Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

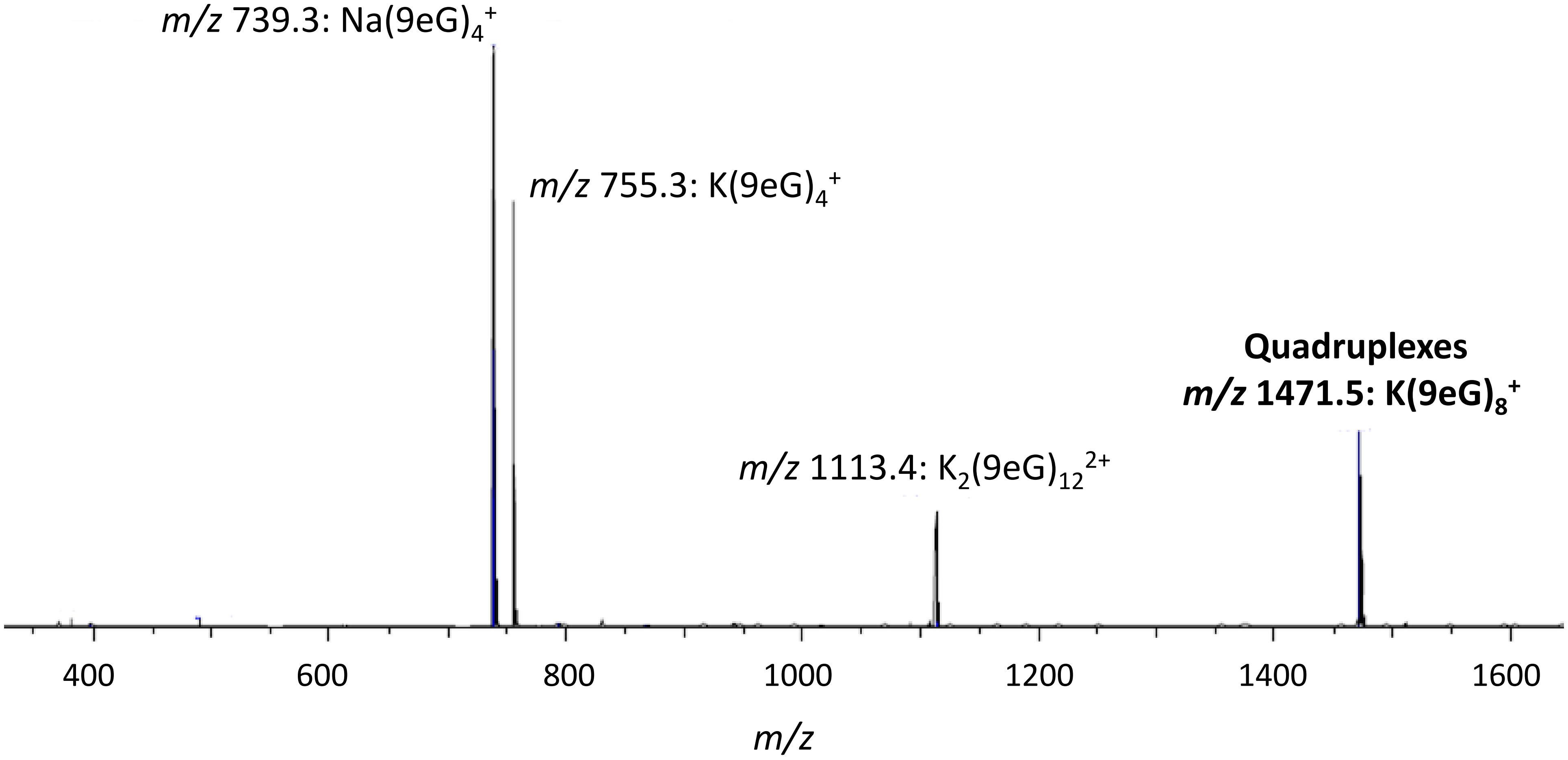
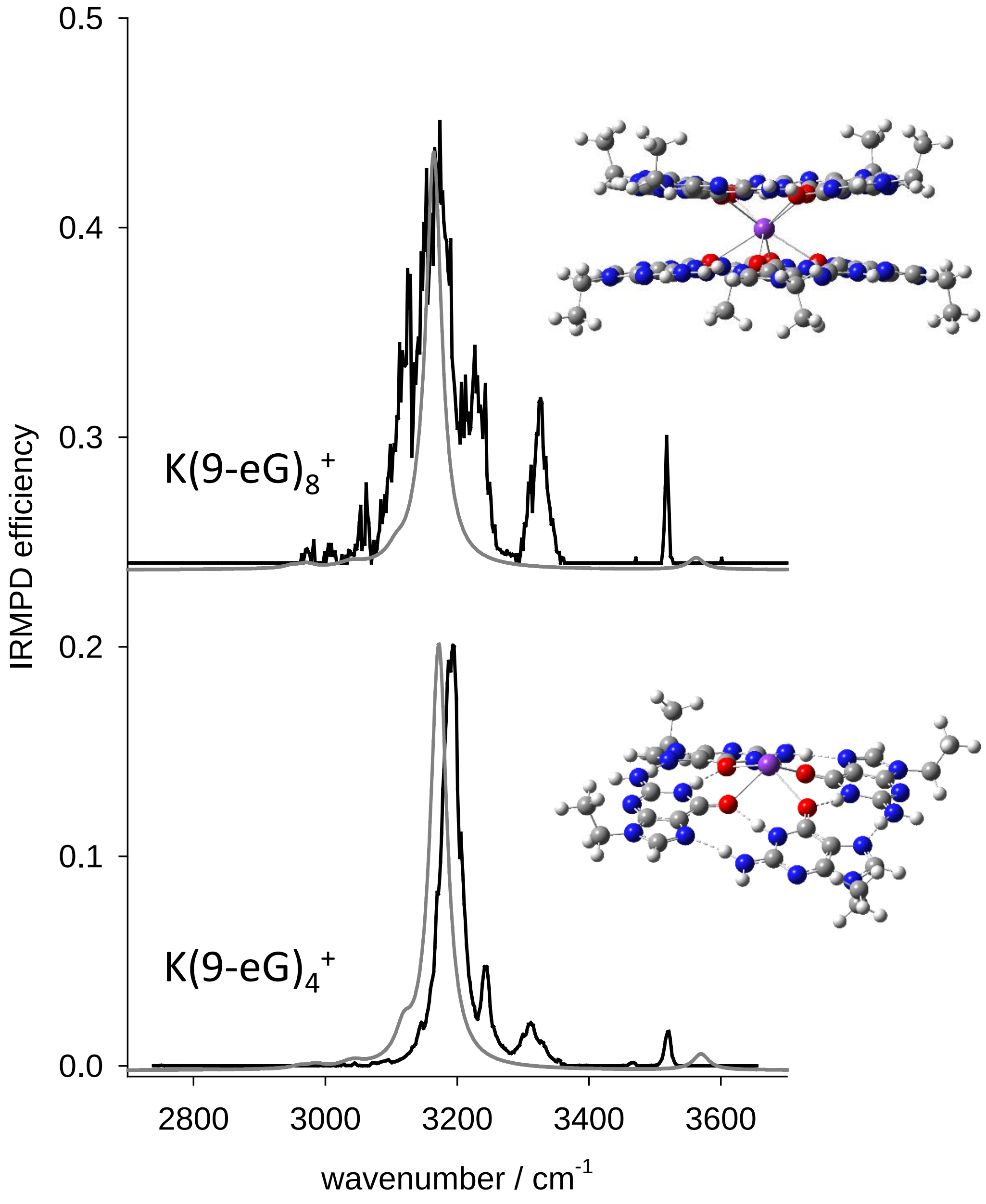



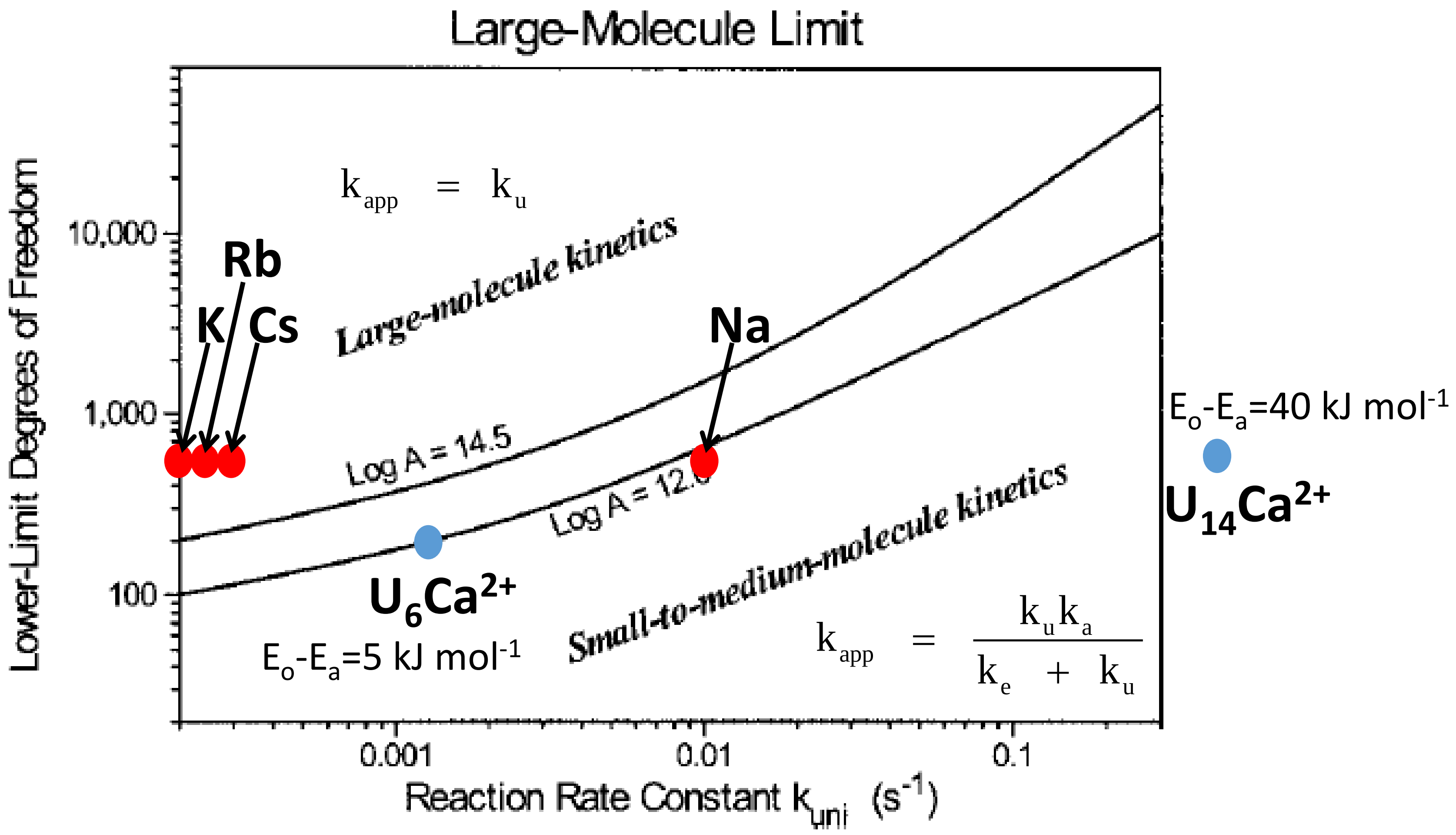

Figure S1

Figure S2



0.5
0.4
0.3
0.2
0.1
0.0
IRMPD efficiency
K(9-eG)$_8^+$
K(9-eG)$_4^+$
2800
3000
3200
3400
3600
wavenumber / cm$^{-1}$

Figure S3





Dunbar, R.C. *Mass Spectrom. Rev.* **2004**, *23*, 127.

E.A.L. Gillis, M. Demireva, K. Nanda, G.J.O. Beran, E. Williams, and T.D. Fridgen *Phys. Chem. Chem. Phys*. **2012**, *14*, 3304.

Na(9-ethylguanine)$_8^+$

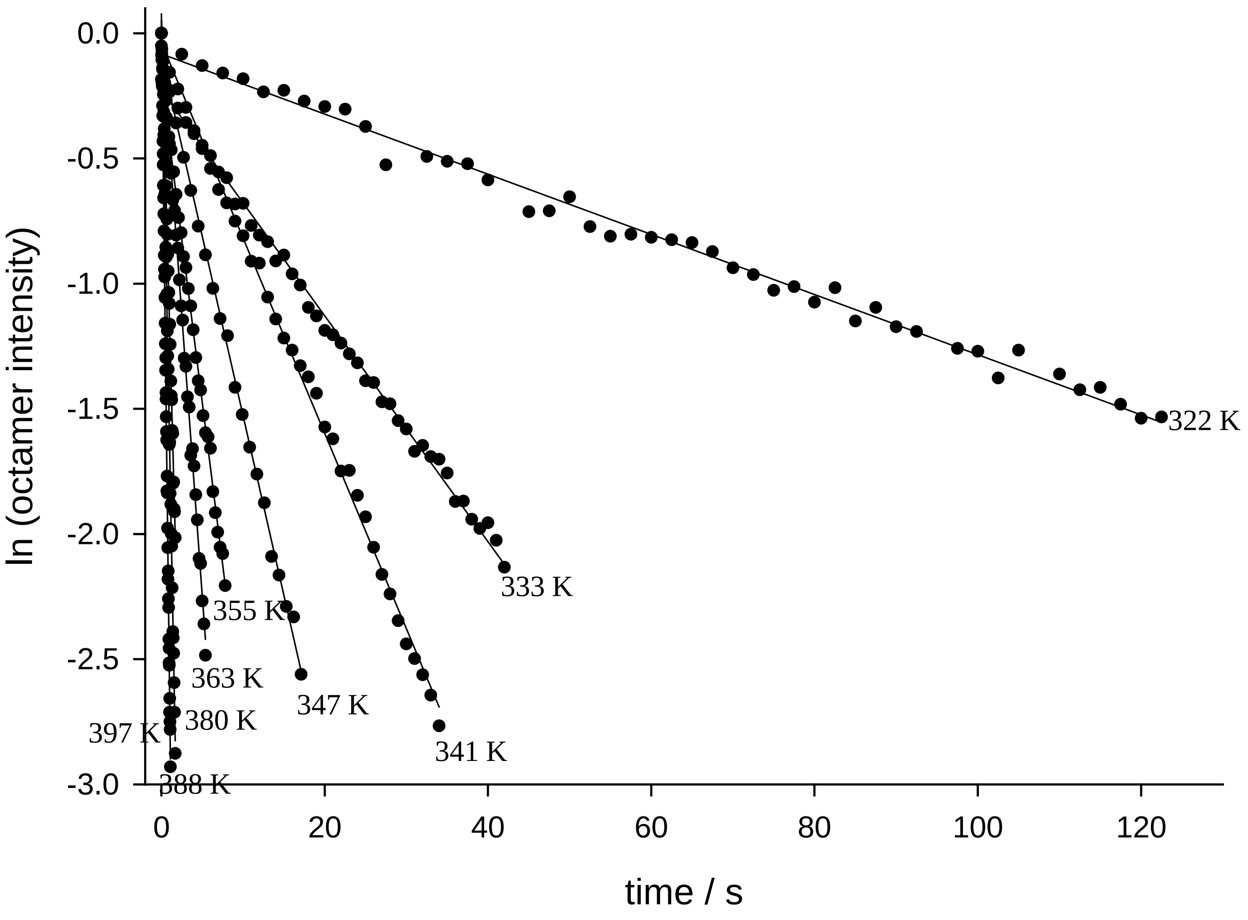
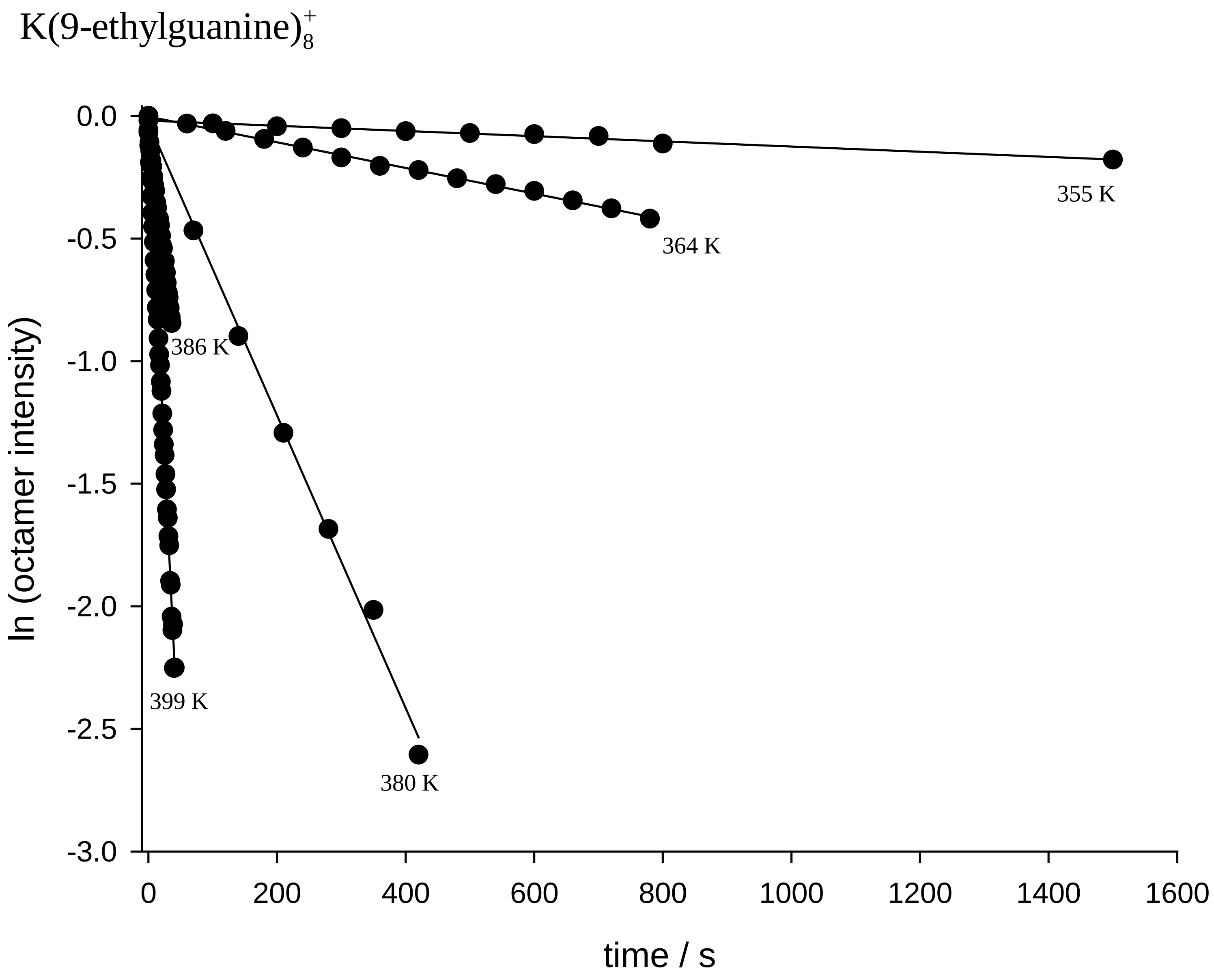
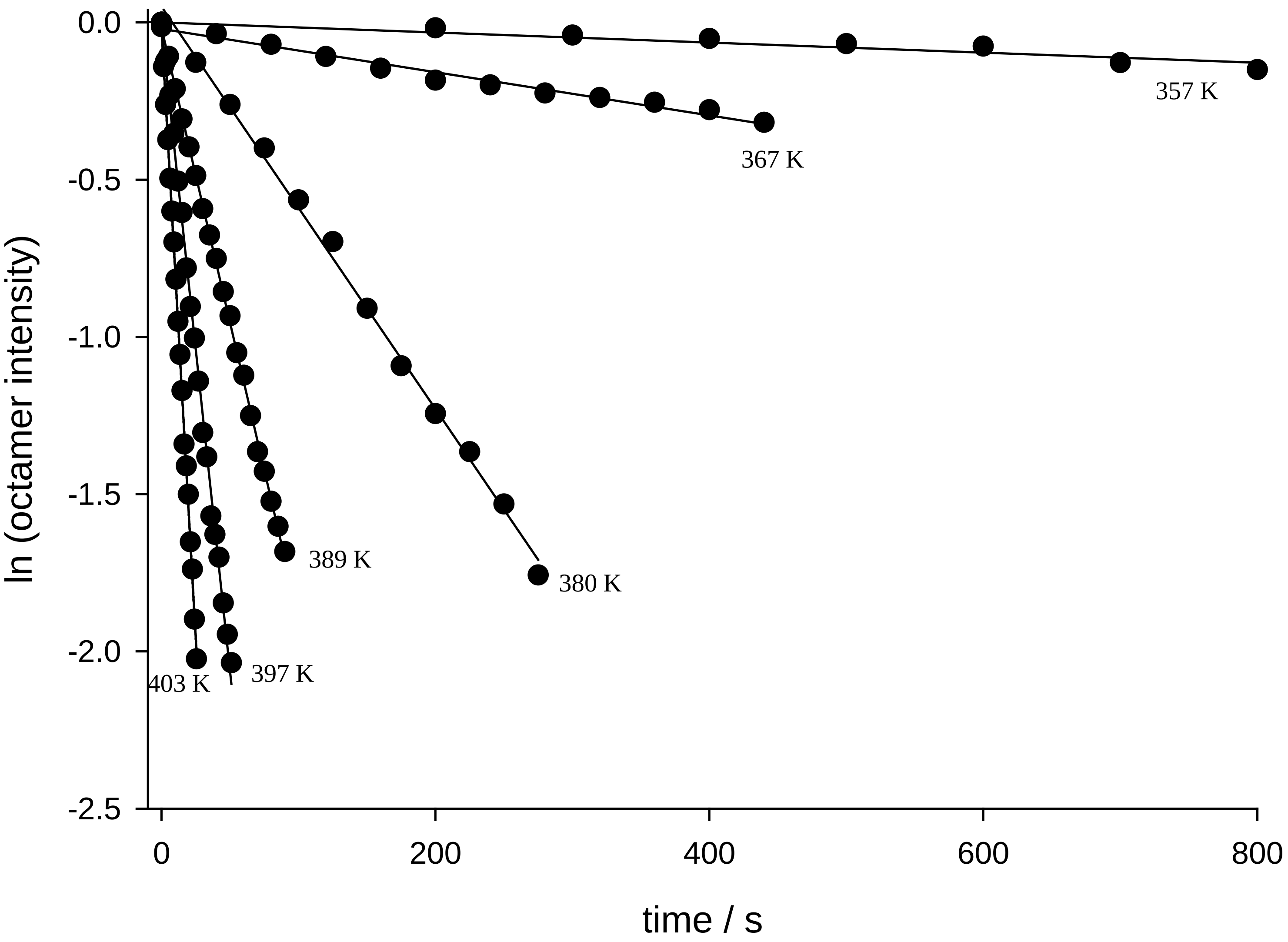


