Electronic Supplementary Information

The adsorption of helium atoms on small cationic gold clusters

Marcelo Goulart,[1] Michael Gatchell,[1,2] Lorenz Kranabetter,[1] Martin Kuhn,[1] Paul Martini,[1] Norbert Gitzl,[1] Manuel Rainer,[1] Johannes Postler,[1] Paul Scheier[1,*] and Andrew M. Ellis[3,*]

[1] Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstr. 25, A-6020 Innsbruck, Austria

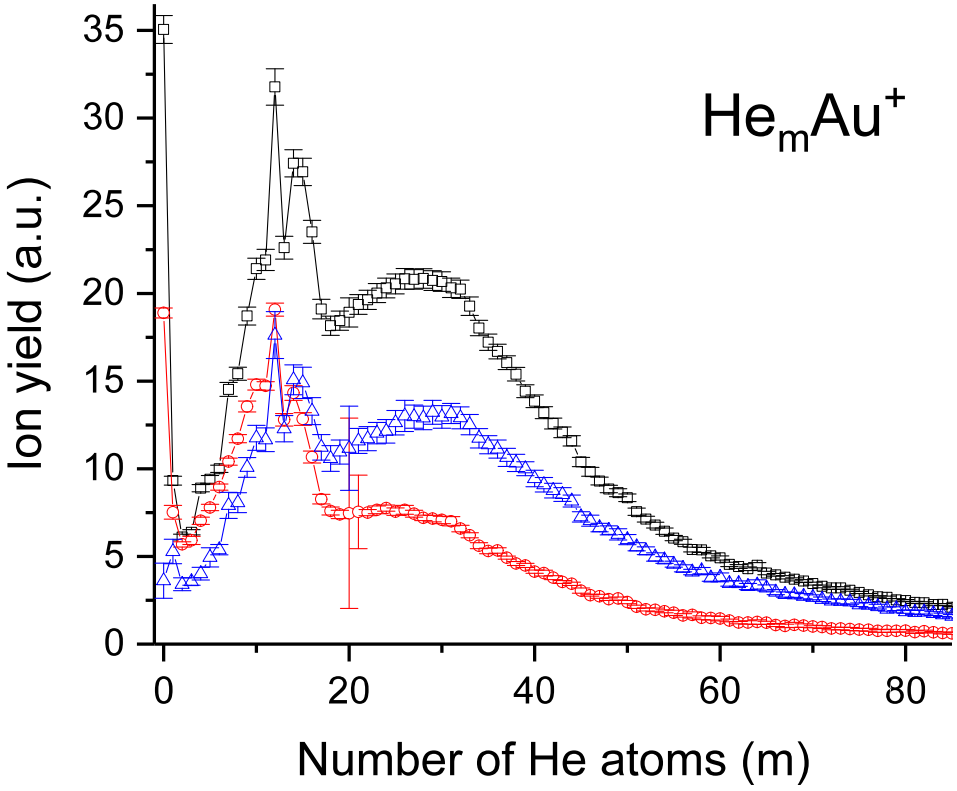
[2] Department of Physics, Stockholm University, 106 91 Stockholm, Sweden

