1 507	-	-	-	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	g	t _		1.527	111.3	111.3	9.3	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g'		1.524	114.9	114.9	117.0	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	_	g		1.528	114.0	114.0	-113.4	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	g_	t		1.524	112.4	112.4	0.0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g⁺		1.526	113.4	114.8	110.9	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		g ⁻		1.526	114.8	113.4	-110.9	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	t	t	g ⁻	1.525	108.3	111.9	1.3	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g^+		-	-	-	-	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		g ⁻		1.524	111.0	115.6	-117.4	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	g^+	t		1.524	112.4	112.4	0.0	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		g^+		1.526	114.8	113.4	110.9	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		g ⁻		1.526	113.4	114.8	-110.9	
g+1.528114.0114.0113.4g-1.524114.9114.9-117.0	g ⁻	t		1.527	111.3	111.3	-9.3	
g ⁻ 1.524 114.9 114.9 -117.0		g^+		1.528	114.0	114.0	113.4	
		g ⁻		1.524	114.9	114.9	-117.0	

^{*a*}For bonds a, b, and c, obtained from $S^{,1}, S^{1}$ -ethane-1,2-diyl 4-dimethyl bis(benzene-1,4-bis(carbodithioate)). For bonds d, e, and f, obtained from EDBS₄. The symbol *j* denotes the current bond. ^{*b*}Length of bond *j*. ^{*c*}Angle formed between bonds *j* – 1 and *j*. ^{*d*}Angle formed between bonds *j* and *j*+1. ^{*e*}Dihedral angle of bond *j*. ^{*f*}Abbreviation: t-t, trans-trans; t-c, trans-cis; c-t, cis-trans; c-c, cis-cis (see Figure 6).