

Supporting Information

Quantitative Collision Cross Sections from FTICR Linewidth Measurements: Improvements in
Theory and Experiment

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Table S-1. Cross sections for the biogenic amino acids (in Å²) calculated at 300 K in He using the projection approximation [1] (PA) and exact hard sphere scattering [1] (EHSS) methods and measured using the corrected CRAFTI technique (1.9 keV in lab frame) and static drift IMS [2].

Amino Acid	PA (He)	EHSS (He)	IMS (Ar)	IMS (He)	CRAFTI (Ar)
Glycine	47.5	48.8	107.1	43.4	35.6 ± 0.6
Alanine	52.6	54.5	109.1	48.3	44.6 ± 0.6
Serine	55.8	57.7	109.9	50.9	47.2 ± 0.5
Proline	59.9	62.7	113.7	55.6	52.9 ± 0.5
Valine	62.4	65.1	116.1	57.5	57.2 ± 0.7
Threonine	60.7	63.1	113.6	55.5	51.8 ± 0.4
Cysteine	58.3	60.7	114.3	55.0	50.1 ± 0.7
Isoleucine	67.5	70.7	120.5	62.5	61.3 ± 0.6
Leucine	69.0	72.3	122.1	63.8	63.8 ± 0.6
Asparagine	62.7	65.6	115.1	58.1	58.1 ± 0.6
Aspartic acid	61.9	64.5	115.7	57.2	57.4 ± 0.5
Glutamine	67.9	71.0	118.6	62.7	61.8 ± 0.6
Lysine	70.5	74.3	121.0	64.2	65.6 ± 0.7
Glutamic acid	67.3	70.2	118.9	61.7	64.9 ± 0.5
Methionine	69.1	72.7	121.5	64.5	61.7 ± 0.6
Histidine	70.0	73.5	120.0	64.6	62.8 ± 0.7
Phenylalanine	75.9	79.8	127.8	70.4	71.5 ± 0.8
Arginine	75.3	79.1	125.6	70.3	71.1 ± 0.6
Tyrosine	79.5	83.6	132.5	73.0	76.3 ± 0.6
Tryptophan	85.0	89.7	138.0	79.0	83.8 ± 0.9

Table S-2. Collision cross sections (in Å²) for 12-crown-4 complexes with various amines, calculated at 300 K in He using the projection approximation (PA) and exact hard sphere scattering (EHSS) methods and measured using CRAFTI (130 eV in center-of-mass frame) and static drift IMS [3].

Guest	PA (He)	EHSS (He)	CRAFTI (Ar)	IMS (N₂)
NH ₄	78.3	82.2	97.1 ± 0.7	109.5
Methyl	84.2	89.7	100.3 ± 1.0	-
Ethyl	88.0	94.0	104.3 ± 1.3	-
n-Propyl	92.5	99.2	111.6 ± 1.1	121.7
n-Butyl	98.0	105.5	118.8 ± 1.3	126.1
t-Butyl	95.1	101.9	123.2 ± 1.3	-
n-Pentyl	103.2	111.5	132.3 ± 1.8	-
n-Hexyl	109.3	118.7	139.5 ± 1.5	-
n-Heptyl	115.5	125.4	145.7 ± 1.4	-
n-Octyl	119.2	129.1	151.5 ± 1.7	-
n-Nonyl	125.0	136.0	115.4 ± 2.4	-

Table S-3. Collision cross sections (in Å²) for 15-crown-5 complexes with various amines, calculated at 300 K in He using the projection approximation (PA) and exact hard sphere scattering (EHSS) methods and measured using CRAFTI (130 eV in center-of-mass frame) and static drift IMS [3].

Guest Amine	PA (He)	EHSS (He)	CRAFTI (Ar)	IMS (N₂)
NH ₄	90.5	96.4	109.2 ± 0.9	118.9
Methyl	94.3	101.2	112.3 ± 0.6	-
Ethyl	98.0	105.2	114.9 ± 0.9	-
n-Propyl	101.8	109.5	119.8 ± 0.9	128.9
n-Butyl	106.8	115.2	133.3 ± 0.7	135.5
t-Butyl	103.1	110.4	129.9 ± 0.9	-
n-Pentyl	111.2	120.4	134.5 ± 1.1	-
n-Hexyl	117.9	128.0	142.9 ± 1.5	-
n-Heptyl	123.4	134.4	148.4 ± 1.2	-
n-Octyl	120.7	130.7	156.3 ± 1.9	-
n-Nonyl	129.7	141.2	160.1 ± 1.7	-

Table S-4. Collision cross sections (in Å²) for 18-crown-6 complexes with various amines, calculated at 300 K in He using the projection approximation (PA) and exact hard sphere scattering (EHSS) methods and measured using CRAFTI (130 eV in center-of-mass frame) and static drift IMS [3].

Guest Amine	PA (He)	EHSS (He)	CRAFTI (Ar)	IMS (N₂)
NH ₄	105.4	113.8	125.5 ± 0.7	132.3
Methyl	106.5	114.7	127.1 ± 0.7	-
Ethyl	109.0	117.6	131.4 ± 0.7	-
n-Propyl	113.7	123.8	134.9 ± 0.5	142.2
n-Butyl	118.8	130.0	144.0 ± 1.2	146.1
t-Butyl	113.1	121.9	140.0 ± 1.1	-
n-Pentyl	123.4	135.5	144.2 ± 1.0	-
n-Hexyl	128.3	140.8	152.6 ± 0.6	-
n-Heptyl	131.4	144.3	159.9 ± 0.7	-
n-Octyl	135.3	148.9	161.7 ± 1.3	-
n-Nonyl	138.6	152.6	168.6 ± 1.4	-

References

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