

Thermochemical Studies of Ni(II) and Zn(II) Ternary Complexes Using Ion Mobility-Mass Spectrometry

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Materials

Name	Company	Catalog Number	Comments
Acetonitrile HPLC-grade	Fisher Scientific (www.Fishersci.com)	A998SK-4	
Alternative metal binding (amb) peptides	PepmicCo (www.pepmic.com)		designed peptides were synthesized by order
Ammonium acetate (ultrapure)	VWR	97061-014	
Ammonium hydroxide (trace metal grade)	Fisher Scientific (www.Fishersci.com)	A512-P500	
Driftscope 2.1 software program	Waters (www.waters.com)		software analysis program
Gaussian 09	Gaussian		Electronic Structure Modeling Software
GaussView	Gaussian		Graphical Interface to Visualize Computations
Glacial acetic acid (Optima grade)	Fisher Scientific (www.Fishersci.com)	A465-250	
Ion-scaled Lennard-Jones (LJ) method	Sigma		Michael T. Bowers' group of University of California at Santa Barbara
MassLynx 4.1	Waters (www.waters.com)		software analysis program
Microcentrifuge Tubes	VWR	87003-294	1.7 mL, polypropylene
Microcentrifuge Tubes	VWR	87003-298	2.0 mL, polypropylene
Ni(II) nitrate hexahydrate (99% purity)	Sigma-Aldrich (www.sigmaaldrich.com)	A15540	
Poly-DL-alanine	Sigma-Aldrich (www.sigmaaldrich.com)	P9003-25MG	
Waters Synapt G1 HDMS	Waters (www.waters.com)		quadrupole - ion mobility- time-of-flight mass spectrometer
Zn(II) nitrate hexahydrate (99%+ purity)	Alfa Aesar (www.alfa.com)	12313	