Electronic Supplementary Material (ESI) for RSC Advances.

Nd-Containing Coordination Ploymer: Syntheses, Crystal Structure and Application as A Nucleating Agent for Isotactic Polypropylene†

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Materials and experiments

1.Materials

Neodymium(III) nitrate hexahydrate ($Nd(NO_3)_3 \cdot 6H_2O$) (purity ≥ 99.99%) was purchased from Jining Zhongkai New Type Material Science Co.,Ltd (P.R. China). N-phthaloylglycine (purity ≥ 99.5%) was bought from TCI (Shanghai) Development Co.,Ltd. CH3OH (AR, Sinopharm Chemical Reagent Co., Ltd). Isotactic polypropylene (iPP, trademarked as T30S) was purchased from Lanzhou Petroleum Chemical Co.,Ltd (P.R. China) with melt flow index (MFI) of 2.3 g/10 min (230 °C, 2.16 kg), weight average molecular weight of ca. 5.869 × 105 g mol^{-1}. The α-nucleating agent TMP-5 was supplied by Shanxi Chemical Research Institute (Co.,Ltd).

2.Experiments

Sample Prepartion and test methods

The nucleating agents (complex **1** and TMP-5) and the iPP were blended by high-speed mixer for 8 min. Then the mixture was extruded by a twin-screw (TDS-35C, Nanjing Norda Extrusion Equipment Co.,Ltd). The extruder barrel was operated at a temperature range of 175 °C to 205 °C and a screw speed of 300 rpm. The extruded pellets were cooled down to the room temperature. Then, the extruded pellets and neat pellets were injection molded using a injection molding machine (Ningbo Haitian Plastic Machinery Co.,Ltd). The injection molding machine barrel temperature ranged from 195 to 205 °C. The mechanical properties were measured according to ATSM test methods, such as D-256-10 for the Izod impact strength, using an impact tester (Chengde Precision Testing Machine Co.,Ltd). The flexural modulus was tested on the basis of D-790-10 and the tensile strength was tested on the basis of D-638-10, using a universal testing machine (Chengde Precision Testing Machine Co.,Ltd). The crosshead speed was 50 mm/min. The values of all the mechanical properties were calculated as averages of over five samples. All the specimens were tested at ambient temperature (about 23 °C). The heat deflection temperature (HDT) was tested on the basis of D-648-10, using a HDT/Vicat tester (Chengde Jinjian Testing Instrument Co.,Ltd). The optical characteristics haze and clarity of the injection-molded samples were tested according to ASTM D-1003-61 (1997) by a light transmittance instrument (WGT-2S, Shanghai Jingke). Reported are the averagesof measured values for at least three samples.

Table S-1 Selected bond lengths (Å) and angles (°) for complex 1.

Nd1-O1W	2.402(2)	Nd1-O5A	2.4305(19)
Nd1-O4	2.4564(19)	Nd1-O1	2.497(2)
Nd1-O3A	2.546(2)	Nd1-O1B	2.551(2)
Nd1-O2B	2.560(2)	Nd1-O6	2.595(2)
Nd1-O5	2.699(2)	Nd1-O4A	2.828(2)
O1W-Nd1-O5A	131.36(8)	O1W-Nd1-O4	143.04(7)
O5A-Nd1-O4	69.88(7)	O1W-Nd1-O1	87.97(7)
O5A-Nd1-O1	68.26(7)	O4-Nd1-O1	71.94(6)
O1W-Nd1-O3A	83.06(7)	O5A-Nd1-O3A	71.42(7)
O4-Nd1-O3A	133.40(7)	O1-Nd1-O3A	115.51(7)
O1W-Nd1-O1B	132.04(7)	O5A-Nd1-O1B	80.06(7)
O4-Nd1-O1B	74.54(6)	O1-Nd1-O1B	139.92(2)
O3A-Nd1-O1B	74.14(7)	O1W-Nd1-O2B	80.76(7)
O5A-Nd1-O2B	120.04(7)	O4-Nd1-O2B	117.26(7)
O1-Nd1-O2B	168.72(6)	O3A-Nd1-O2B	63.83(7)
O1B-Nd1-O2B	51.36(6)	O1W-Nd1-O6	70.86(7)
O5A-Nd1-O6	137.88(7)	O4-Nd1-O6	75.04(7)
O1-Nd1-O6	79.36(7)	O3A-Nd1-O6	149.81(7)
O1B-Nd1-O6	112.36(7)	O2B-Nd1-O6	96.31(7)
O1W-Nd1-O5	101.15(7)	O5A-Nd1-O5	127.40(6)
O4-Nd1-O5	64.86(6)	O1-Nd1-O5	118.31(6)
O3A-Nd1-O5	126.11(6)	O1B-Nd1-O5	63.50(6)

