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

Magic Cluster Sizes of Cationic and Anionic Sodium Chloride Clusters Explained by Statistical Modeling of the Complete Phase Space

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Supplementary Material

1. Optimized Structures

1.1 Cationic Clusters

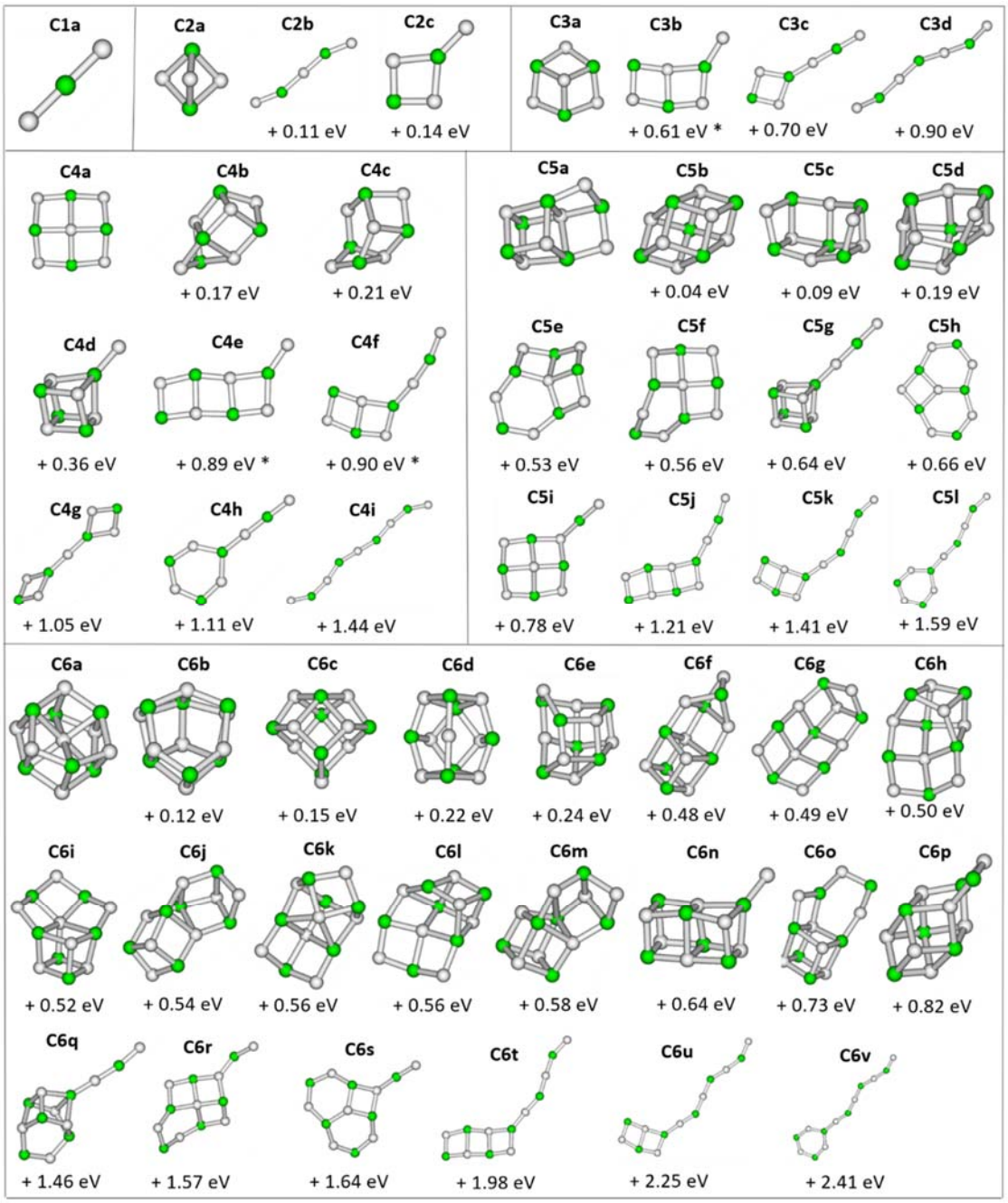

Figure S1: Overview of the lowest-energy isomers with relative energies calculated at the CCSD/DZ//B3LYP-D3 level of theory for the cationic clusters $(NaCl)_xNa^+$, x = 1–6. Energies marked with * are obtained by using the ωB97XD functional for the geometrical optimization due to the presence of an imaginary frequency using the B3LYP-D3 functional.

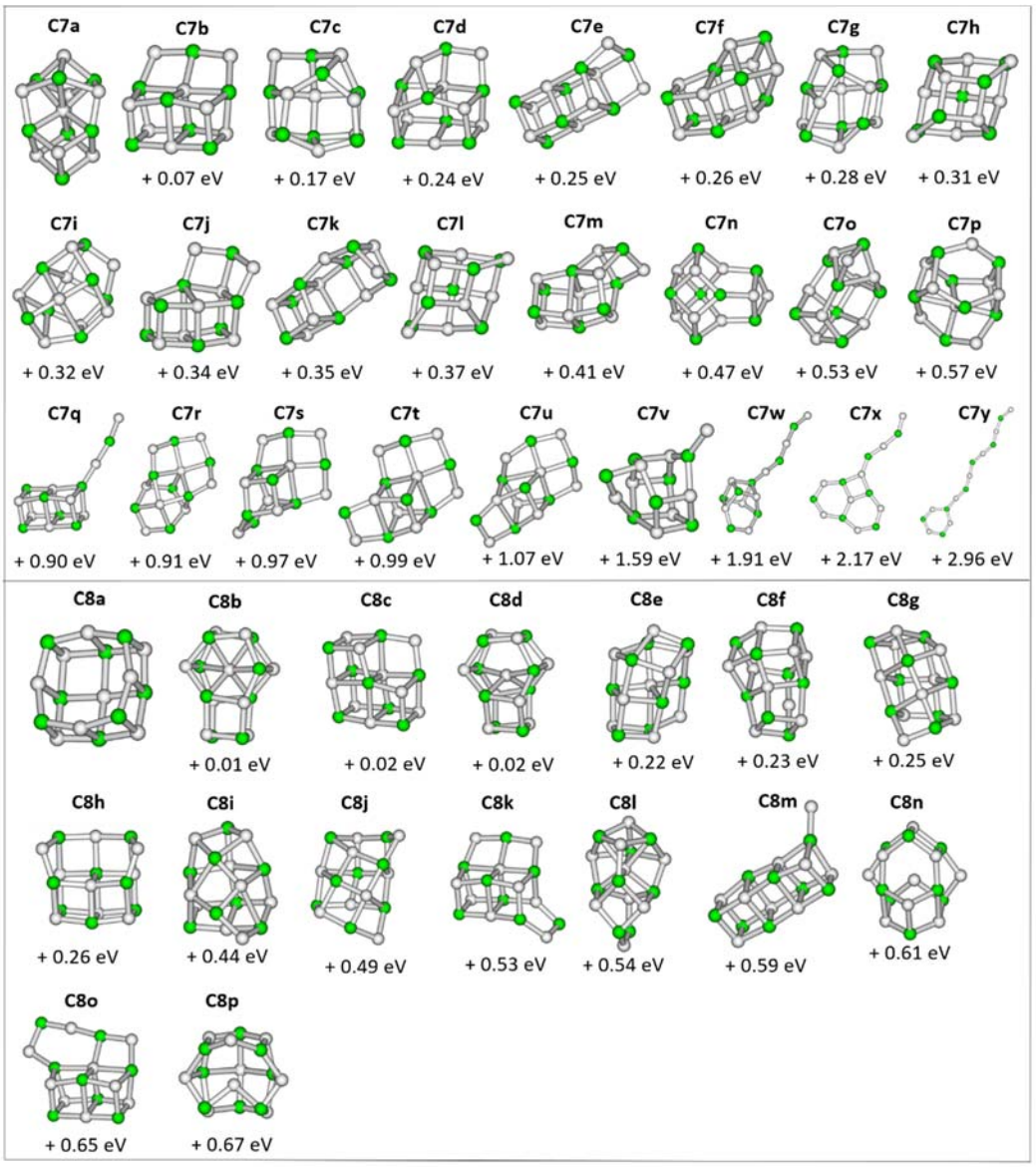

Figure S2: Overview of the lowest-energy isomers with relative energies calculated at the CCSD/DZ//B3LYP-D3 level of theory for the cationic clusters $(NaCl)_xNa^+$ with x = 7,8.

Table S1: Overview of the lowest-energy isomers including symmetry groups and relative energies of $(NaCl)_xNa^+$. Isomers whose energy is marked with * have one imaginary frequency within the listed symmetry group and thus, the listed energy corresponds to a structure with lower symmetry. Imaginary frequency for given functional: i. f.

Isomer	Symmetry Group	B3LYP-D3/ aug-cc-pVDZ	CCSD/DZ// B3LYP-D3	CCSD/TZ// B3LYP-D3	CCSD(T)/TZ/ /B3LYP-D3	ωB97XD/ aug-cc-pVDZ	CCSD/DZ// ωB97XD	CCSD/TZ// ωB97XD	CCSD(T)/TZ/ /ωB97XD
C1a	$D_{\infty h}$	0.00	0.00	0.00	0.00	0.00		0.00	0.00
C2a	D_{3h}	0.00	0.00	0.00	0.00	0.00		0.00	0.00
C2b	C_2 (°$D_{\infty h}$)	0.19	0.11	0.04	0.06	0.20°		0.01°	0.03°
C2c	C_{2v}	0.16	0.14	0.10	0.11	0.19		0.09	0.10
C3a	C_{3v}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C3b	C_1	i. f.				0.65	0.61	0.59	0.60
C3c	C_{2v}	0.84	0.70	0.64	0.66	0.77	0.70	0.66	0.67
C3d	C_2	1.07	0.90	0.83	0.85	0.99	0.87	0.79	0.81
C4a	C_{2v}	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C4b	C_s	0.00	0.17	0.24	0.22	0.06	0.17	0.24	0.23
C4c	C_2	0.02	0.21	0.26	0.25	0.15	0.20	0.25	0.24
C4d	C_{3v}	0.23	0.36	0.44	0.42	0.27	0.37	0.45	0.44
C4e	C_s	i. f.				0.89	0.89	0.90	0.91
C4f	C_s	i. f.				0.93	0.90	0.89	0.91
C4g	D_{2d}	1.11	1.05	1.06	1.07	i. f.			
C4h	C_{2v}	1.11	1.11	1.10	1.12	i. f.			
C4i	C_s	1.58	1.44	1.41	1.44	1.50		1.35	1.38
C5a	C_s	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
C5b	D_{3h}	0.05	0.04	0.04	0.03	0.00	0.09	0.08	0.08
C5c	C_{2v}	0.13	0.09	0.08	0.08	0.15	0.09	0.07	0.08
C5d	C_1	0.14	0.19	0.19	0.19	i. f.			
C5e	C_2	0.68	0.53	0.46	0.49	0.67		0.44	0.46
C5f	C_1	0.72	0.56	0.50	0.52	0.67		0.50	0.52
C5g	C_{3v}	0.83	0.64	0.61	0.62	0.71		0.62	0.64
C5h	C_{2v}	0.80	0.66	0.57	0.61	i. f.			
C5i	C_1	1.05	0.78	0.70	0.72	0.91		0.66	0.68
C5j	C_1	1.54	1.21	1.11	1.15	1.37		1.12	1.15
C5k	C_s	1.77	1.41	1.31	1.35	1.58*		1.29*	1.33*
C5l	C_s	1.87	1.59	1.48	1.54	i. f.			
C6a	D_{3d}	0.00	0.00	0.00	0.00	0.00		0.00	0.00
C6b	C_{3v}	0.10	0.12	0.12	0.15	0.29		0.09	0.12
C6c	C_{2v}	0.13	0.15	0.14	0.17	0.36		0.10	0.13
C6d	C_{2v}	0.14	0.22	0.21	0.23	0.32		0.21	0.23
C6e	C_1	0.17	0.24	0.23	0.25	0.38		0.21	0.23
C6f	C_s	0.48	0.48	0.48	0.50	0.60		0.47	0.49
C6g	C_s	0.69	0.49	0.43	0.47	0.75		0.40	0.44
C6h	C_1	0.59	0.50	0.47	0.50	0.68		0.43	0.46
C6i	C_s	0.58	0.52	0.47	0.50	0.72		0.42	0.45
C6j	C_1	0.56	0.54	0.52	0.55	0.69		0.49	0.52
C6k	C_s	0.59	0.56	0.52	0.54	0.68		0.47	0.49
C6l	C_1	0.65	0.56	0.51	0.54	0.70		0.49	0.51
C6m	C_1	0.53	0.58	0.56	0.59	i. f.			
C6n	C_s	0.67	0.64	0.64	0.66	0.79		0.63	0.65
C6o	C_1	0.77	0.73	0.70	0.73	0.90		0.67	0.71
C6p	C_s	0.84	0.82	0.79	0.82	0.91		0.77	0.79
C6q	C_s	1.60	1.46	1.39	1.44	i. f.			

Isomer	Symmetry Group	B3LYP-D3/ aug-cc-pVDZ	CCSD/DZ// B3LYP-D3	CCSD/TZ// B3LYP-D3	CCSD(T)/TZ/ /B3LYP-D3	ωB97XD/ aug-cc-pVDZ	CCSD/DZ// ωB97XD	CCSD/TZ// ωB97XD	CCSD(T)/TZ/ /ωB97XD
C6r	C_1	1.87	1.57	1.48	1.54	1.87		1.43	1.49
C6s	C_s	1.89	1.64	1.54	1.61	2.00		1.44	1.51
C6t	C_s	2.44	1.98	1.85	1.92	2.32*		1.79*	1.87*
C6u	C_1	2.72	2.25	2.11	2.19	2.60		2.04	2.12
C6v	C_s	2.81	2.41	2.27	2.37	i. f.			
C7a	C_{3v}	0.00	0.00			0.00			
C7b	C_{2v}	0.10	0.07			0.20			
C7c	C_1	0.08	0.17			0.24			
C7d	C_1	0.14	0.24			0.24			
C7e	C_s	0.26	0.25			0.35			
C7f	C_s	0.22	0.26			0.28			
C7g	C_1	0.16	0.28			i. f.			
C7h	C_{2v}	0.26	0.31			i. f.			
C7i	C_1	0.12	0.32			0.25			
C7j	C_1	0.27	0.34			0.42			
C7k	C_s	0.40	0.35			0.47			
C7l	C_s	0.19	0.37			0.42			
C7m	C_1	0.31	0.41			0.28			
C7n	C_s	0.40	0.47			0.53			
C7o	C_s	0.53	0.53			i. f.			
C7p	C_2	0.45	0.57			0.56			
C7q	C_s	1.08	0.90			1.05			
C7r	C_s	0.95	0.91			1.05			
C7s	C_s	1.00	0.97			1.12			
C7t	C_1	1.02	0.99			i. f.			
C7u	C_1	1.14	1.07			1.13			
C7v	C_s	1.54	1.59			i. f.			
C7w	C_s	2.17	1.91			2.17			
C7x	C_s	2.54	2.17			2.54*			
C7y	C_s	3.46	2.96			i. f.			
C8a	C_{4v}	0.10	0.00			0.23	0.00		
C8b	C_2	0.04	0.01			0.00	0.02		
C8c	C_s	0.00	0.02			0.14	0.02		
C8d	C_2	0.02	0.02			i. f.			
C8e	C_1	0.29	0.22			0.31			
C8f	C_s	0.21	0.23			0.33			
C8g	C_1	0.27	0.25			0.38			
C8h	C_s	0.24	0.26			0.38			
C8i	C_1	0.37	0.44			0.42			
C8j	C_2	0.42	0.49			0.48			
C8k	C_1	0.70	0.53			0.75			
C8l	C_s	0.56	0.54			i. f.			
C8m	C_s	0.77	0.59			0.75			
C8n	C_s	0.40	0.61			i. f.			
C8o	C_s	0.79	0.65			0.86			
C8p	C_s	0.49	0.67			i. f.			

