

Electronic Supplementary Information

**Computational design of polymers:
poly(ester amide) and polyurethane**

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Table S1 Stable conformations, intramolecular interactions, and effectual MO theories found for various functional units and characteristic ratios of the corresponding polymers

Polymer type	Included element	Corresponding polymer	Functional unit	Stable conformation	Intramolecular interaction ^a	Characteristic ratio ($\langle r^2 \rangle_0 / \langle r^2 \rangle_b$) ^b	Effectual MO theory ^c	Reference no.	
Polyether	C, H, O	poly(methylene oxide) poly(ethylene oxide) poly(trimethylene oxide) poly(propylene oxide) poly(tetramethylene oxide)	[O-CH ₂ -]	gg	dipole-dipole, $n_0 \rightarrow \sigma_{C,O}^*$, $E_p \approx -1.7$	9.2	B3LYP	1,2	
			[O-CH ₂ -CH ₂ -]	ttt, tgt	C-H...O, $E_p \approx -1.5$ to $+0.1$	5.1 (40 °C)	MP2	2-4	
			[O-CH ₂ -CH ₂ -CH ₂ -]	tggt	$E_p \approx -0.7$	3.7	MP2	5	
			[O-CH ₂ -CH(CH ₃)-]	tg ⁺ g ⁺ [(R) form], ttt	C-H...O	5.9 (isotactic, 50 °C)	MP2	2,6-8	
Polyamine	C, H, N	poly(ethylene imine) poly(trimethylene imine)	[O-CH ₂ -CH ₂ -CH ₂ -]	tggt	C-H...O, $E_p \approx -0.6$	5.7 (30 °C)	MP2	9,10	
			[NH-CH ₂ -CH ₂ -]	tgt [meso]	N-H...N	3.1	MP2	11,12	
Polyphosphine	C, H, P	poly(1-methylphosphirane) poly(1-phenylphosphirane)	[NH-CH ₂ -CH ₂ -CH ₂ -]	tg ⁺ g ⁺ t [racemo]	N-H...N	3.5	MP2	13	
			[P(CH ₃)-CH ₂ -CH ₂ -]	ttt [meso]	$\pi - \pi$	7.0 [atactic]	MP2	14	
Polysulfide (Polythioether)	C, H, S	poly(methylene sulfide) poly(ethylene sulfide) poly(trimethylene sulfide) poly(propylene sulfide)	[P(CH ₃)-CH ₂ -CH ₂ -]	ttt [racemo]	$\pi - \pi$	13.0 [atactic]	MP2	14	
			[S-CH ₂ -]	gg	dipole-dipole, $n_s \rightarrow \sigma_{C,S}^*$, $E_p \approx -1.5$	7.6	B3LYP	1,2	
			[S-CH ₂ -CH ₂ -]	g ⁺ tg ⁺	dipole-dipole, $E_p \approx -0.4$, [S...S]	3.1	MP2	2,3	
			[S-CH ₂ -CH ₂ -CH ₂ -]	gggg	$E_p \approx -0.2$, $E_p \approx -0.3$	3.6	MP2	5	
Polyselenide (Polyselenoether)	C, H, Se	poly(methylene selenide) poly(ethylene selenide) poly(trimethylene selenide)	[S-CH ₂ -CH(CH ₃)-]	g ⁺ tg ⁺ [(R) form]	$E_p \approx -0.5$	4.0 (isotactic)	MP2	2,15	
			[Se-CH ₂ -]	gg	dipole-dipole, $n_{se} \rightarrow \sigma_{C,Se}^*$, $E_p \approx -1.2$	7.3	MP2	16	
			[Se-CH ₂ -CH ₂ -]	g ⁺ tg ⁺	$E_p \approx -0.3$, [Se...Se]	5.4	MP2	16	
			[Se-CH ₂ -CH ₂ -CH ₂ -]	g ⁺ tg ⁺	$E_p \approx -0.4$	5.3	MP2	16	
Copolymer	C, H, N, O	poly(ethylene imine- <i>alt</i> -ethylene oxide) poly(ethylene imine- <i>alt</i> -ethylene sulfide) poly(ethylene oxide- <i>alt</i> -ethylene sulfide)	[NH-CH ₂ -CH ₂ -O-CH ₂ -CH ₂ -]	tg ⁻ t [form] in N-C-C-O	N-H...O, C-H...N, C-H...O	1.3	MP2	12,17	
