

Supporting Information

Polymerization of 1,3-Butadiene Catalyzed by Co(II) and Ni(II) Complexes of 6,6'-dihydroxy -2,2'-bipyridine Ligands. 1,4-*cis*-Polymerization versus Isospecific 1,2-Polymerization

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Table S1. Synthesis of isospecific-1,2-polybutadiene^a

Run	F _{NBA} ^b	F _{MAO} ^c	Yield % ^d	Microstructure (%) ^e				M _n ^f	M _w /M _n ^f
				<i>cis</i> - 1,4	<i>trans</i> - 1,4	1,2	rr/mr/mm		
1	9	100	92	91.8	4.3	3.9	-	380,000	1.16
								11,000	2.91
2	18	100	59	72.0	3.0	25.0	<1/<1/>99	8,000	3.72
3	33	100	20	8.7	0	91.3	<1/<1/>99	510,000	2.58
								3,800	1.71
4	40	100	Trace	-	-	-	-	-	-
5	50	100	Trace	-	-	-	-	-	-
6	25	50	Trace	-	-	-	-	-	-
7	25	150	64	63.1	2.9	34.0	<1/<1/>99	140,000	2.06
								6,600	2.16
8	25	200	82	87.7	4.7	7.6	-	190,000	1.37
								7,800	2.61
9 ^g	25	100	26	6.5	0	93.5	<1/<1/>99	549,000	2.61

^a[BD]/[Ni]/[MAO] = 500/1/100, [1-Ni] = 0.02 mmol, toluene = 10 mL, 30 °C, 1 h.

NBA purchased from TCI was used. ^bF_{NBA} = [NBA]/[Ni] ratio. ^cF_{MAO} =

[MAO]/[Ni] ratio. ^dMethanol insoluble part. ^eDetermined by NMR (C₂D₂Cl₄, 100

°C). ^fDetermined by SEC. ^gNBA purchased from Enamine Ltd. was used.

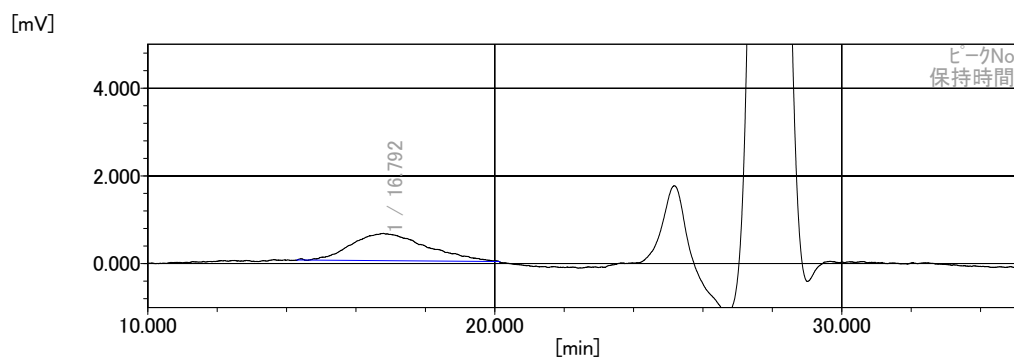


Figure S1. GPC profile of polybutadiene

(run 9 in Table 1, eluent: 1,2,4-trichlorobenzene, 140 °C)

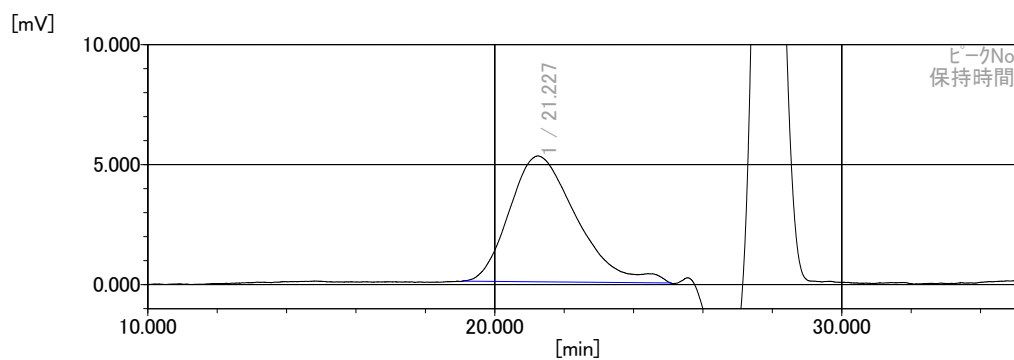


Figure S2. GPC profile of polybutadiene

(run 11 in Table 1, eluent: 1,2,4-trichlorobenzene, 140 °C)