1.2 Anionic Clusters

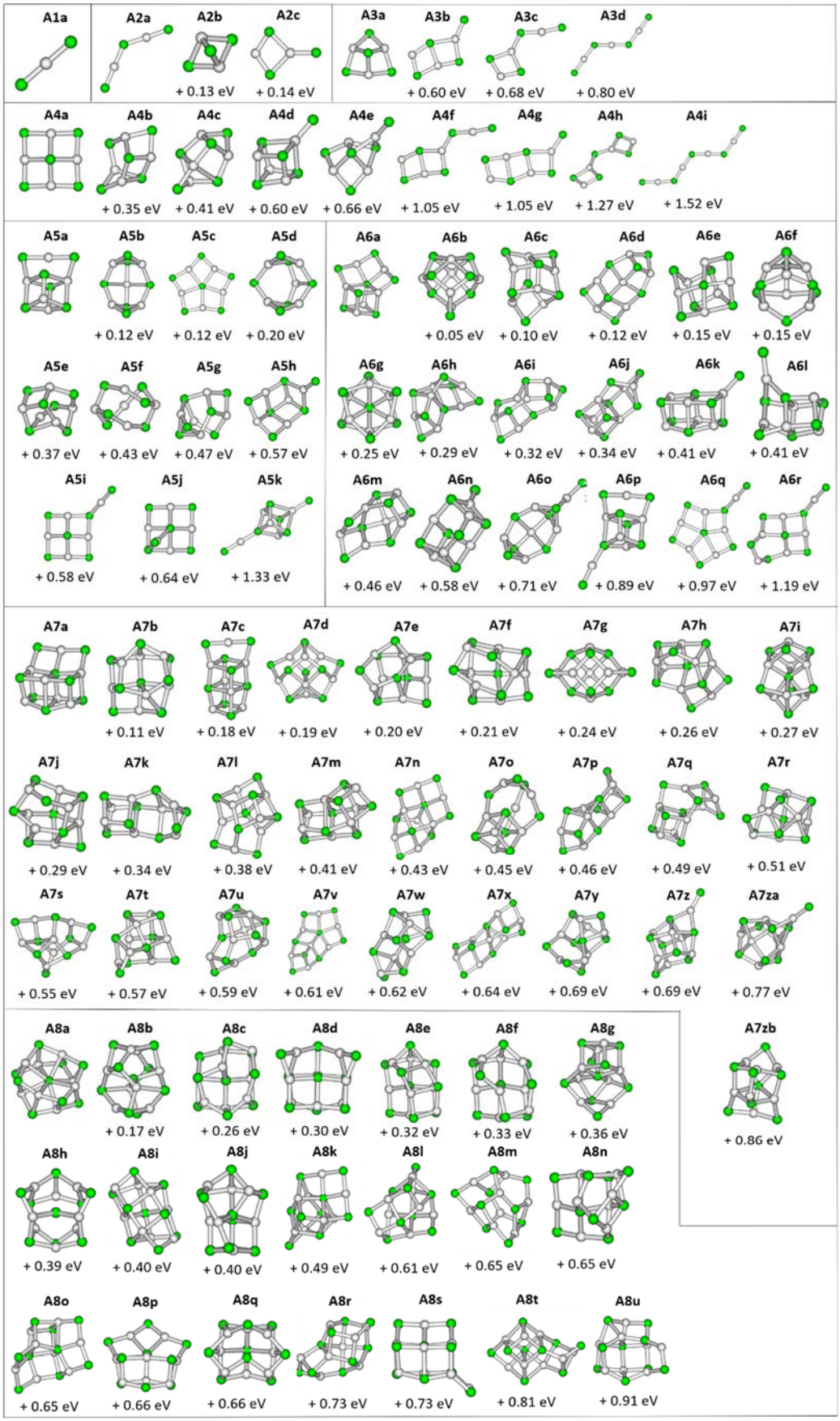

Figure S3: Overview of the lowest-energy isomers with relative energies calculated at the CCSD/DZ//B3LYP-D3 level of theory for the anionic clusters $(NaCl)_xNa^+$ with x = 1–8.

Table S2: Overview of the lowest-energy isomers including symmetry groups and relative energies of $(NaCl)_xCl^-$. Isomers whose energy is marked with * have one imaginary frequency within the listed symmetry group and thus, the listed energy corresponds to a structure with lower symmetry. Imaginary frequency for given functional: i. f.

Isomer	Symmetry Group	B3LYP-D3/ aug-cc-pVDZ	CCSD/DZ// B3LYP-D3	CCSD/TZ// B3LYP-D3	CCSD(T)/TZ/ /B3LYP-D3	ωB97XD/ aug-cc-pVDZ	CCSD/DZ// ωB97XD	CCSD/TZ// ωB97XD	CCSD(T)/TZ/ /ωB97XD
A1a	$D_{\infty h}$	0.00	0.00	0.00	0.00	0.00		0.00	0.00
A2a	C_{2v}	0.00	0.00	0.00	0.00	0.00		0.00	0.00
A2b	D_{3h}	0.15	0.13	0.11	0.09	0.05		0.14	0.12
A2c	C_{2v}	0.13	0.14	0.15	0.14	0.11		0.17	0.16
A3a	C_{3v}	0.00	0.00	0.00	0.00	0.00		0.00	0.00
A3b	C_s	0.58	0.60	0.59	0.60	0.64		0.58	0.59
A3c	C_s	0.68	0.68	0.66	0.68	0.72		0.64	0.65
A3d	C_{2h}	0.80	0.80	0.77	0.80	0.87		0.73	0.75
A4a	C_{4v}	0.00	0.00	0.00	0.00	0.00		0.00	0.00
A4b	C_2	0.27	0.35	0.34	0.33	0.31		0.35	0.34
A4c	C_s	0.28	0.41	0.39	0.38	0.28		0.37	0.35
A4d	C_{3v}	0.47	0.60	0.63	0.62	0.51		0.63	0.62
A4e	C_s	0.62	0.66	0.67	0.66	0.61		0.68	0.68
A4f	C_s	1.09	1.05	1.02	1.03	1.07*		1.01*	1.02*
A4g	C_s	1.05	1.05	1.03	1.04	1.05*		1.02*	1.03*
A4h	C_s	1.31	1.27	1.24	1.25	1.27*		1.23*	1.24*
A4i	C_{2v}	1.58	1.52	1.48	1.51	1.59		1.44	1.47
A5a	C_{2v}	0.00	0.00	0.00	0.00	0.00		0.00	0.00
A5b	C_{2v}	0.21	0.12	0.09	0.11	0.20		0.06	0.08
A5c	D_{5h}	0.21	0.12	0.10	0.14	0.28		0.09	0.13
A5d	C_s	0.25	0.20	0.17	0.19	i. f.			
A5e	C_1	0.28	0.37	0.35	0.35	0.35		0.33	0.32
A5f	D_3	0.29	0.43	0.42	0.41	0.29		0.32	0.30
A5g	C_1	0.40	0.47	0.44	0.43	0.34		0.39	0.38
A5h	C_s	0.63	0.57	0.55	0.58	0.70		0.53	0.56
A5i	C_s	0.73	0.58	0.54	0.58	0.75		0.51	0.54
A5j	C_s	0.71	0.64	0.62	0.65	0.77		0.62	0.65
A5k	C_{3v}	1.32	1.33	1.30	1.33	1.40		1.28	1.30
A6a	C_s	0.07	0.00	0.00	0.00	0.05	0.00	0.00	0.00
A6b	C_{2v}	0.00	0.05	0.04	0.03	0.09	0.06	0.05	0.04
A6c	C_s	0.02	0.10	0.09	0.07	0.00	0.09	0.09	0.08
A6d	C_s	0.30	0.12	0.08	0.09	0.20		0.08	0.08
A6e	C_1	0.05	0.15	0.13	0.11	0.03		0.13	0.10
A6f	C_{3v}	0.03	0.15	0.14	0.12	0.09		0.10	0.08
A6g	D_{3d}	0.22	0.25	0.25	0.19	0.12		0.26	0.21
A6h	C_2	0.28	0.29	0.26	0.24	0.19		0.27	0.25
A6i	C_1	0.32	0.32	0.29	0.29	0.27		0.24	0.24
A6j	C_s	0.33	0.34	0.32	0.30	0.27		0.30	0.28
A6k	C_s	0.36	0.41	0.42	0.41	0.37		0.42	0.40
A6l	C_1	0.40	0.41	0.42	0.41	i. f.			
A6m	C_1	0.41	0.46	0.44	0.42	0.37		0.43	0.41
A6n	C_s	0.50	0.58	0.58	0.58	i. f.			
A6o	C_s	0.83	0.71	0.69	0.69	0.74		0.68	0.68
A6p	C_s	0.88	0.89	0.87	0.87	0.84		0.85	0.84
A6q	C_s	1.10	0.97	0.93	0.96	1.07*		0.89*	0.92*
A6r	C_1	1.31	1.19	1.14	1.16	i. f.			

Isomer	Symmetry Group	B3LYP-D3/ aug-cc-pVDZ	CCSD/DZ// B3LYP-D3	CCSD/TZ// B3LYP-D3	CCSD(T)/TZ/ /B3LYP-D3	ωB97XD/ aug-cc-pVDZ	CCSD/DZ// ωB97XD	CCSD/TZ// ωB97XD	CCSD(T)/TZ/ /ωB97XD
A7a	C_{2v}	0.00	0.00			0.00			
A7b	C_1	0.09	0.11			0.07			
A7c	C_{2v}	0.23	0.18			0.12			
A7d	C_s	0.11	0.19			0.08*			
A7e	C_1	0.11	0.20			i. f.			
A7f	C_1	0.17	0.21			0.08			
A7g	C_{2v}	0.24	0.24			i. f.			
A7h	C_1	0.28	0.26			0.24			
A7i	C_{3v}	0.23	0.27			0.16			
A7j	C_s	0.23	0.29			0.25			
A7k	C_s	0.49	0.34			0.34			
A7l	C_1	0.32	0.38			i. f.			
A7m	C_s	0.40	0.41			i. f.			
A7n	C_s	0.55	0.43			0.48			
A7o	C_s	0.41	0.45			0.30			
A7p	C_1	0.62	0.46			0.45			
A7q	C_1	0.52	0.49			0.48			
A7r	C_1	0.48	0.51			0.41			
A7s	C_1	0.56	0.55			0.52			
A7t	C_1	0.53	0.57			0.44			
A7u	C_1	0.56	0.59			0.54			
A7v	C_1	0.92	0.61			0.75			
A7w	C_s	0.62	0.62			0.58			
A7x	C_1	0.77	0.64			0.60			
A7y	C_1	0.62	0.69			0.67			
A7z	C_{2v}	0.73	0.69			0.78			
A7za	C_s	0.78	0.77			0.78			
A7zb	C_s	0.83	0.86			0.84			
A8a	D_{4d}	0.00	0.00			0.00			
A8b	S_4	0.02	0.17			0.14			
A8c	C_1	0.17	0.26			0.29			
A8d	C_s	0.27	0.30			0.29			
A8e	C_s	0.25	0.32			0.31			
A8f	C_1	0.24	0.33			0.36			
A8g	C_s	0.35	0.36			0.37			
A8h	C_s	0.29	0.39			0.45			
A8i	C_1	0.45	0.40			0.50			
A8j	C_1	0.39	0.40			0.31			
A8k	C_{2v}	0.58	0.49			0.57			
A8l	C_1	0.60	0.61			0.58			
A8m	C_2	0.55	0.65			0.56			
A8n	C_1	0.66	0.65			0.57			
A8o	C_1	0.80	0.65			0.85			
A8p	C_{2v}	0.71	0.66			0.78			
A8q	C_s	0.50	0.66			0.63			
A8r	C_1	0.77	0.73			i. f.			
A8s	C_1	0.82	0.73			0.89			
A8t	C_1	0.85	0.81			0.88			
A8u	C_1	1.00	0.91			1.05			

1.3 Neutral Clusters

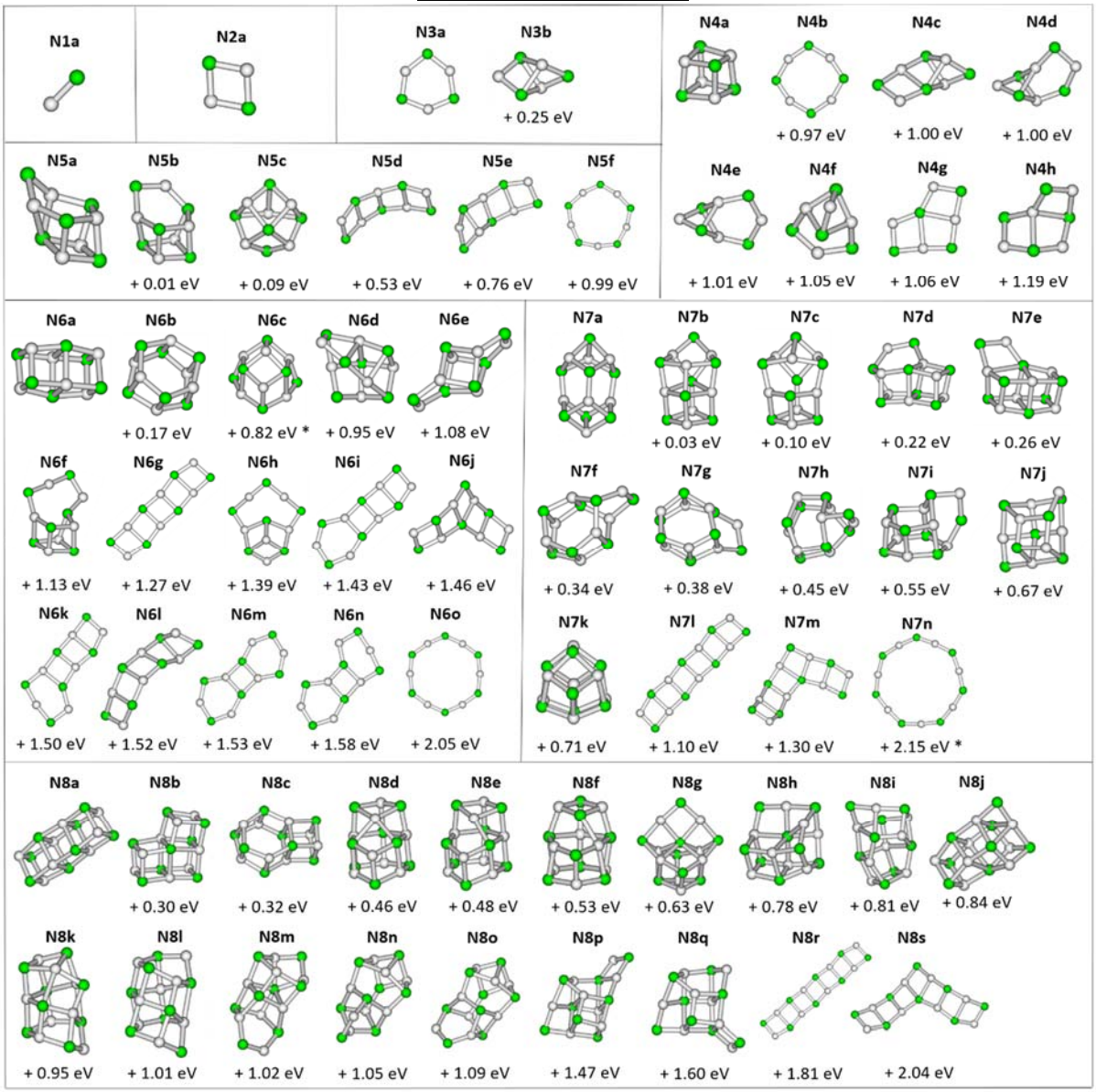

Figure S4: Overview of the lowest energy isomers with relative energies calculated at the CCSD/DZ//B3LYP-D3 level of theory for the neutral clusters $(NaCl)_x$ with x = 1–8. Energies marked with * are obtained by using the ωB97XD functional for the geometrical optimization due to the presence of an imaginary frequency using the B3LYP-D3 functional.