O2B-Nd1-O5	64.02(6)	O6-Nd1-O5	48.95(6)
O1W-Nd1-O4A	68.96(7)	O5A-Nd1-O4A	63.10(6)
O4-Nd1-O4A	126.99(6)	O1-Nd1-O4A	69.13(6)
O3A-Nd1-O4A	48.10(6)	O1B-Nd1-O4A	117.72(6)
O2B-Nd1-O4A	106.82(6)	O6-Nd1-O4A	128.95(6)
O5-Nd1-O4A	168.12(6)		

Symmetry codes: A, -x+1,y+1/2,-z+1/2; B, -x+1,y-1/2,-z+1/2.

Table S-2 H-bonds lengths (Å) and angles(°) for complex 1.

D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)
O(1W)-H(1WA)...O(3W)#3	0.86	1.89	2.679(4)	152.8
O(1W)-H(1WB)...O(2W)#1	0.86	2.00	2.704(4)	138.4
O(1W)-H(1WB)...O(4)#1	0.86	2.52	2.981(3)	114.5
O(2W)-H(2WA)...O(3W)#4	0.92	2.22	3.133(6)	169.8
O(2W)-H(2WB)...O(2)	0.82	2.33	3.064(3)	148.2
O(2W)-H(2WB)...O(5)#1	0.82	2.45	3.062(3)	132.0
O(2W)-H(2WB)...O(4)	0.82	2.54	3.079(3)	123.9
O(3W)-H(3WA)...O(8)#5	0.95(7)	1.90(7)	2.795(5)	157(6)

Symmetry codes: #1, -x+1,y+1/2,-z+1/2; #2, -x+1,y-1/2,-z+1/2; #3, x,y,z-1;

#4, -x+1,y+1/2,-z+3/2; #5, x,y,z+1

Table S-3 Short ring π-π interactions with Cg-Cg Distances for complex 1

Cg(I)->Cg(J)	Distance between ring centroids (Å)	Dihedral angle (°)	Perpendicular distance of Cg(I) on Cg(J) (Å)	Perpendicular distance of Cg(J) on Cg(I) (Å)	Slippage
Cg(1)->Cg(3) (-x,-y,-z)	3.6141(1)	1	-3.4454	-3.4551	
Cg(3)->Cg(1) (-x,1-y,-z)	3.5758(1)	1	3.3932	3.3954	
Cg(3)->Cg(3) (-x,1-y,-z)	3.6075(1)	0	3.3920	3.3920	1.228

Cg(1): N1-->C9-->C10-->C15-->C16--> ; Cg(3): C10 -->C11-->C12-->C13--> C14-->C15-->

Table S-4 Effect of α-nucleating agent on HDT of iPP

Content (wt%) / HDT (°C) / Composition	0	0.05	0.10	0.15	0.20	0.25
NA	79.9	97.4	101.5	104.5	105.3	104.6
TMP-5				105.4		

Table S-5 The calculated peaks and the experimental ones of XRD

(hkl)	2Theta(°)(simulated)	Intensity(simulated)	2Theta(°)(PWXRD)	Intensity(PWXRD)
(100)	6.340	10000	6.338	99342.67
(002)	9.625	4892.62	9.564	4348.13
(200)	12.699	2083.66	12.695	2076.83
(102)	13.119	2525.26	13.019	2564.77
(111)	15.413	782.483	15.343	787.733
(113)	21.569	1199.46	21.407	1191.77
(021)	25.448	974.955	25.327	1164