			[NH-CH ₂ -CH ₂ -S-CH ₂ -CH ₂ -]	tg ⁺ g ⁺ [form] in N-C-C-S	N-H...S, $E_p(CS) = -0.4$	5.2	MP2	12	
			[O-CH ₂ -CH ₂ -S-CH ₂ -CH ₂ -]	ttg in O-C-C-S	C-H...O, dipole-dipole, $E_p(CS) = -0.4$	6.0	MP2	18	
Polyester	C, H, O	poly(ethylene terephthalate) poly(trimethylene terephthalate) poly(butylene terephthalate) poly(ethylene naphthalate) poly(L-lactide), poly(D)-lactic acid poly((R)-3-hydroxybutyrate) poly(ethylene succinate)	[CO ₂ C ₆ H ₄ COO-(CH ₂) ₂ -O-]	trans-tgt ^d	C-H...O, dipole-dipole, $E_p \approx -1.2$	2.6 ^e	MP2	19	
			[CO ₂ C ₆ H ₄ COO-(CH ₂) ₃ -O-]	trans-tggt, tggg ^d	$\pi - \pi$, C-H...O, dipole-dipole, $E_p \approx -0.6$	4.1 ^e	MP2, MP3 ^f	20,21	
			[CO ₂ C ₆ H ₄ COO-(CH ₂) ₄ -O-]	trans-tgtgt, tgggg, tg ⁺ tg ⁺ t ^d	$\pi - \pi$, C-H...O, dipole-dipole, $E_p \approx -0.3$	3.8 ^e	MP2, MP3 ^f	21	
			[CO ₂ C ₁₀ H ₆ COO-(CH ₂) ₂ -O-]	gt	C-H...O, dipole-dipole, $E_p \approx -1.2$	2.4 ^e	MP2	19	
			[CO-O-CH(CH ₃)-]	tg ⁺ t	O...H, [O...O]	11.8	MP2 or B3LYP ^g	22	
			[CO-O-CH(CH ₃)-CH ₂ -]	ttg ⁺ g ⁺	O...H	5.6	MP2	23	
			[COO-(CH ₂) ₂ -O-]	tgt	$E_p \approx -1.3$	6.2	MP2, M06-2X	24	
			[COO-(CH ₂) ₄ -O-]	ttt	$E_p \approx -0.2$	7.1	MP2, M06-2X	24	
			[COO-(CH ₂) ₂ -CH ₂ -]	tg ⁺ tg ⁺ t					
			[COO-(CH ₂) ₃ -NH-]	ttt					
Polyamide	C, H, N	aromatic polyamide 2T aromatic polyamide 3T	[CO ₂ C ₆ H ₄ CONH-(CH ₂) ₂ -NH-]	cis-trans-tg ⁺ g ⁺ t ^d	N-H...O	3.2 ^e	B3LYP	25	
			[CO ₂ C ₆ H ₄ CONH-(CH ₂) ₃ -NH-]	cis-trans-ttg ^d	C-H...O	3.7 ^e	B3LYP	25	
Polythioester	C, H, O, S	poly(ethylene dithioester) poly(trimethylene dithioester)	[CO ₂ C ₆ H ₄ COS-(CH ₂) ₂ -S-]	trans-g ⁺ tg ⁺ t ^d	dipole-dipole, $E_p \approx -1.5$, [S...S]	16.7 ^e	MP2	25-28	
			[CO ₂ C ₆ H ₄ COS-(CH ₂) ₃ -S-]	trans-gtgg ^d	dipole-dipole, $E_p \approx -1.0$ to -1.4	10.5 ^e	MP2	25,27,28	
Polythioamide	C, H, N, S	aromatic polythioamide 2T aromatic polythioamide 3T	[CSC ₆ H ₄ CSSNH-(CH ₂) ₂ -NH-]	cis-trans-tg ⁺ g ⁺ t ^d , g ⁺ tg ⁺ , ggg ^d	N-H...S	3.6 ^e	B3LYP	25	
			[CSC ₆ H ₄ CSSNH-(CH ₂) ₃ -NH-]	cis-trans-tttt ^d		5.7 ^e	B3LYP	25	
Polydithioester	C, H, S	poly(ethylene tetrahydroester) poly(trimethylene tetrahydroester)	[CSC ₆ H ₄ CSS-(CH ₂) ₂ -S-]	trans-cis-g ⁺ tg ⁺ t ^d	dipole-dipole, $E_p \approx -1.0$, [S...S]	5.2 ^e	MP2	25-28	
			[CSC ₆ H ₄ CSS-(CH ₂) ₃ -S-]	trans-cis-gtgg ^d	dipole-dipole, $E_p \approx -0.8$	6.1 ^e	MP2	25,27,28	
Polysilane	C, H, Si	poly(methyl- <i>n</i> -propylsilane) poly(di- <i>n</i> -butylsilane) poly(di- <i>n</i> -hexylsilane)	[Si(CH ₃)(C ₃ H ₇)-]	[repulsion between the side chains] [as above]	19.9	(MD) ^h	29,30		
			[Si(C ₄ H ₉) ₂ -]	[as above]	42.3 (19.1 °C)	(MD) ^h	29,30		
			[Si(C ₆ H ₁₃) ₂ -]	[as above]	42.5	(MD) ^h	29,30		