Table S3: Overview of the lowest energy isomers including symmetry groups and relative energies of $(NaCl)_x$. Isomers whose energy is marked with * have one imaginary frequency within the listed symmetry group and thus, the listed energy corresponds to a structure with lower symmetry. Imaginary frequency for given functional: i. f.

Isomer	Symmetry Group	B3LYP-D3/ aug-cc-pVDZ	CCSD/DZ// B3LYP-D3	CCSD/TZ// B3LYP-D3	CCSD(T)/TZ/ /B3LYP-D3	ωB97XD/ aug-cc-pVDZ	CCSD/DZ// ωB97XD	CCSD/TZ// ωB97XD	CCSD(T)/TZ/ /ωB97XD
N1a	$C_{\infty v}$	0.00	0.00	0.00	0.00	0.00		0.00	0.00
N2a	D_{2h}	0.00	0.00	0.00	0.00	0.00		0.00	0.00
N3a	D_{3h}	0.00	0.00	0.00	0.00	0.00		0.00	0.00
N3b	C_{2v}	0.27	0.25	0.26	0.24	0.14		0.28	0.26
N4a	T_d	0.00	0.00	0.00	0.00	0.00		0.00	0.00
N4b	D_{4h}	0.97	0.97	0.90	0.94	1.09		0.82	0.86
N4c	C_s	0.97	1.00	0.95	0.95	0.96		0.89	0.90
N4d	C_s	0.97	1.00	0.96	0.97	0.95		0.89	0.90
N4e	C_{2v}	0.97	1.01	0.98	0.99	1.02		0.93	0.94
N4f	C_s	0.98	1.05	1.02	1.02	i. f.			
N4g	C_{2v}	1.00	1.06	1.00	1.03	1.09		0.94	0.96
N4h	C_2	1.09	1.19	1.13	1.15	i. f.			
N5a	C_s	0.00	0.00	0.00	0.00	0.00		0.01	0.00
N5b	C_s	0.02	0.01	0.00	0.01	0.06*		0.00*	0.00*
N5c	C_{2v}	0.04	0.09	0.10	0.09	0.01		0.10	0.08
N5d	C_s	0.73	0.53	0.48	0.50	0.62		0.44	0.46
N5e	C_1	0.87	0.76	0.72	0.73	0.76		0.68	0.68
N5f	D_{5h}	1.19	0.99	0.91	0.96	1.19		0.86	0.90
N6a	D_{2h}	0.00	0.00			0.00	0.00		
N6b	D_{3d}	0.14	0.17			0.25	0.13		
N6c	C_1	i. f.				0.88	0.82		
N6d	C_1	0.84	0.95			0.81			
N6e	C_s	1.00	1.08			1.16			
N6f	C_s	1.12	1.13			1.18			
N6g	C_2	1.53	1.27			1.40			
N6h	C_1	1.40	1.39			1.47			
N6i	C_s	1.62	1.43			i. f.			
N6j	C_2	1.65	1.46			1.58			
N6k	C_s	1.66	1.50			1.63			
N6l	C_1	1.67	1.52			1.55			
N6m	C_s	1.66	1.53			i. f.			
N6n	C_s	1.68	1.58			1.74			
N6o	D_{6h}	2.34	2.05			2.30			
N7a	C_{3v}	0.01	0.00			0.08	0.00		
N7b	C_s	0.00	0.03			0.00	0.06		
N7c	C_s	0.00	0.10			0.00	0.13		
N7d	C_s	0.24	0.22			0.24			
N7e	C_s	0.26	0.26			0.26			
N7f	C_s	0.32	0.34			i. f.			
N7g	C_1	0.43	0.38			i. f.			
N7h	C_s	0.35	0.45			0.39			
N7i	C_s	0.48	0.55			0.54			
N7j	C_1	0.52	0.67			0.54			
N7k	C_{3v}	0.41	0.71			0.29			

Isomer	Symmetry Group	B3LYP-D3/ aug-cc-pVDZ	CCSD/DZ// B3LYP-D3	CCSD/TZ// B3LYP-D3	CCSD(T)/TZ/ /B3LYP-D3	ωB97XD/ aug-cc-pVDZ	CCSD/DZ// ωB97XD	CCSD/TZ// ωB97XD	CCSD(T)/TZ/ /ωB97XD
N7l	C_{2v}	1.50	1.10			1.25			
N7m	C_1	1.62	1.30			1.42			
N7n	C_s					2.49			
N8a	D_{2d}	0.00	0.00			0.00			
N8b	C_s	0.17	0.30			0.27			
N8c	C_2	0.25	0.32			i. f.			
N8d	C_s	0.35	0.46			0.48			
N8e	C_1	0.36	0.48			0.47			
N8f	C_1	0.41	0.53			0.53			
N8g	C_{2v}	0.53	0.63			0.59			
N8h	C_s	0.61	0.78			0.74			
N8i	C_1	0.65	0.81			i. f.			
N8j	C_s	0.64	0.84			0.74			
N8k	C_1	0.71	0.95			i. f.			
N8l	C_1	0.81	1.01			0.90			
N8m	C_1	0.87	1.02			1.04			
N8n	C_s	0.82	1.05			1.01			
N8o	C_1	0.87	1.09			1.06			
N8p	C_1	1.32	1.47			1.40			
N8q	C_1	1.38	1.60			1.51			
N8r	C_{2h}	2.24	1.81			2.01*			
N8s	C_2	2.36	2.04			2.21			

2. Cluster Stability and Dissociation Energies

2.1 Dissociation of NaCl and the Atomic Ion

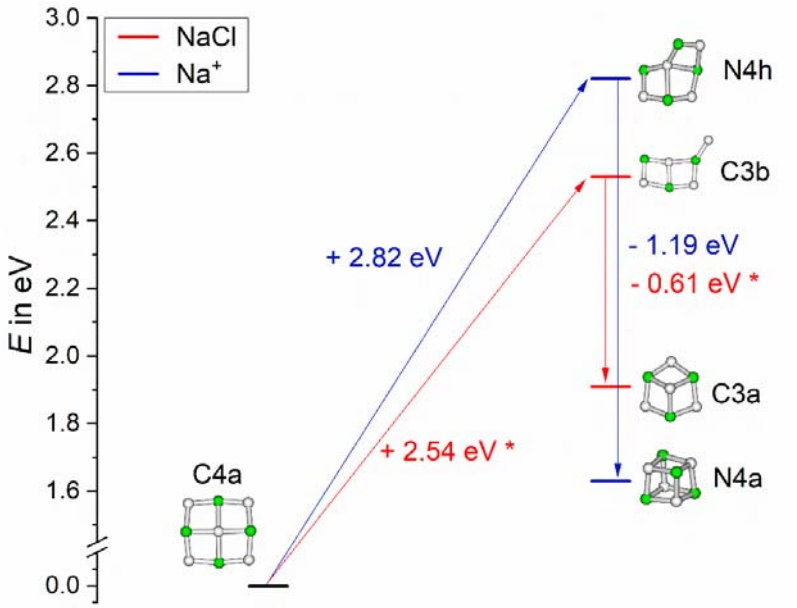

Figure S5: Energy scheme for the cationic magic cluster $(NaCl)_4Na^+$ when no isomerization before fragmentation is allowed. Thus, dissociation of NaCl or Na^+ occurs directly from the minimum energy structure C4a and proceeds via a higher lying isomer of the product. Given energies are calculated at the CCSD/DZ//B3LYP-D3 level of theory. Energies marked with * are obtained by using the ωB97XD functional for the geometrical optimization due to the presence of an imaginary frequency using the B3LYP-D3 functional.

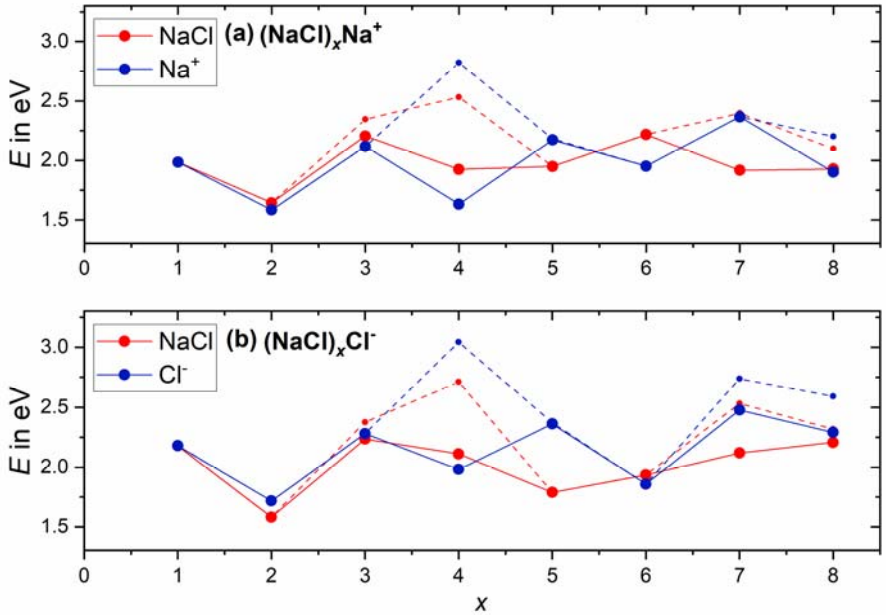

Figure S6: Energy needed to remove NaCl or the respective atomic ion (Cl^- and Na^+) from the ionic clusters $(NaCl)_xCl^-$ (a) and $(NaCl)_xNa^+$ (b). Solid lines, large symbols: isomerization before dissociation and thus, fragmentation into lowest lying product isomers, see Figure 3 for x = 4. Dashed lines, small symbols: no isomerization before dissociation, resulting in higher lying product isomers, see Figure S5 for x = 4. Given energies are calculated at the CCSD/DZ//B3LYP-D3 level of theory.

2.1 Benchmarking Dissociation Energies

The dissociation energies of the loss channels described by equation (2), (3) and (4) are plotted in Figure S7. All Methods used in Table S4, Figure S7 and Figure 4 provide similar results. The dissociation energies calculated with CCSD(T)/TZ//B3LYP-D3 (Figure S7: lower-left) and CCSD(T)/TZ//ωB97XD (Figure S7: lower-right) are almost identical, reflecting the insensitivity of the results to the method employed. For CCSD(T), only ions up to x = 6 and neutrals up to x = 5 are calculated.

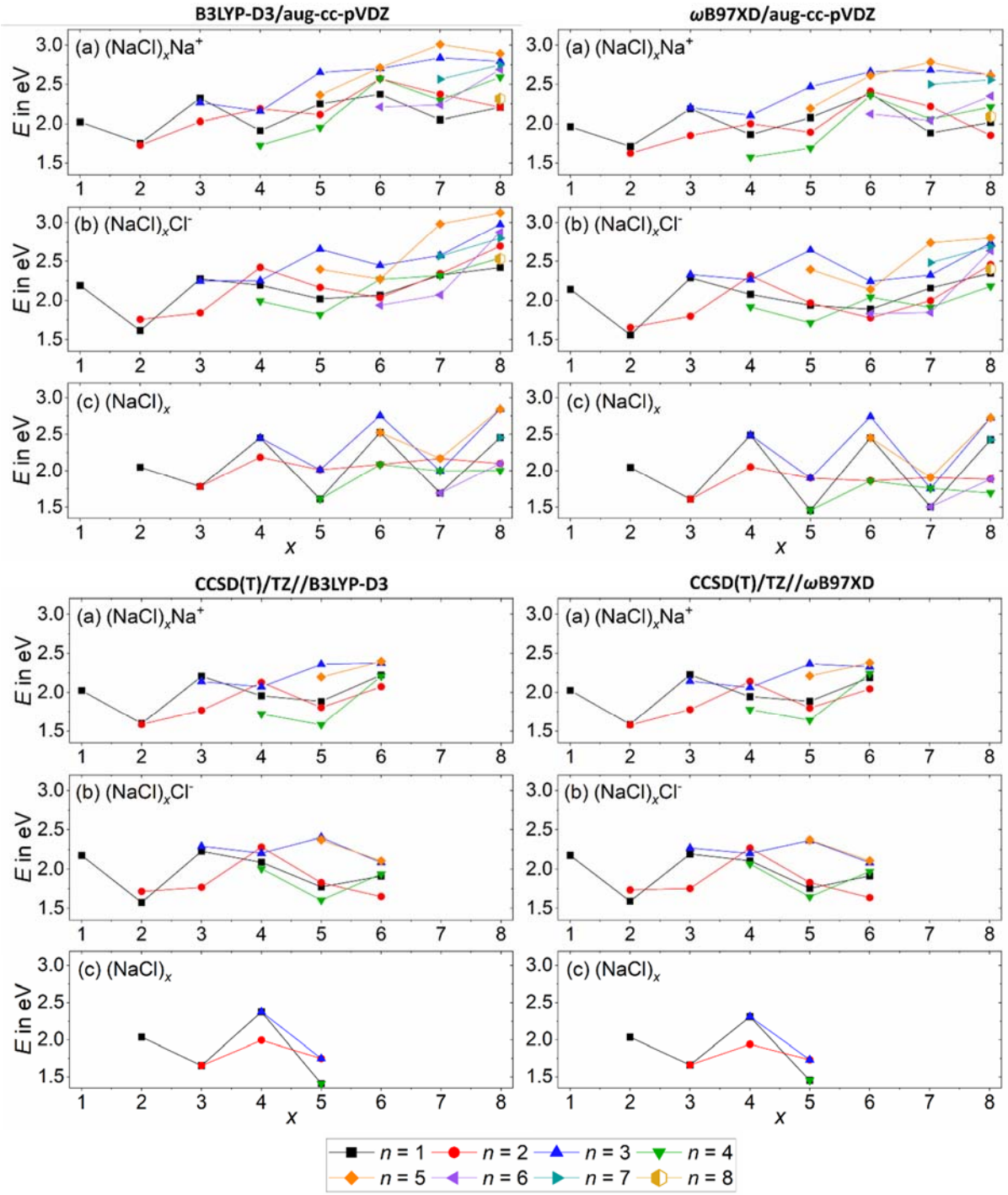

Figure S7: Dissociation energies of the a) cations, reaction (2); b) anions, reaction (3) and c) neutrals, reaction (4) as a function of cluster size x. Dissociation from the lowest energy isomer of the precursor to the lowest energy isomer of the products is assumed, including isomerization of the precursor. Calculations are performed at the B3LYP-D3/aug-cc-pVDZ (upper-left), the ωB97XD/aug-cc-pVDZ

(upper-right), the CCSD(T)/TZ//B3LYP-D3 (lower-left) and the CCSD(T)/TZ//ωB97XD (lower-right) level of theory.