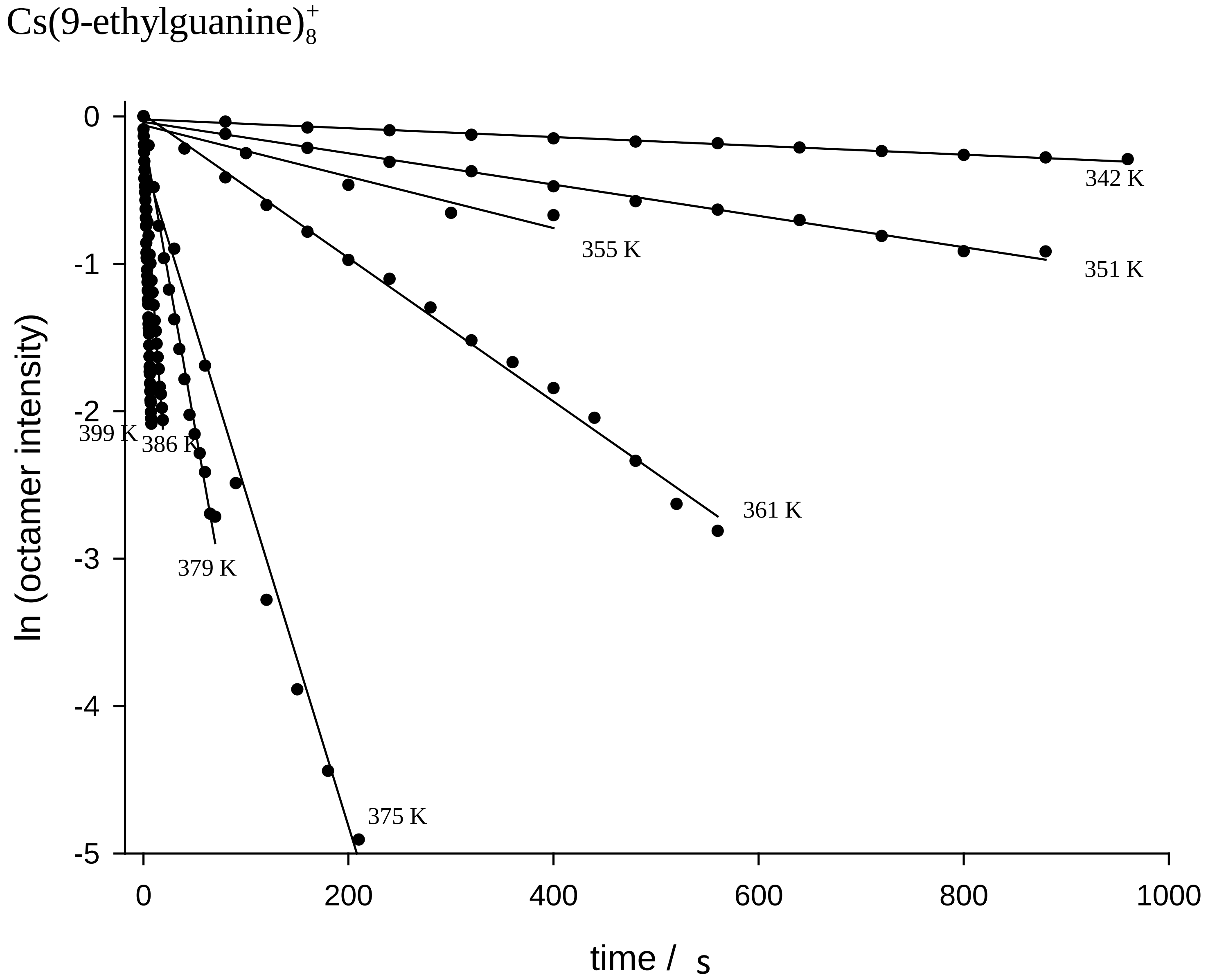

Figure S4.



K(9-ethylguanine)$_8^+$
ln (octamer intensity)
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
0
200
400
600
800
1000
1200
1400
1600
time / s
355 K
364 K
386 K
380 K
399 K

$Rb(9\text{-ethylguanine})_8^+$

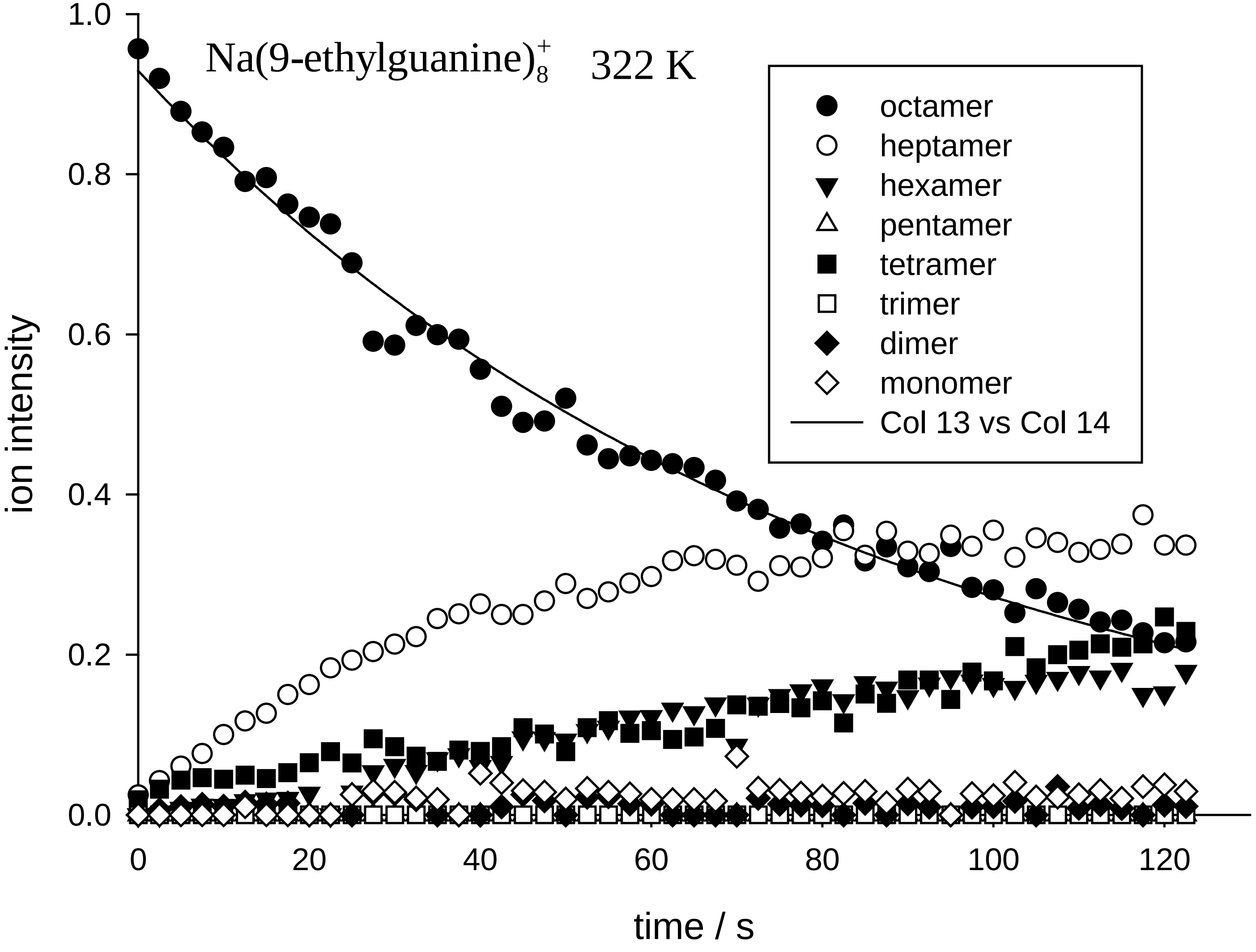


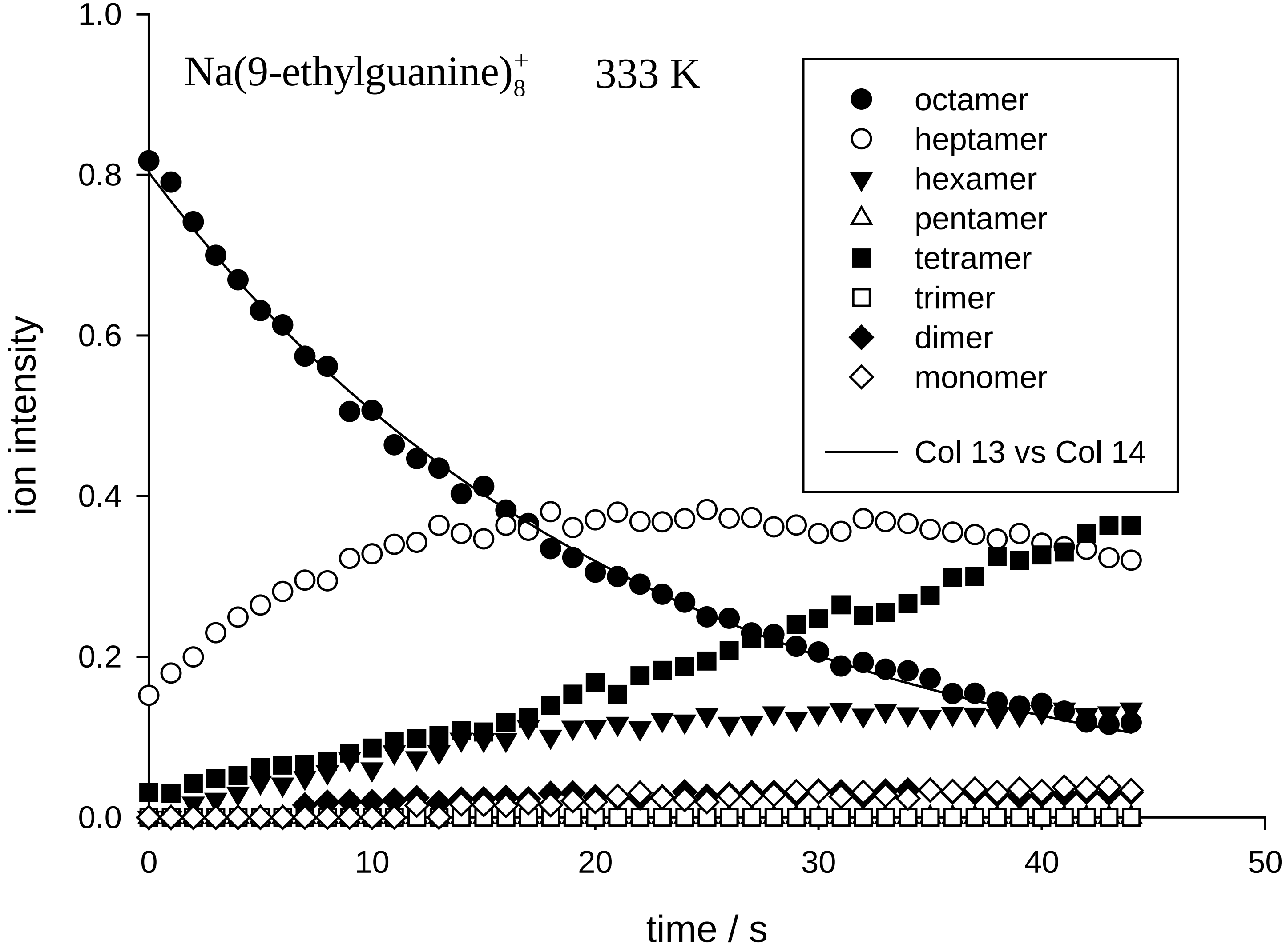


Cs(9-ethylguanine)$_8^+$
ln (octamer intensity)
time / s
0
-1
-2
-3
-4
-5
0
200
400
600
800
1000
342 K
351 K
355 K
361 K
375 K
379 K
386 K
399 K

