Electronic Supplementary Material (ESI) for Dalton Transactions.

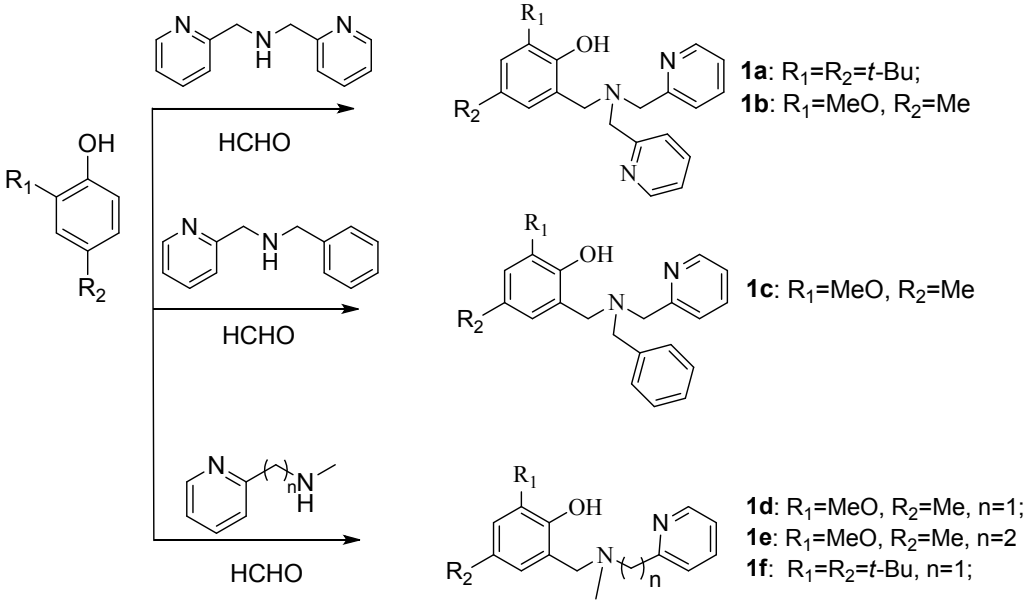
Supporting Information

[ONN]-Type amine pyridine(s) phenolate-based oxovanadium(V) catalysts for ethylene homo- and copolymerization

Jia-Bao Wang,[†,‡] Ling-Pan Lu,[†,‡] Jing-Yu Liu,[*,†] Yue-Sheng Li[*,†]

State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, China

and University of the Chinese Academy of Sciences, Changchun Branch, Changchun 130022, China



Scheme S1. General synthetic route of tridentate amine pyridine(s) phenolate ligands **1a-f.**

[*] Corresponding Author. E-mail: ljy@ciac.ac.cn and ysli@ciac.ac.cn,

[†] State Key Laboratory of Polymer Physics and Chemistry

‡ Graduate School of the Chinese Academy of Sciences

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Table S1. Crystal data and structure refinements of complexes **2a**, **2c**, and **2d**.

	2a	**2c**	**2d**
Empirical formula	$C_{33}H_{48}N_3O_4V$	$C_{28}H_{37}N_2O_5V$	$C_{23}H_{35}Cl_2N_2O_5V$
Formula weight	601.68	532.54	541.37
Crystal system	hexagonal	monoclinic	triclinic
Space group	R-3	P2(1)/n	P-1
a (Å)	40.3177(11)	14.0405(7)	13.2554(5)
b (Å)	40.3177(11)	16.1686(8)	19.2889(8)
c (Å)	11.1035(6)	25.3609(12)	23.4680(9)
α (°)	90.00	90.00	110.70
β (°)	90.00	106.07	102.62
γ (°)	120.00	90.00	91.40
V (Å^3), Z	15630.8(10), 18	5532.3(5), 8	5443.2(4), 8
$Density_{calcd}$ (Mg/m^3)	1.151	1.279	1.321
Absorption coefficient (mm^{-1})	0.322	0.397	0.594
F (000)	5796	2256	2272
Crystal size (mm)	0.39×0.26×0.19	0.33×0.25×0.17	0.35×0.27×0.14
θ range for data collection (°)	1.75 to 25.03	1.51 to 26.05	1.58 to 25.75
Reflections collected	6143	10929	20425
Independent reflections	4687 (R_{int}= 0.0669)	7309 (R_{int}= 0.0492)	12242 (R_{int}= 0.0827)
Data/restraints/ parameters	6143/0/378	10929/84/729	20425/9/1228
Goodness-of-fit on F^2	1.050	1.045	1.036
Final R indices [I>2σ (I)]: R1, wR2	0.0607, 0.1350	0.0627, 0.1469	0.0827, 0.1860
Largest diff. Peak and hole (e Å^{-3})	0.490 and -0.259	0.719 and -0.333	0.628 and -0.379