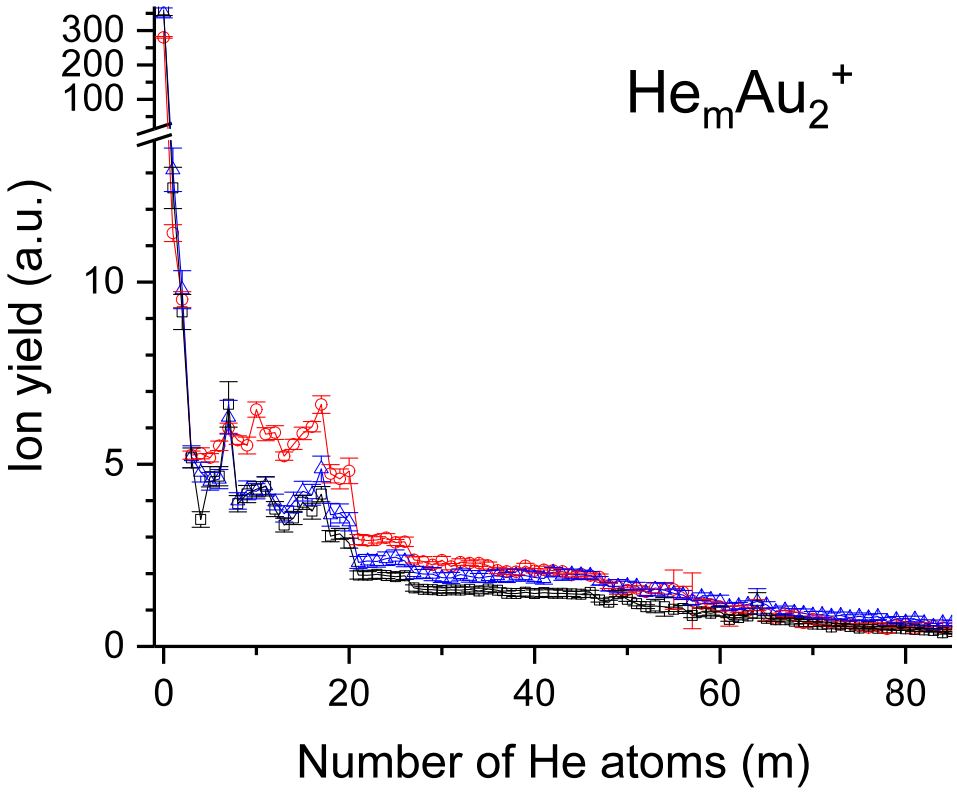
[3] Department of Chemistry, University of Leicester, University Road, Leicester, LE1 7RH, UK

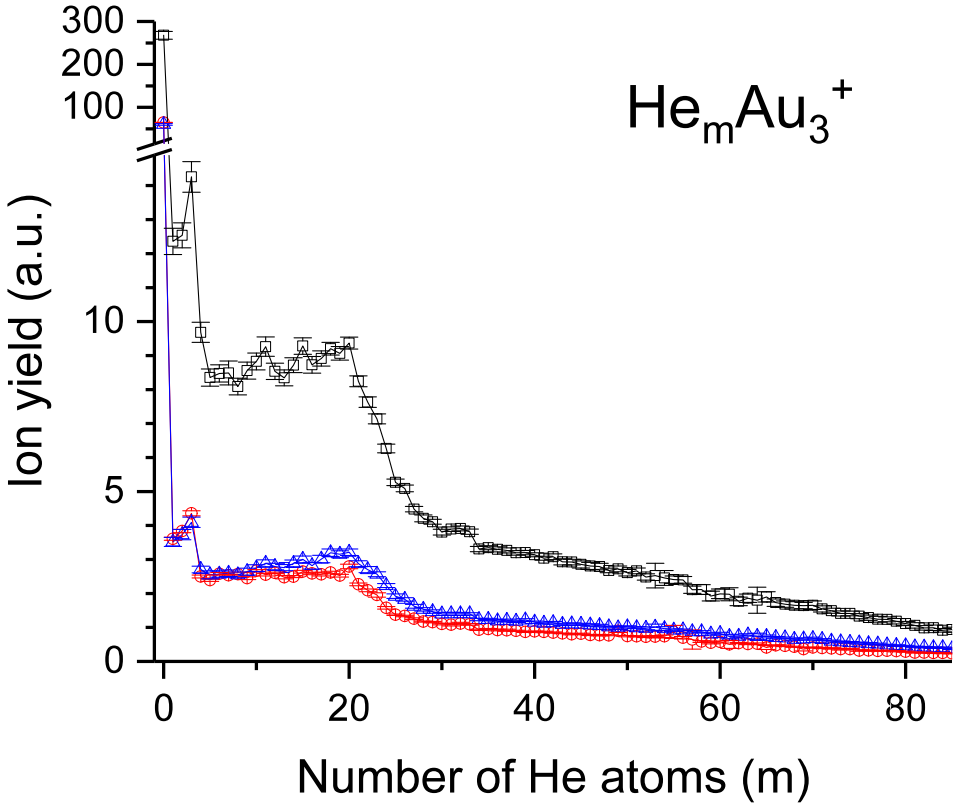
Email: paul.scheier@uibk.ac.at; andrew.ellis@le.ac.uk