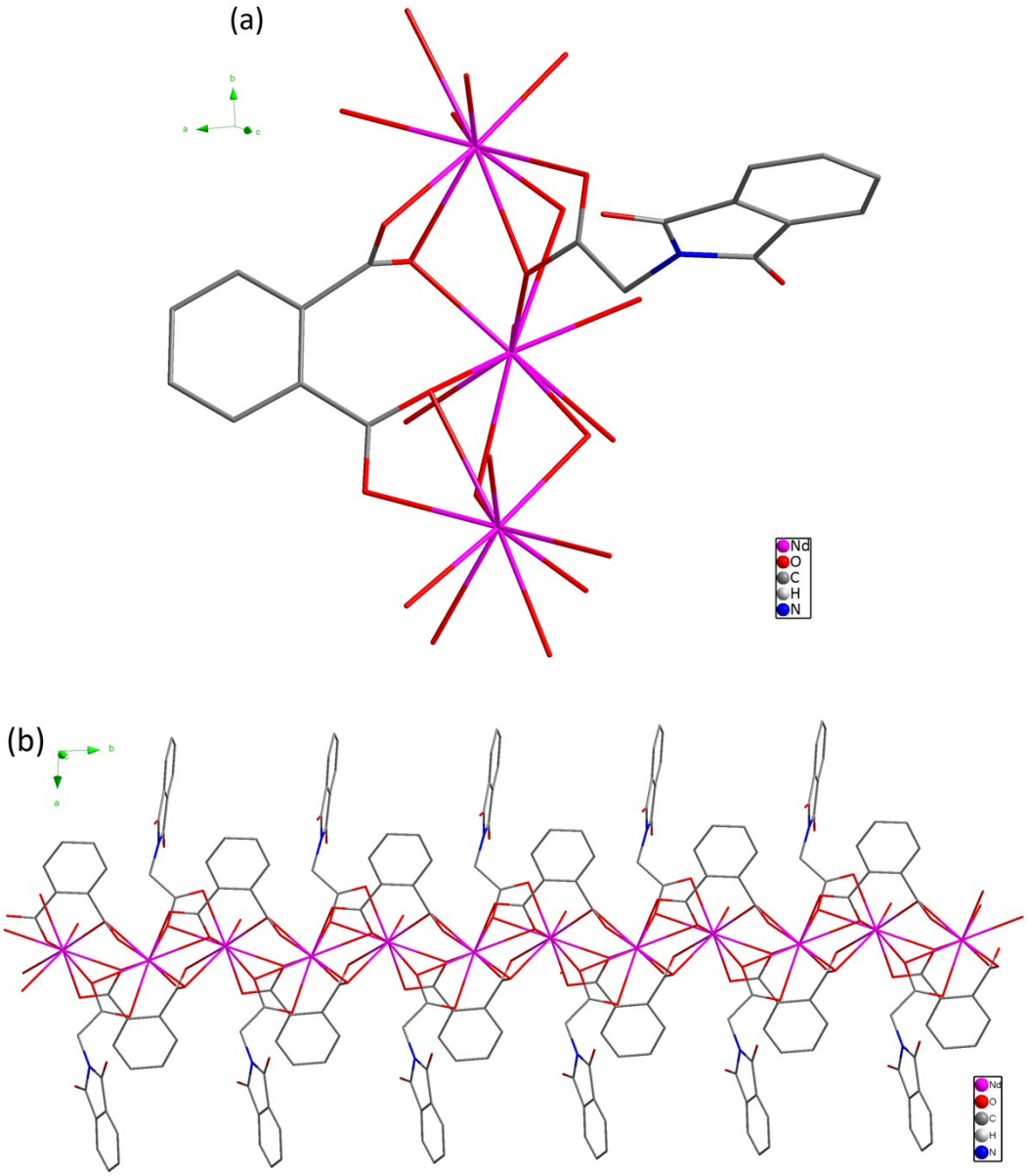


Fig.S1 (a) the coordination modes of complex 1, (b) 1D infinite O-Nd-O chain along the b-axis of complex 1