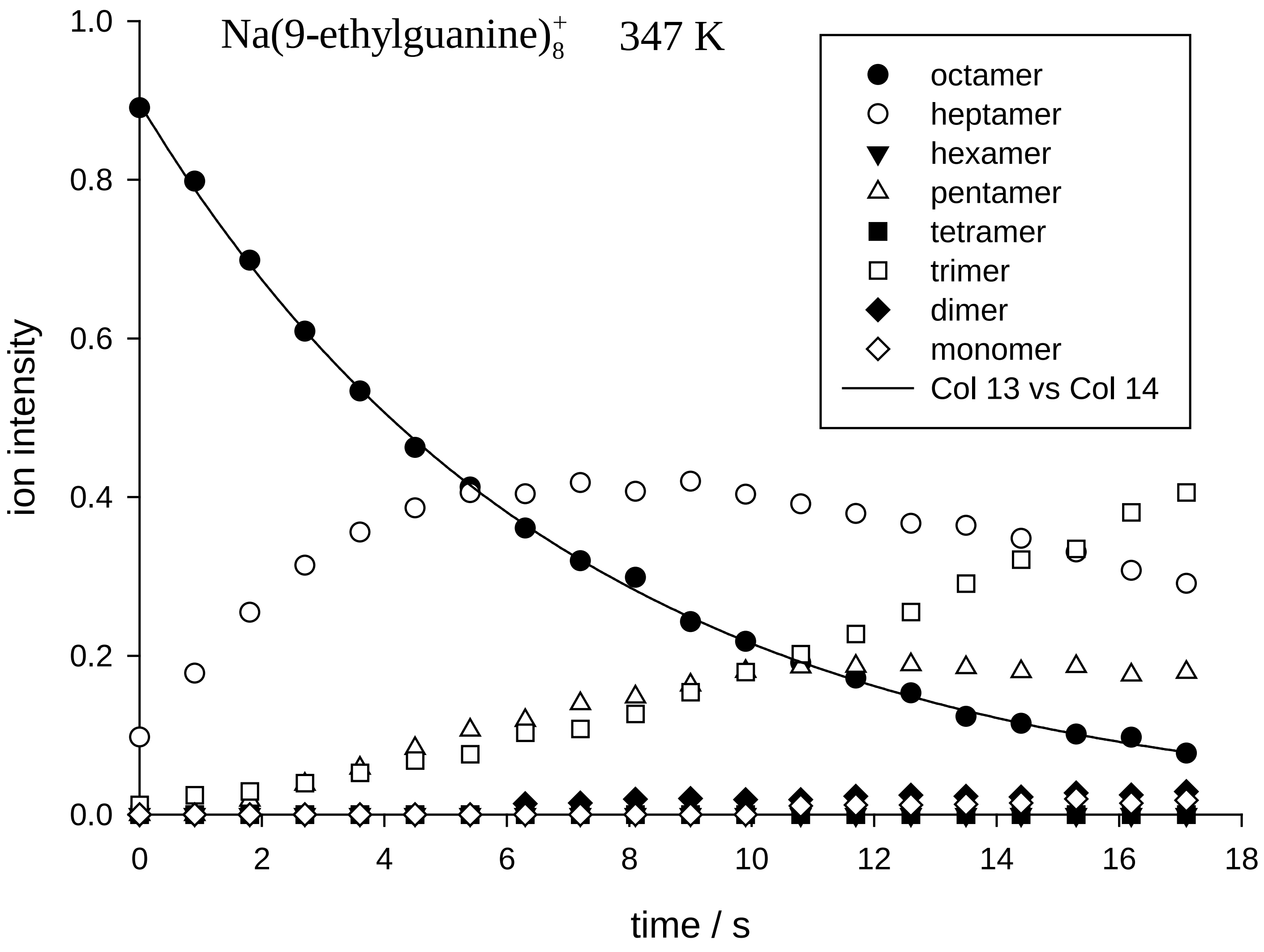
| $Na(9eG)_8^+$ | $K(9eG)_8^+$ | $Rb(9eG)_8^+$ | $Cs(9eG)_8^+$ |
|---|---|---|---|
| $k_{322}$ =1.20(±0.02)×10$^{-2}$ s$^{-1}$ | — | — | — |
| $k_{333}$ =4.45(±0.04)×10$^{-2}$ s$^{-1}$ | — | — | — |
| $k_{341}$ =7.48(±0.07)×10$^{-2}$ s$^{-1}$ | — | — | $k_{342}$ =1.98(±0.09)×10$^{-4}$ s$^{-1}$ |
| $k_{347}$ =1.42(±0.02)×10$^{-1}$ s$^{-1}$ | — | — | $k_{351}$ =1.06 (±0.03)×10$^{-3}$ s$^{-1}$ |
| $k_{355}$ =2.60(±0.02)×10$^{-1}$ s$^{-1}$ | $k_{355}$ =1.06(±0.03)×10$^{-4}$ s$^{-1}$ | $k_{357}$ =2.13(±0.16)×10$^{-4}$ s$^{-1}$ | $k_{355}$ =1.63(±0.22)×10$^{-3}$ s$^{-1}$ |
| $k_{363}$ =4.47(±0.04)×10$^{-1}$ s$^{-1}$ | $k_{364}$ =5.24(±0.07)×10$^{-4}$ s$^{-1}$ | $k_{367}$ =6.88(±0.32)×10$^{-4}$ s$^{-1}$ | $k_{361}$ =4.87(±0.10)×10$^{-3}$ s$^{-1}$ |
| $k_{380}$ =1.21(±0.02) s$^{-1}$ | $k_{380}$ =5.70(±0.02)×10$^{-3}$ s$^{-1}$ | $k_{380}$ =6.40(±0.11)×10$^{-3}$ s$^{-1}$ | $k_{379}$ =3.97(±0.11)×10$^{-2}$ s$^{-1}$ |
| $k_{388}$ =1.73(±0.02) s$^{-1}$ | $k_{386}$ =2.10(±0.03)×10$^{-2}$ s$^{-1}$ | $k_{389}$ =1.88(±0.01)×10$^{-2}$ s$^{-1}$ | $k_{386}$ =9.19(±0.09)×10$^{-2}$ s$^{-1}$ |
| $k_{397}$ =2.68(±0.02) s$^{-1}$ | $k_{398}$ =5.36(±0.04)×10$^{-2}$ s$^{-1}$ | $k_{403}$ =7.77(±0.06)×10$^{-2}$ s$^{-1}$ | $k_{399}$ =267(±0.02)×10$^{-1}$ s$^{-1}$ |

Table 1

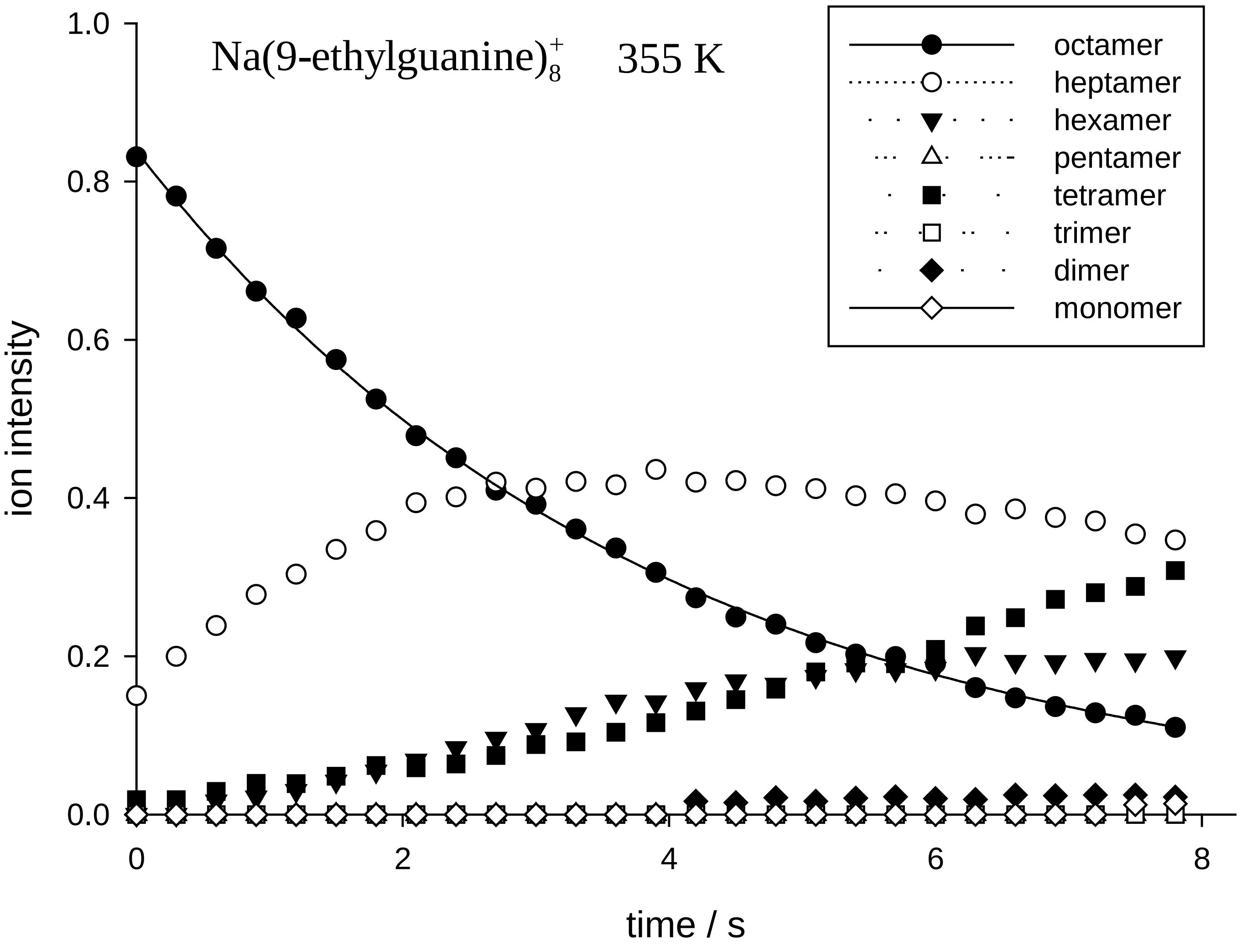

Na(9-ethylguanine)$_8^+$ 322 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
Col 13 vs Col 14
ion intensity
time / s
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
120



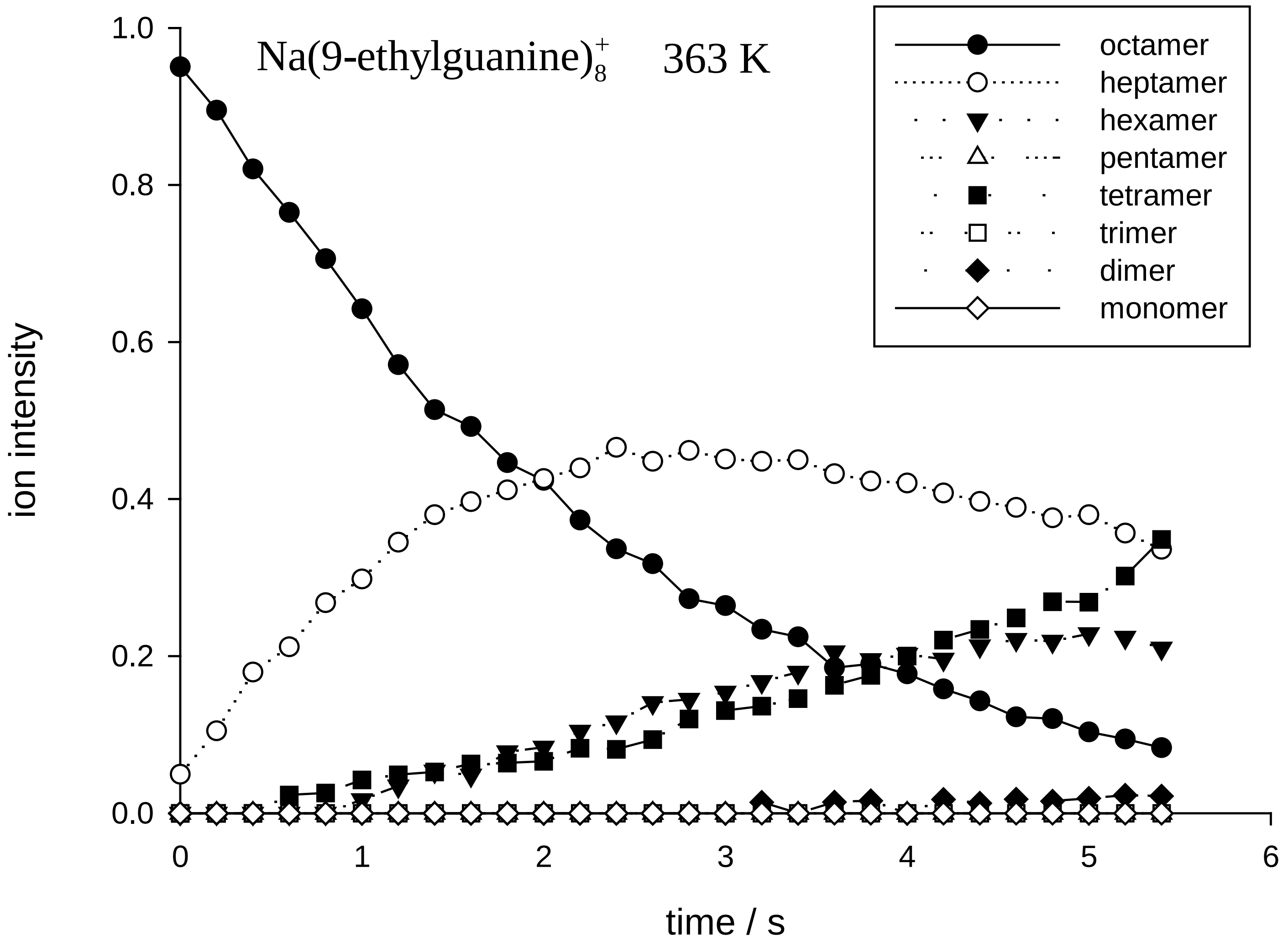
Na(9-ethylguanine)$_8^+$
333 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
Col 13 vs Col 14
ion intensity
time / s
1.0
0.8
0.6
0.4
0.2
0.0
0
10
20
30
40
50

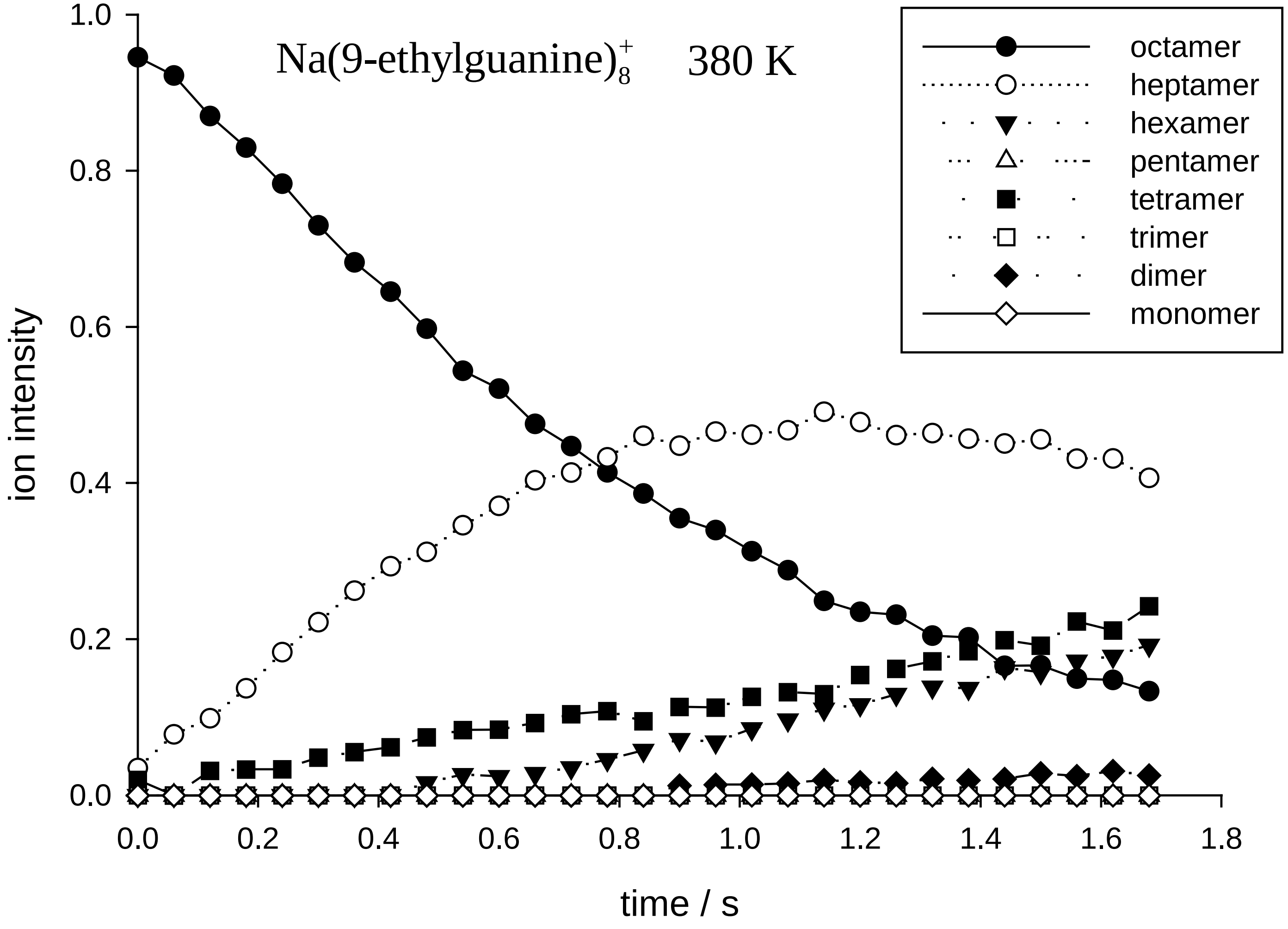


Na(9-ethylguanine)$_8^+$ 347 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
Col 13 vs Col 14
ion intensity
time / s
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
10
12
14
16
18

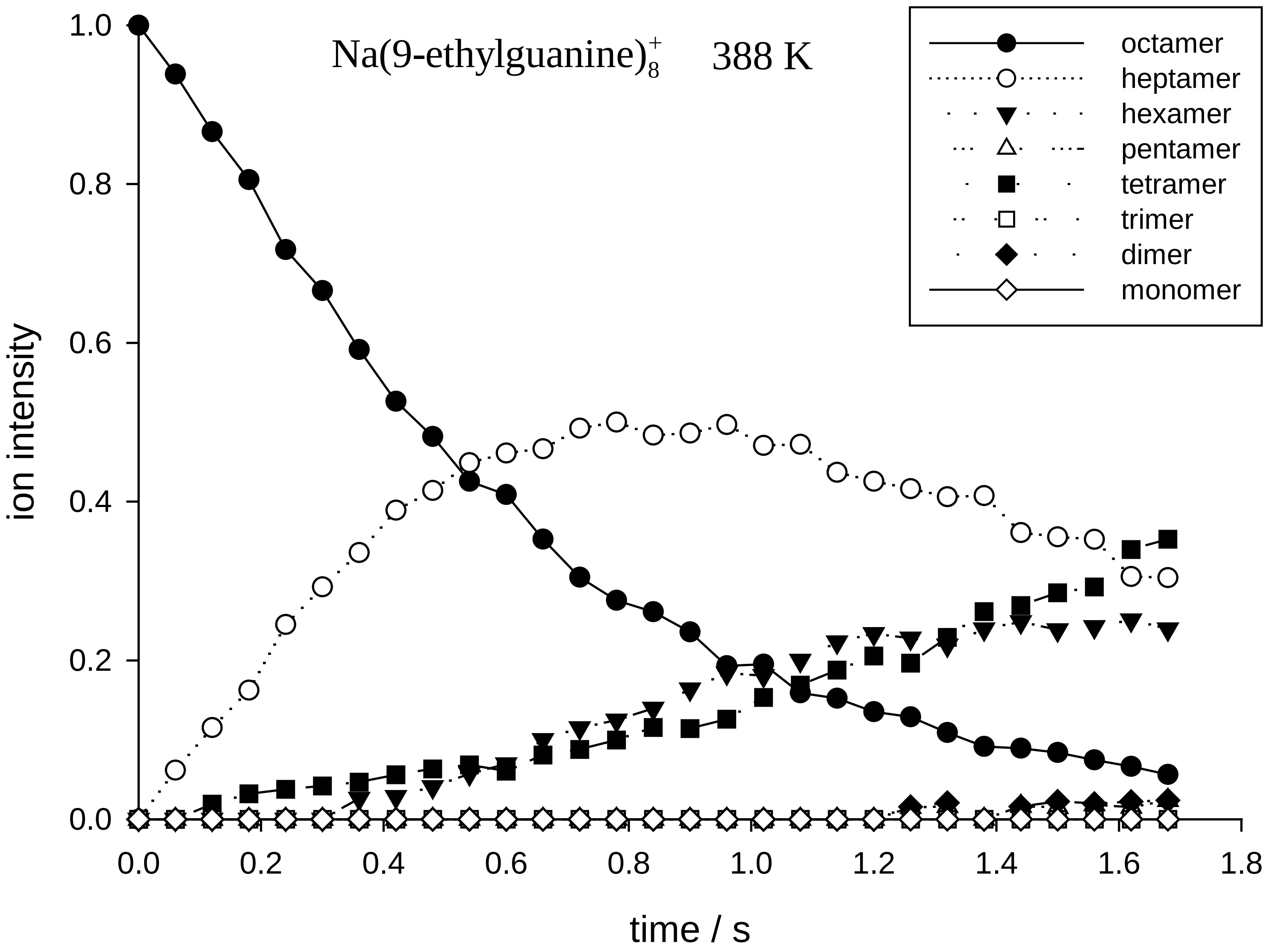


Na(9-ethylguanine)$_8^+$ 355 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
time / s