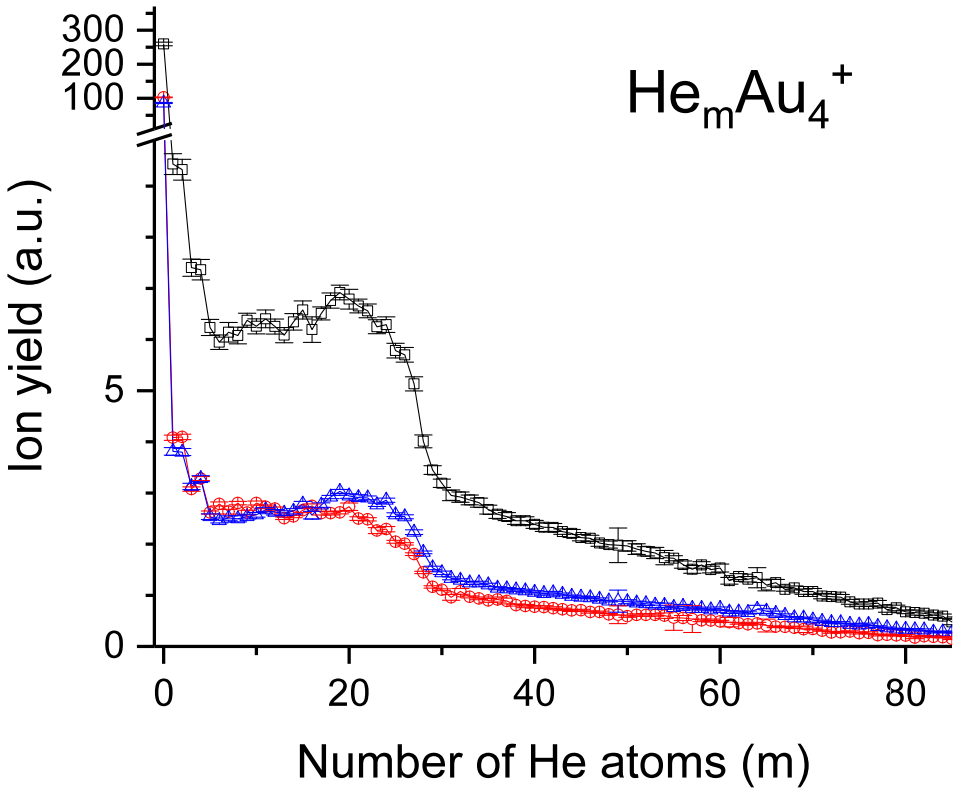
Experimental data

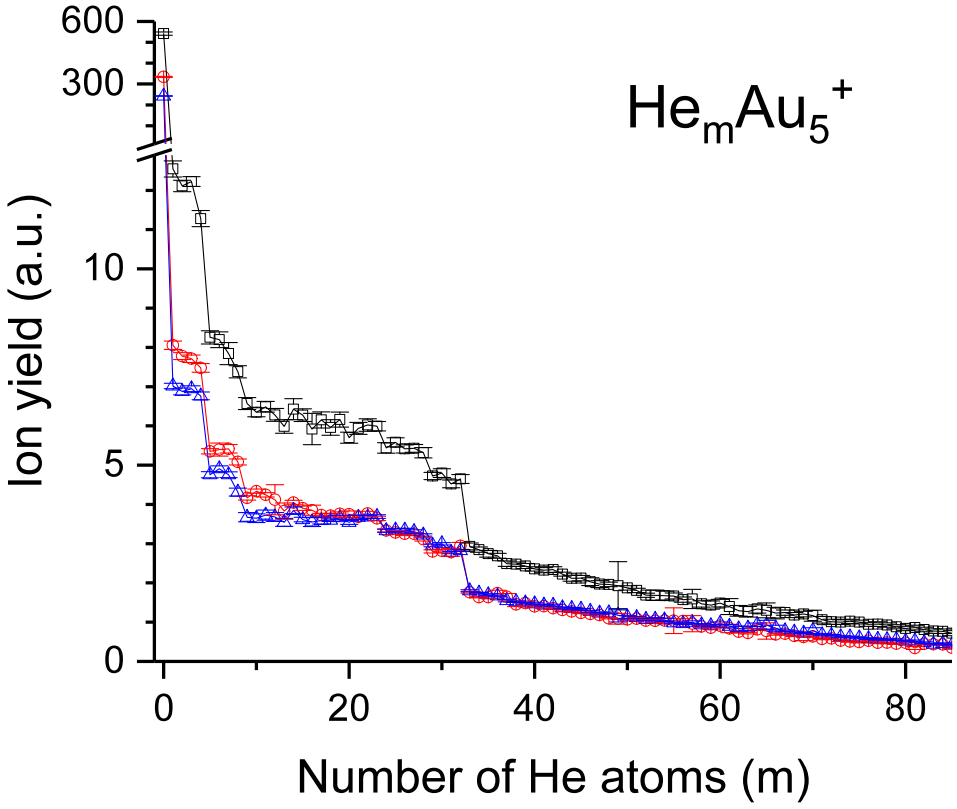
A complete set of the ion abundance plots determined from mass spectrometry of gold-doped helium droplets is provided below.