Table S4: Dissociation energies for the loss channels (2), (3) and (4) of the cationic, anionic and neutral clusters, respectively. The energies are calculated by considering the minimum energy structures of reactant and products.

Charge	*x*	*n*	B3LYP-D3/ aug-cc-pVDZ	CCSD/DZ// B3LYP-D3	CCSD/TZ// B3LYP-D3	CCSD(T)/TZ/ /B3LYP-D3	ωB97XD/ aug-cc-pVDZ	CCSD/TZ// ωB97XD	CCSD(T)/TZ/ /ωB97XD
$(NaCl)_xNa^+$	1	1	2.02	1.98	2.03	2.03	1.96	2.03	2.03
	2	1	1.75	1.64	1.58	1.60	1.71	1.57	1.59
		2	1.73	1.58	1.58	1.58	1.63	1.57	1.58
	3	1	2.32	2.21	2.21	2.21	2.19	2.23	2.23
		2	2.03	1.81	1.75	1.77	1.85	1.76	1.78
		3	2.27	2.12	2.13	2.14	2.20	2.13	2.14
	4	1	1.91	1.92	1.96	1.96	1.86	1.95	1.95
		2	2.19	2.09	2.13	2.13	2.00	2.14	2.14
		3	2.16	2.06	2.05	2.07	2.10	2.04	2.06
		4	1.73	1.63	1.74	1.72	1.58	1.80	1.78
	5	1	2.25	1.95	1.86	1.89	2.08	1.86	1.89
		2	2.11	1.83	1.78	1.81	1.89	1.77	1.80
		3	2.65	2.36	2.33	2.36	2.47	2.34	2.37
		4	1.95	1.60	1.57	1.58	1.69	1.62	1.64
		5	2.36	2.17	2.20	2.20	2.19	2.21	2.21
	6	1	2.37	2.22	2.19	2.22	2.38	2.15	2.19
		2	2.57	2.12	2.01	2.07	2.41	1.98	2.04
		3	2.70	2.38	2.31	2.38	2.66	2.26	2.33
		4	2.57	2.17	2.17	2.21	2.36	2.21	2.25
		5	2.71	2.41	2.35	2.40	2.61	2.33	2.38
		6	2.21	1.95			2.12		
	7	1	2.05	1.92			1.88		
		2	2.37	2.09			2.22		
		3	2.84	2.37			2.68		
		4	2.30	1.88			2.06		
		5	3.01	2.68			2.78		
		6	2.24	1.88			2.04		
		7	2.57	2.37			2.50		
	8	1	2.21	1.93			2.02		
		2	2.21	1.80			1.85		
		3	2.79	2.35			2.62		

Charge	*x*	*n*	B3LYP-D3/ aug-cc-pVDZ	CCSD/DZ// B3LYP-D3	CCSD/TZ// B3LYP-D3	CCSD(T)/TZ/ /B3LYP-D3	ωB97XD/ aug-cc-pVDZ	CCSD/TZ// ωB97XD	CCSD(T)/TZ/ /ωB97XD
		4	2.59	1.88			2.21		
		5	2.89	2.40			2.62		
		6	2.69	2.17			2.35		
		7	2.75	2.31			2.56		
		8	2.31	1.90			2.09		
$(NaCl)_xCl^-$	1	1	2.19	2.18	2.18	2.18	2.14	2.18	2.18
	2	1	1.62	1.58	1.58	1.58	1.56	1.59	1.59
		2	1.76	1.72	1.73	1.72	1.65	1.74	1.74
	3	1	2.28	2.24	2.21	2.23	2.29	2.17	2.20
		2	1.84	1.77	1.75	1.77	1.80	1.74	1.75
		3	2.25	2.28	2.27	2.29	2.33	2.25	2.27
	4	1	2.20	2.11	2.09	2.09	2.08	2.11	2.11
		2	2.42	2.30	2.26	2.28	2.32	2.25	2.27
		3	2.25	2.21	2.18	2.21	2.27	2.18	2.20
		4	1.99	1.98	2.02	2.01	1.92	2.08	2.07
	5	1	2.02	1.79	1.74	1.77	1.94	1.72	1.76
		2	2.17	1.86	1.80	1.83	1.97	1.80	1.83
		3	2.66	2.42	2.34	2.40	2.64	2.31	2.37
		4	1.82	1.59	1.58	1.60	1.71	1.62	1.65
		5	2.40	2.36	2.36	2.37	2.40	2.35	2.37
	6	1	2.07	1.94	1.92	1.91	1.89	1.92	1.91
		2	2.04	1.68	1.62	1.65	1.78	1.61	1.64
		3	2.45	2.12	2.05	2.09	2.24	2.05	2.09
		4	2.27	1.94	1.91	1.94	2.04	1.94	1.97
		5	2.27	2.12	2.09	2.11	2.14	2.09	2.11
		6	1.94	1.86			1.83		
	7	1	2.33	2.12			2.16		
		2	2.34	2.01			2.00		
		3	2.58	2.13			2.32		
		4	2.32	1.83			1.91		
		5	2.98	2.66			2.74		
		6	2.07	1.80			1.85		
		7	2.57	2.48			2.48		
	8	1	2.42	2.21			2.35		
		2	2.69	2.28			2.46		
		3	2.98	2.55			2.73		
		4	2.54	1.92			2.18		

Charge	*x*	*n*	B3LYP-D3/ aug-cc-pVDZ	CCSD/DZ// B3LYP-D3	CCSD/TZ// B3LYP-D3	CCSD(T)/TZ/ /B3LYP-D3	ωB97XD/ aug-cc-pVDZ	CCSD/TZ// ωB97XD	CCSD(T)/TZ/ /ωB97XD
		5	3.13	2.63			2.80		
		6	2.88	2.42			2.64		
		7	2.80	2.50			2.69		
		8	2.53	2.29			2.40		
$(NaCl)_x$	2	1	2.05	2.04	2.04	2.04	2.05	2.03	2.03
	3	1	1.79	1.67	1.66	1.65	1.61	1.67	1.66
		2	1.79	1.67	1.66	1.65	1.61	1.67	1.66
	4	1	2.45	2.41	2.34	2.38	2.49	2.28	2.31
		2	2.19	2.04	1.97	1.99	2.05	1.91	1.94
		3	2.45	2.41	2.34	2.38	2.49	2.28	2.31
	5	1	1.61	1.41	1.40	1.41	1.46	1.45	1.45
		2	2.02	1.78	1.71	1.75	1.90	1.70	1.73
		3	2.02	1.78	1.71	1.75	1.90	1.70	1.73
		4	1.61	1.41	1.40	1.41	1.46	1.45	1.45
	6	1	2.53	2.44			2.45		
		2	2.09	1.80			1.86		
		3	2.76	2.54			2.74		
		4	2.09	1.80			1.86		
		5	2.53	2.44			2.45		
	7	1	1.70	1.50			1.51		
		2	2.17	1.90			1.91		
		3	2.00	1.63			1.76		
		4	2.00	1.63			1.76		
		5	2.17	1.90			1.91		
		6	1.70	1.50			1.51		
	8	1	2.46	2.39			2.43		
		2	2.10	1.85			1.89		
		3	2.84	2.62			2.73		
		4	2.00	1.61			1.70		
		5	2.84	2.62			2.73		
		6	2.10	1.85			1.89		
		7	2.46	2.39			2.43		

3. Collision Induced Dissociation Experiments

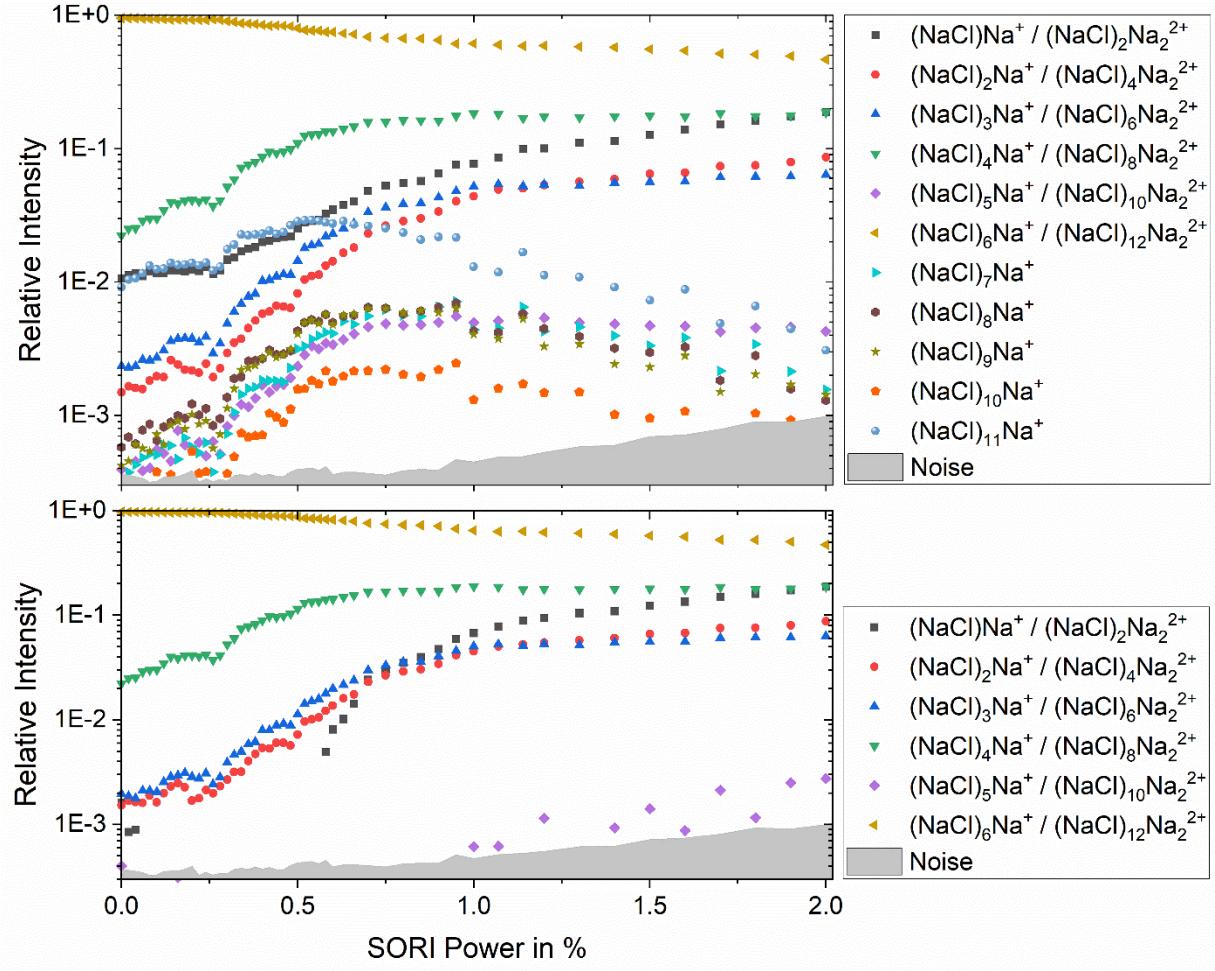

Figure S8: Due to an overlap of the precursor ion $(NaCl)_6Na^+$ with the doubly charged cluster $(NaCl)_{12}Na_2^{2+}$, a correction has been made in the CID spectrum of the cluster size $x = 6$ based on the intensities of the fragment peaks originating from the doubly charged species, which occur at higher mass to charge ratios than the precursor ion peak $(NaCl)_6Na^+$ / $(NaCl)_{12}Na_2^{2+}$. The loss of odd-numbered neutrals from $(NaCl)_{12}Na_2^{2+}$ is not observed, while the loss of even-numbered neutrals from $(NaCl)_{12}Na_2^{2+}$ would be overlapped with the fragment peaks of $(NaCl)_6Na^+$ and thus, cannot be ruled out. However, we assume main fragmentation of $(NaCl)_{12}Na_2^{2+}$ into two singly charged species, e.g. $(NaCl)_{12}Na_2^{2+} \rightarrow (NaCl)_8Na^+ + (NaCl)_4Na^+$, whereby the intensity of the $(NaCl)_8Na^+$ peak should equal the intensity of the corresponding second product $(NaCl)_4Na^+$ originating from $(NaCl)_{12}Na_2^{2+}$. By subtracting the intensity of one product (e.g. $(NaCl)_8Na^+$) - originating from $(NaCl)_{12}Na_2^{2+}$ - from the corresponding second product peak (e.g. $(NaCl)_4Na^+$), we correct for the contribution of the doubly charged species. Since we cannot rule out the loss of even-numbered neutrals from $(NaCl)_{12}Na_2^{2+}$, the fragment peaks might be slightly overestimated, whereby the single contribution to each peak cannot be determined.

4. Statistical Analysis

4.1 DOS: Cations

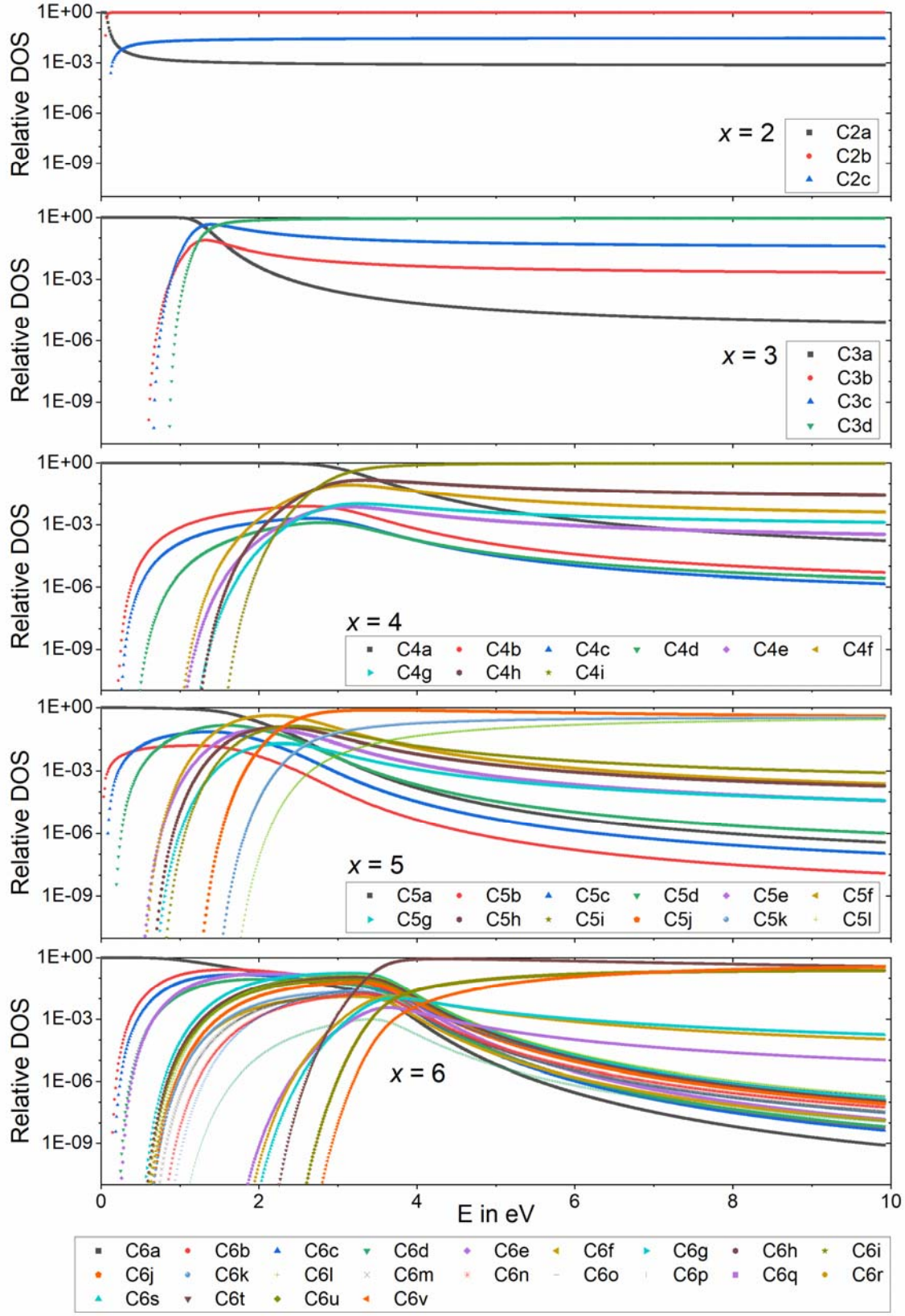

Figure S9: Relative DOS for the cationic clusters $(NaCl)_xNa^+$ with $x = 2–6$, calculated at the CCSD(T)/TZ//B3LYP-D3 level of theory. The isomers C3b, C4e and C4f have one imaginary frequency using the B3LYP-D3 functional and thus, the ωB97XD optimized frequencies and energies are used for an approximation of the DOS of these isomers.

