

Table 1. List of ion parameters of ions that were used to validate the SIMION-SDS-FDMC.

Chemical	Ion	Mass (amu)	K_0 ($10^{-4} \text{ m}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$)	α_2 (Td^{-2})	α_4 (Td^{-4})
1. Hydrated Proton	$\text{H}^+(\text{H}_2\text{O})_3$	55.00	2.34	1.78×10^{-5}	-4.91×10^{-10}
2. Hydroxyproline	$(\text{C}_5\text{H}_9\text{NO}_3)\text{H}^+$	131.13	2.18	5.82×10^{-6}	-1.09×10^{-10}
3. Leucine	$(\text{C}_6\text{H}_{13}\text{NO}_2)\text{H}^+$	131.17	2.17	4.06×10^{-6}	0.79×10^{-10}
4. Hydrated Oxygen	$\text{O}_2^-(\text{H}_2\text{O})_3$	86.00	2.13	1.93×10^{-5}	-4.30×10^{-10}
5. 2-Propanone (dimer)	$(\text{C}_3\text{H}_6\text{O})_2\text{H}^+$	116.16	1.85	7.44×10^{-6}	-6.94×10^{-10}
6. 2-Dodecanone (dimer)	$\text{C}_{12}\text{H}_{24}\text{O})_2\text{H}^+$	368.62	1.39	-2.16×10^{-6}	-0.84×10^{-10}