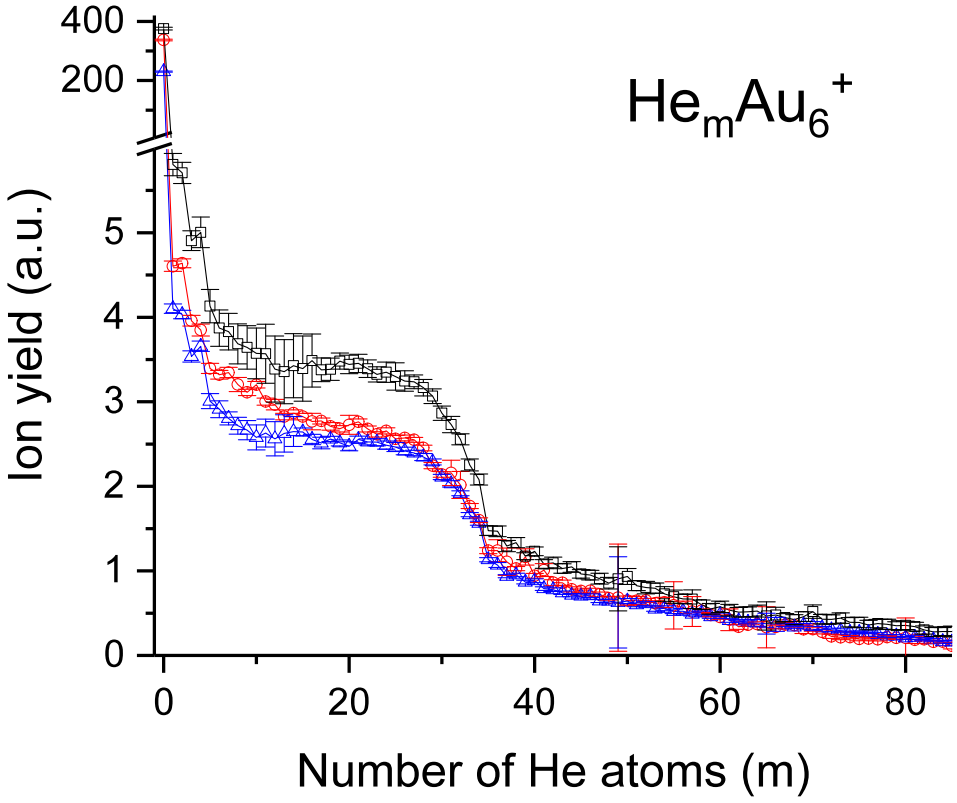


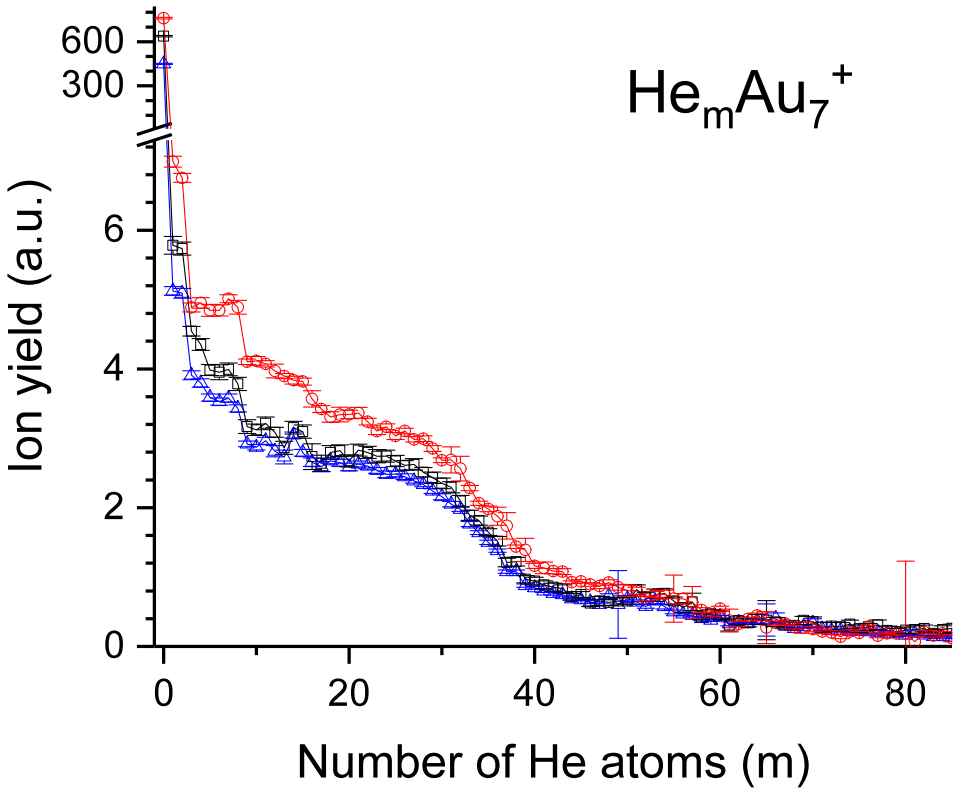

300
200
100
10
5
0
Ion yield (a.u.)
0
20
40
60
80
Number of He atoms (m)