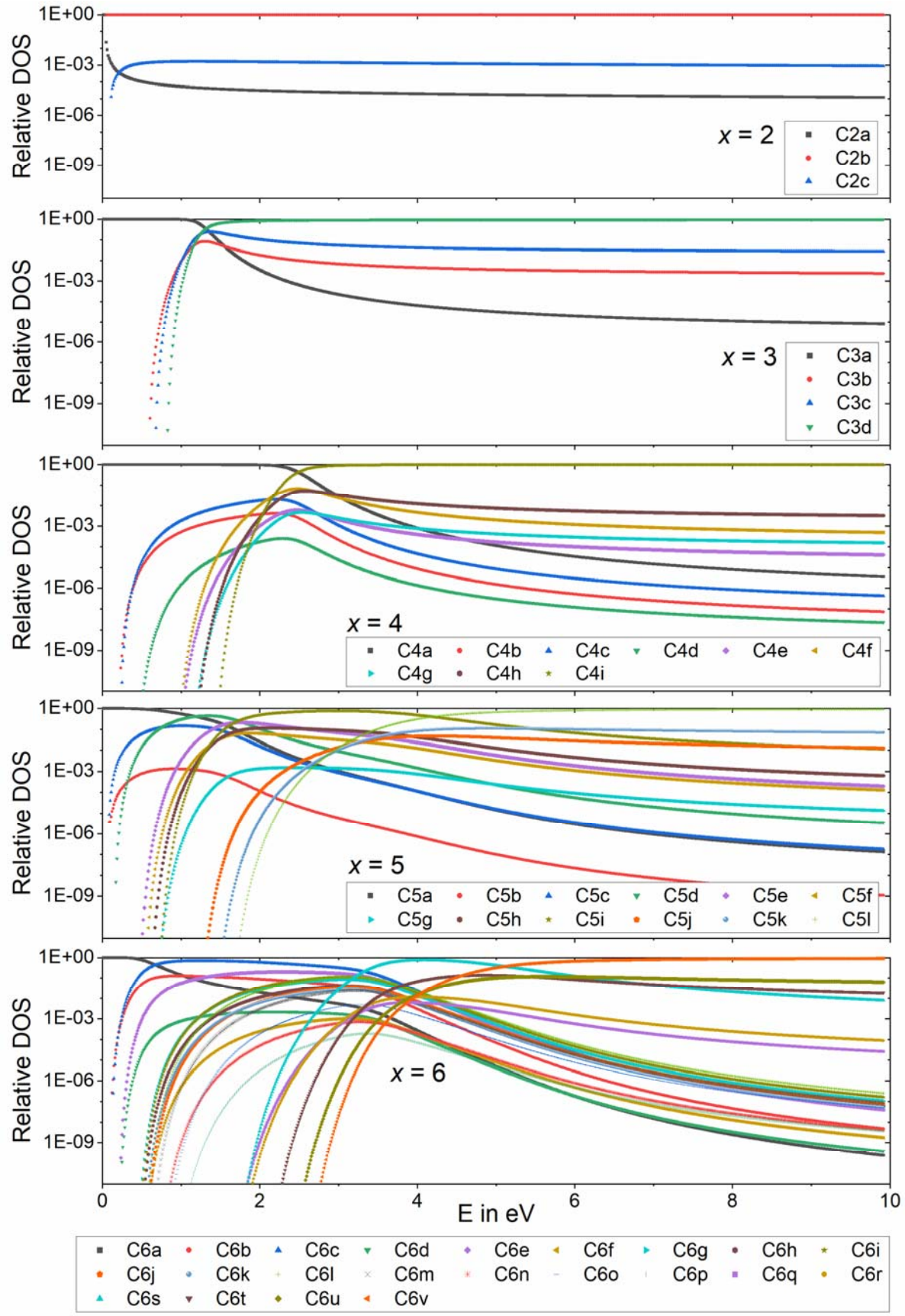

Figure S10: Relative DOS for the cationic clusters $(NaCl)_xNa^+$ with $x = 2–6$, calculated at the CCSD(T)/TZ//ωB97XD level of theory. The isomers C4g, C4h, C5d, C5h, C5l, C6m, C6q and C6v have one imaginary frequency using the ωB97XD functional and thus, the B3LYP-D3 optimized frequencies and energies are used for an approximation of the DOS of these isomers.

4.2 DOS: Anions

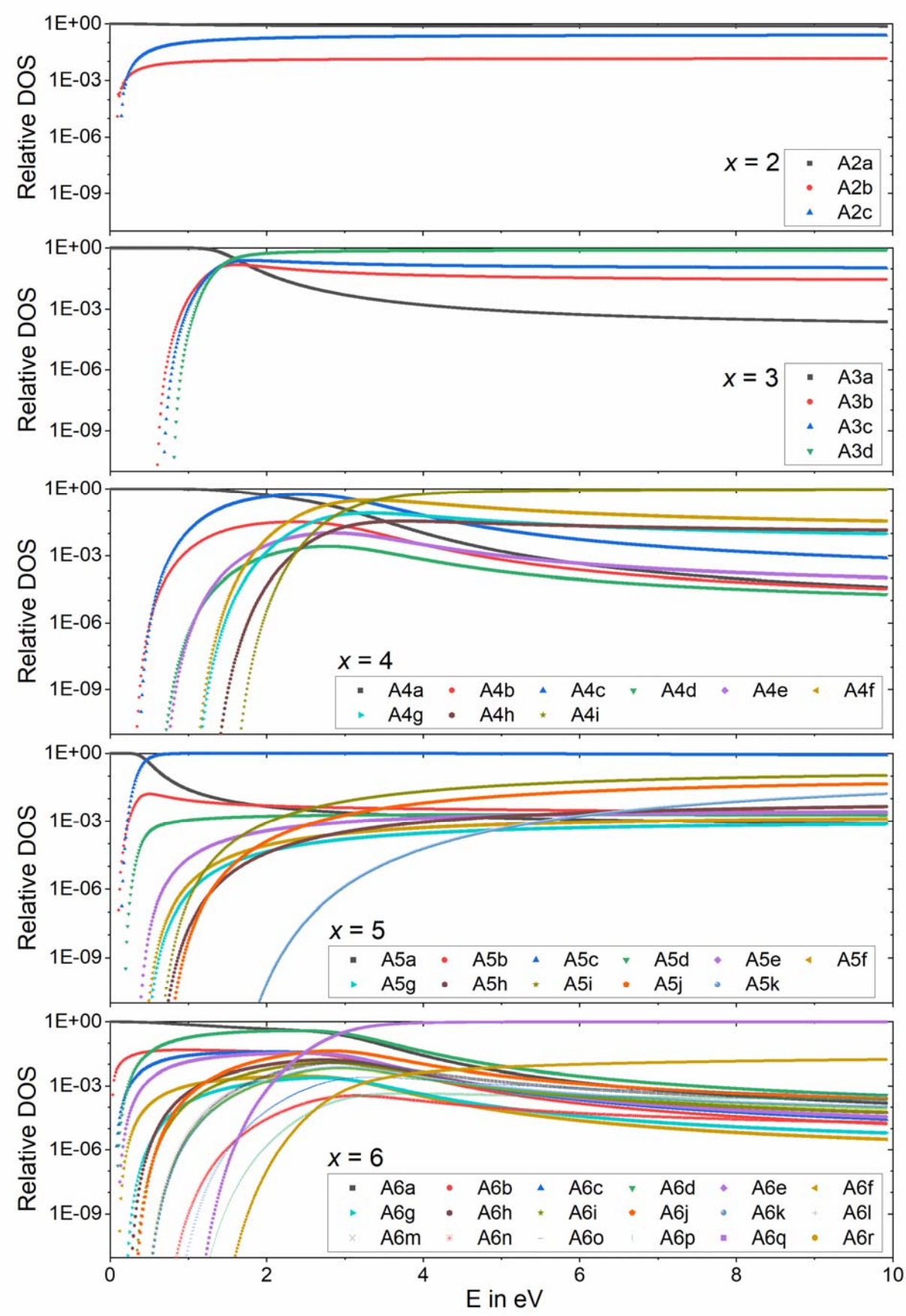

Figure S11: Relative DOS for the anionic clusters $(NaCl)_xCl^-$ with $x = 2–6$, calculated at the CCSD(T)/TZ//B3LYP-D3 level of theory.

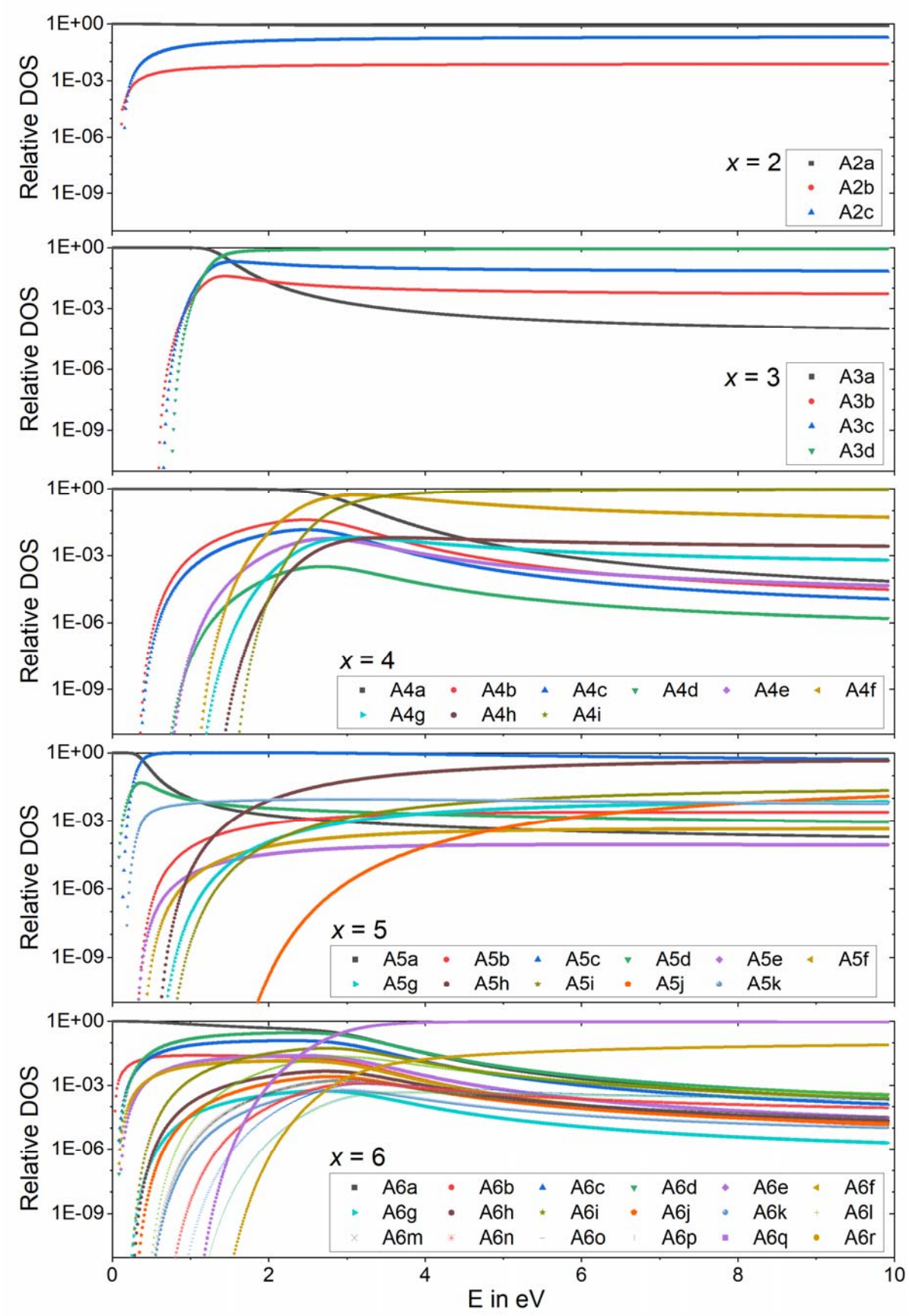

Figure S12: Relative DOS for the anionic clusters $(NaCl)_xCl^-$ with $x = 2–6$, calculated at the CCSD(T)/TZ//ωB97XD level of theory. The isomers A5d, A6l, A6n and A6r have one imaginary frequency using the ωB97XD functional and thus, the B3LYP-D3 optimized frequencies and energies are used for an approximation of the DOS of these isomers.

4.3 Benchmarking RRKM Rate Constants: Cations

Figures S13-S17 show the calculated RRKM rate constants $k^+_{x,n}$ for the loss channels (2) of the precursor ions $(NaCl)_xNa^+$ with x = 3–5 (a)–(c) and the total fragmentation rate constants $\sum_n k^+_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5 (d), calculated at different levels of theory. The results are similar for aug-cc-pVDZ and aug-cc-pVTZ basis sets, see Figures S13 and S14. Furthermore, single-point calculations employing CCSD and CCSD(T) also provide similar results, see Figures S14–S17. The only factor that causes slightly different results is the functional used for the frequency and geometry optimization, see again Figures S14–S17.