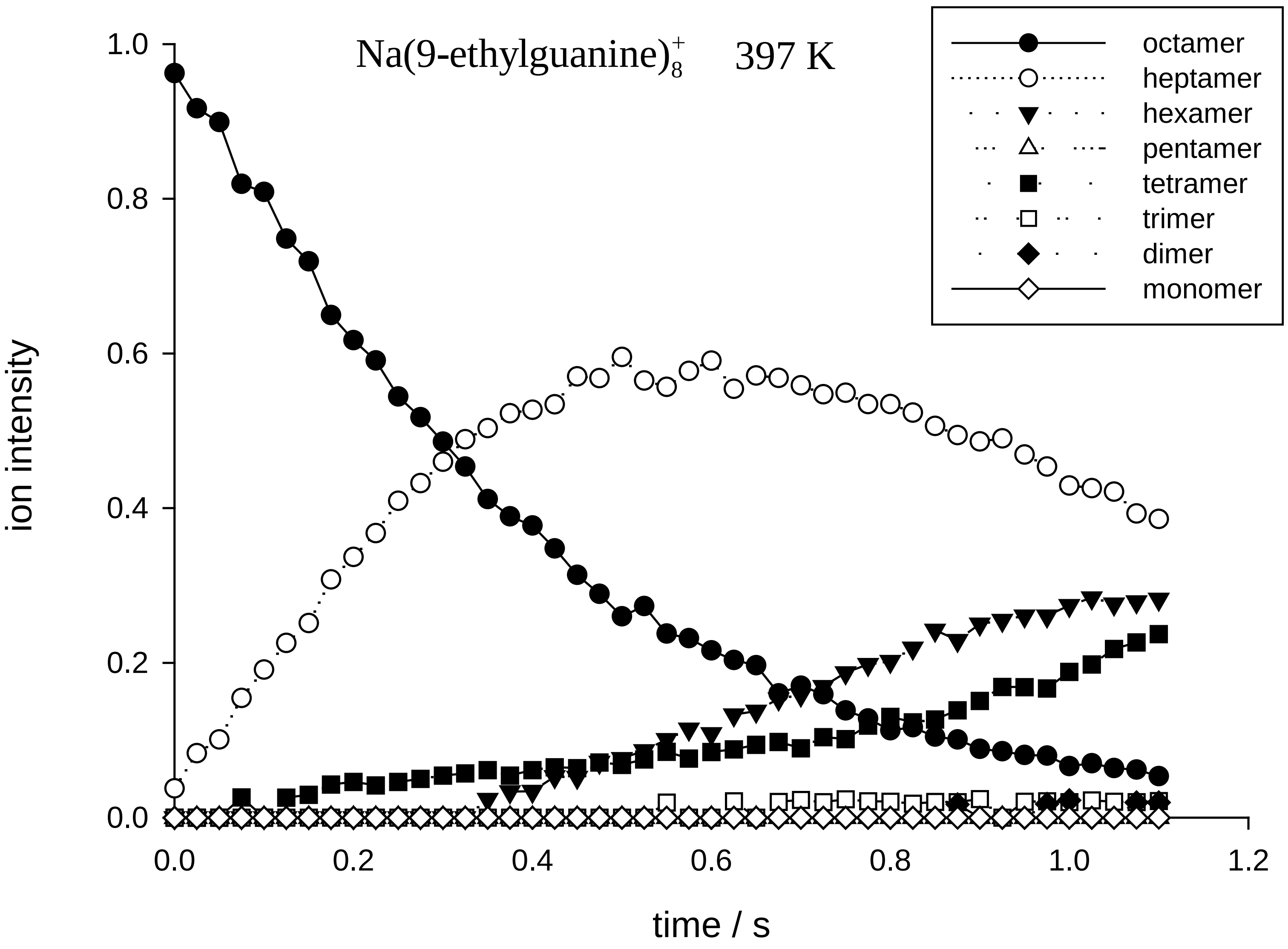

Na(9-ethylguanine)$_8^+$ 363 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
time / s
1.0
0.8
0.6
0.4
0.2
0.0
0
1
2
3
4
5
6

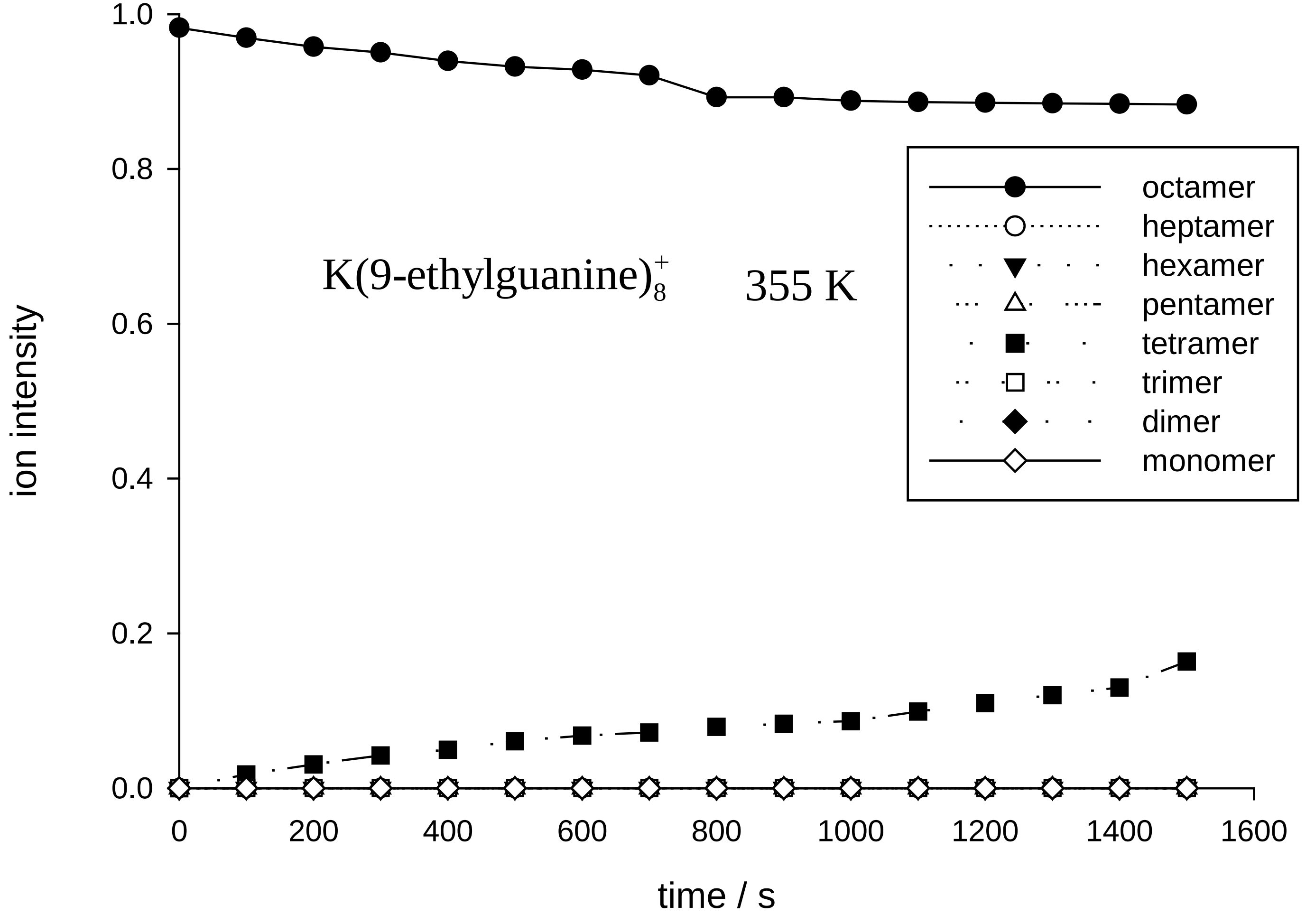


Na(9-ethylguanine)$_8^+$ 380 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
time / s
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8

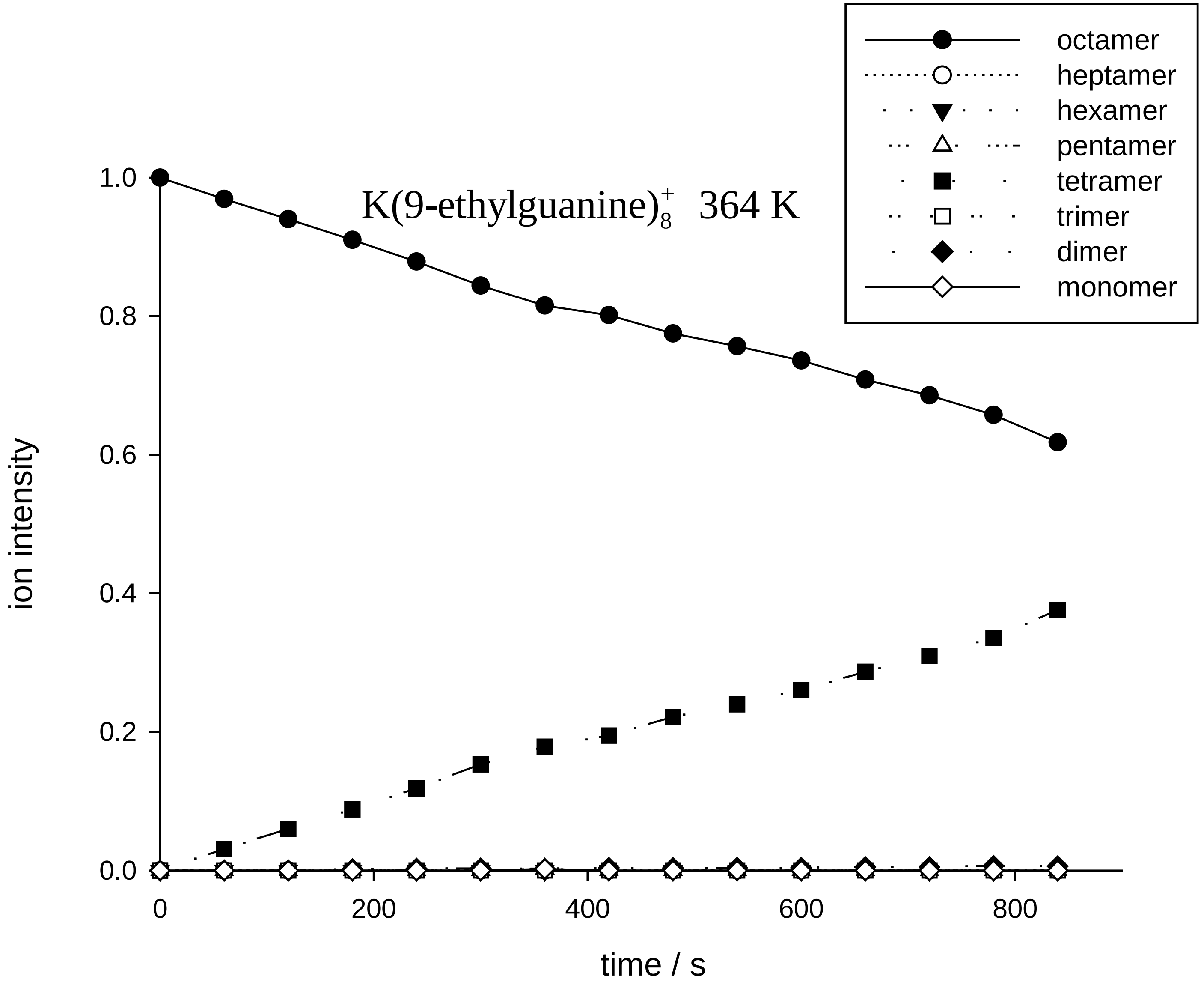


Na(9-ethylguanine)$_8^+$ 388 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
time / s
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8

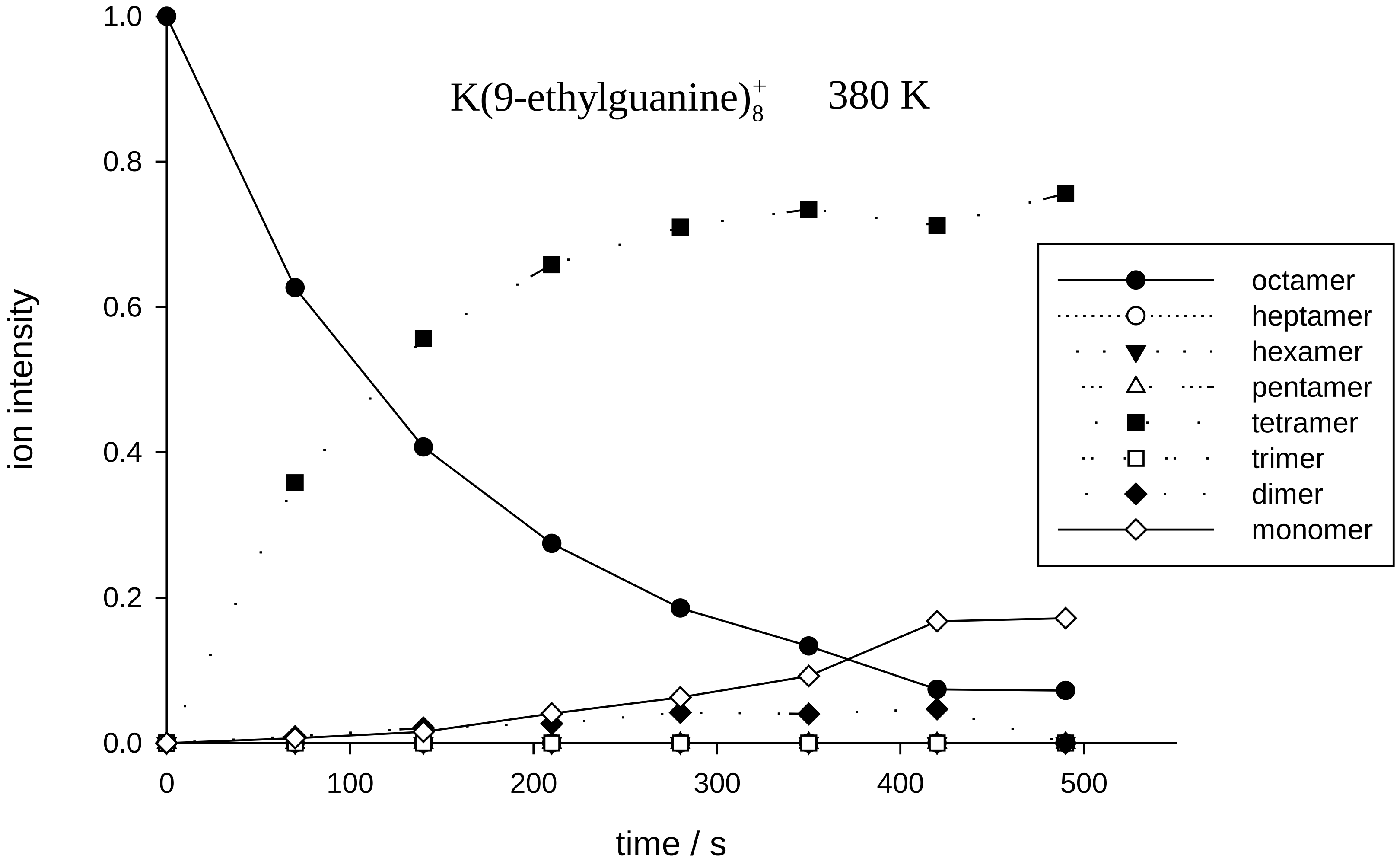

Na(9-ethylguanine)$_8^+$ 397 K
ion intensity
time / s
0.0
0.2
0.4
0.6
0.8
1.0
1.2
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer



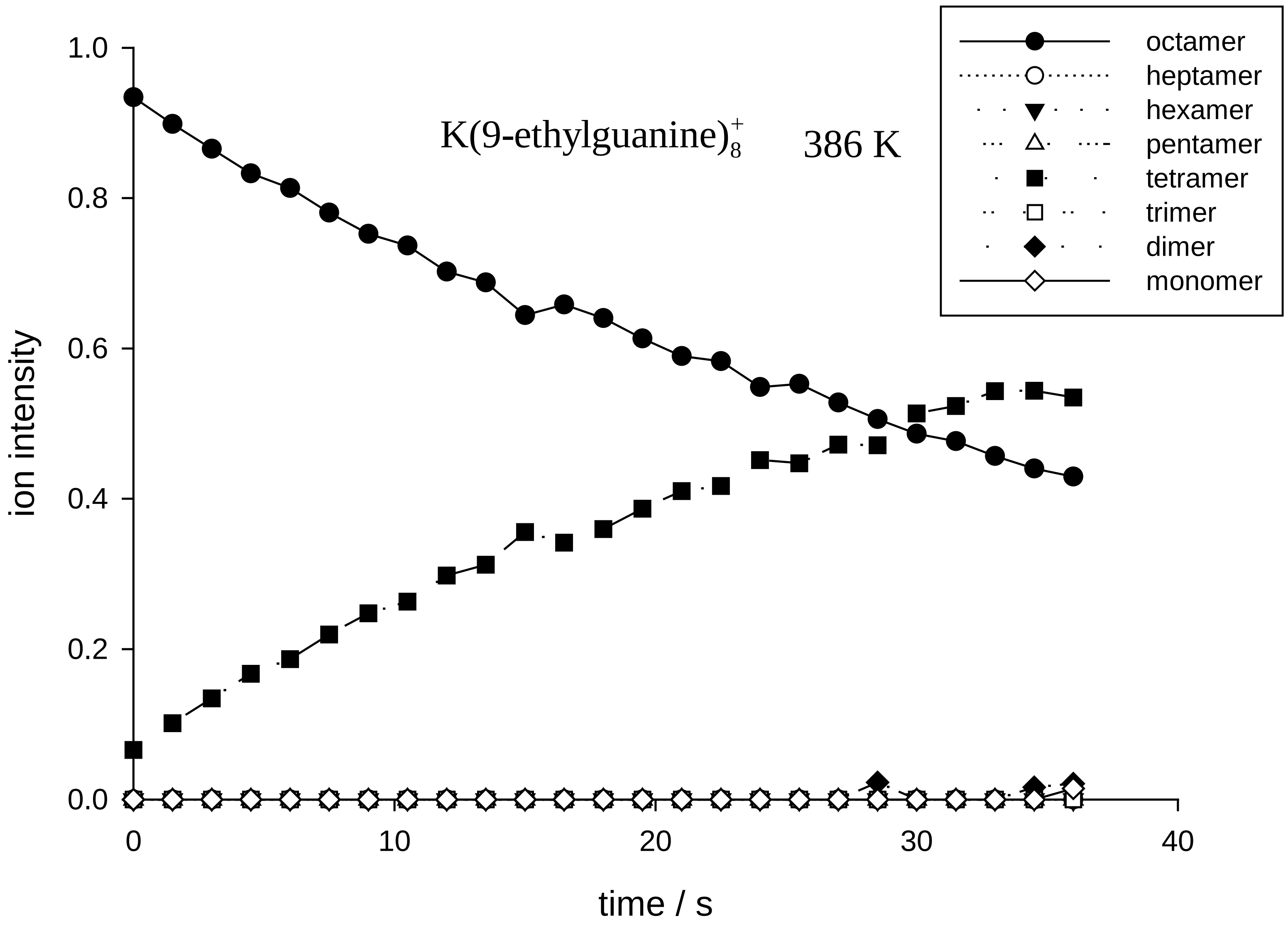
K(9-ethylguanine)$_8^+$
355 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
0.0
0.2
0.4
0.6
0.8
1.0
0
200
400
600
800
1000
1200
1400
1600
time / s