$He_mAu_2^+$

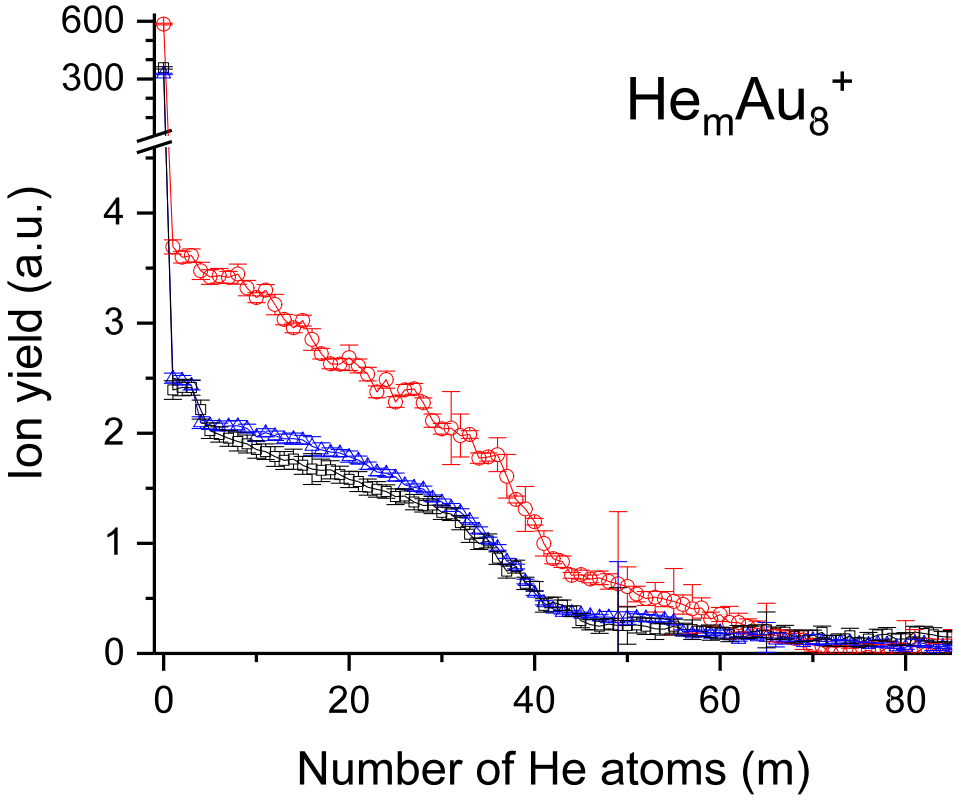

300
200
100
10
5
0
Ion yield (a.u.)
0
20
40
60
80
Number of He atoms (m)
$He_mAu_3^+$