^a Attractive interactions are mainly specified, and repulsions are written in the square brackets. E_p and E_o are conformational energies (in kcal mol⁻¹) of the gauche states in C-X and XC-C bonds (X: heteroatom), respectively. The designations are not necessarily consistent with those in the original papers. ^b At 25 °C when the temperature is not indicated. ^c Abbreviations: B3LYP, Becke's three parameter hybrid functional with the correlation functional of Lee, Yang, and Parr; ³¹ MP2 or MP3, a Hartree-Fock calculation followed by the Miller-Plesset correlation energy correction truncated at second-order (MP2) or third order (MP3); ³² M06-2X, the hybrid functional of Zhao and Truhlar. ³³ *d* Trans and cis represent the relative orientations between two carbonyl or thiocarbonyl groups bonded to the benzene ring. ^e The virtual bond was used to represent the benzene or naphthalene ring. ^f The extrapolation to the complete basis set ^{34,35} and the compensation for the higher-order correlations ^{36,37} are required for proper evaluation of $\pi - \pi$ interaction energies of these aromatic polyesters. ^g The MP2 energies reproduced NMR experiments on the model compounds better than the B3LYP ones, whereas the latter energies yielded better agreement with experimental configurational properties of poly(L-lactide) and poly(DL-lactide). ^h By the rotational isomeric state (RIS) scheme with molecular dynamic simulations.

Table S2 Observed vicinal ^1H – ^1H and ^{13}C – ^1H coupling constants of EA-1 and EA-1– ^{13}C ^a

Solvent ^b	Temp (°C)	J_{CH}^{O}	J_{HH}	J'_{HH}	J_{CH}^{N}	J_{HH}^{N}
C_6D_6	15	3.33	6.66	4.72	3.50	5.85
	25	3.33	6.66	4.72	3.50	5.85
	35	3.35	6.60	4.72	3.50	5.85
	45	3.36	6.60	4.78	3.50	5.85
	55	3.38	6.60	4.79	3.50	5.85
CDCl_3	15	3.12	6.79	3.87	3.32	5.74
	25	3.18	6.78	3.90	3.32	5.74
	35	3.19	6.78	3.93	3.32	5.74
	45	3.24	6.78	3.98	3.31	5.74
	55	3.27	6.75	4.02	3.31	5.74
$(\text{CD}_3)_2\text{SO}$	25	3.19	6.52	4.96	3.76	5.70
	35	3.20	6.52	5.02	3.76	5.70
	45	3.24	6.52	5.08	3.76	5.70
	55	3.25	6.48	5.14	3.76	5.72
D_2O	15	3.10	6.77	3.80	3.80	– ^c
	25	3.13	6.76	3.80	3.80	–
	35	3.15	6.75	3.91	3.80	–
	45	3.17	6.74	3.95	3.78	–
	55	3.17	6.74	3.97	3.78	–

^aIn Hz. ^b Symbols: C_6D_6 , benzene-*d*₆; CDCl_3 , chloroform-*d*; $(\text{CD}_3)_2\text{SO}$, dimethyl-*d*₆ sulfoxide (abbreviated as DMSO-*d*₆); D_2O , deuterium oxide (water-*d*₂). ^c Not available.