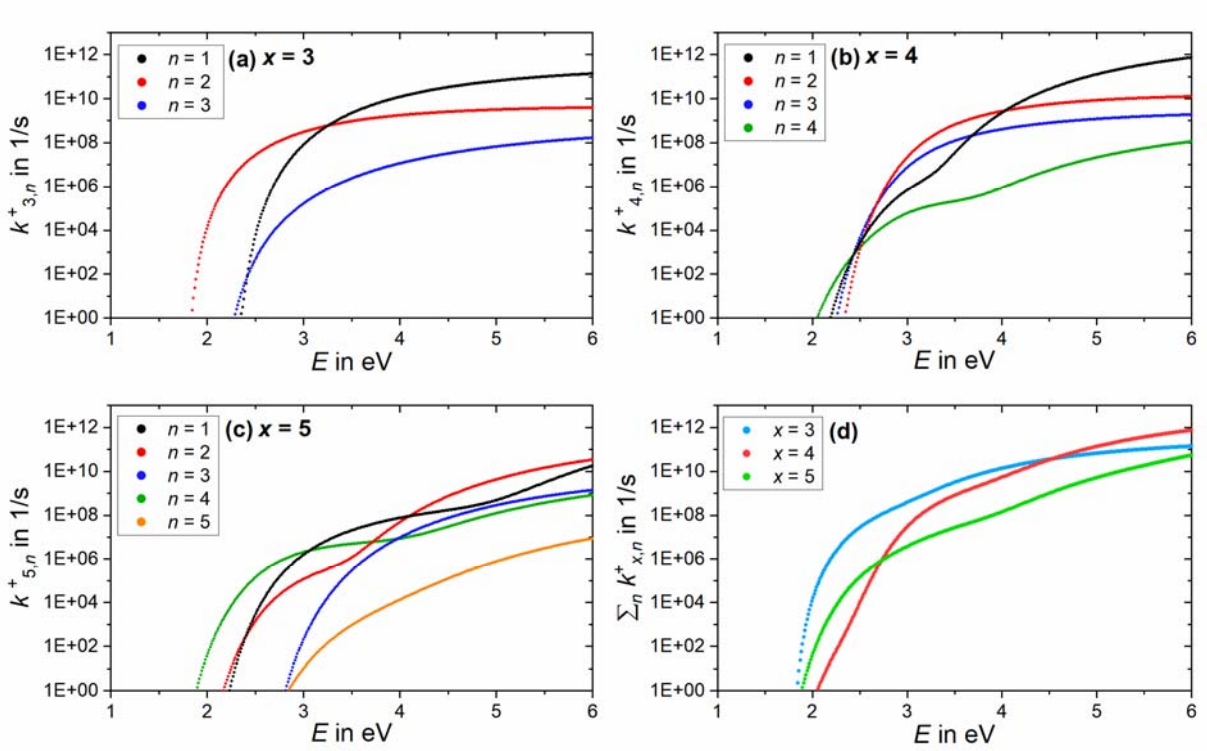

Figure S13: Method: CCSD/DZ//B3LYP-D3. (a)–(c) Calculated RRKM rate constants $k^+_{x,n}$ for the loss channels (2) of the precursor ions $(NaCl)_xNa^+$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^+_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

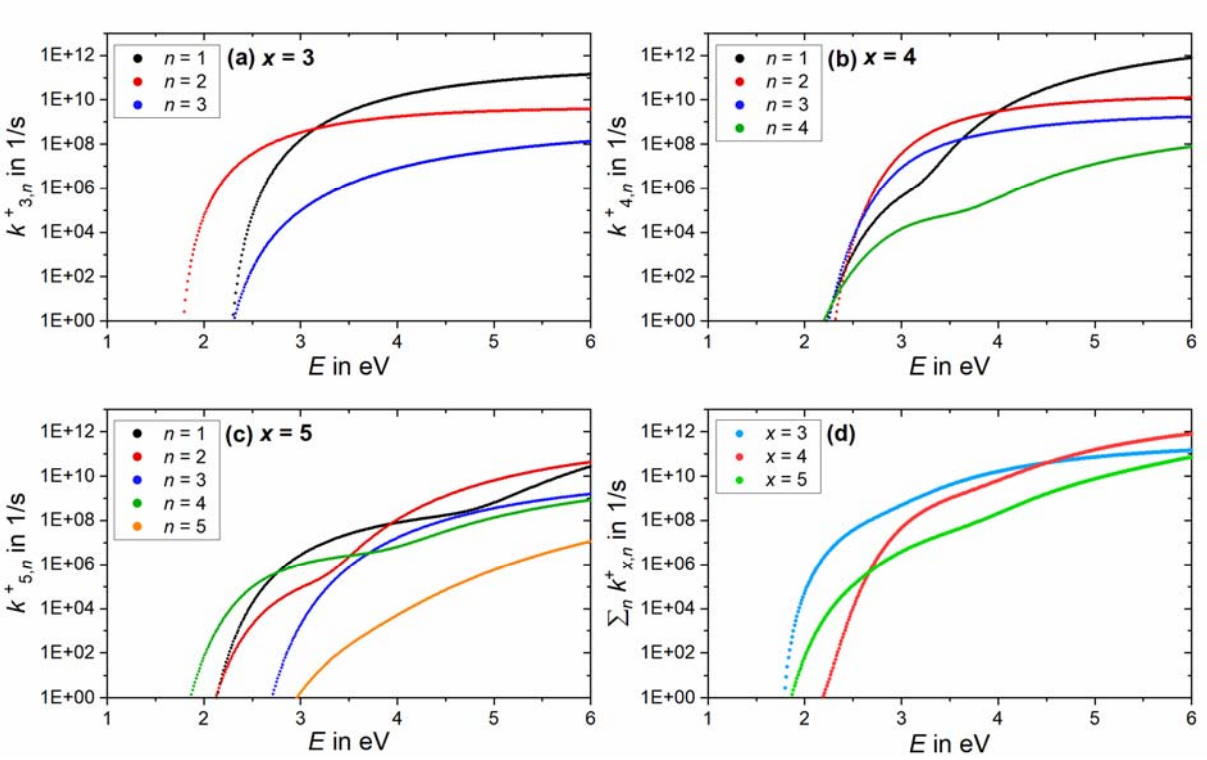

Figure S14: Method: CCSD/TZ//B3LYP-D3. (a)–(c) Calculated RRKM rate constants $k^{+}_{x,n}$ for the loss channels (2) of the precursor ions $(NaCl)_xNa^+$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^{+}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

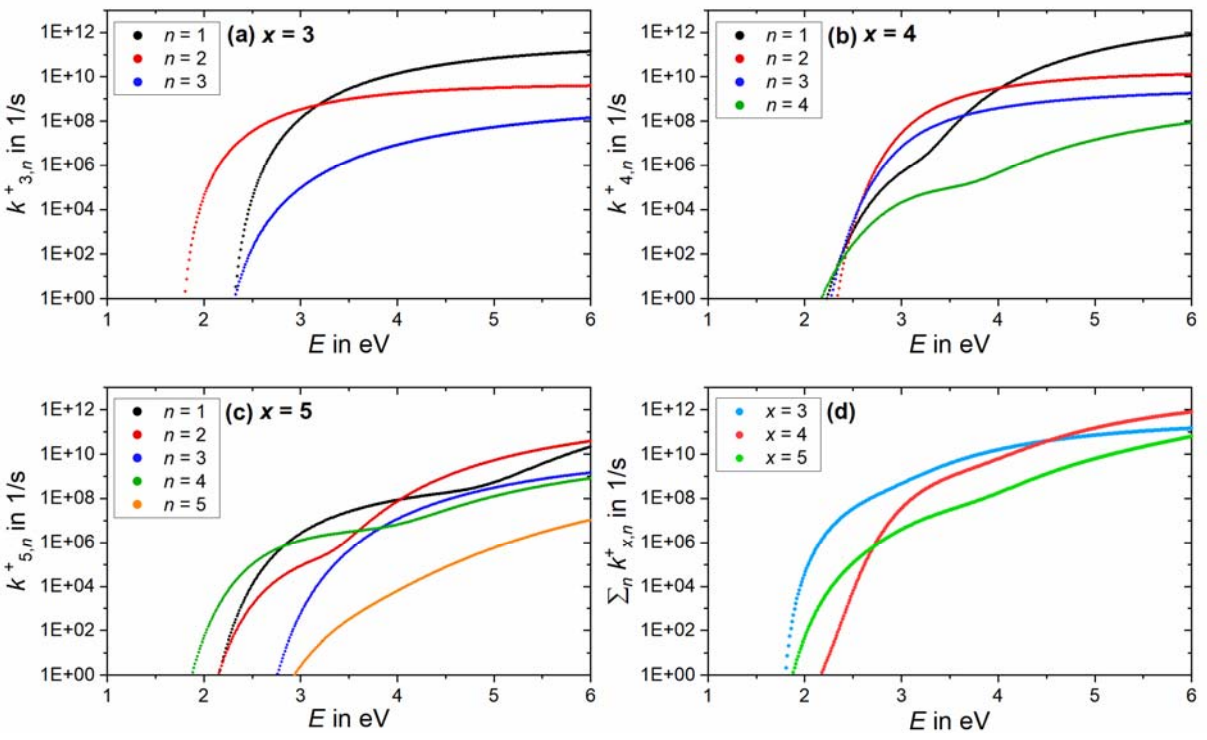

Figure S15: Method: CCSD(T)/TZ//B3LYP-D3. (a)–(c) Calculated RRKM rate constants $k^{+}_{x,n}$ for the loss channels (2) of the precursor ions $(NaCl)_xNa^+$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^{+}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

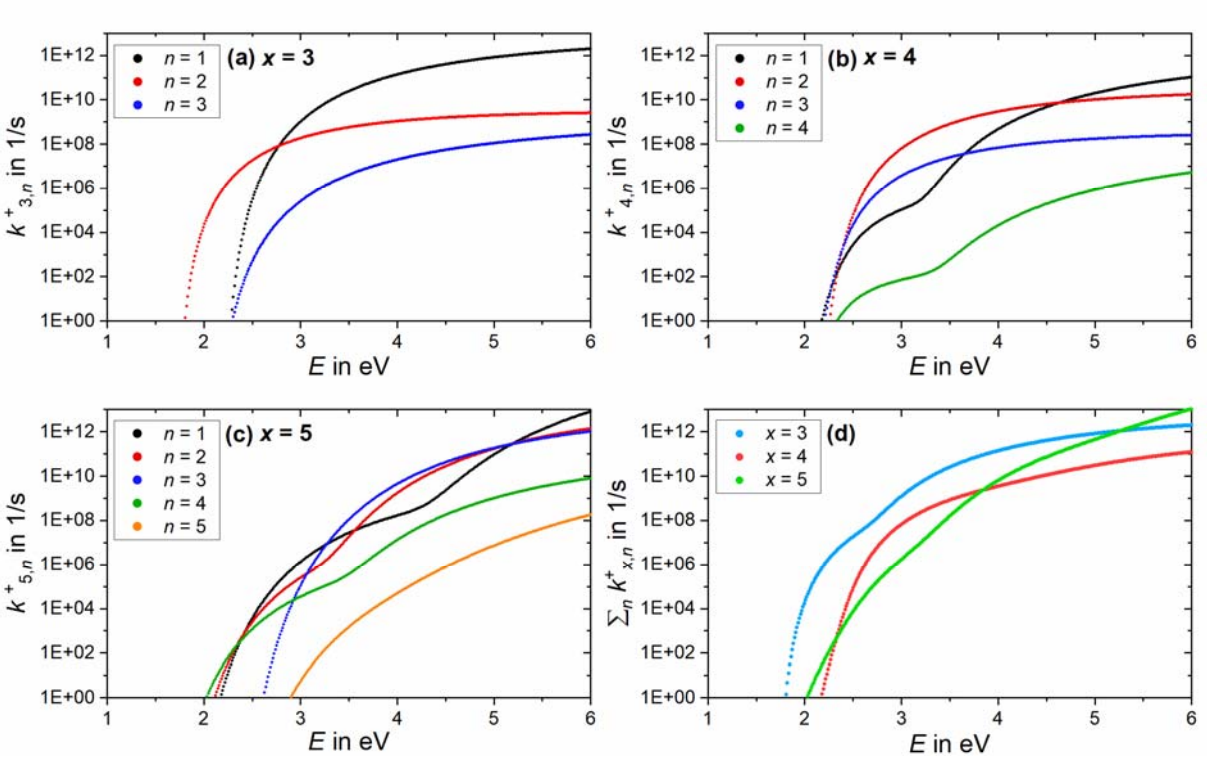

Figure S16: Method: CCSD/TZ//ωB97XD (a)–(c) Calculated RRKM rate constants $k^{+}_{x,n}$ for the loss channels (2) of the precursor ions $(NaCl)_xNa^+$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^{+}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

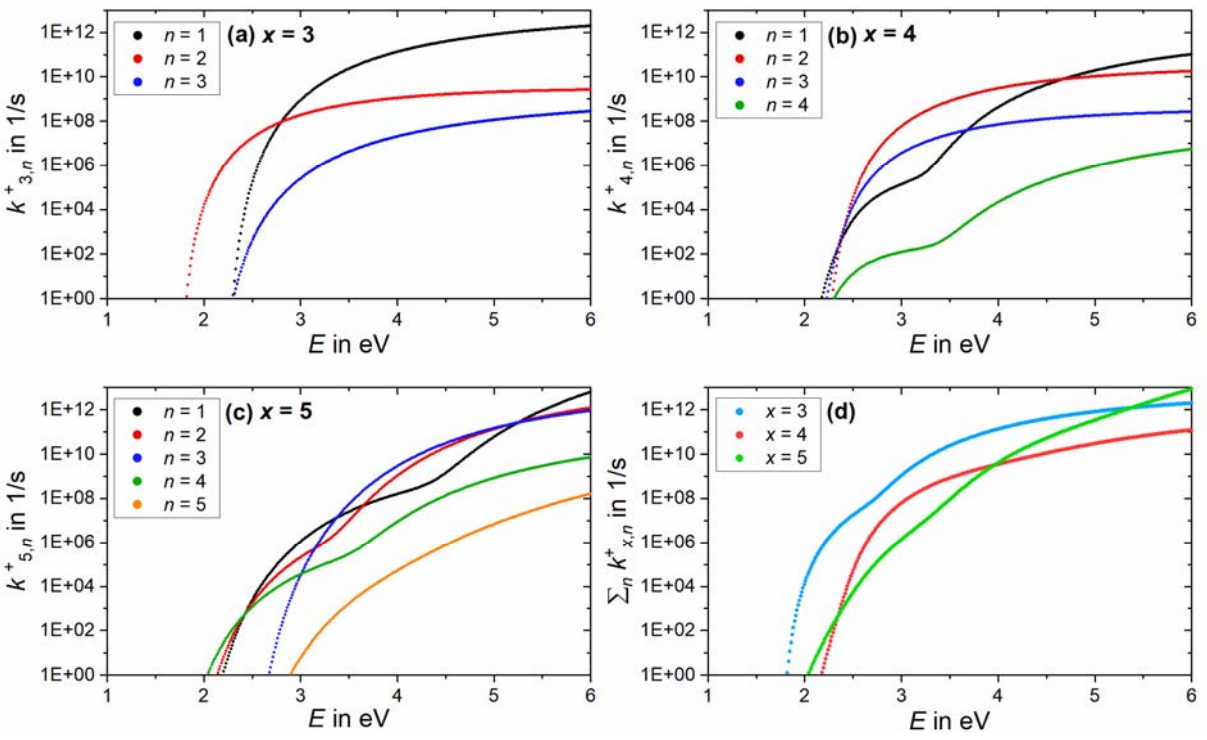

Figure S17: Method: CCSD(T)/TZ//ωB97XD. (a)–(c) Calculated RRKM rate constants $k^{+}_{x,n}$ for the loss channels (2) of the precursor ions $(NaCl)_xNa^+$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^{+}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

4.4 Benchmarking RRKM Rate Constants: Anions

Figures S18-S22 show the calculated RRKM rate constants $k^{-}_{x,n}$ for the loss channels (3) of the precursor ions $(NaCl)_xNa^-$ with x = 3–5 (a)–(c) and the total fragmentation rate constants $\sum_n k^{-}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5 (d), calculated at different levels of theory. The results are similar for the basis sets aug-cc-pVDZ and aug-cc-pVTZ, see Figures S18 and S19. Furthermore, single-point calculations employing CCSD and CCSD(T) also provide similar results, see Figures S19–S22. The only factor that causes slightly different results is the functional used for the frequency and geometry optimization, see again Figures S19–S22.

