Electronic Supplementary Material (ESI) for Polymer Chemistry

Supplementary Information

Molecular Design, Synthesis and Characterization of Aromatic Polythioester and Polydithioester

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Table S1. Geometrical parameters of $PETS_2$, used in the refined RIS calculations[a]

conformation						
	bond					
$j-1$	j	$j+1$	l_j [b]	$\angle(j-1)\wedge j$ [c]	$\angle j\wedge(j+1)$ [d]	ϕ_j [e]
				bond a (c)		
t	t	t	1.803	98.5	117.3	0.0
g^+			1.802	99.4	117.3	0.4
g^-			1.802	99.4	117.3	−0.4
t	t	cis	1.804	98.7	118.5	0.0
g^+			1.803	99.3	118.7	−0.4
g^-			1.803	99.3	118.7	0.4
				bond b		
t	t	t	5.787	117.3	117.3	−0.7
	cis		5.786	118.5	118.5	178.7
				bond d (f)		
t	t	t	1.835	98.6	108.6	−0.2
	g^+		1.833	99.4	112.3	99.4
	g^-		1.833	99.4	112.3	−99.4
	t	g^+	–	–	–	–
	g^+		1.829	99.3	115.0	99.1
	g^-		1.830	100.6	114.0	−69.4
	t	g^-	–	–	–	–
	g^+		1.830	100.6	114.0	69.4
	g^-		1.830	99.3	115.0	−99.1
				bond e		
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		–	–	–	–
	g^+		–	–	–	–
	g^-		–	–	–	–
g^-	t		–	–	–	–
	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

[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 $EDBS_2$. 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.

Table S2. Geometrical parameters of $PETS_4$, used in the refined RIS calculations[a]

conformation						
bond						
$j-1$	j	$j+1$	l_j [b]	$\angle(j-1)\wedge j$ [c]	$\angle j\wedge(j+1)$ [d]	ϕ_j [e]
			bond a (c) [f]			
t	t	t-t	1.760	103.5	112.7	3.1
g^+			1.762	104.4	112.7	−3.7
g^-			1.762	104.4	112.7	3.7
t	t	t-c	1.761	103.5	112.9	−4.3
g^+			1.762	104.5	112.6	−3.6
g^-			1.762	104.5	112.6	3.6
t	t	c-t	1.760	103.4	113.1	2.9
g^+			1.763	104.5	112.8	−2.9
g^-			1.763	104.5	112.8	2.9
t	t	c-c	1.761	103.5	113.2	3.5
g^+			1.763	104.4	113.0	−3.8
g^-			1.763	104.4	113.0	3.8
			bond b [f]			
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	177.8
			bond d (f)			
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^-	1.829	103.4	111.0	−4.6
	g^+		1.828	105.6	113.4	64.8
	g^-		1.824	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^-		1.523	111.0	111.0	−111.3
g^+	t		1.525	111.9	108.3	1.3
	g^+		1.524	115.6	111.0	117.4
	g^-		–	–	–	–
g^-	t		1.525	111.9	108.3	−1.3
	g^+		–	–	–	–
	g^-		1.524	115.6	111.0	−117.4
t	t	g^+	1.525	108.3	111.9	1.3
	g^+		1.524	111.0	115.6	117.4
	g^-		–	–	–	–
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^-	t		1.524	112.4	112.4	0.0
	g^+		1.526	113.4	114.8	110.9
	g^-		1.526	114.8	113.4	−110.9
t	t	g^-	1.525	108.3	111.9	1.3
	g^+		–	–	–	–
	g^-		1.524	111.0	115.6	−117.4
g^+	t		1.524	112.4	112.4	0.0
	g^+		1.526	114.8	113.4	110.9
	g^-		1.526	113.4	114.8	−110.9
g^-	t		1.527	111.3	111.3	−9.3
	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 $EDBS_4$. 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).