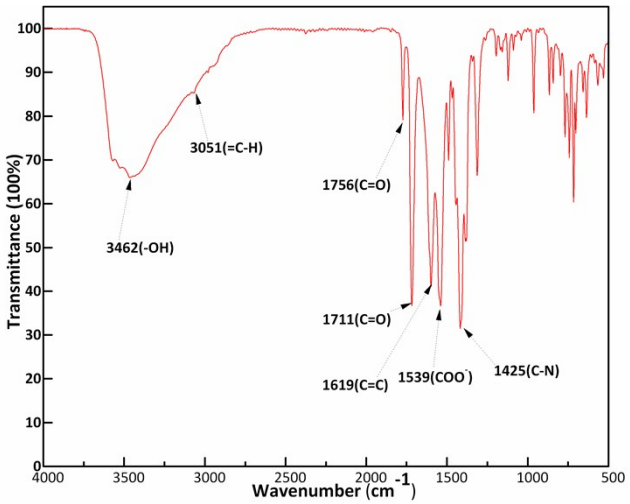


Fig.S2 IR Spectra of complex 1

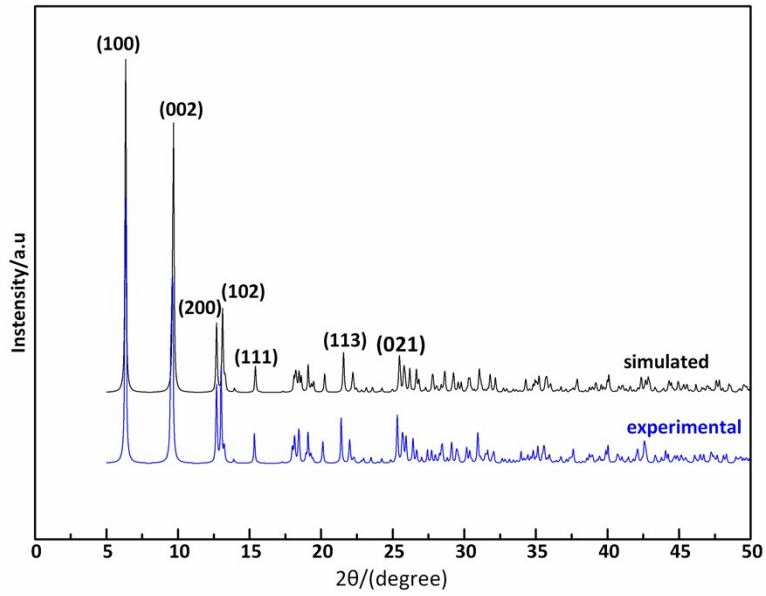


Fig.S3 Experimental and simulated PXRD patterns for complex 1

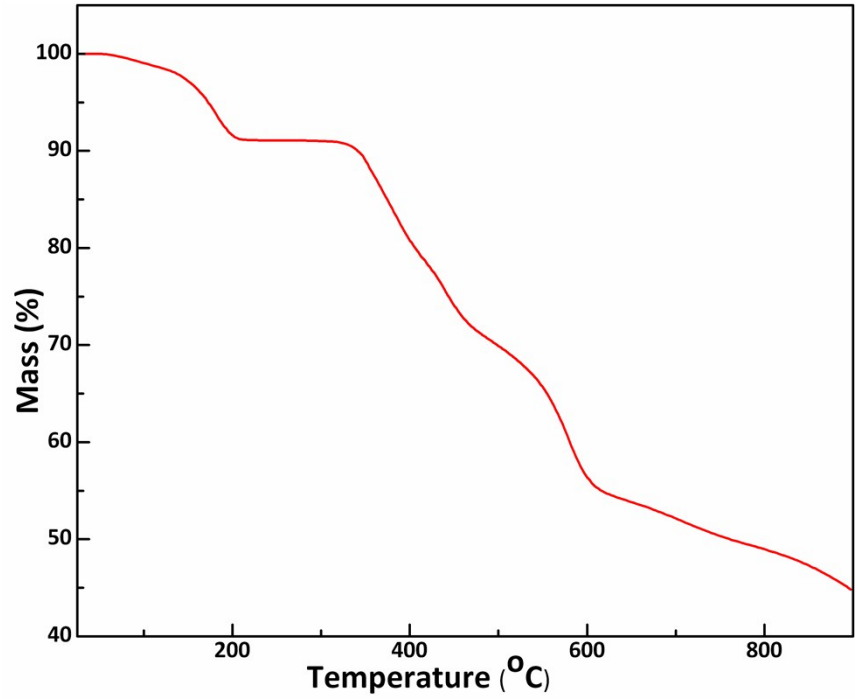
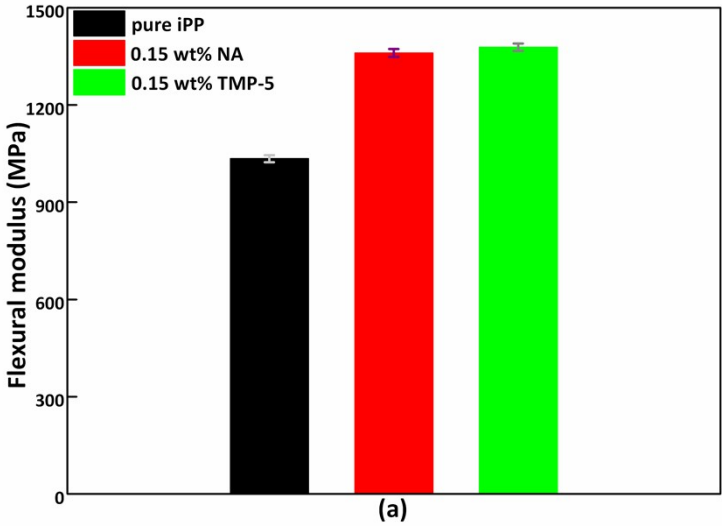