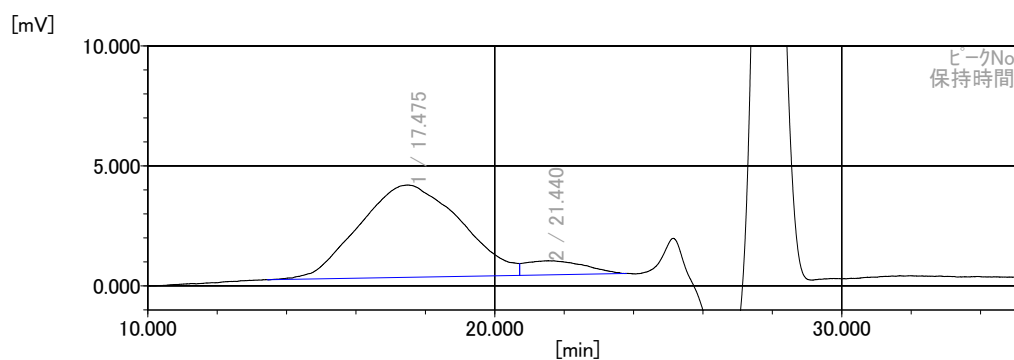


Figure S3. GPC profile of polybutadiene

(run 12 in Table 1, eluent: 1,2,4-trichlorobenzene, 140 °C)

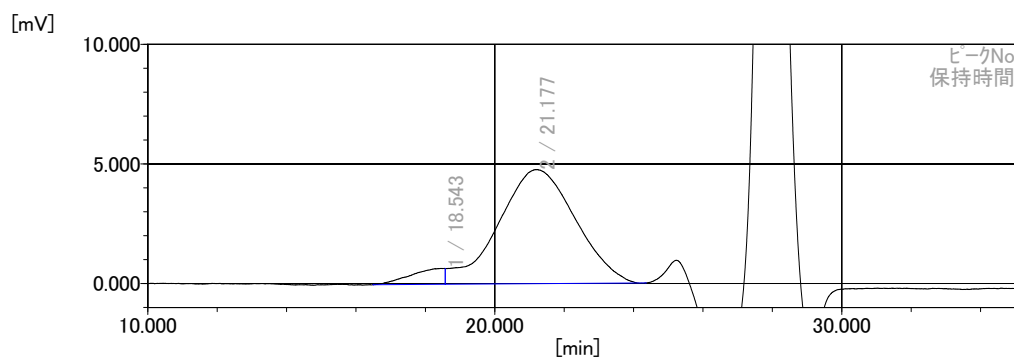


Figure S4. GPC profile of polybutadiene
(run 1 in Table S1, eluent: 1,2,4-trichlorobenzene, 140 °C)

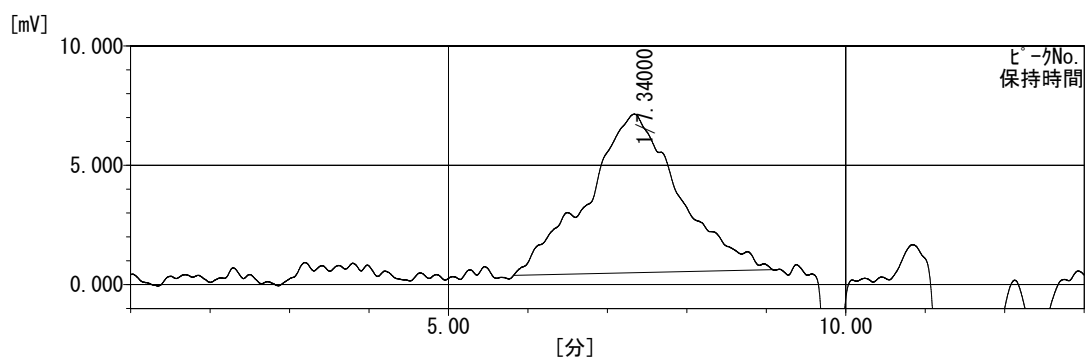


Figure S5. GPC profile of polybutadiene
(run 2 in Table S1, eluent: THF, 40 °C)