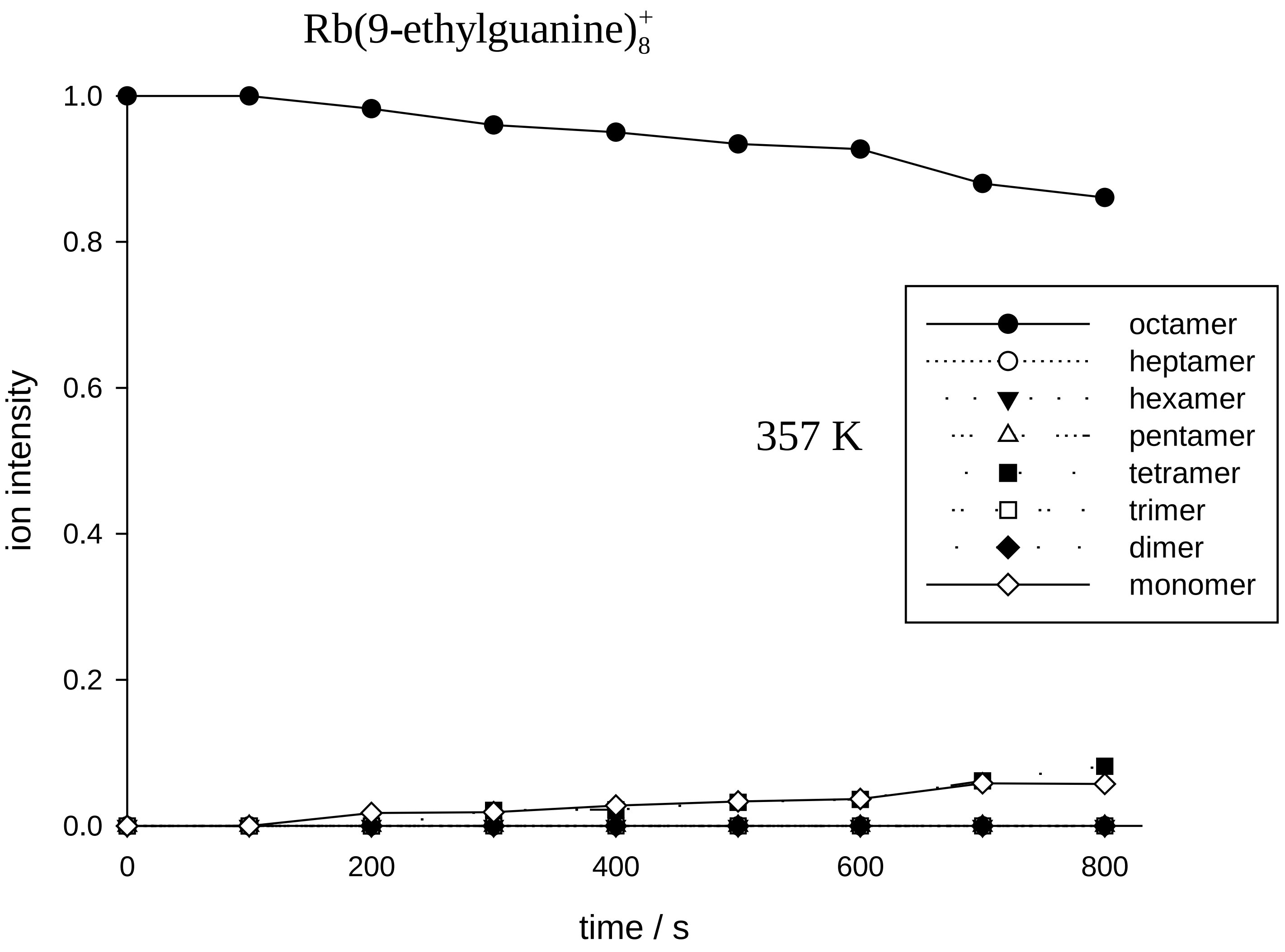
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
$K(9\text{-ethylguanine})_8^+$ 364 K
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
200
400
600
800
time / s



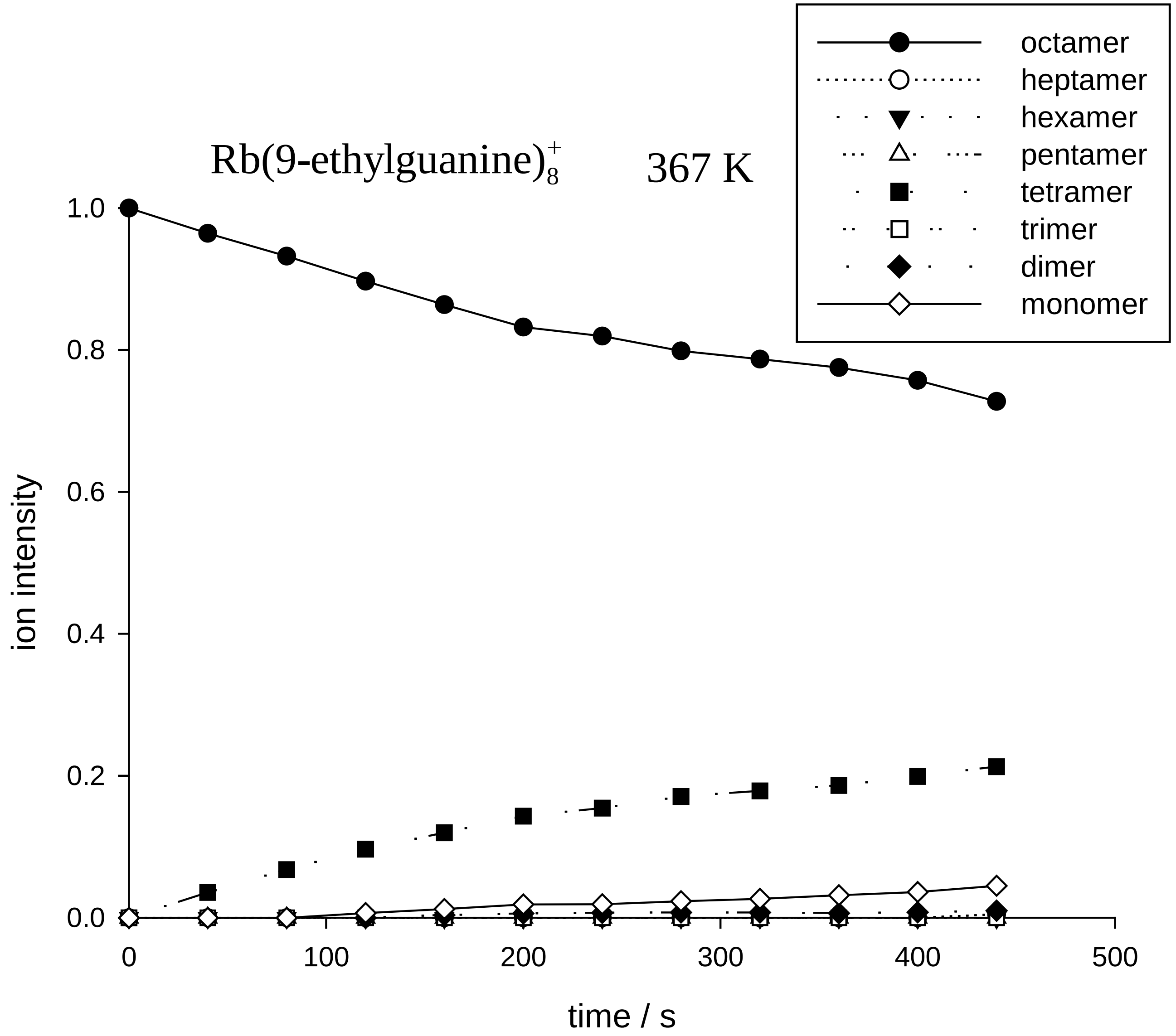
K(9-ethylguanine)$_8^+$ 380 K
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400
500
time / s
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer



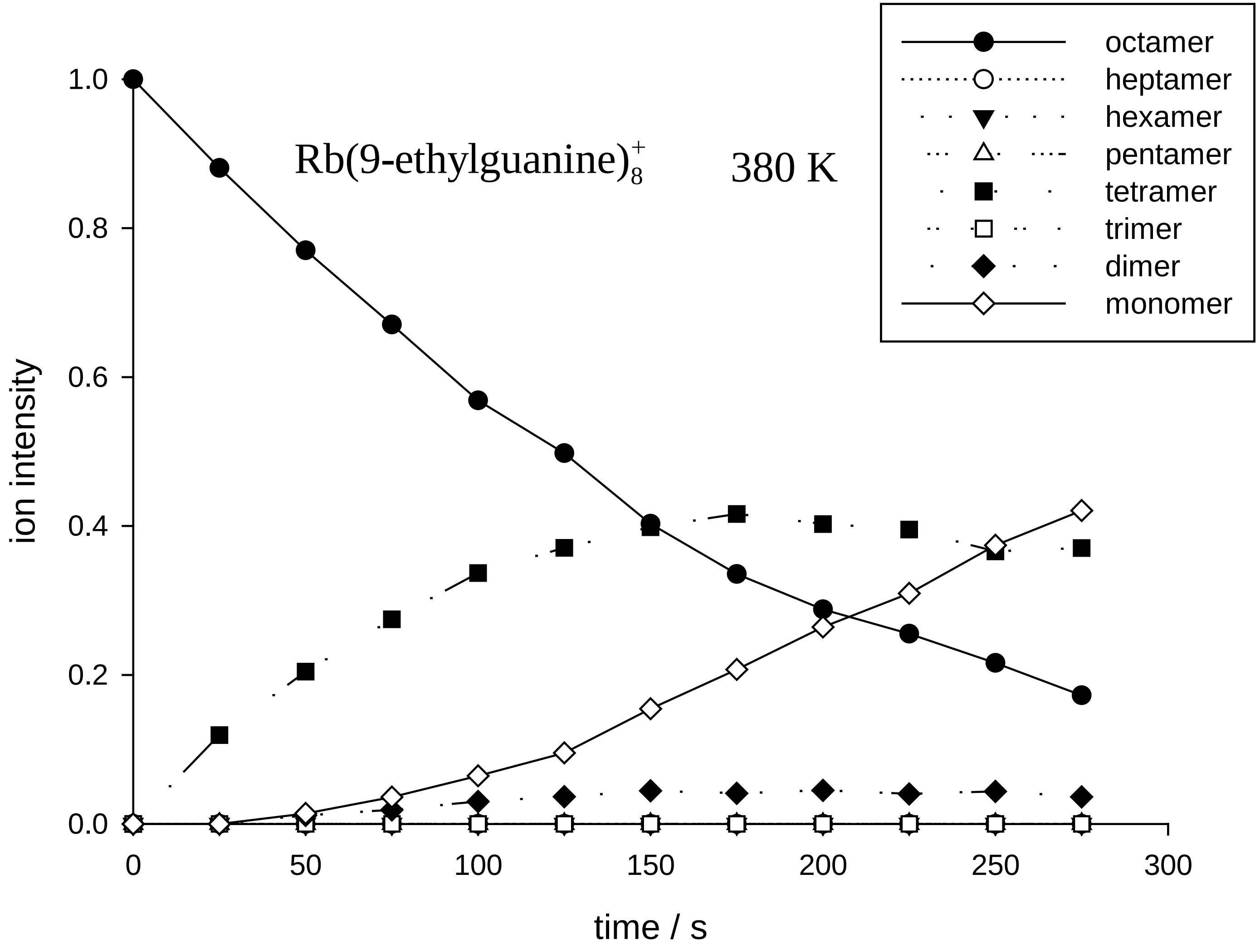
K(9-ethylguanine)$_8^+$
386 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
time / s
0.0
0.2
0.4
0.6
0.8
1.0
0
10
20
30
40



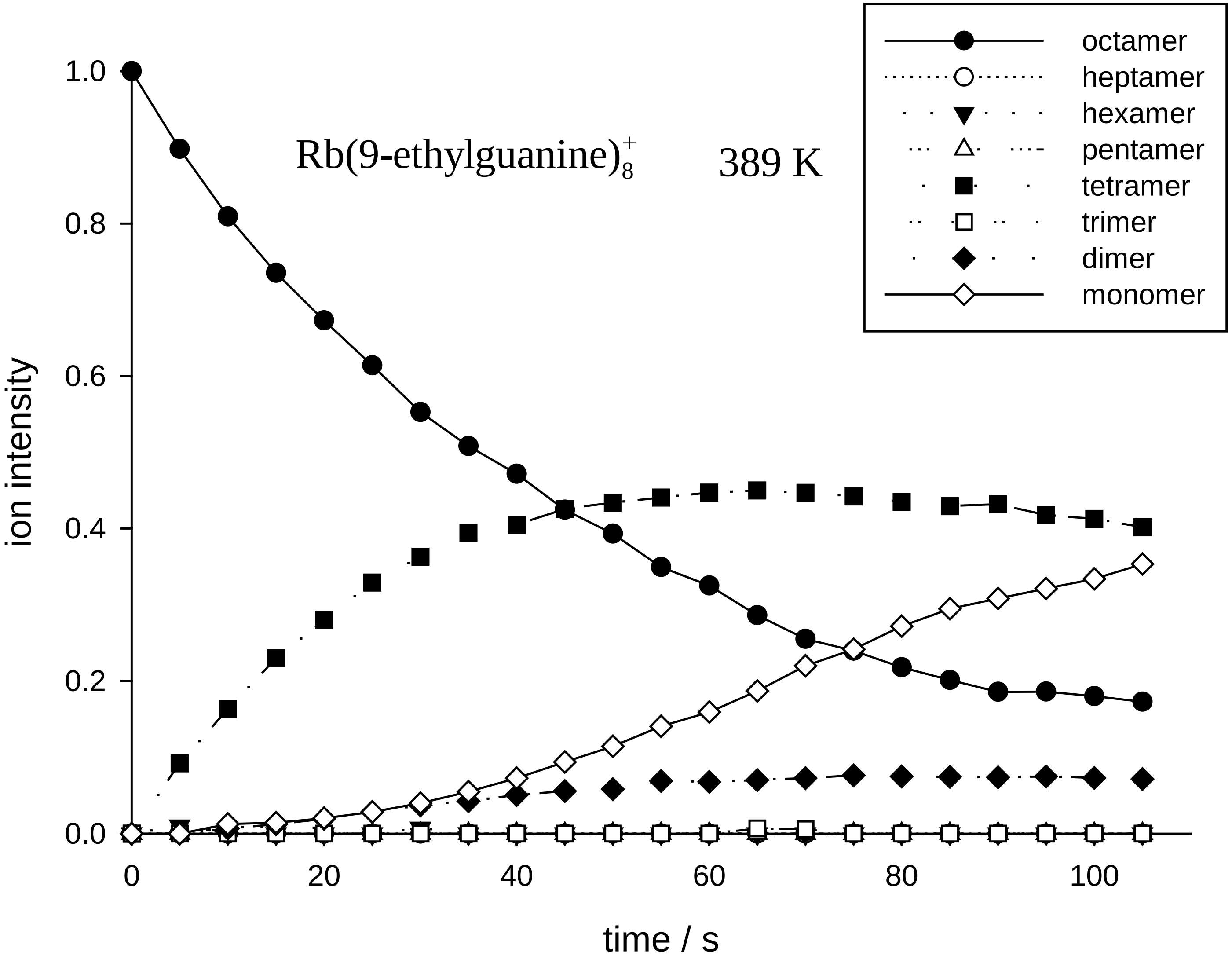
Rb(9-ethylguanine)$_8^+$
357 K
ion intensity
time / s
1.0
0.8
0.6
0.4
0.2
0.0
0
200
400
600
800
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer



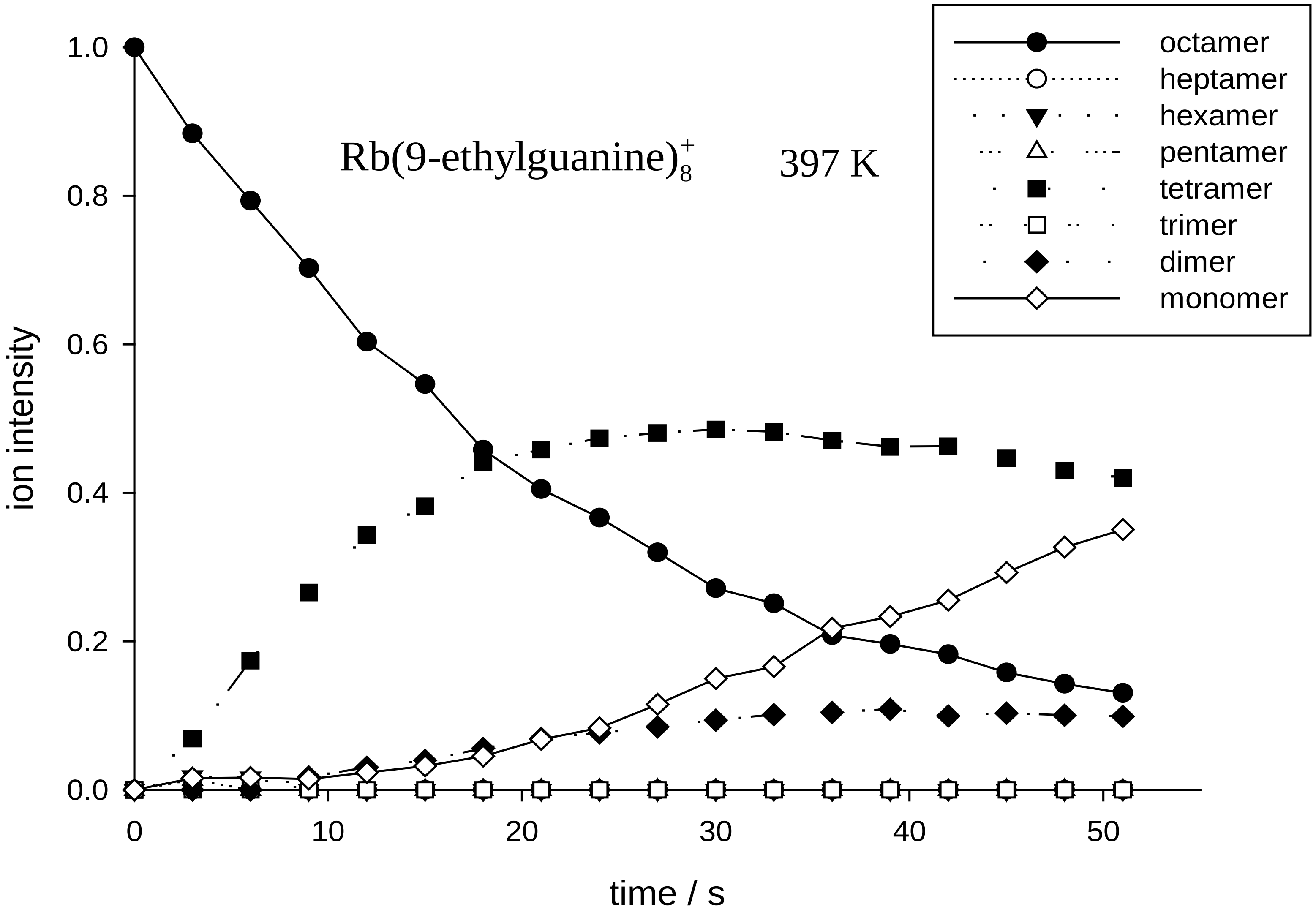
Rb(9-ethylguanine)$_8^+$
367 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400
500
time / s