Table S3 Trans fractions of the O–C, C–C, and C–N bonds of EA-1, determined from NMR experiments

		Bond ^a							
		b: O–C		c: C–C		d: C–N			
		J_{CH}^{O}		J_{HH} and J'_{HH}		J_{CH}^{N}		J_{HH}^{N}	
Solvent	Temp (°C)	Set A ^b	Set B ^c	Set C ^d	Set D ^e	Set E ^f	Set F ^g	Set G ^h	Set H ⁱ
C ₆ D ₆	15	0.40	0.42	0.14	0.22	0.10	0.16	0.10	0.11
	25	0.40	0.42	0.14	0.22	0.10	0.16	0.10	0.11
	35	0.40	0.42	0.14	0.23	0.10	0.16	0.10	0.11
	45	0.40	0.41	0.15	0.23	0.10	0.16	0.10	0.11
	55	0.39	0.41	0.15	0.23	0.10	0.16	0.10	0.11
CDCl ₃	15	0.46	0.48	0.07	0.14	0.16	0.22	0.15	0.14
	25	0.45	0.46	0.07	0.15	0.16	0.22	0.15	0.14
	35	0.44	0.46	0.07	0.15	0.16	0.22	0.15	0.14
	45	0.43	0.45	0.08	0.15	0.17	0.22	0.15	0.14
	55	0.42	0.44	0.08	0.16	0.17	0.22	0.15	0.14
(CD ₃) ₂ SO	25	0.44	0.46	0.17	0.25	0.01	0.08	0.17	0.15
	35	0.44	0.46	0.17	0.26	0.01	0.08	0.17	0.15
	45	0.43	0.45	0.18	0.27	0.01	0.08	0.17	0.15
	55	0.43	0.44	0.19	0.27	0.01	0.08	0.16	0.14
D ₂ O	15	0.47	0.48	0.06	0.14	0.00	0.07	– ^j	– ^j
	25	0.46	0.47	0.07	0.14	0.00	0.07	–	–
	35	0.45	0.47	0.07	0.15	0.00	0.07	–	–
	45	0.45	0.46	0.08	0.15	0.00	0.07	–	–
	55	0.45	0.46	0.08	0.15	0.00	0.07	–	–

^a See Fig. 2a. ^b With the coupling constants calculated from a Karplus equation proposed by Tvaroška and Gajdoš:³⁸ $J_{\text{G}_1} + J_{\text{G}_2} = 2.42$ Hz and $J'_{\text{T}} + J'_{\text{G}} = 9.53$ Hz. ^c With the coupling constants calculated from MO calculations at the B3LYP/6-311++G(3df,3pd) level: $J_{\text{G}_1} + J_{\text{G}_2} = 2.26$ Hz and $J'_{\text{T}} + J'_{\text{G}} = 9.87$ Hz. ^d With the coupling constants of 2-methylmorpholine: e.g., $J_{\text{T}} = 11.62$, $J_{\text{G}} = 2.35$, $J'_{\text{T}} = 11.62$, $J'_{\text{G}} = 3.33$, $J''_{\text{G}} = 1.21$, and $J'''_{\text{G}} = 2.51$ Hz for the chloroform solution. For the details, see reference¹⁷. ^e With the coupling constants calculated from MO calculations at the B3LYP/6-311++G(3df,3pd) level: $J_{\text{T}} = 11.12$, $J_{\text{G}} = 4.82$, $J'_{\text{T}} = 10.07$, $J'_{\text{G}} = 2.25$, $J''_{\text{G}} = 1.96$, and $J'''_{\text{G}} = 1.82$ Hz. ^f With the coupling constants calculated from a Karplus equation proposed by Kao and Barfield:³⁹ $J_{\text{G}_1} + J_{\text{G}_2} = 1.96$ Hz and $J'_{\text{T}} + J'_{\text{G}} = 7.56$ Hz. ^g With the coupling constants calculated from MO calculations at the B3LYP/6-311++G(3df,3pd) level: $J_{\text{G}_1} + J_{\text{G}_2} = 1.57$ Hz and $J'_{\text{T}} + J'_{\text{G}} = 8.03$ Hz. ^h With the coupling constants calculated from a Karplus equation proposed by Ludvigsen *et al.*:⁴⁰ $J_{\text{C}_1} + J_{\text{C}_2} = 8.13$ Hz and $J'_{\text{E}} + J'_{\text{C}} = 12.09$ Hz. ⁱ With the coupling constants calculated from MO calculations at the B3LYP/6-311++G(3df,3pd) level: $J_{\text{C}_1} + J_{\text{C}_2} = 5.16$ Hz and $J'_{\text{E}} + J'_{\text{C}} = 12.48$ Hz. ^j Not available.