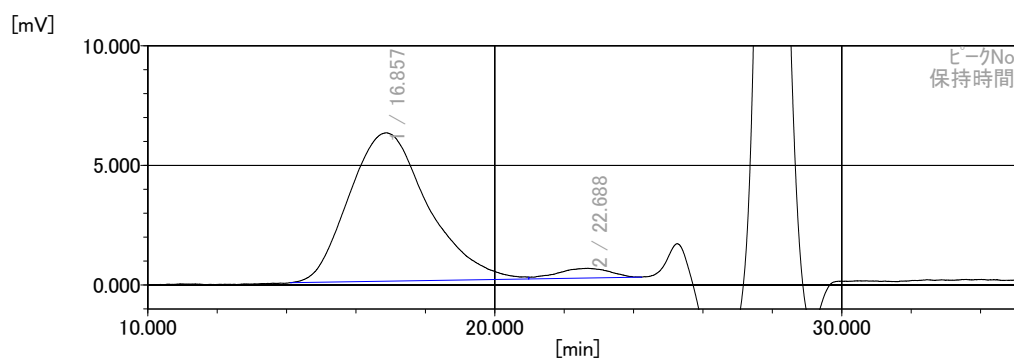


Figure S6. GPC profile of polybutadiene
(run 3 in Table S1, eluent: 1,2,4-trichlorobenzene, 140 °C)

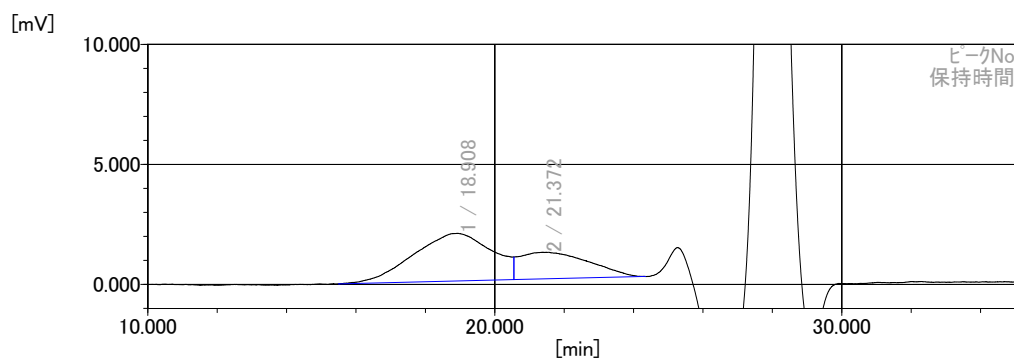


Figure S7. GPC profile of polybutadiene
(run 7 in Table S1, eluent: 1,2,4-trichlorobenzene, 140 °C)

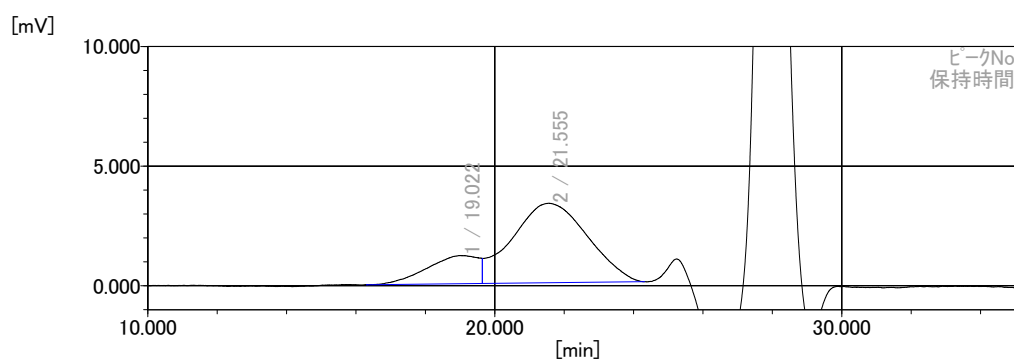


Figure S8. GPC profile of polybutadiene
(run 8 in Table S1, eluent: 1,2,4-trichlorobenzene, 140 °C)