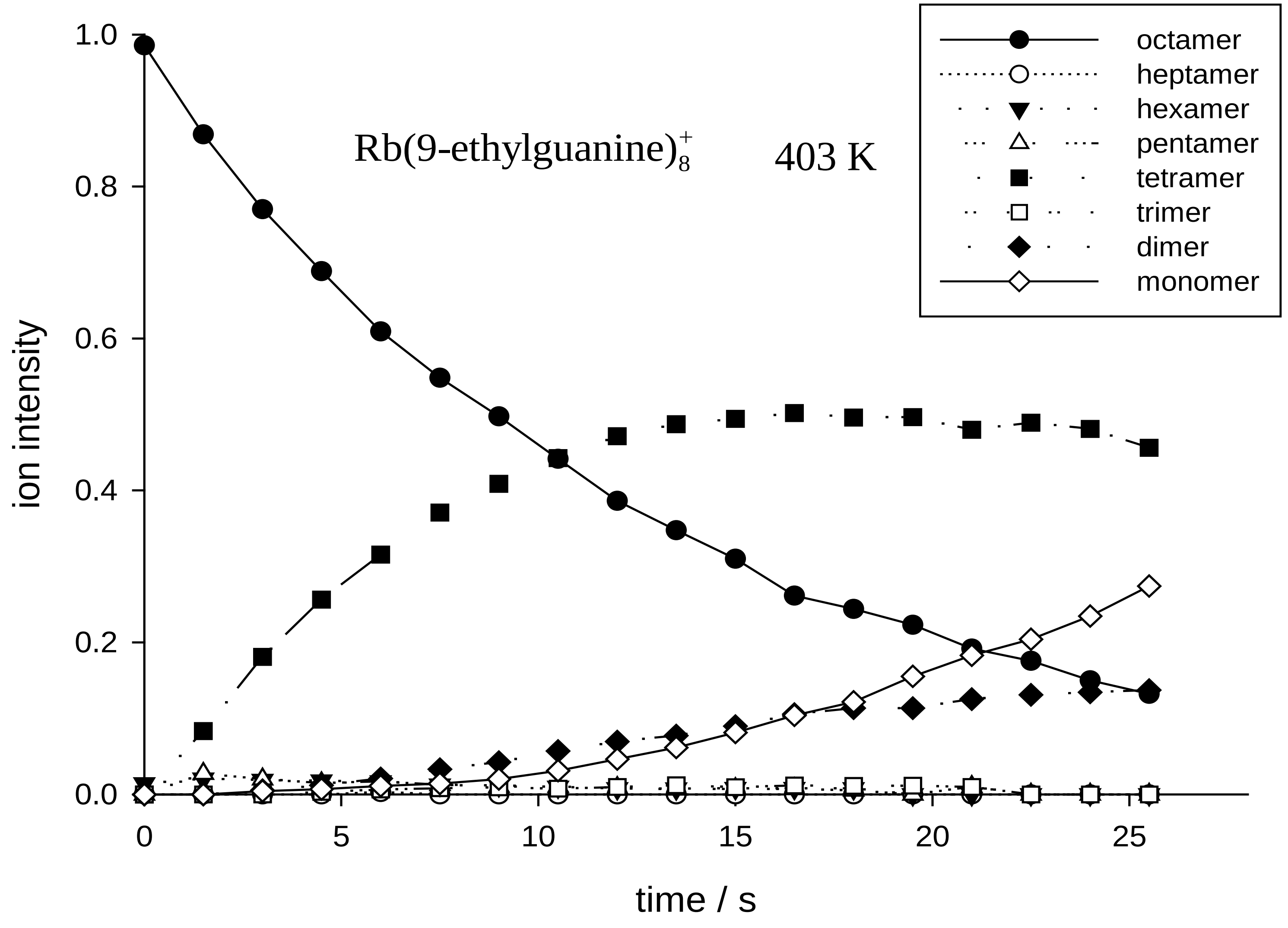
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
Rb(9-ethylguanine)$_8^+$
380 K
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
time / s



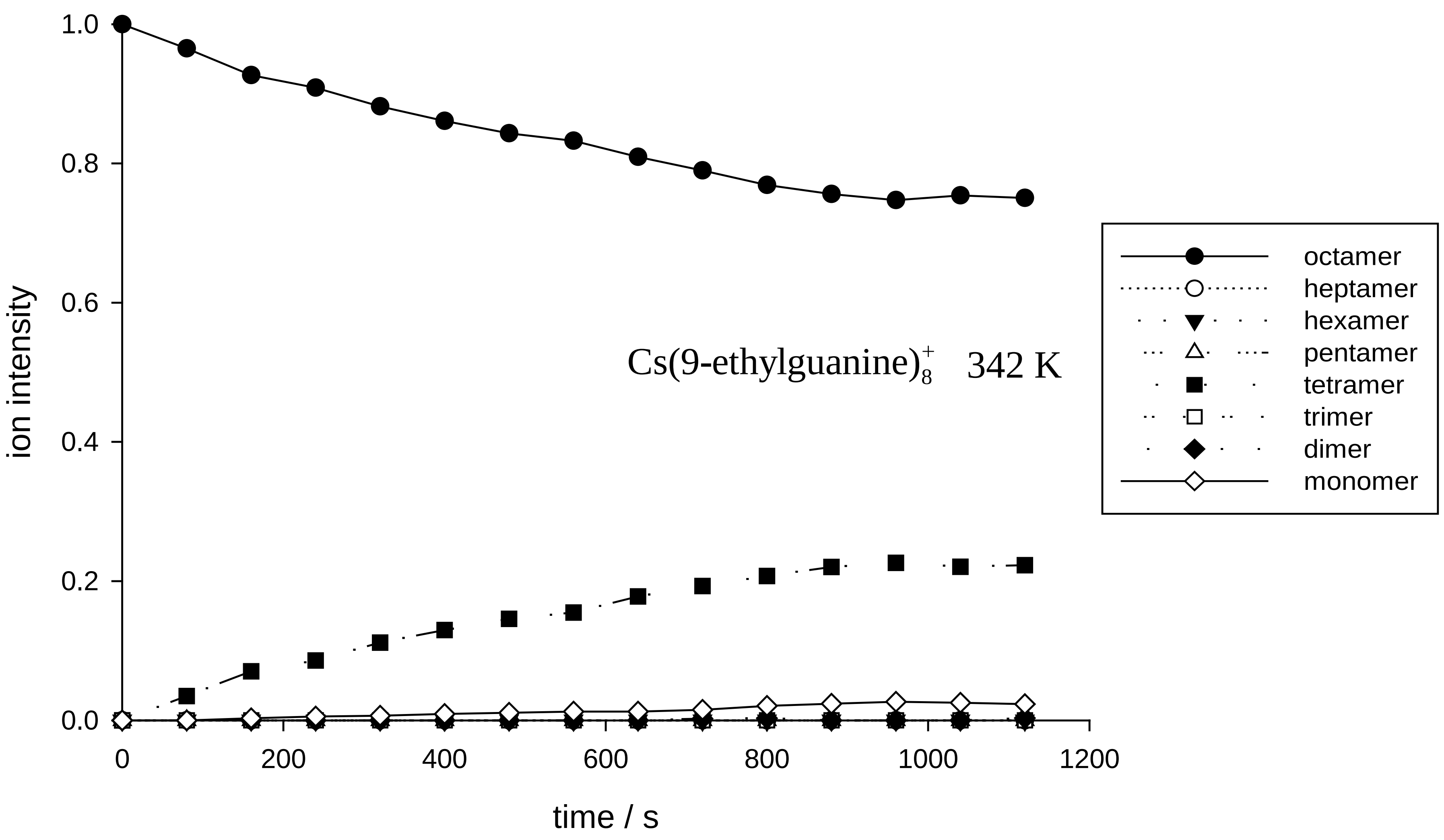
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
Rb(9-ethylguanine)$_8^+$
389 K
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
time / s



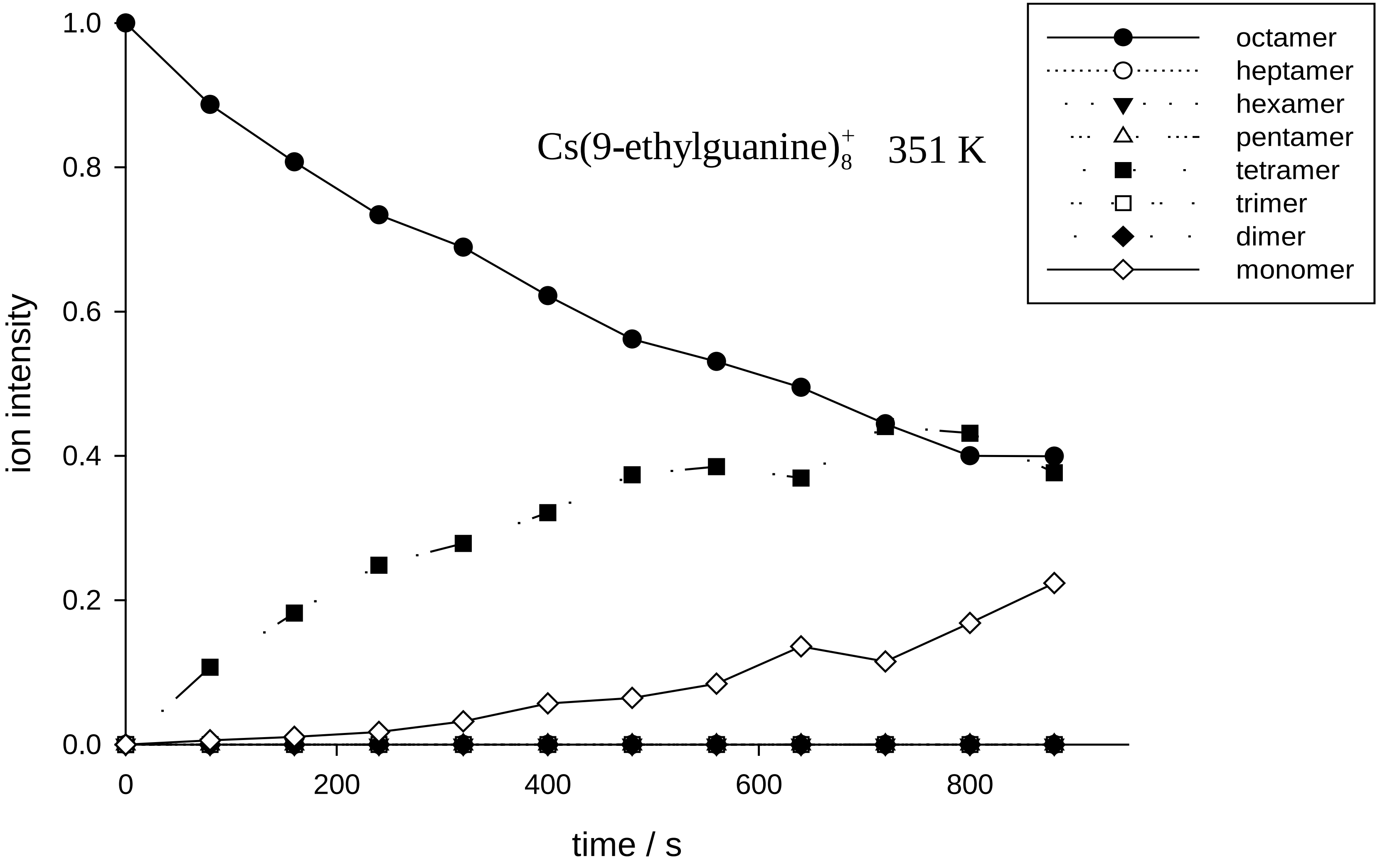
Rb(9-ethylguanine)$_8^+$
397 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
10
20
30
40
50
time / s



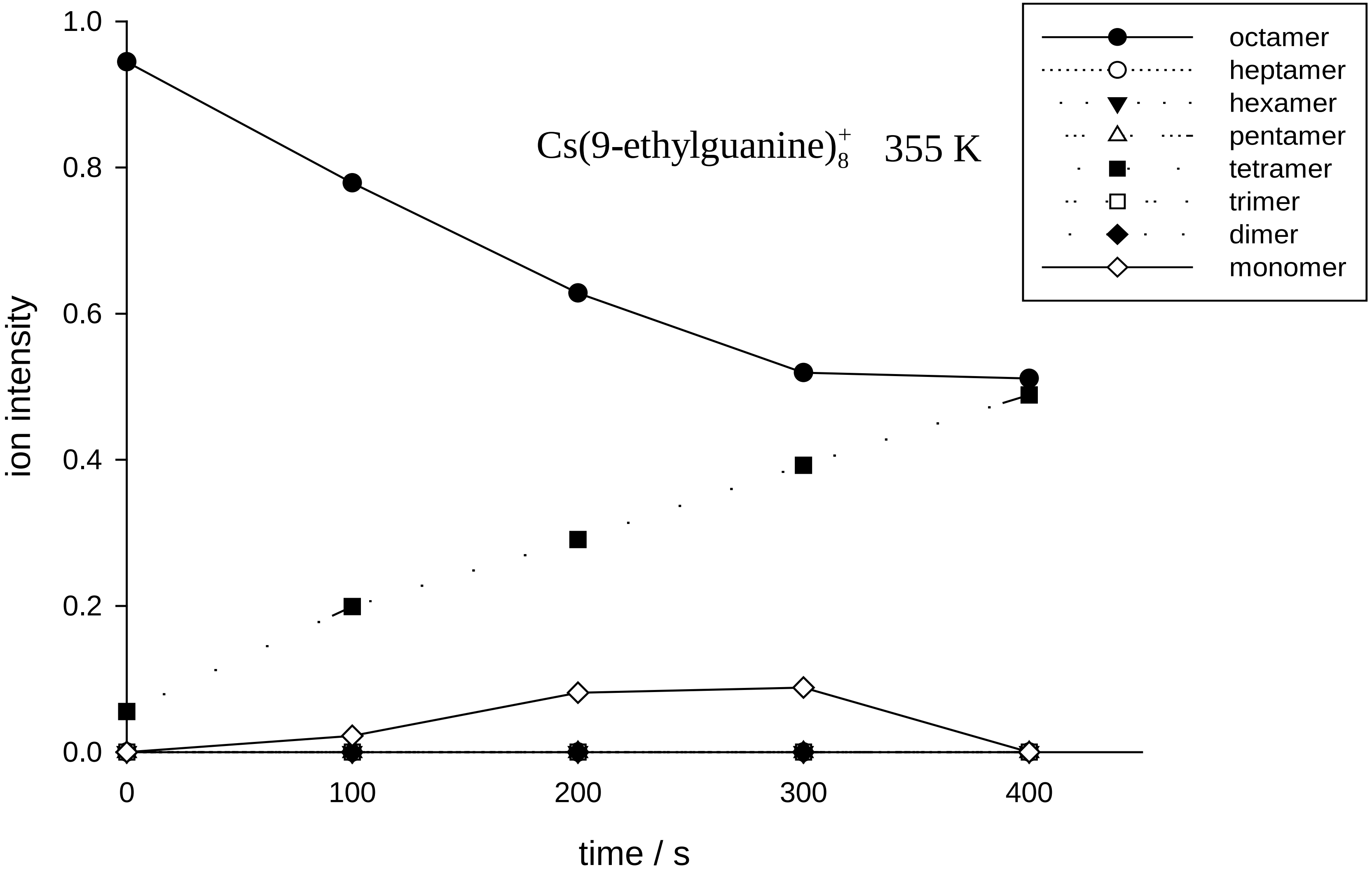
Rb(9-ethylguanine)$_8^+$
403 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
5
10
15
20
25
time / s



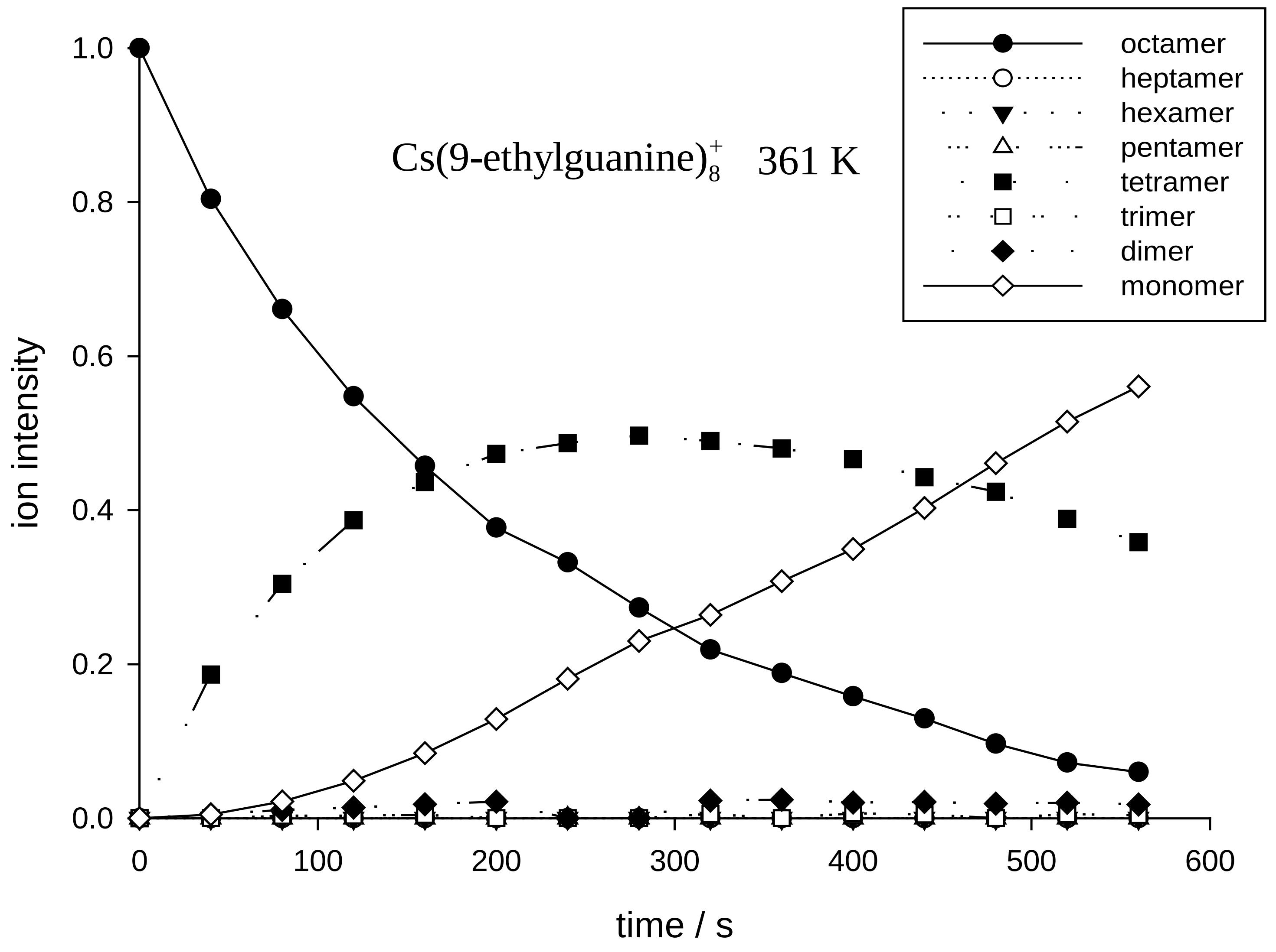
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
200
400
600
800
1000
1200
time / s
Cs(9-ethylguanine)$_8^+$ 342 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer



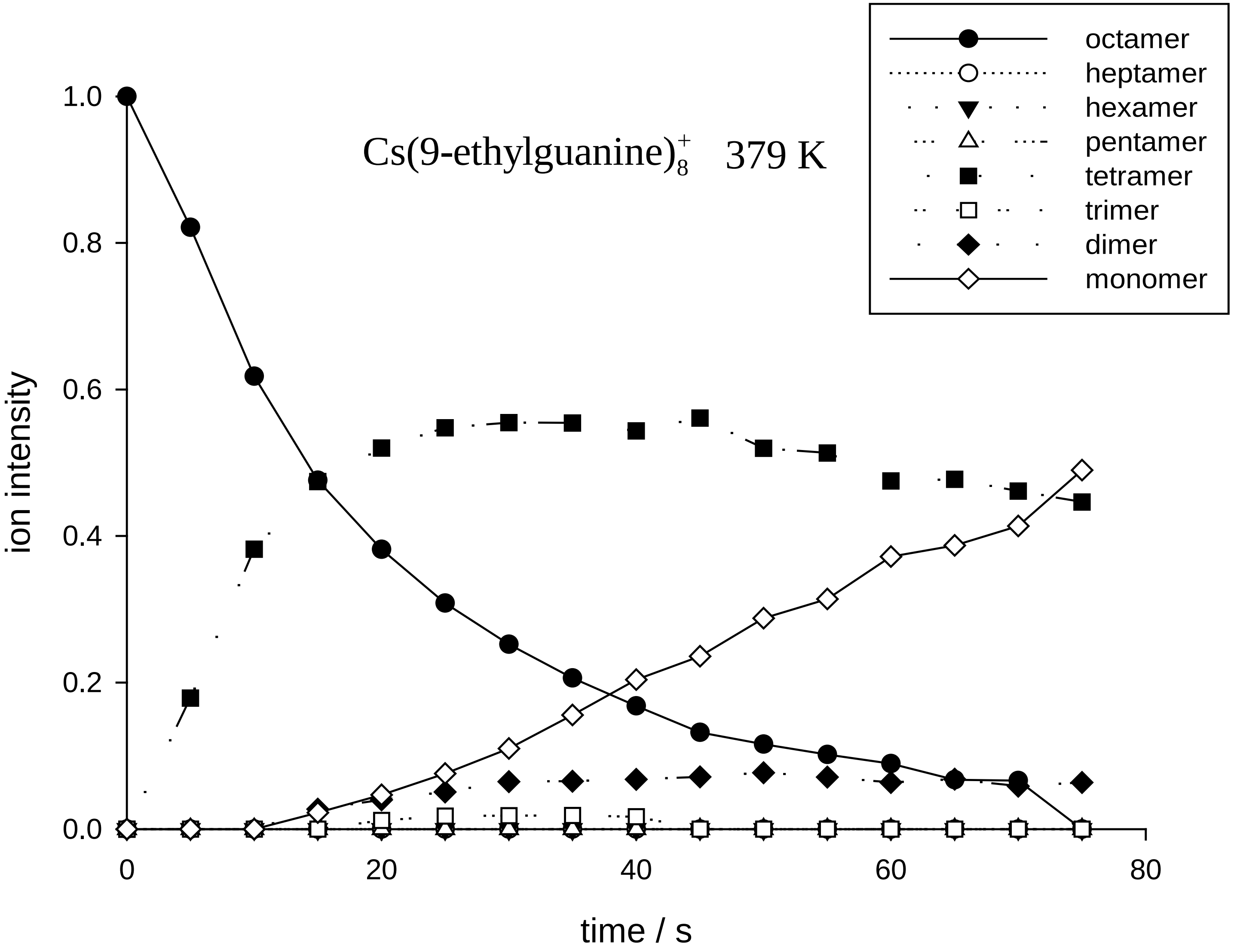
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
Cs(9-ethylguanine)$_8^+$ 351 K
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
200
400
600
800
time / s



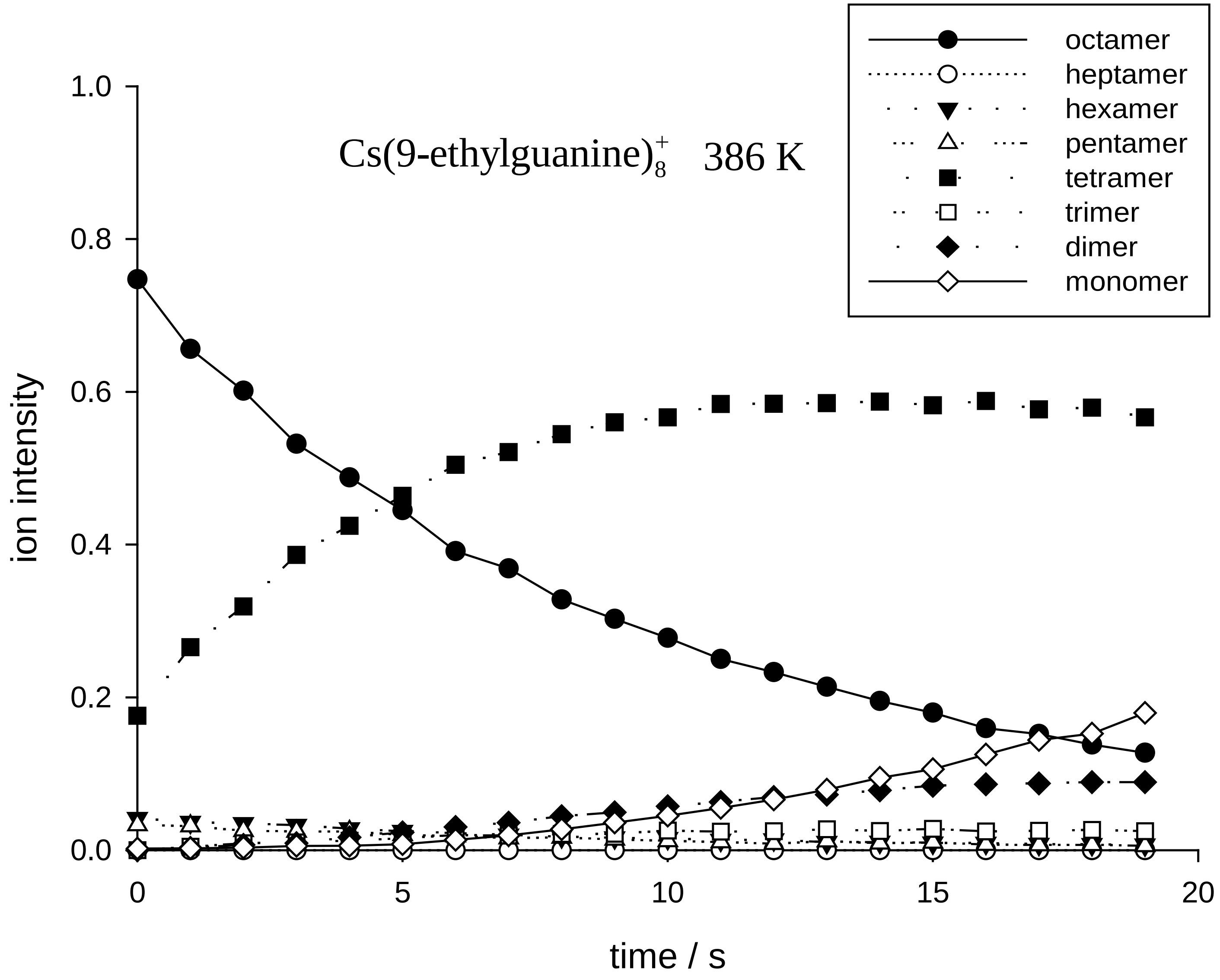
Cs(9-ethylguanine)$_8^+$ 355 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
time / s
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400



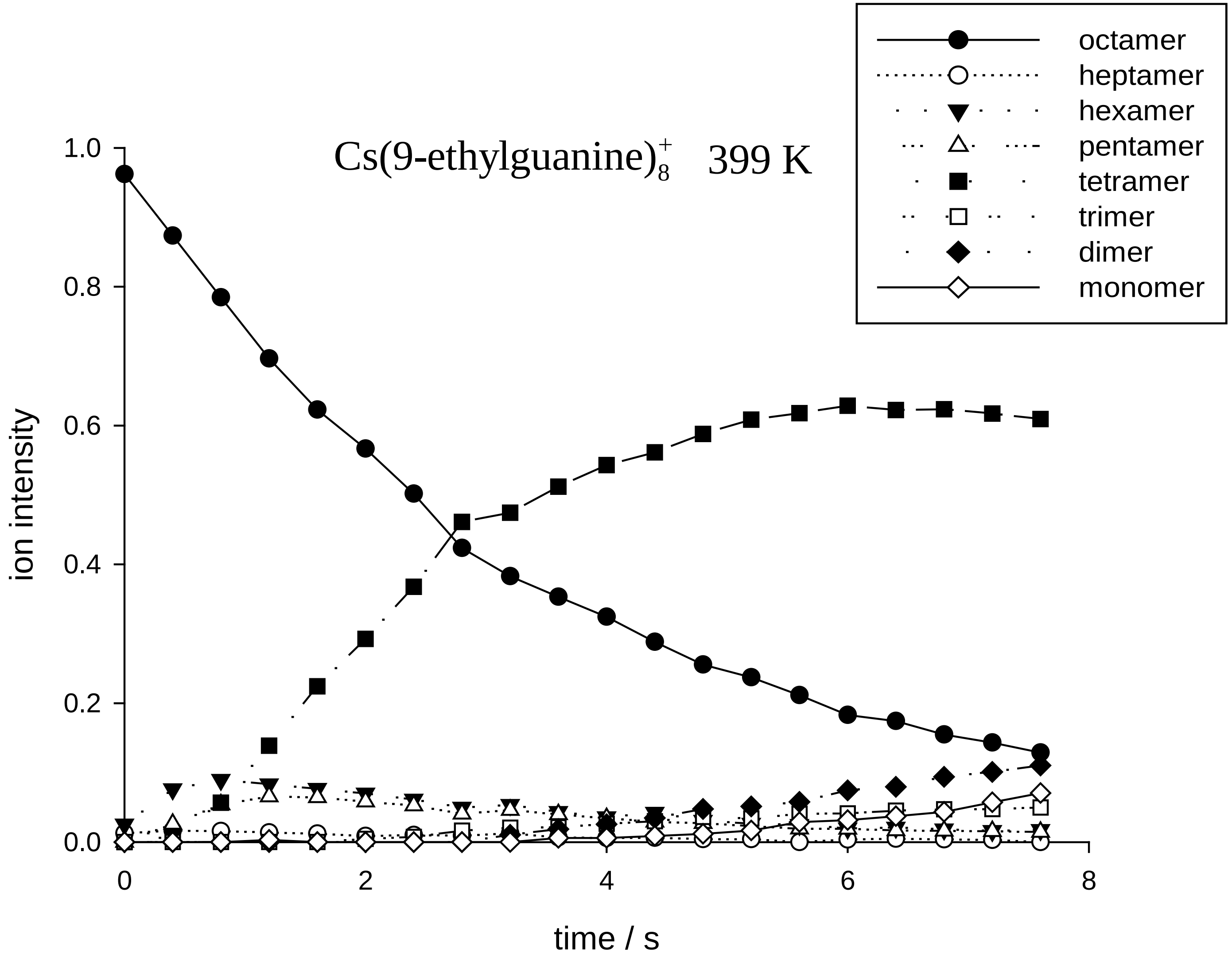
Cs(9-ethylguanine)$_8^+$ 361 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
0.0
0.2
0.4
0.6
0.8
1.0
0
100
200
300
400
500
600
time / s



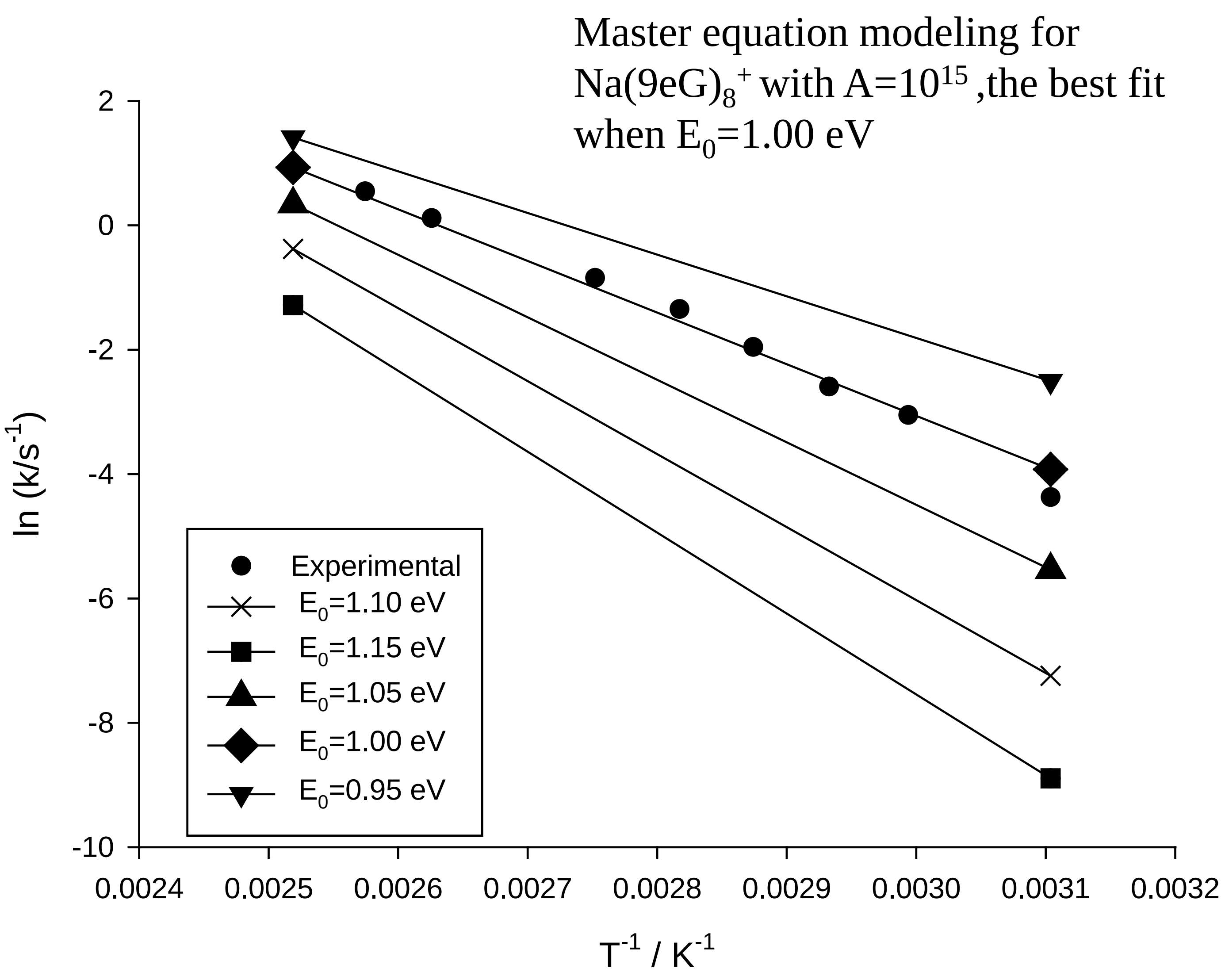
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
Cs(9-ethylguanine)$_8^+$ 379 K
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
time / s



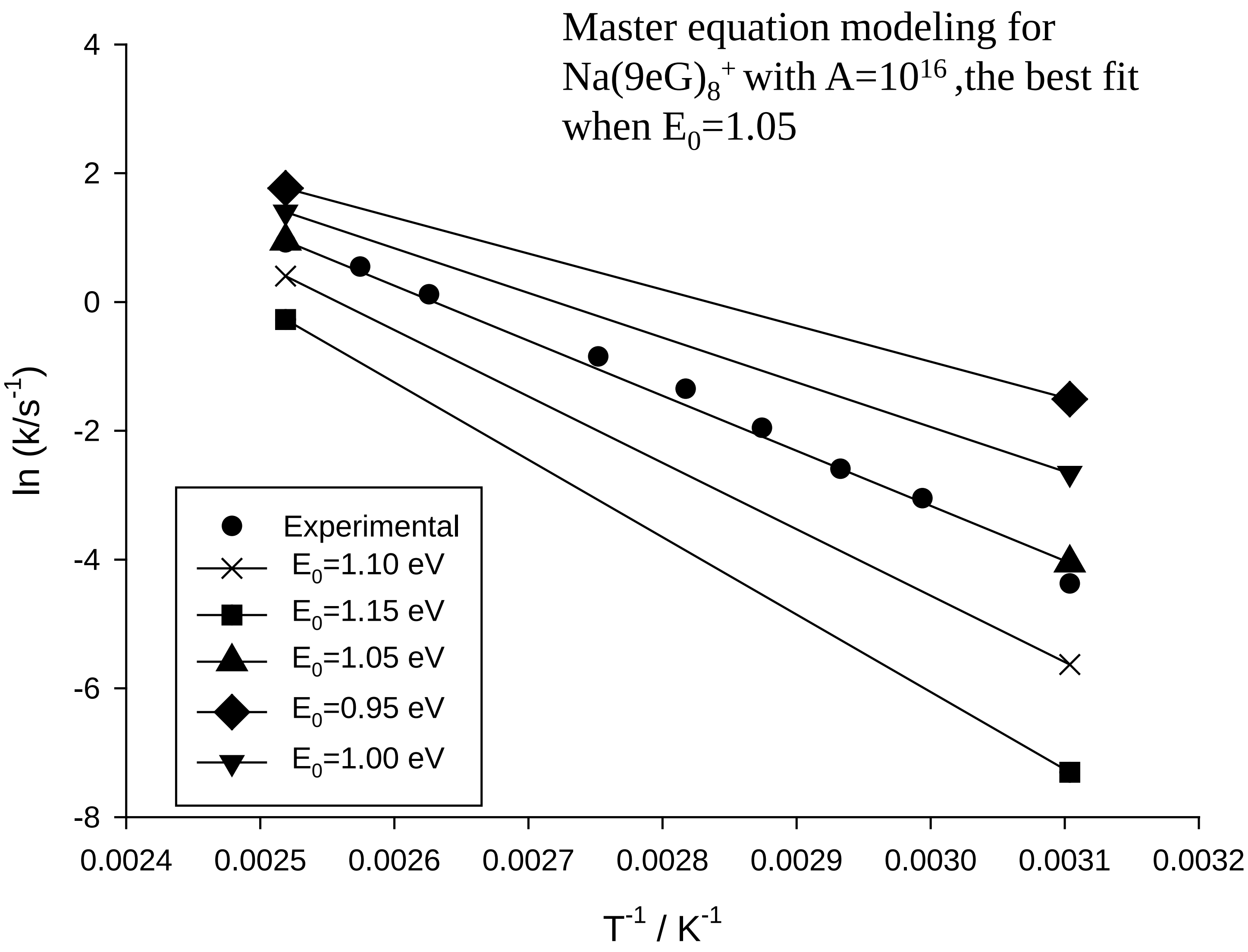
Cs(9-ethylguanine)$_8^+$ 386 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
5
10
15
20
time / s



