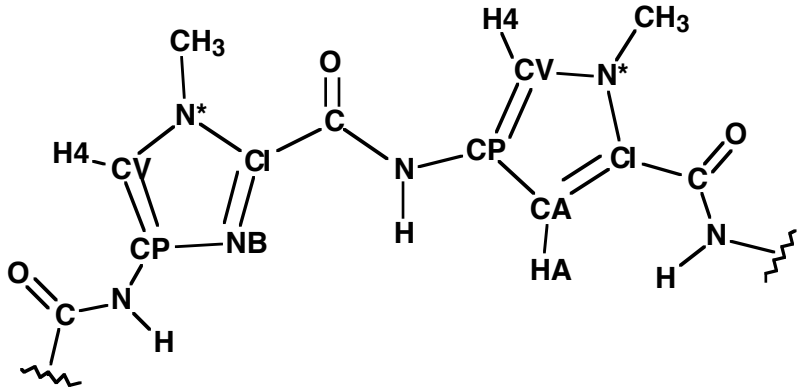
Supplementary Information:
AMBER Force field Parameter Development

The electrostatic charges for the ligand atoms were calculated using model fragments of imidazole or pyrrole rings flanked by amide groups. The charges reported for the amide group atoms represent averages over all such atoms in each fragment. The calculations were performed at the HF/6-31G* level using Gaussian98. The charges are reported in the following table:

Table of Electrostatic Charges Developed for Polyamide Ligands

Amide		Pyrrole			Imidazole		
C	0.7106	Methyl	CT	-0.1861	Methyl	CT	-0.1675
O	-0.5752		H1	0.1017		H1	0.0942
H	0.3439		H1	0.0975		H1	0.0984
N	-0.4793		H1	0.0922		H1	0.1057
		Ring	N*	0.1266	Ring	N*	0.1624
			CI	-0.1523		CI	0.0472
			CA	-0.4104		NB	-0.6138
			HA	0.1813		CP	0.3857
			CP	0.1794		CV	-0.3129
			CV	-0.2409		H4	0.2006
			H4	0.2109			

AMBER atom types defined for a representative polyamide ligand fragment (CP and CI are new atom types):



The pyrrole and imidazole constructs were not adequately represented by the existing AMBER atoms types and parameters. Bond lengths, bond angles and dihedral angles (torsions) were taken from optimized geometries of model fragments at the B3LYP/6-31G* level using Gaussian98 (Frisch *et al.*, 1998). The force constants for the new torsions involving CI and CP were calculated by evaluating the rotational energy barrier (difference between energy at 0° and 90°.) In most other cases, the values for the force constants were taken by comparison with

similar bonds and angles. The parameters cited for the torsions are defined in the AMBER manual.

AMBER Parameters Developed for Polyamide Ligands

Parameter	Force Constant	Bond Length (Å)
C-CR	469.0	1.460
CI-C	469.0	1.470
CI-N*	427.0	1.380
CI-NB	488.0	1.340
CI-CA	469.0	1.400
CP-N	490.0	1.390
CP-CV	469.0	1.390
CP-NB	488.0	1.380
CV-N*	410.0	1.370
CV-CV	469.0	1.390
Parameter	Force Constant	Angle (°)
NB-CI-C	70.0	122.76
NB-CI-N*	70.0	111.18
N -C -CI	70.0	110.70
CI-C -O	70.0	125.26
C -N -CP	70.0	123.29
CI-NB-CV	70.0	105.82
CI-N*-CV	70.0	106.83
CI-N*-CT	70.0	126.72
N*-CV-CV	70.0	106.38
N*-CV-H4	70.0	121.91
NB-CV-CV	70.0	109.78
CV-N*-CT	70.0	124.06
CV-CV-H4	70.0	128.31
CV-CP-CA	70.0	107.03
N*-CV-CP	70.0	108.53
CV-CP-NB	70.0	110.30
N- CP-CV	70.0	129.87
N -CP-NB	70.0	119.83
CP-NB-CI	70.0	105.63
N -CP-CV	70.0	126.98
N -CP-CA	70.0	125.68
H -N -CP	70.0	120.76
CP-CV-H4	70.0	128.36
CP-CA-HA	70.0	125.55
CP-CA-CI	70.0	107.57
CA-CI-N*	70.0	107.55
C -CI-CA	70.0	130.71

CI-CA-HA	70.0	128.89		
C -CI-N*	70.0	126.05		
Parameter	IDIVF	PK	Phase	PN
X-CI-C -X	4	6.95	180.0	2
X-N -CP-X	4	2.45	180.0	2
X-CV-N*-X	4	7.40	180.0	2
X-CI-N*-X	4	7.40	180.0	2
X-CI-NB-X	2	10.00	180.0	2
X-CA-CI-X	4	20.60	180.0	2
X-CP-CV-X	4	20.60	180.0	2
X-CP-NB-X	2	4.80	180.0	2
X-CP-CA-X	4	20.60	180.0	2
X-CV-CV-X	4	14.50	180.0	2