Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Modeling the interactions between peptide functions and Sr^{2+}: Formamide-Sr^{2+} reactions in the Gas Phase

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Supporting Information (A total of 2 pages)

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Table S1. Energies were calculated with G96LYP functional and with an expanded LAN2DZ basis set for the Sr^{2+} cation, and 6-311+G(3df,2p) basis set for C, O, N and H atoms. Zero-Point Vibrational energies were calculated with G96LYP functional and an improved LAN2DZ basis set for the Sr^{2+} cation and with 6-31+G(d,p) basis set for C, O, N and H atoms. All values are in hartrees.

	Energy	**ZPVE**
1	-199.8266053	0.047084
2	-199.7446179	0.044135
3	-199.7906672	0.046499
4	-199.7822307	0.046538
5	-199.805685	0.041279
6	-199.7807166	0.040973
7	-199.7721218	0.043414
8	-199.7520549	0.045105
TS11	-199.771644	0.045178
TS12	-199.7259154	0.040471
TS23	-199.7404989	0.043550
TS34	-199.7370156	0.044236
TS45	-199.6973997	0.039367
TS56	-199.7782474	0.041239
TS17	-199.7015365	0.039623
TS18	-199.6802649	0.039372
TS2A	-199.7378161	0.040304
TS6A	-199.7540128	0.039662