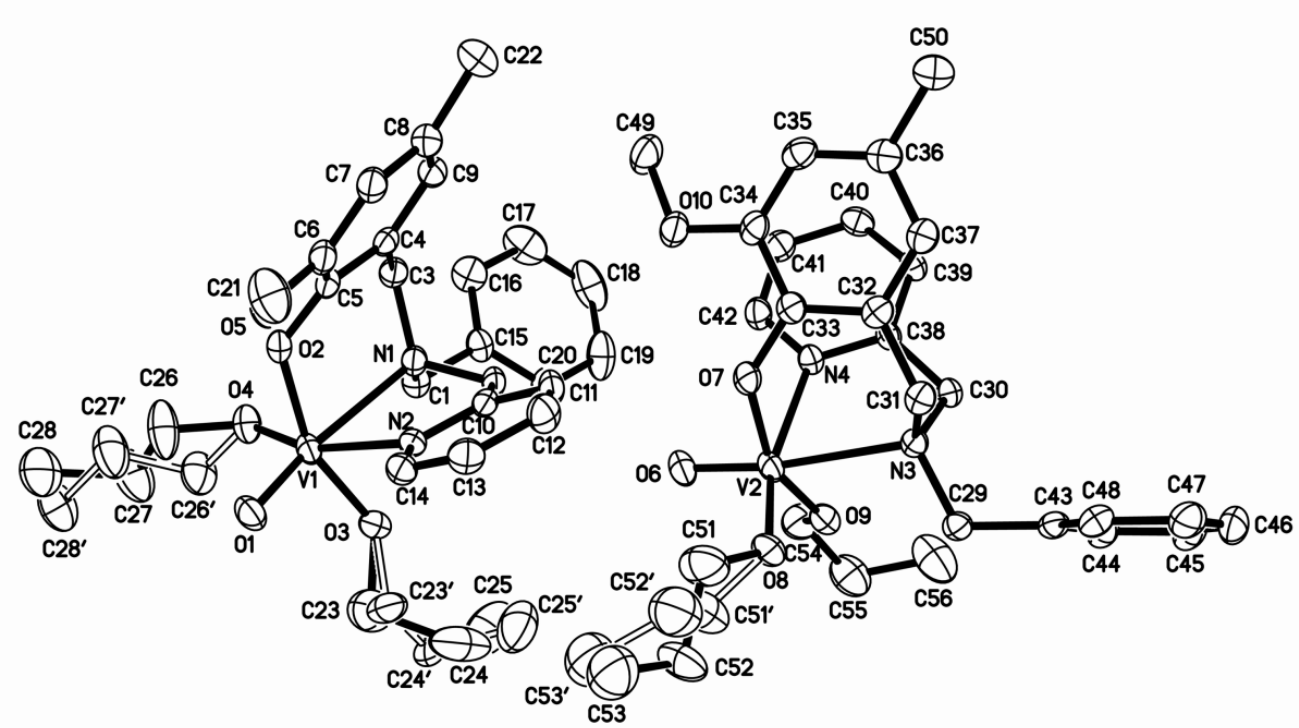

Figure S1. Molecular structure of complex **2c** with thermal ellipsoids at 30% probability level. Hydrogen atoms are omitted for clarity.

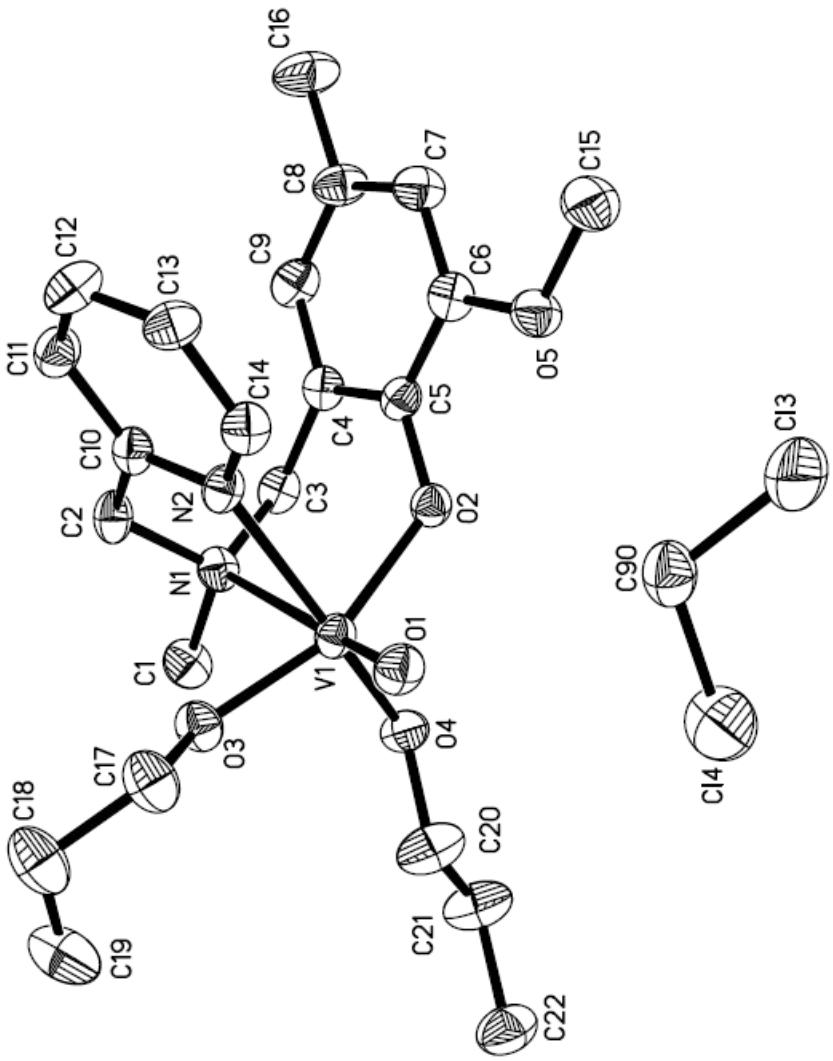

Figure S2. Molecular structure of complex **2d** with thermal ellipsoids at 30% probability level. Hydrogen atoms are omitted for clarity.（one of the four crystallographic molecules）