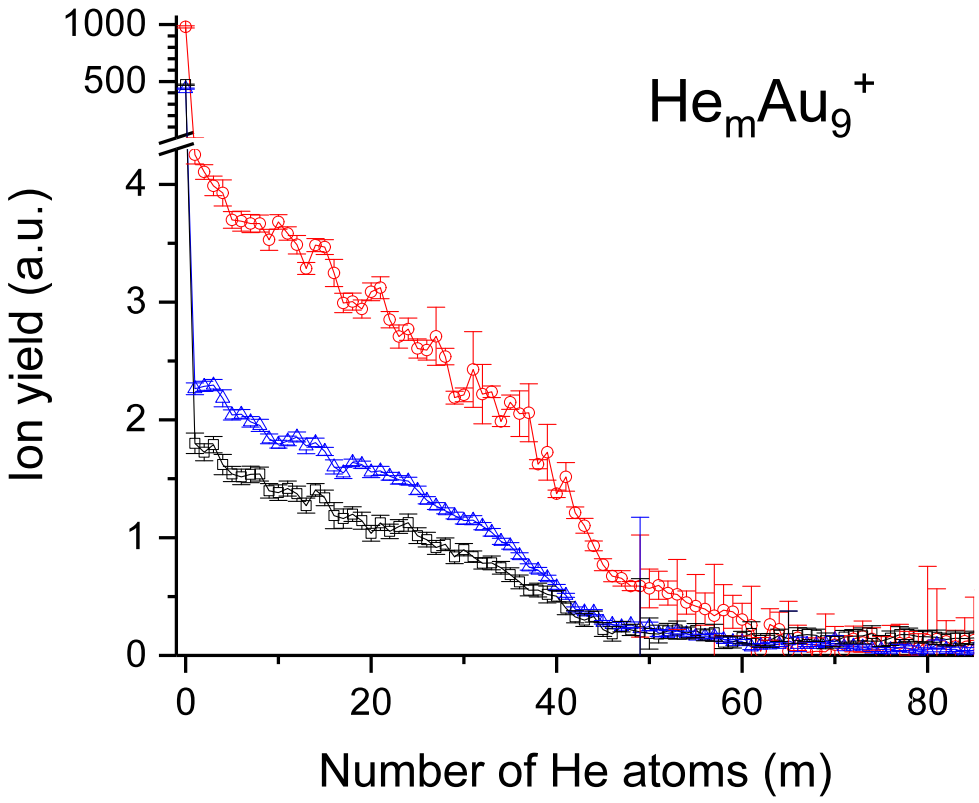

300
200
100
5
0
Ion yield (a.u.)
0
20
40
60
80
Number of He atoms (m)
$He_mAu_4^+$

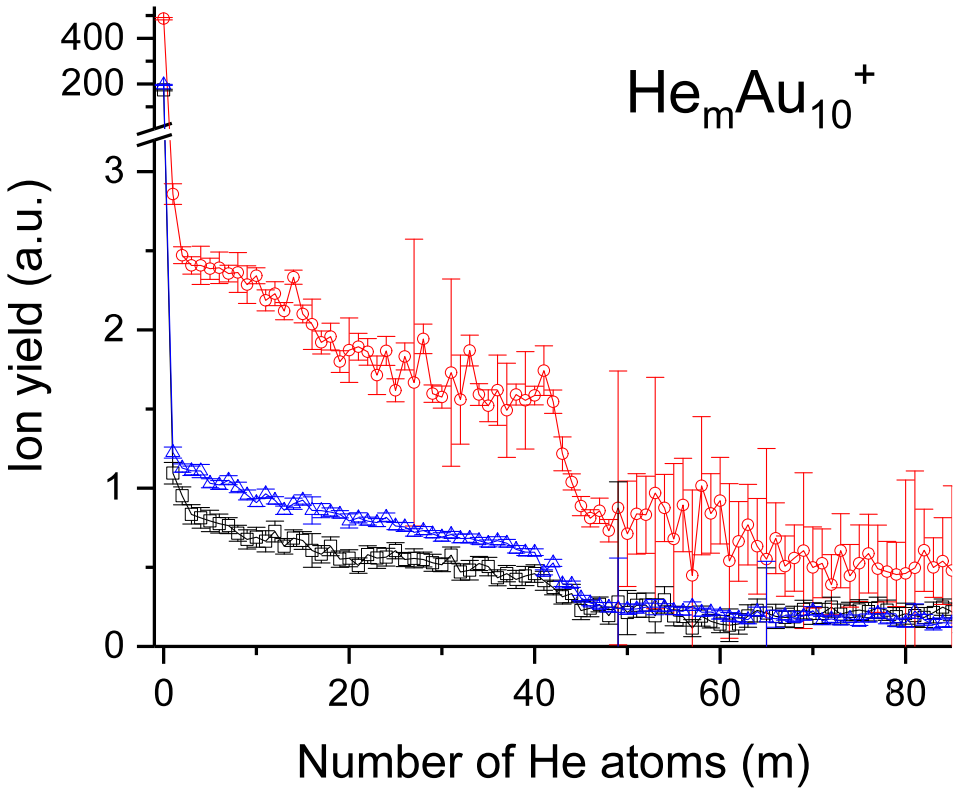

600
300
10
5
0
Ion yield (a.u.)
0
20
40
60
80
Number of He atoms (m)
$He_mAu_5^+$

