Table S1. Probability of TM-TM pairs in NMC333

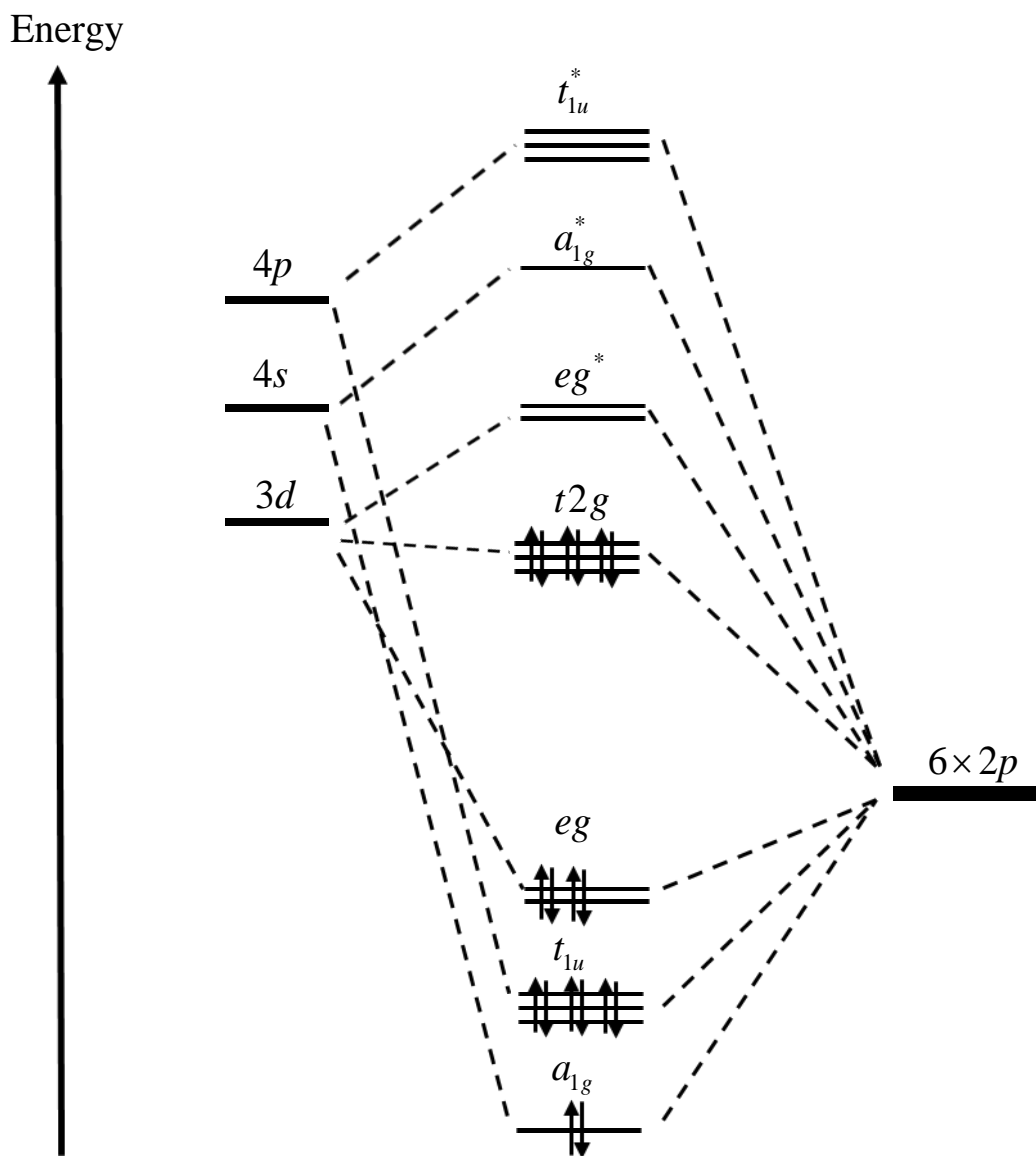| TM	Ni	Mn	Co
Ni	20.6%	35.3%	44.1%
Mn	35.5%	25.8%	38.7%
Co	41.6%	33.4%	25.0%

Figure S1. Molecular orbital diagram of the transition metal complex showing the d orbital electron population of Co^{3+} and O $2p$ orbital.
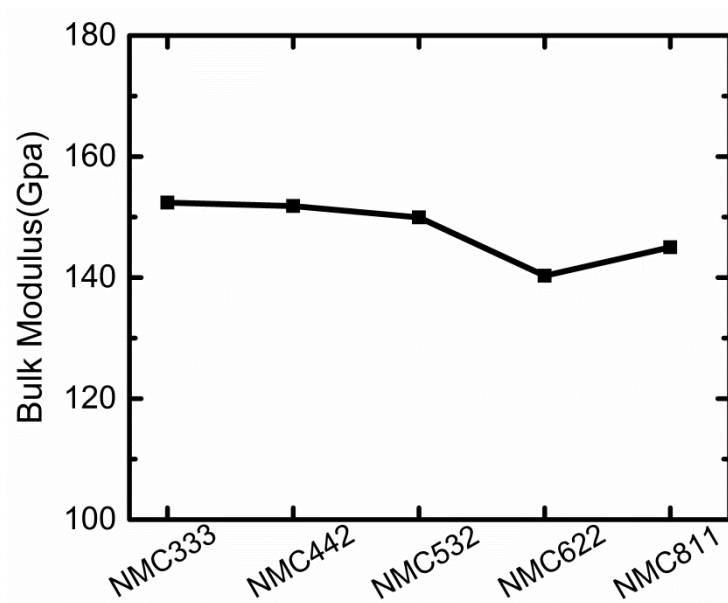
Figure S2. Bulk modulus of the five NMC compositions calculated from the VCA model.