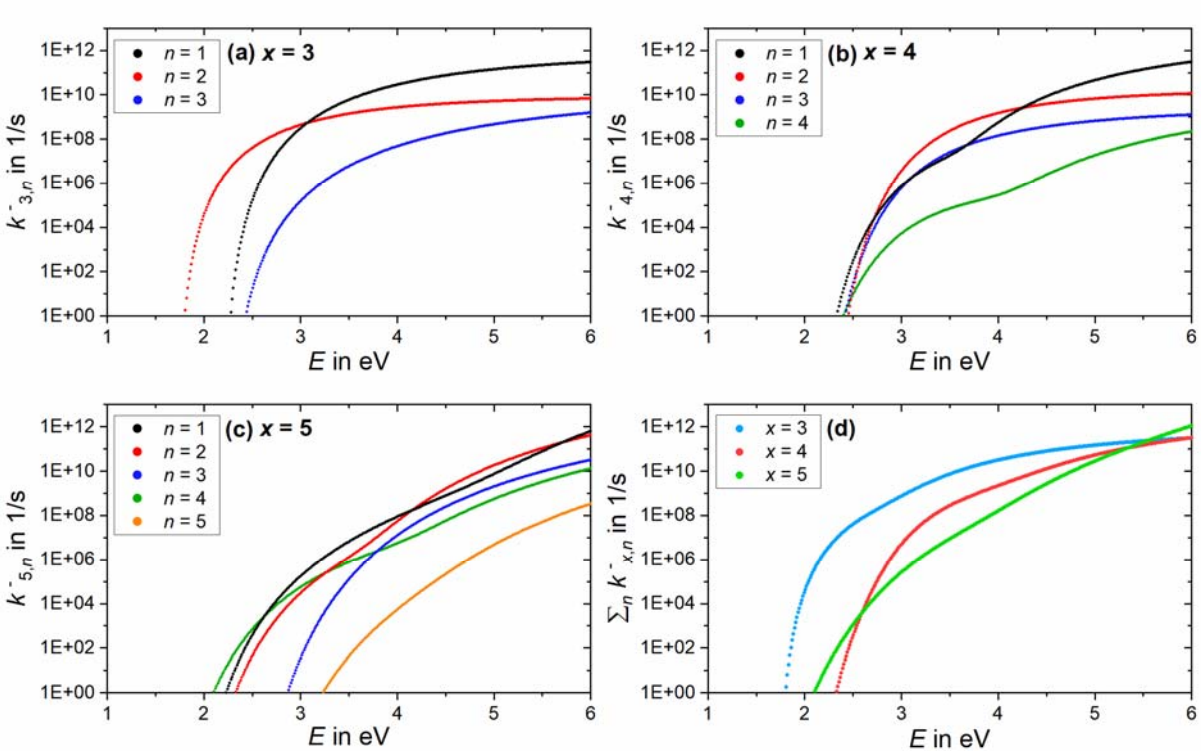

Figure S18: Method: CCSD/DZ//B3LYP-D3. (a)–(c) Calculated RRKM rate constants $k^{-}_{x,n}$ for the loss channels (3) of the precursor ions $(NaCl)_xCl^-$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^{-}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

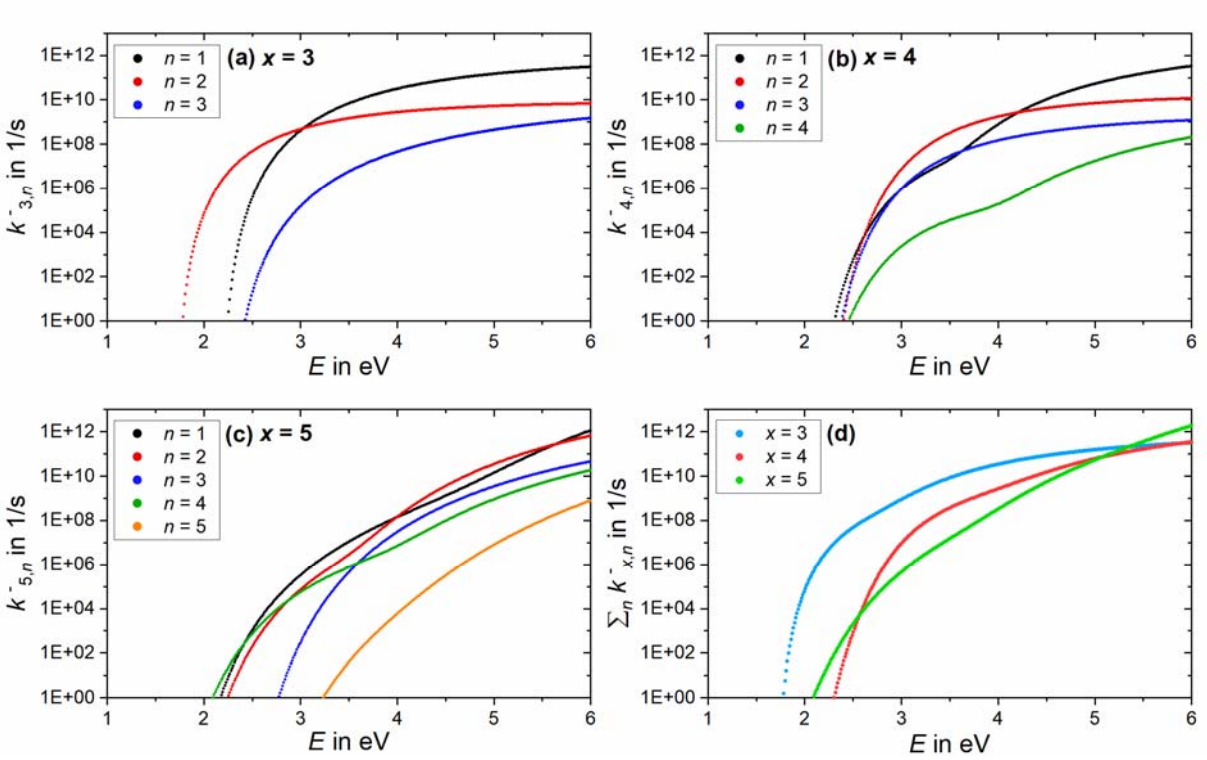

Figure S19: Method: CCSD/TZ//B3LYP-D3. (a)–(c) Calculated RRKM rate constants $k^{-}_{x,n}$ for the loss channels (3) of the precursor ions $(NaCl)_xCl^-$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^{-}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

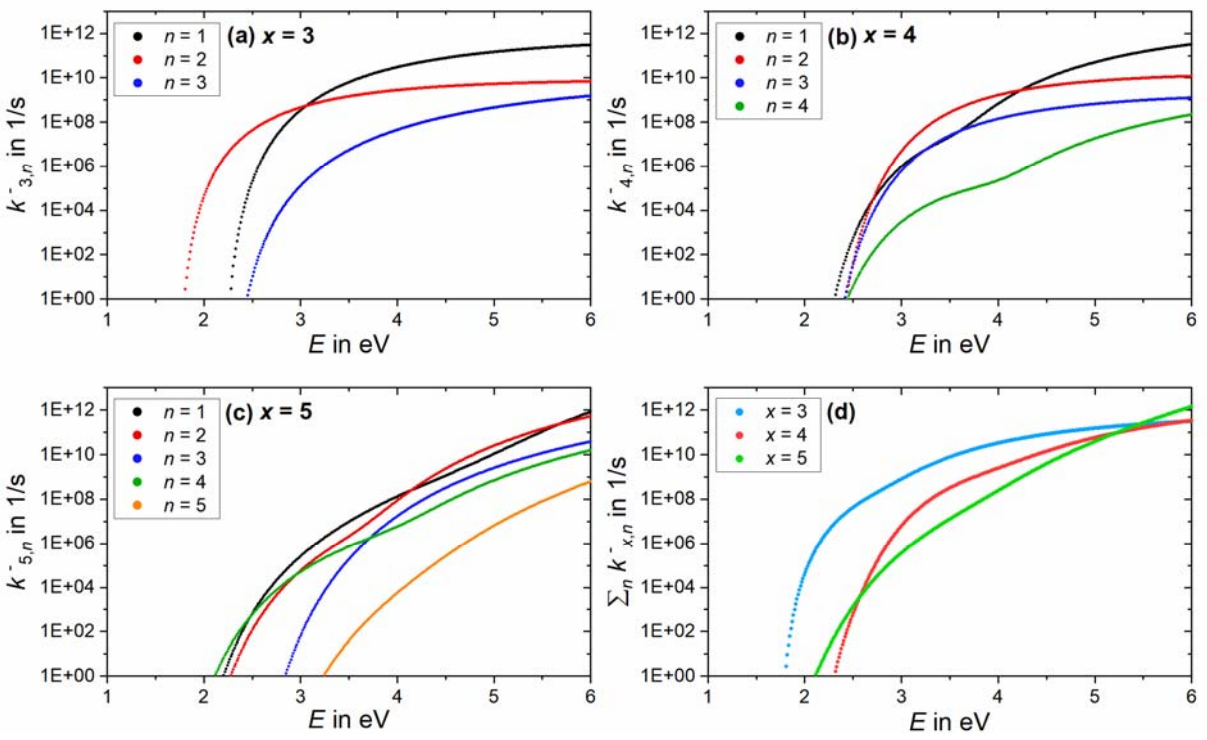

Figure S20: Method: CCSD(T)/TZ//B3LYP-D3. (a)–(c) Calculated RRKM rate constants $k^{-}_{x,n}$ for the loss channels (3) of the precursor ions $(NaCl)_xCl^-$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^{-}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

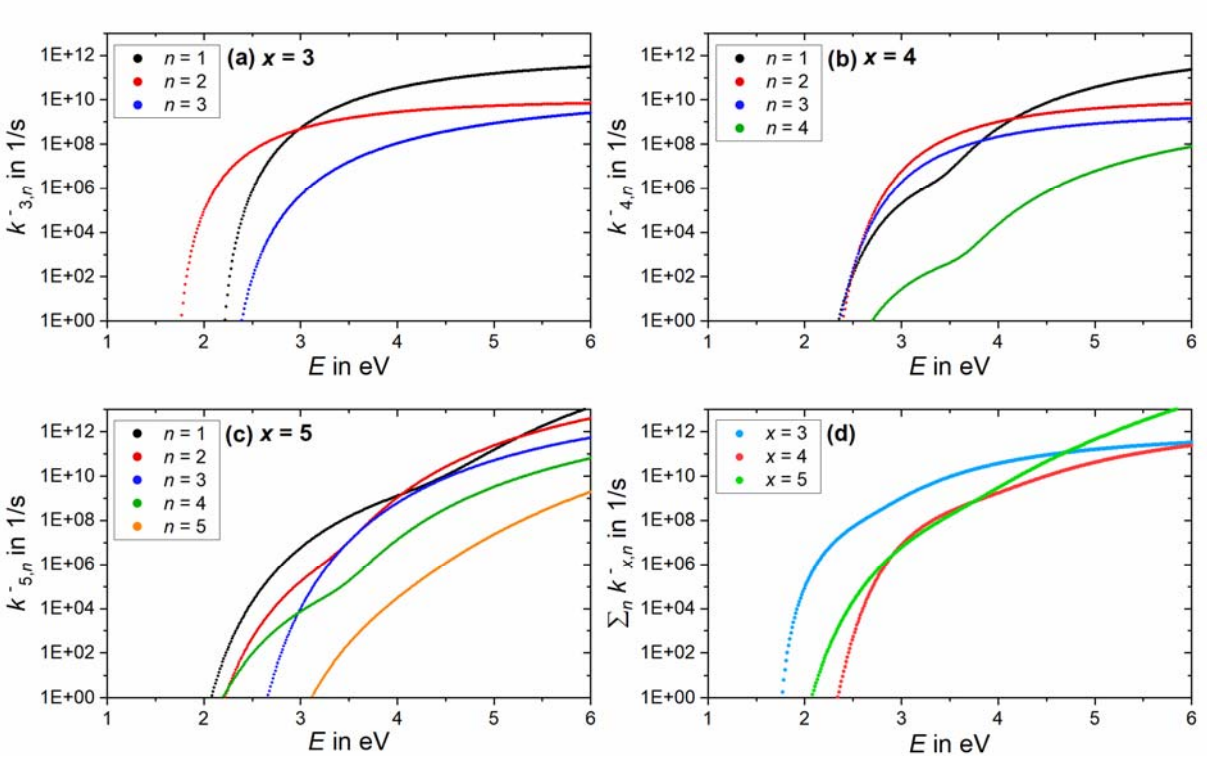

Figure S21: Method: CCSD/TZ//ωB97XD. (a)–(c) Calculated RRKM rate constants $k^{-}_{x,n}$ for the loss channels (3) of the precursor ions $(NaCl)_xCl^-$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^{-}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

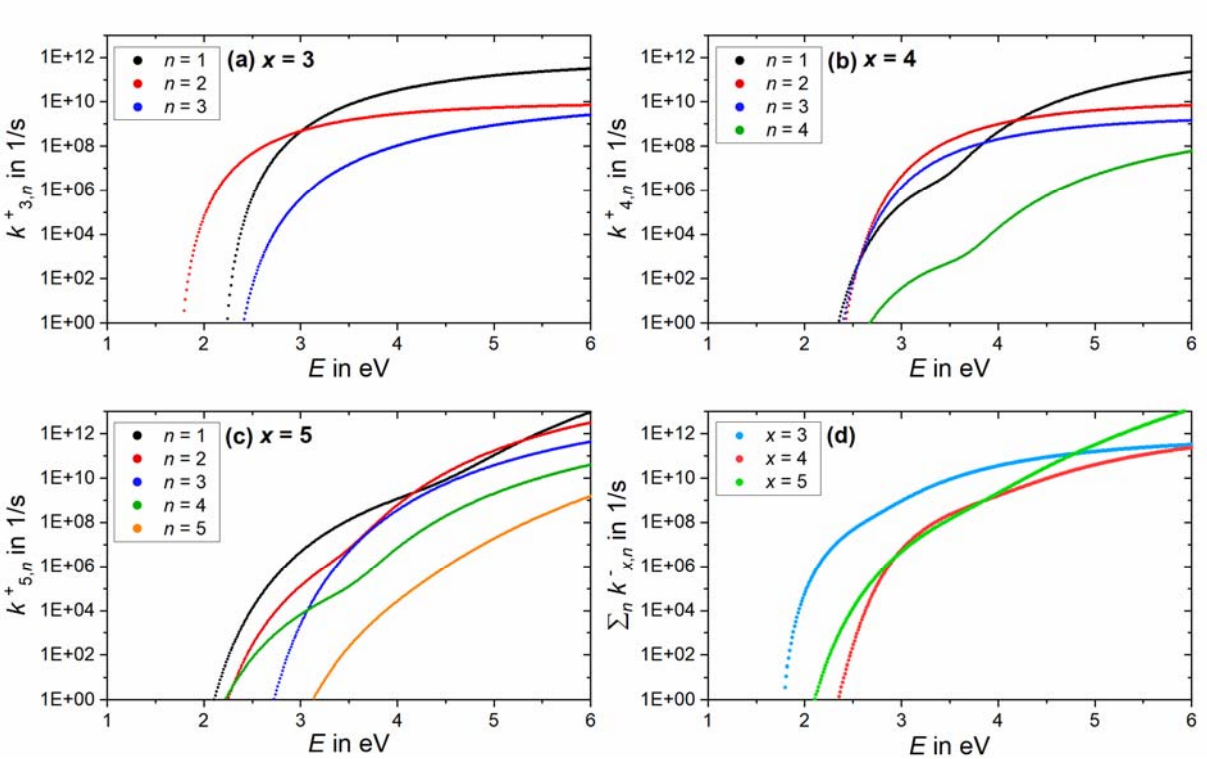

Figure S22: Method: CCSD(T)/TZ//ωB97XD. (a)–(c) Calculated RRKM rate constants $k^{-}_{x,n}$ for the loss channels (3) of the precursor ions $(NaCl)_xCl^-$ with x = 3–5. (d) Total fragmentation rate constants $\sum_n k^{-}_{x,n}$ as sum of all loss channels n for cluster sizes x = 3–5.