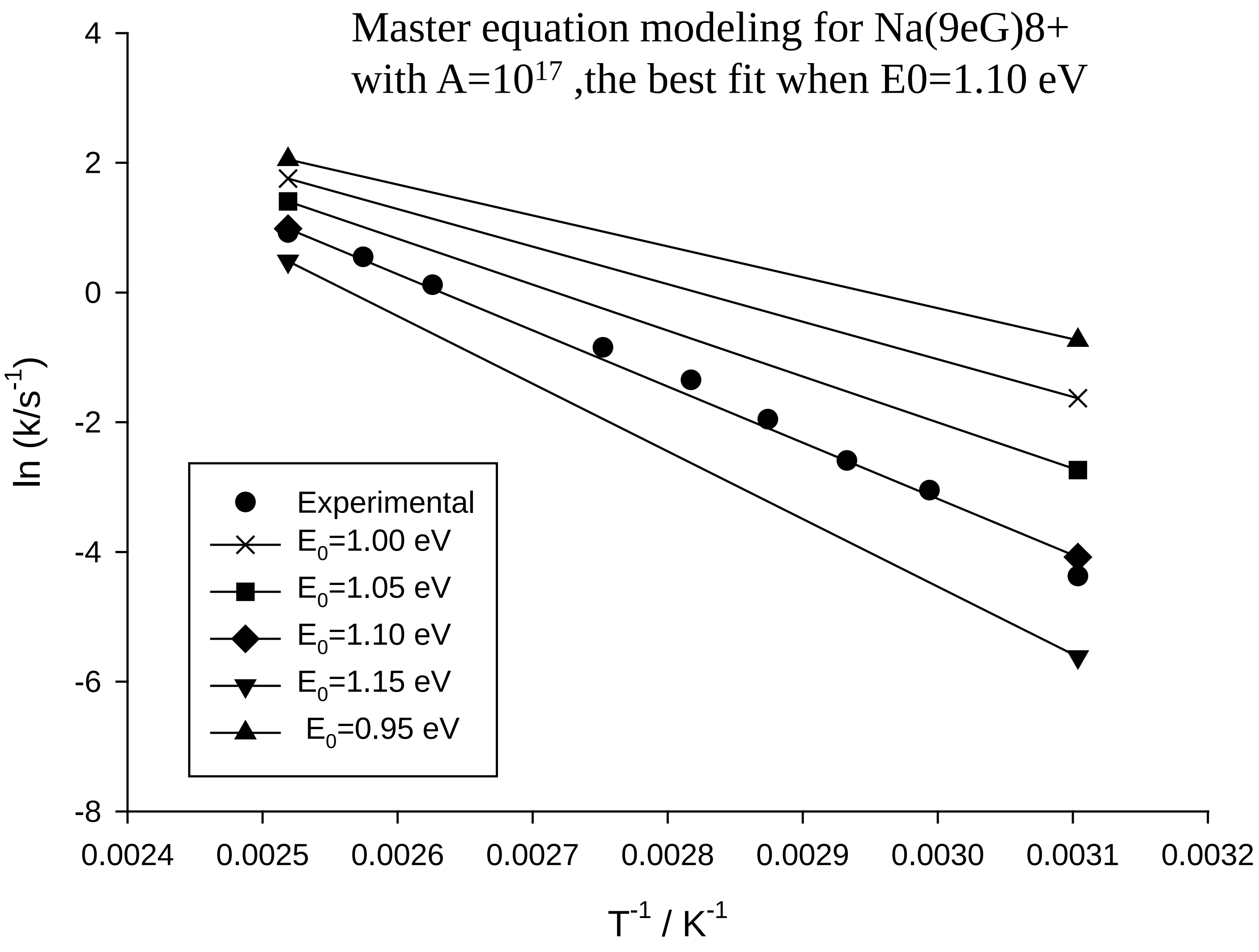
Cs(9-ethylguanine)$_8^+$ 399 K
octamer
heptamer
hexamer
pentamer
tetramer
trimer
dimer
monomer
ion intensity
time / s
0.0
0.2
0.4
0.6
0.8
1.0
0
2
4
6
8



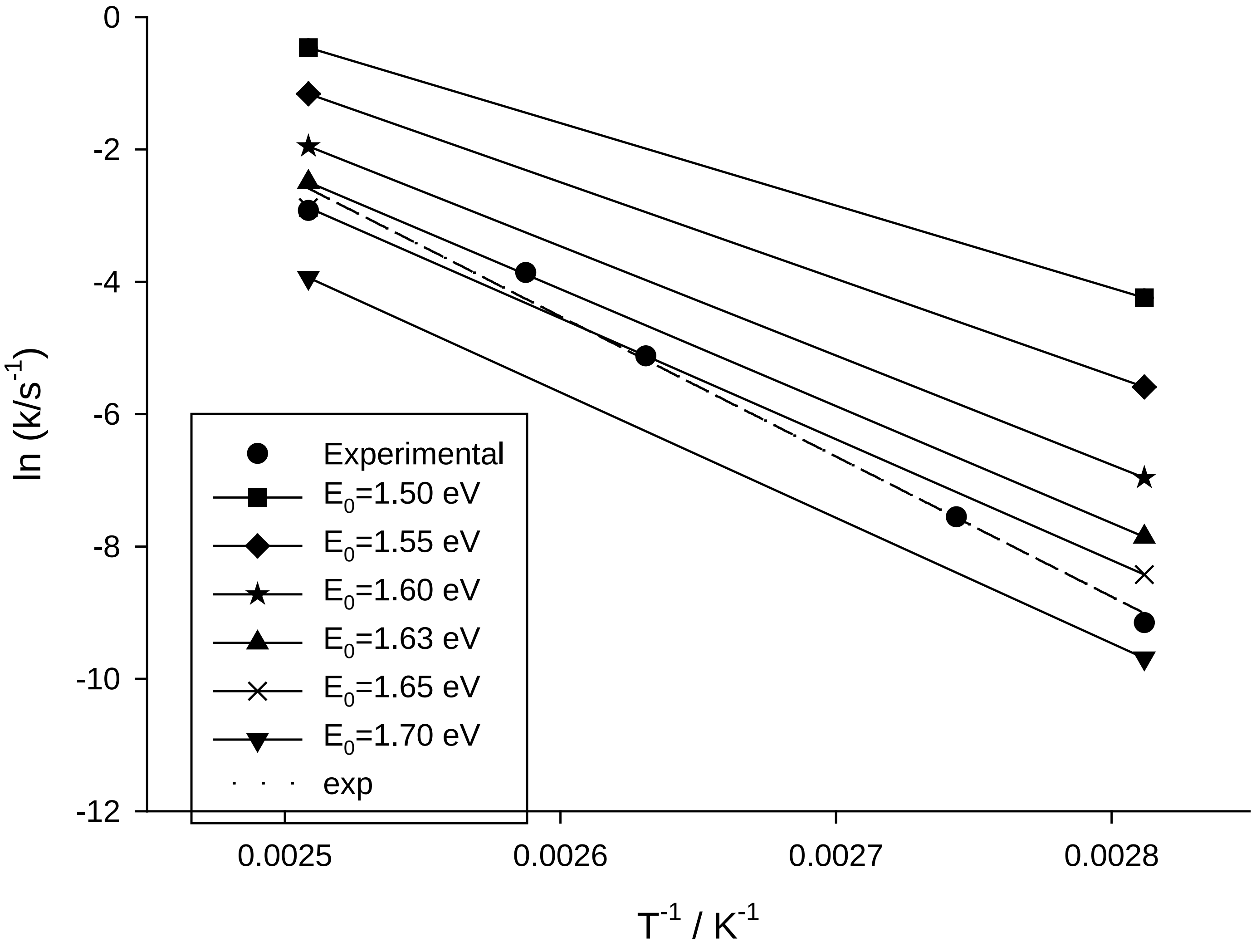
Master equation modeling for $Na(9eG)_8^+$ with $A=10^{15}$ ,the best fit when $E_0$=1.00 eV
ln (k/s$^{-1}$)
$T^{-1}$ / $K^{-1}$
2
0
-2
-4
-6
-8
-10
0.0024
0.0025
0.0026
0.0027
0.0028
0.0029
0.0030
0.0031
0.0032
Experimental
$E_0$=1.10 eV
$E_0$=1.15 eV
$E_0$=1.05 eV
$E_0$=1.00 eV
$E_0$=0.95 eV

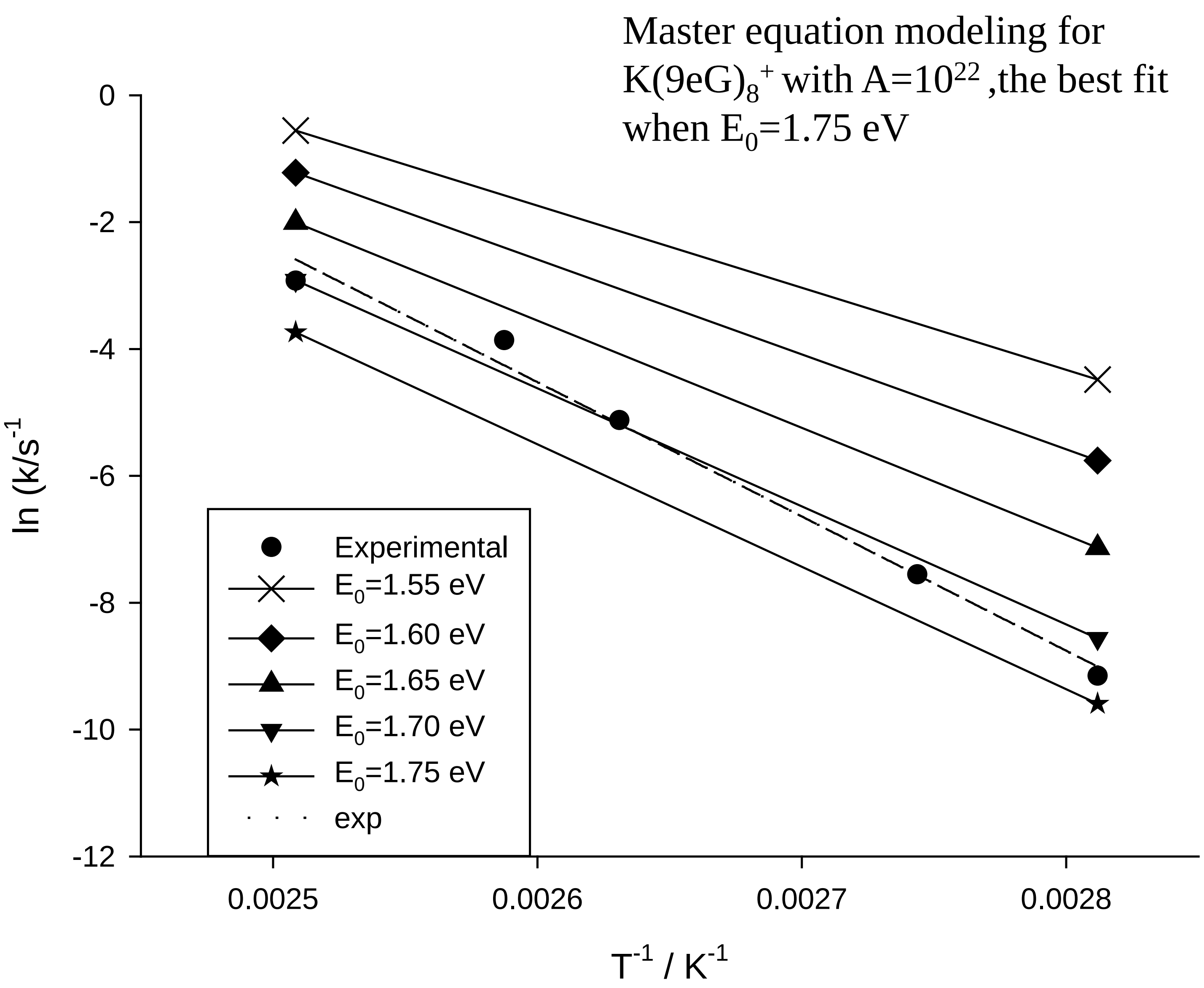


Master equation modeling for
$Na(9eG)_8^+$ with $A=10^{16}$ ,the best fit
when $E_0$=1.05
ln $(k/s^{-1})$
$T^{-1}$ / $K^{-1}$
4
2
0
-2
-4
-6
-8
0.0024
0.0025
0.0026
0.0027
0.0028
0.0029
0.0030
0.0031
0.0032
Experimental
$E_0$=1.10 eV
$E_0$=1.15 eV
$E_0$=1.05 eV
$E_0$=0.95 eV
$E_0$=1.00 eV

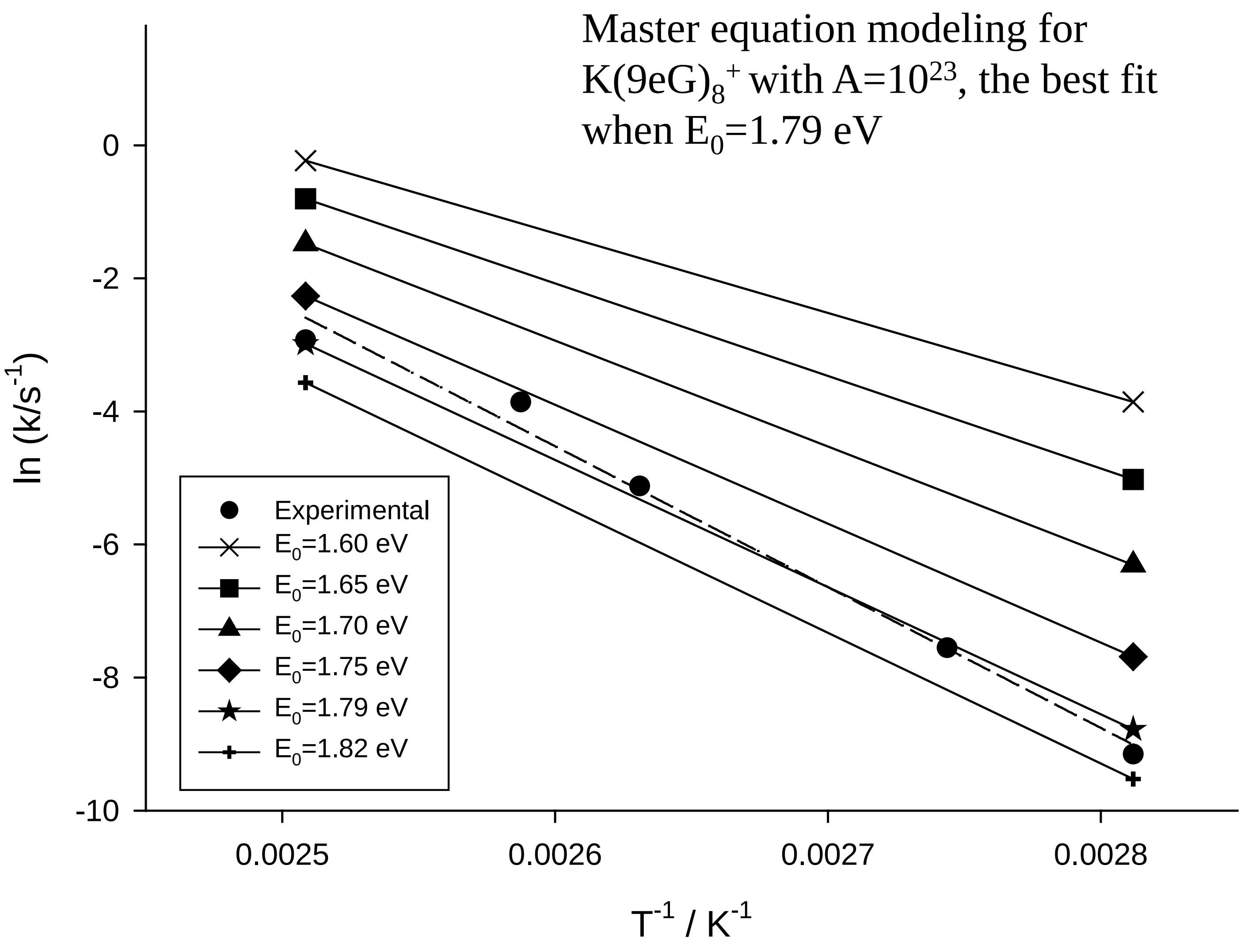

Master equation modeling for Na(9eG)8+
with A=10^17 ,the best fit when E0=1.10 eV
ln (k/s^-1)
T^-1 / K^-1
4
2
0
-2
-4
-6
-8
0.0024
0.0025
0.0026
0.0027
0.0028
0.0029
0.0030
0.0031
0.0032
Experimental
E0=1.00 eV
E0=1.05 eV
E0=1.10 eV
E0=1.15 eV
E0=0.95 eV

Master equation modeling for $K(9eG)_8^+$ with $A=10^{21}$, the best fit when $E_0$=1.70 eV





Master equation modeling for
K(9eG)8+ with A=10^22 ,the best fit
when E0=1.75 eV
ln (k/s-1)
T-1 / K-1
0
-2
-4
-6
-8
-10
-12
0.0025
0.0026
0.0027
0.0028
Experimental
E0=1.55 eV
E0=1.60 eV
E0=1.65 eV
E0=1.70 eV
E0=1.75 eV
exp



Master equation modeling for
K(9eG)8+ with A=10^23, the best fit
when E0=1.79 eV
ln (k/s-1)
0
-2
-4
-6
-8
-10
0.0025
0.0026
0.0027
0.0028
T-1 / K-1
Experimental
E0=1.60 eV
E0=1.65 eV
E0=1.70 eV
E0=1.75 eV
E0=1.79 eV
E0=1.82 eV