Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Probing electrostatic interactions and structural changes in highly charged protein polyanions by conformer-selective photoelectron spectroscopy †

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Electronic supplementary information (ESI)

Table S1 / S2

EXTENDED CYTO C

Charge state	PA (Å^2)	EHSS (Å^2)
2	2335	2759
3	2331	2764
4	2378	2815
5	2379	2816
6	2387	2820
7	2331	2760
8	2372	2806
9	2384	2824
10	2376	2807
11	2380	2816
12	2376	2813
13	2378	2814

PBD NATIVE CYTO C

Charge state	PA (Å^2)	EHSS (Å^2)
2	1086	1353
3	1093	1366
4	1083	1363
5	1084	1363
6	1083	1351
7	1076	1342
8	1074	1339
9	1076	1342
10	1068	1332
11	1070	1340
12	1080	1343
13	1065	1333

We have calculated the average values of the collision cross sections for the different charge states of cytochrome C using two different types of model structures : (S1) fully extended structures and (S2) pdb native structures (1CYC). For each charge state, the initial structures were subjected to a relaxation using the AMBER force field. For the cross-section calculation, we used the projection approximation (PA)(Ref. 1) and exact hard sphere model (EHSS) (Ref. 2) which treats the atoms as hard spheres. Note that these models do not take into account the charge of the molecule.

References:

(1) von Helden, G.; Wyttenbach, T.; Bowers, M. T. Int. J. Mass Spectrom. 1995, 146, 349;
(2) Shvartsburg, AA; Jarrold, MF; Chem. Phys. Lett. 261: 86-91 (1996)
(3) M. F. Mesleh, J. M. Hunter, A. A. Shvartsburg, G. C. Schatz, and M. F. Jarrold, J. Phys. Chem. 1996, 100, 16082.

Fig. S1

Correlation plot between collision cross sections of cytochrome c for helium (from Ref. 29&30) and nitrogen as collision gas (this work) in $Å^2$. Numbers given at the data points indicate the charge state of the ion. The fit parameters obtained from the regression were used to linearly scale the nitrogen values into helium values. (Data points marked in green were not used for the fit).