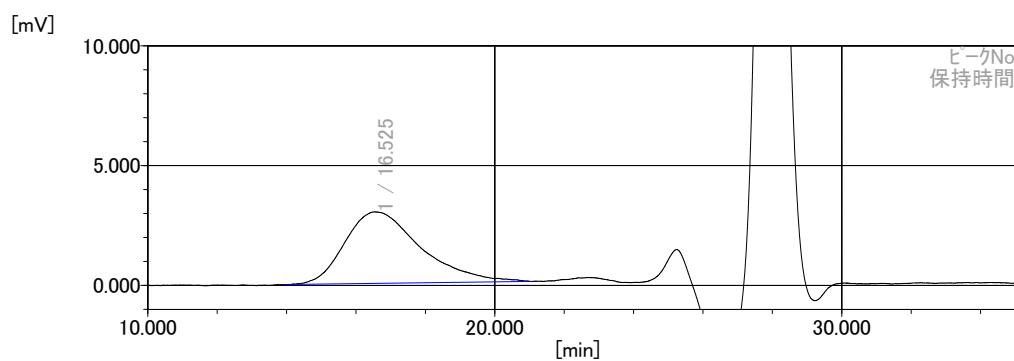


Figure S9. GPC profile of polybutadiene
(run 9 in Table S1, eluent: 1,2,4-trichlorobenzene, 140 °C)

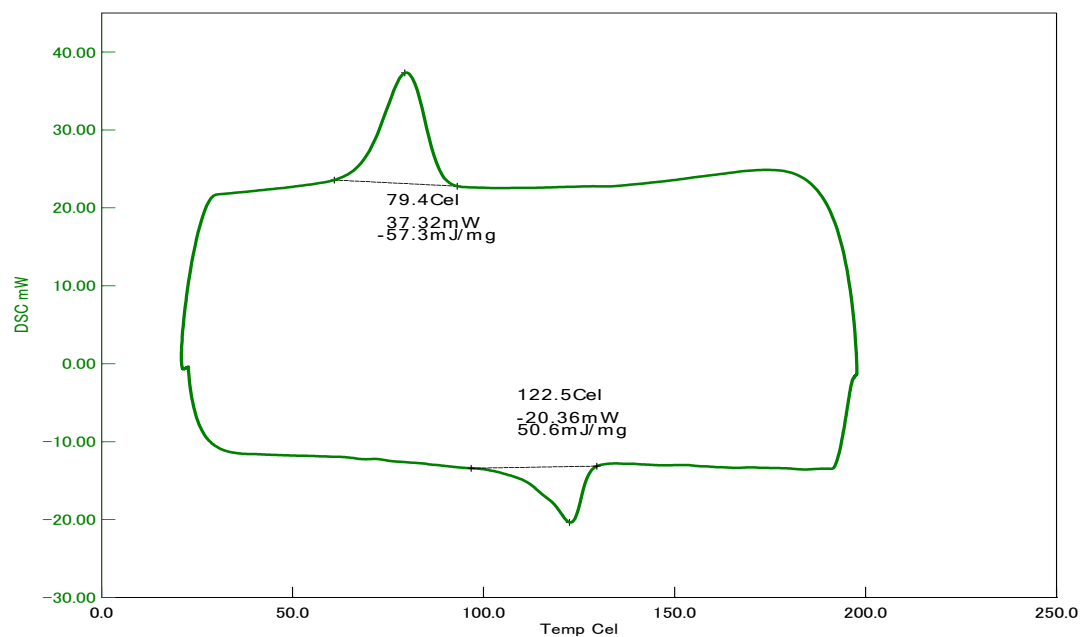


Figure S10. DSC profile of *iso*-1,2-polybutadiene (run 9 in table 1)

25 - 200 °C, 2nd scan, heating rate = 10 °C/min, cooling rate = 20 °C/min.