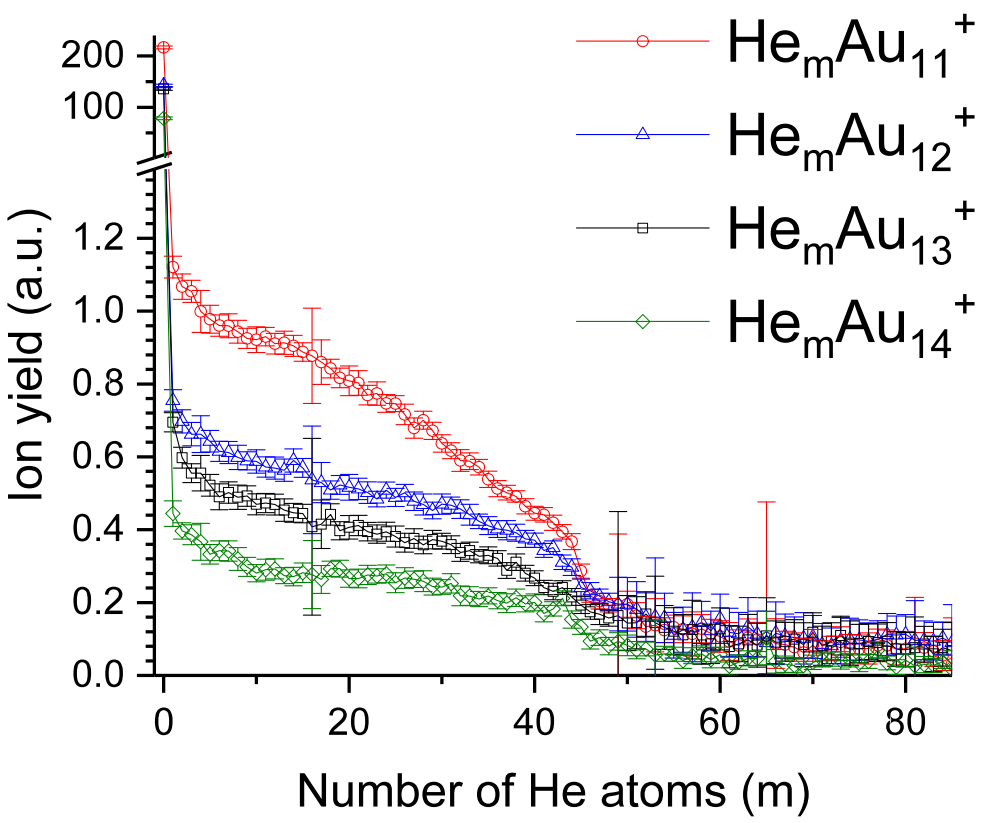

400
200
5
4
3
2
1
0
Ion yield (a.u.)
0
20
40
60
80
Number of He atoms (m)
$He_mAu_6^+$


600
300
6
4
2
0
0
20
40
60
80
Ion yield (a.u.)
Number of He atoms (m)
$He_mAu_7^+$


600
300
4
3
2
1
0
Ion yield (a.u.)
0
20
40
60
80
Number of He atoms (m)
$He_mAu_8^+$


1000
500
4
3
2
1
0
0
20
40
60
80
Ion yield (a.u.)
Number of He atoms (m)
$He_mAu_9^+$


400
200
3
2
1
0
0
20
40
60
80
Ion yield (a.u.)
Number of He atoms (m)
$He_mAu_{10}^+$


200
100
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Ion yield (a.u.)
0
20
40
60
80
Number of He atoms (m)
$He_mAu_{11}^+$
$He_mAu_{12}^+$
$He_mAu_{13}^+$
$He_mAu_{14}^+$

Calculated (MP2) helium binding sites and binding energies for Au_n^+ ions up to and including n = 6