Table S4 Trans fractions of the O–C, C–C, and C–N bonds of EA-1, evaluated from MO calculations

Solvent	Solvation model	Temp (°C)	Bond ^a									
			b: O–C			c: C–C			d: C–N			
			B3LYP ^b	M06-2X ^c	MP2 ^d	B3LYP ^b	M06-2X ^c	MP2 ^d	B3LYP ^b	M06-2X ^c	MP2 ^d	
Benzene	IEFPCM	15		0.34	0.37		0.13	0.11		0.19	0.17	
		25		0.34	0.37		0.14	0.11		0.20	0.17	
		35		0.34	0.37		0.14	0.12		0.20	0.17	
		45		0.34	0.37		0.15	0.12		0.20	0.17	
		55		0.34	0.37		0.15	0.13		0.20	0.18	
Chloroform	IEFPCM	15	0.66	0.39	0.41	0.19	0.16	0.13	0.07	0.13	0.12	
		25	0.65	0.39	0.41	0.19	0.16	0.14	0.08	0.14	0.12	
		35	0.64	0.39	0.41	0.20	0.17	0.14	0.08	0.14	0.13	
		45	0.63	0.39	0.41	0.20	0.17	0.15	0.08	0.14	0.13	
		55	0.63	0.39	0.40	0.21	0.18	0.15	0.09	0.14	0.13	
	CPCM	15	0.66	0.40	0.41	0.20	0.16	0.14	0.06	0.11	0.10	
		25	0.66	0.40	0.41	0.20	0.17	0.14	0.06	0.11	0.10	
		35	0.65	0.40	0.41	0.21	0.17	0.15	0.07	0.11	0.11	
		45	0.64	0.40	0.41	0.21	0.18	0.15	0.07	0.12	0.11	
		55	0.64	0.40	0.41	0.22	0.18	0.16	0.07	0.12	0.11	
DMSO	IEFPCM	25	0.70	0.45	0.45	0.24	0.20	0.17	0.04	0.08	0.08	
		35	0.70	0.45	0.45	0.24	0.21	0.17	0.05	0.08	0.08	
		45	0.69	0.45	0.45	0.25	0.21	0.18	0.05	0.08	0.08	
		55	0.68	0.44	0.45	0.25	0.21	0.18	0.05	0.09	0.08	
		CPCM	25	0.70	0.45	0.45	0.24	0.20	0.17	0.04	0.08	0.07
	35		0.70	0.45	0.45	0.25	0.21	0.17	0.04	0.08	0.08	
	45		0.69	0.45	0.45	0.25	0.21	0.18	0.05	0.08	0.08	
	55		0.68	0.45	0.45	0.25	0.21	0.18	0.05	0.08	0.08	
	Water		IEFPCM	15		0.45	0.45		0.20	0.17		0.07
		25			0.45	0.45		0.20	0.17		0.08	0.07
35				0.45	0.45		0.21	0.17		0.08	0.08	
45				0.45	0.45		0.21	0.18		0.08	0.08	
55				0.45	0.45		0.22	0.18		0.08	0.08	

^a See Fig. 2a. ^b At the B3LYP/6-311+G(2d,p)//B3LYP/6-311+G(2d,p) level. ^c At the M06-2X/6-311+G(2d,p)//B3LYP/6-311+G(2d,p) level. ^d At the MP2/6-311+G(2d,p)//B3LYP/6-311+G(2d,p) level.