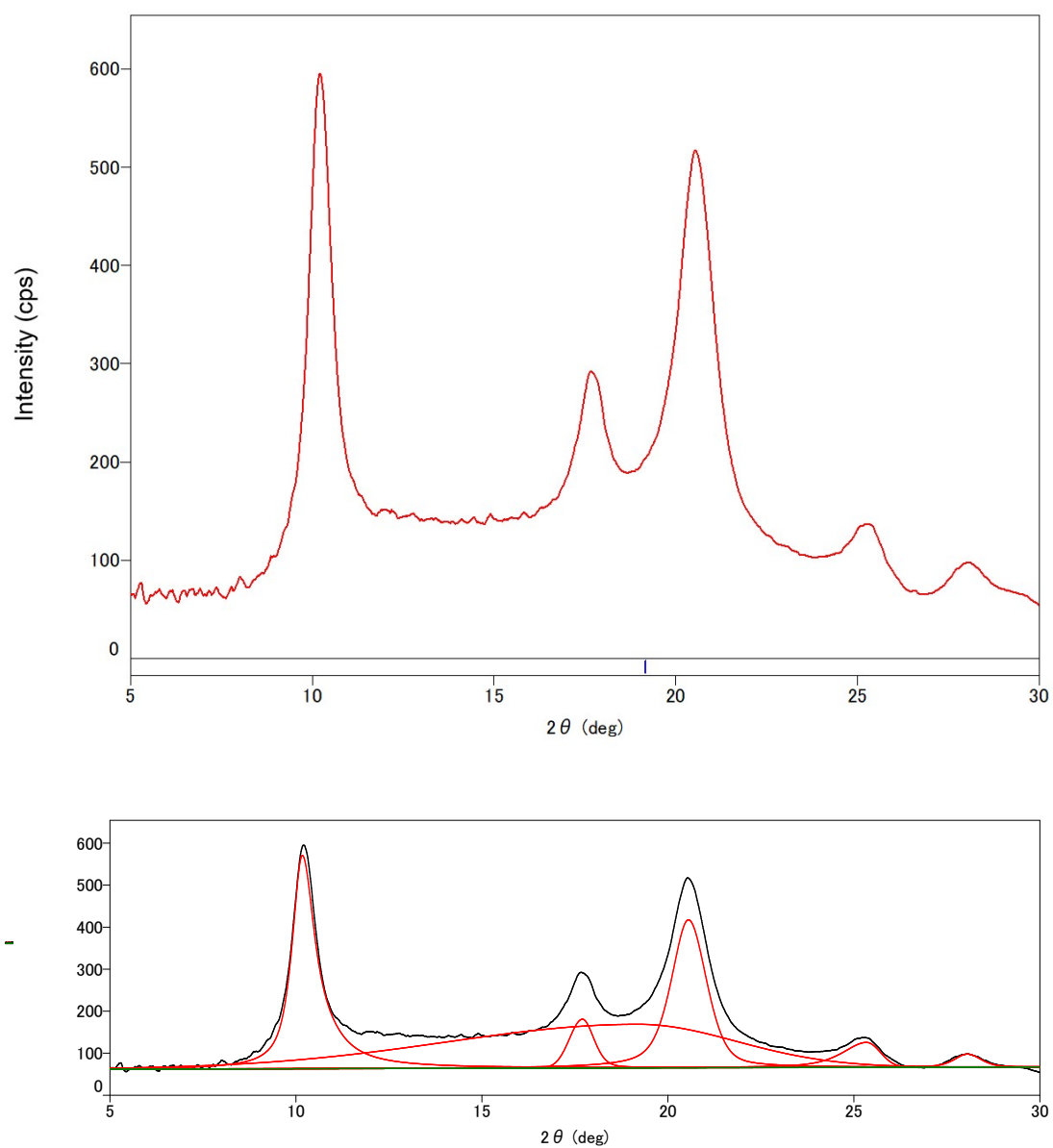


Figure S11. XRD profile of *iso*-1,2-polybutadiene (run 9 in table 1) and peak separation into crystalline and amorphous part.