Fig.S4 The TGA curve of complex 1



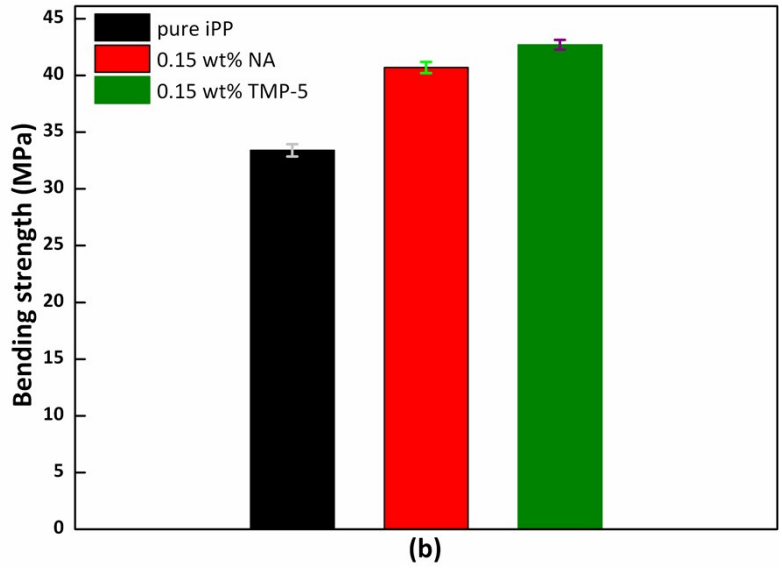


Fig.S5 Effect of 0.15 wt% NA and 0.15 wt% TMP-5 on flexural modulus and bending strength of iPP

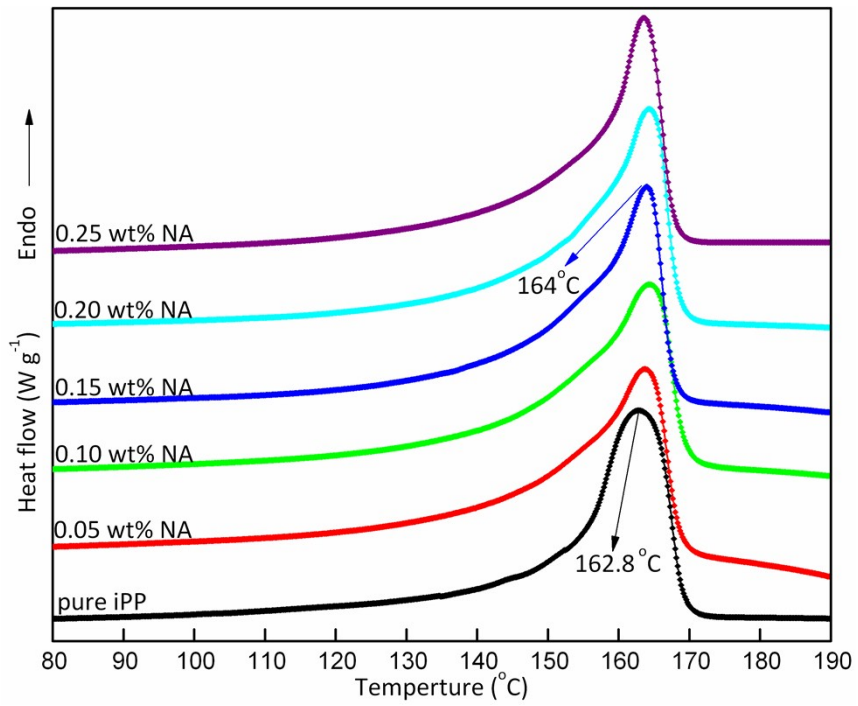


Fig.S6 Effect of NA content on the melting behaviors of iPP