Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Collision Induced Dissociation of Doubly-charged Ions: Coulomb Explosion vs Neutral Loss in $[Ca(urea)]^{2+}$ Gas Phase Reactivity via Chemical Dynamics Simulations

Riccardo Spezia, Alvaro Cimas, Marie-Pierre Gaigeot, Jean-Yves Salpin, Kihyung Song and William H. Hase

Supporting Information

Canonical kinetics

On the basis of Figure 4, the steady-state solution of the master equation leads to the microcanonical expression of the overall rate coefficient:

$$k_{overall} = k_a + k_b + k_c + k_d + k_e + k_f + k_g + k_h \tag{S1}$$

where the individual coefficients for the different channels (*a*: Ca^{2+} + H_2NCONH_2, *b*: $CaNH_2^+$ + H_2NCO^+, *c*: NH_4^+ + $CaNCO^+$, *d*: NH_4^+ + $CaOCN^+$, *e*: NH_3 + $CaNHCO^{2+}$, *f*: $CaNH_3^{2+}$ + HNCO, *g*: NH_3 + $CaOCNH^{2+}$, *h*: CaO^+ + $H_2NCNH_2^+$) are given by the following formulas:

$$k_a = k_1$$

$$k_b = k_3 \frac{H}{G}$$

$$k_c = \frac{k_6}{C}\left[\frac{k_4 H}{G} + k_{12}\left(\frac{k_{11}}{E} + \frac{k_{-12}k_4 H}{CEG}\right)\right]$$

$$k_d = \frac{k_5}{C}\left[\frac{k_4 H}{G} + k_{12}\left(\frac{k_{11}}{E} + \frac{k_{-12}k_4 H}{CEG}\right)\right]$$

$$k_e = \frac{k_{17}}{C}\left[\frac{k_4 H}{G} + k_{12}\left(\frac{k_{11}}{E} + \frac{k_{-12}k_4 H}{CEG}\right)\right] + k_9\frac{k_8 k_7}{ABC}\left[\frac{k_4 H}{G} + k_{12}\left(\frac{k_{11}}{E} + \frac{k_{-12}k_4 H}{CEG}\right)\right]$$

$$k_f = k_{10}\frac{k_8 k_7}{ABC}\left[\frac{k_4 H}{G} + k_{12}\left(\frac{k_{11}}{E} + \frac{k_{-12}k_4 H}{CEG}\right)\right] + k_{15}\frac{k_{13}}{D}\left(\frac{k_{11}}{E} + \frac{k_{-12}k_4 H}{CEG}\right)$$

$$k_g = k_{14}\frac{k_{13}}{D}\left(\frac{k_{11}}{E} + \frac{k_{-12}k_4H}{CEG}\right)$$

$$k_h = k_{16}$$

where

$$A = k_{-8} + k_9 + k_{10}$$

$$B = k_{-7} + k_8 - \frac{k_{-8}k_8}{A}$$

$$C = k_{-4} + k_5 + k_6 + k_7 + k_{-12} + k_{17} - \frac{k_{-7}k_7}{B}$$

$$D = k_{-13} + k_{14} + k_{15}$$

$$E = k_{-11} + k_{12} + k_{13} - \frac{k_{-13}k_{13}}{D} - \frac{k_{-12}k_{12}}{C}$$

$$F = \frac{k_{-4}k_{12}k_{-12}k_4}{C^2E}$$

$$G = k_{-2} + k_3 + k_4 - \frac{k_{-4}k_4}{C} - F$$

$$H = k_2 - \frac{k_{-4}k_{12}k_{11}}{CE}$$

Moments of inertia

We list in the following table the moments of inertia of the different species (nomenclature is the same as figures 4 and 5)

	I_x	I_y	I_z
I1	1193.24482	1366.24066	172.99583
TS12	995.49589	1147.17729	193.75419
I2	886.67005	1053.57113	176.47050
TS-Caurea	4789.74996	4940.40803	195.32315
I4	1228.93498	1395.03437	176.05148
I5	2027.05738	2027.05819	9.37091
I6	901.17519	1054.80669	163.64409
I7	1314.71574	1496.33263	191.71093
I8	1899.14769	1980.68061	90.90100
TS14	1292.75424	1435.25169	152.63944
TS26	882.97310	1032.88317	178.62098
TS46	1180.37308	1362.98012	192.49185
TS67	1242.61093	1371.52970	208.55866
TS78	1216.51335	1460.62832	253.65370
TS45	1324.80884	1580.84352	265.58398
TS1a	2036.71553	2180.37138	149.52077
TS2a	1567.46849	1814.33958	256.22200
TS6a	1677.04393	1966.80662	299.16193
TS6b	1485.56321	1718.12189	241.99901
k17-TS	1448.93537	1616.89627	177.95623
k14-TS	3091.47747	3091.47747	9.44571
k15-TS	6744.19776	6779.27460	44.44682

Table S1. Inertia moments in amu*bohr^2 .