Table S5 Observed vicinal ^1H - ^1H coupling constants of U-1 and U-2 ^a

Solvent	Temp (°C)	U-1			U-2	
		J_{HH}^{N}	J_{HH}	J'_{HH}	J_{HH}	J'_{HH}
CD ₃ OD	15	– ^b	6.89	5.34	6.49	2.92
	25	–	6.89	5.41	6.44	2.95
	35	–	6.87	5.47	– ^b	– ^b
	45	–	6.81	5.54	–	–
	55	–	6.74	5.59	–	–
(CD ₃) ₂ SO	25	5.81	7.20	5.39	6.65	2.61
	35	5.76	7.15	5.40	– ^b	– ^b
	45	5.70	7.14	5.51	–	–
	55	5.70	7.02	5.57	–	–

^a In Hz. ^b The satellite of U-2 was broadened at temperatures above 25 °C.

Table S6 Trans fractions (p_t 's) of U-1 and U-2: Comparison between NMR experiments and MO calculations

Medium	Temp (°C)	U-1 ^a				U-2 ^a					
		c & e: N–C		d: C–C		h & j: O–C	i: C–C				
		NMR	MO ^b	NMR	MO ^b	MO ^b	NMR	MO ^b			
		Set A ^c	Set B ^d	Set C ^e	Set D ^f		Set E ^g	Set F ^h			
Gas	15		0.16		0.13		0.47			0.24	
	25		0.16		0.14		0.46			0.24	
	35		0.16		0.14		0.46			0.25	
	45		0.17		0.14		0.46			0.25	
	55		0.17		0.14		0.45			0.25	
Methanol	15		0.19	0.18	0.23	0.14	0.65	0.07	0.15	0.12	
	25		0.19	0.19	0.24	0.15	0.64	0.08	0.15	0.13	
	35		0.19	0.19	0.24	0.15	0.63	– ^j	– ^j	0.14	
	45		0.19	0.20	0.25	0.16	0.62	–	–	0.14	
	55		0.19	0.21	0.26	0.16	0.62	–	–	0.15	
DMSO	25	0.18	0.17	0.19	0.18	0.21	0.15	0.64	0.04	0.11	0.13
	35	0.21	0.18	0.19	0.18	0.22	0.15	0.63	– ^j	– ^j	0.13
	45	0.23	0.20	0.19	0.19	0.23	0.16	0.63	–	–	0.14
	55	0.23	0.20	0.19	0.20	0.24	0.16	0.62	–	–	0.14

^a For the bond symbols, see Figs. 2c and 2d. ^b At the MP2/6-311+G(2d,p)//B3LYP/6-311+G(2d,p) level with the IEFPCM solvation model. ^c With the coupling constants calculated from a Karplus equation proposed by Ludvigsen *et al.*:⁴⁰ $J_{C_1} + J_{C_2} = 7.98$ Hz and $J'_E + J'_C = 12.44$ Hz. ^d With the coupling constants calculated from MO calculations at the B3LYP/6-311++G(3df,3pd) level: $J_{C_1} + J_{C_2} = 4.77$ Hz and $J'_E + J'_C = 13.03$ Hz. ^e With the coupling constants of 2-methylpiperazine:¹¹ $J_T = 11.92$, $J_G = 2.77$, $J'_T = 11.92$, $J'_G = 3.19$, and $J''_G = 1.92$ Hz for the methanol solution; $J_T = 11.49$, $J_G = 2.74$, $J'_T = 11.49$, $J'_G = 3.05$, and $J''_G = 2.14$ Hz for the DMSO solution. ^f With the coupling constants calculated from MO calculations at the B3LYP/6-311++G(3df,3pd) level: $J_T = 10.33$, $J_G = 4.51$, $J'_T = 10.38$, $J'_G = 2.62$, and $J''_G = 1.65$ Hz. ^g With the coupling constants optimized for ethylene oxides:⁴¹ $J_T = J'_T = 11.4$ Hz and $J_G = J'_G = J''_G = 2.3$ Hz. ^h With the coupling constants calculated from MO calculations at the B3LYP/6-311++G(3df,3pd) level: $J_T = 11.33$, $J_G = 4.96$, $J'_T = 10.73$, $J'_G = 1.39$, and $J''_G = 2.49$ Hz. ⁱ Not available.

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