Supplementary Materials: Quantitative Structure-Thermostability Relationship of Late Transition Metal Catalysts in Ethylene Oligo/Polymerization

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Table S1. The catalytic activities for complexes **1**–**20** at different temperatures along with the reaction time.

Cat.	*T*/°C	Act. [a]	Cat.	*T*/°C	Act. [a]	Time/min
1	20	49.9	**1**	60	315	15
2	20	29.9	**2**	60	200	15
3	20	9.3	**3**	60	81	15
4	20	48.0	**4**	60	352	15
5	20	42.9	**5**	60	218	15
Cat.	***T*/°C**	**Act. [a]**	**Cat.**	***T*/°C**	**Act. [a]**	**Time/min**
6	20	32.0	**6**	80	119	30
7	20	42.7	**7**	60	247	30
8	20	38.0	**8**	60	246	30
9	20	47.8	**9**	60	146	30
10	20	68.2	**10**	60	134.6	30
Cat.	***T*/°C**	**Act. [a]**	**Cat.**	***T*/°C**	**Act. [a]**	**Time/min**
11	20	0.478	**11**	40	26.9	30
12	20	0.163	**12**	40	4.79	30
13	20	0.0199	**13**	40	0.19	30
14	20	2.64	**14**	40	21.1	30
15	20	0.513	**15**	40	5.43	30
Cat.	***T*/°C**	**Act. [a]**	**Cat.**	***T*/°C**	**Act. [a]**	**Time/min**
16	20	44.2	**16**	60	59.1	30
17[b]	20	2352	**17**[b]	60	4340	15
18[b]	25	1331	**18**[b]	75	1882	180
19	20	44.9	**19**	60	103	30
20	20	56.0	**20**	60	76.7	30

[a] 10^5 g mol^{-1} h^{-1}; [b] h^{-1}.

Table S2. The bond lengths and bond angles for metal atoms and atoms coordinated with central metal, which were used as parameters of modified Dreiding force field.

Bond	**Bond Lengths (Å)**				
	Fe4	**Fe8**	**Fe12**	**Bond**	**Ni19**
Fe–N1	2.228	2.283	2.391	**Ni–N1**	2.010
Fe–N2	2.061	2.091	2.100	**Ni–N2**	2.031
Fe–N3	2.178	2.209	2.298	**Ni–Br1**	2.336
Fe–Cl1	2.319	2.331	2.341	**Ni–Br2**	2.317
Fe–Cl2	2.264	2.276	2.249	-	-
Angle	**Bond Angles (°)**				
	Fe4	**Fe8**	**Fe12**	**Angle**	**Ni19**
N1–Fe–N2	72.82	72.00	73.77	**N1–Ni–N2**	82.71
N2–Fe–N3	74.02	73.32	73.18	**N1–Ni–Br1**	114.83
N1–Fe–N3	141.12	140.40	145.86	**N1–Ni–Br2**	104.14
N1–Fe–Cl1	101.72	106.60	93.70	**N2–Ni–Br1**	105.89
N2–Fe–Cl1	91.72	92.97	98.23	**N2–Ni–Br2**	115.67
N3–Fe–Cl1	99.02	93.72	99.19	**Br1–Ni–Br2**	125.62
N1–Fe–Cl2	98.72	94.78	104.73	-	-
N2–Fe–Cl2	151.12	155.68	141.53	-	-
N3–Fe–Cl2	100.62	10.967	95.87	-	-
Cl1–Fe–Cl2	117.19	110.59	120.09	-	-

Table S3. The correlation coefficient (R^2) results for the models of Fe and Ni-based complexes which were fitted by one, two and three parameters, respectively.

Complexes 1–5 (Fe)		
No.	**MLRA Equation**	R^2
1	$A_T = 150.262 - 1385.43 \cdot B$	0.786
2	$A_T = 1.459 + 1.940 \cdot D$	0.038
3	$A_T = 17.786 - 1.457 \cdot \alpha$	0.090
4	$A_T = 151.583 - 1393.55 \cdot B - 0.213 \cdot D$	0.787
5	$A_T = 21.314 - 0.674 \cdot D - 1.703 \cdot \alpha$	0.092
6	$A_T = 158.693 - 1366.69 \cdot B - 1.261 \cdot \alpha$	0.854
7	$A_T = 204.655 - 1541.56 \cdot B - 5.326 \cdot D - 3.184 \cdot \alpha$	0.970
Complexes 16–20 (Ni)		
No.	**MLRA Equation**	R^2
8	$A_T = 4.020 - 33.095 \cdot B$	0.884
9	$A_T = -0.588 + 0.470 \cdot D$	0.073
10	$A_T = 0.608 + 0.035 \cdot \alpha$	0.022
11	$A_T = 2.681 - 33.412 \cdot B + 0.519 \cdot D$	0.973
12	$A_T = -1.033 + 0.609 \cdot D + 0.061 \cdot \alpha$	0.132
13	$A_T = 3.984 - 32.902 \cdot B + 0.013 \cdot \alpha$	0.887
14	$A_T = 2.344 - 32.898 \cdot B + 0.072 \cdot D + 0.039 \cdot \alpha$	0.998