5. Mass Spectra

Figures S23 and S24 show mass spectra of the sodium chloride cluster cations and anions without any isolation. These mass spectra demonstrate, that only the pure sodium chloride cluster ions without contamination (e.g., water) are observed in the mass spectra. Figures S25–S30 show mass spectra of specific cluster sizes for a SORI Power of 1 %, representing the mass spectra used to obtain the SORI CID breakdown curves in Figures 4 and 5.

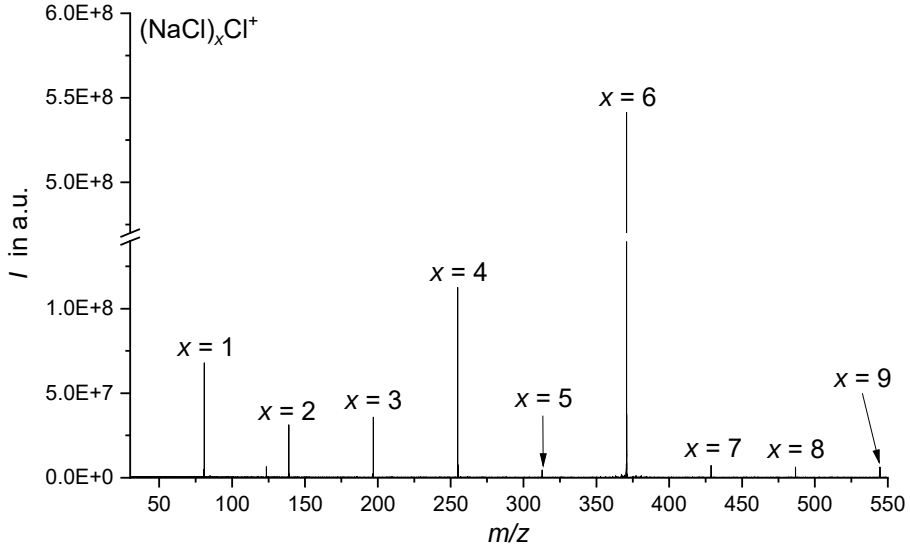

Figure S23: Mass spectrum of the sodium chloride cluster cations. The peak at $m/z \approx 123.6$ is the third harmonic of the $x = 6$ peak. Only the pure sodium chloride cluster cations without contamination (e.g., water) are observed in the mass spectra. The intensity distribution of the peaks depends significantly on the settings of the FT-ICR MS and does not represent the inherent stability of specific cluster sizes.

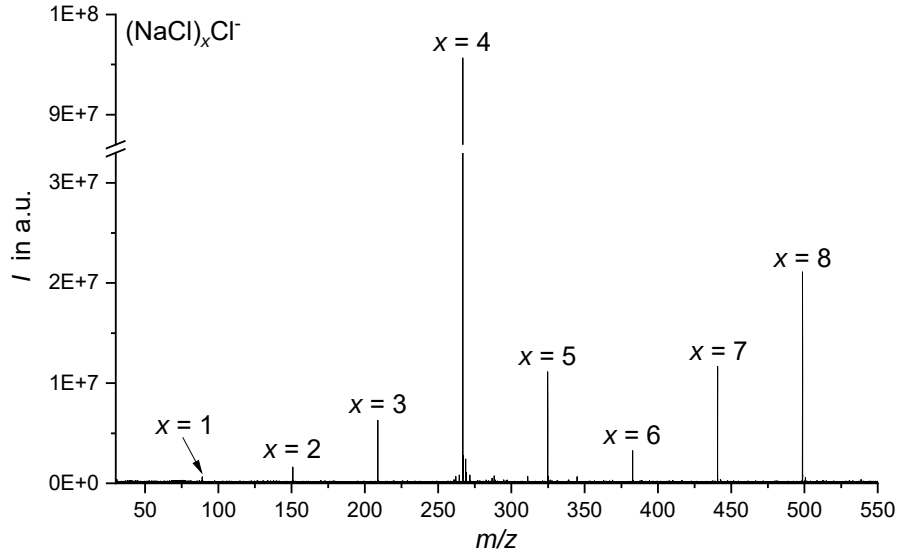

Figure S24: Mass spectrum of the sodium chloride cluster anions. Only the pure sodium chloride cluster anions without contamination (e.g. water) are observed in the mass spectra. The intensity distribution of the peaks depends significantly on the settings of the FT-ICR MS and does not represent the inherent stability of specific cluster sizes.

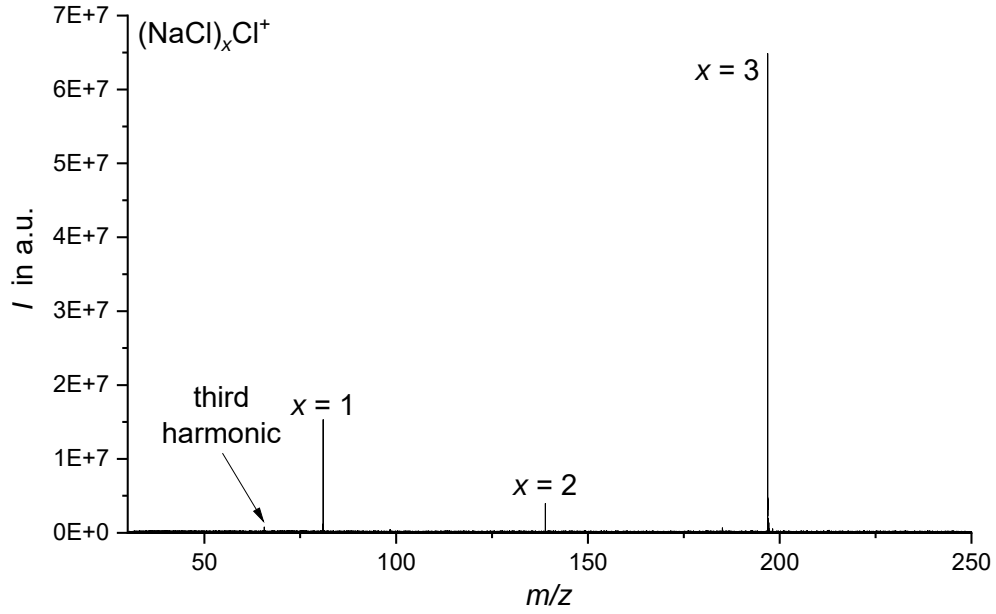

Figure S25: Mass spectrum of the cationic cluster size *x* = 3 at 1 % SORI Power.

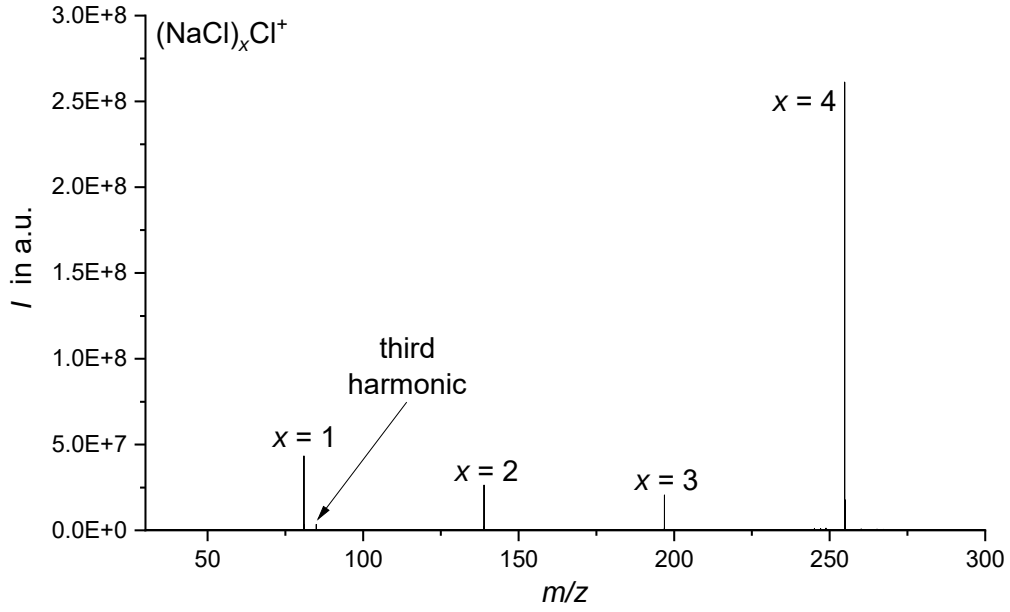

Figure S26: Mass spectrum of the cationic cluster size *x* = 4 at 1 % SORI Power.

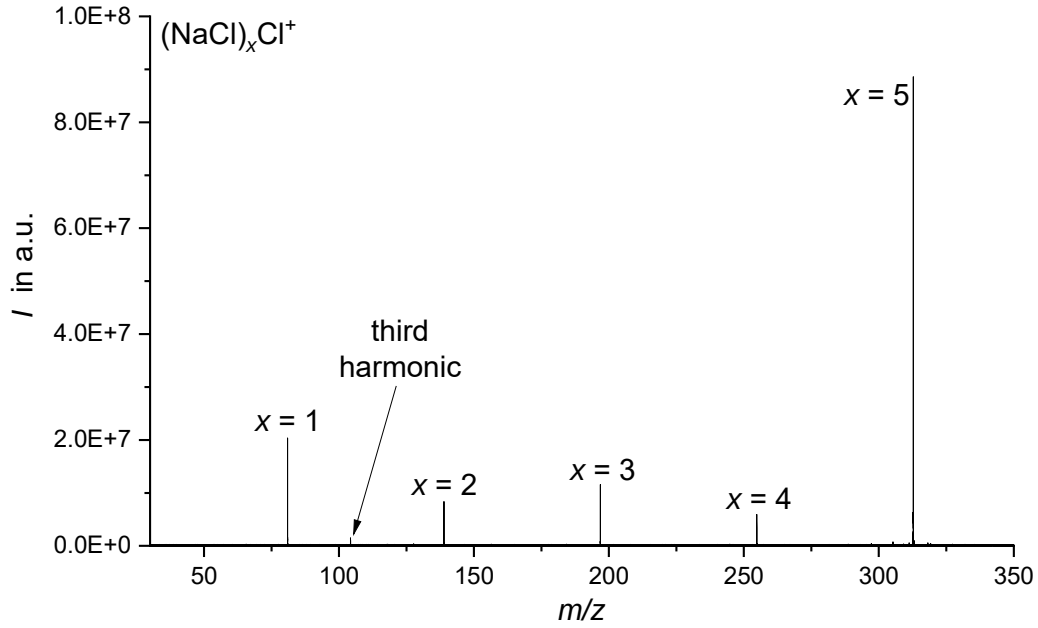

Figure S27: Mass spectrum of the cationic cluster size *x* = 5 at 1 % SORI Power.

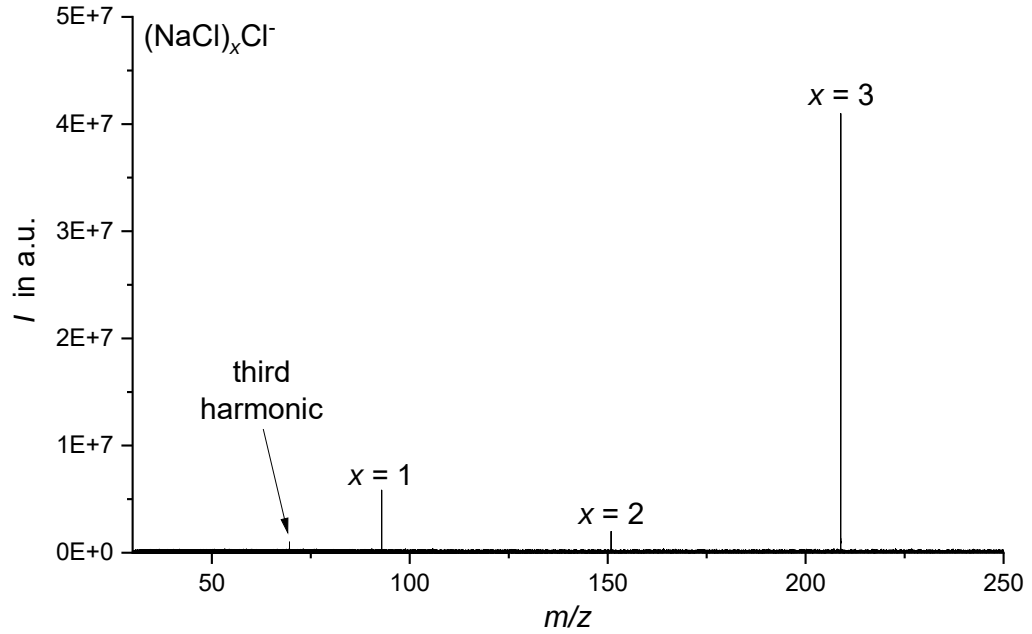

Figure S28: Mass spectrum of the anionic cluster size *x* = 3 at 1 % SORI Power.

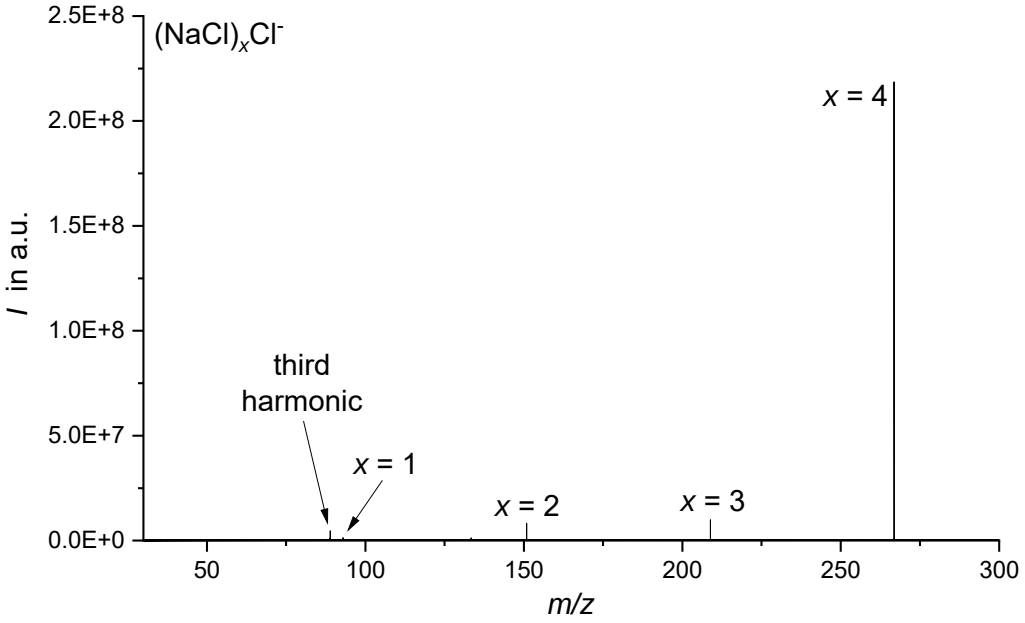

Figure S29: Mass spectrum of the anionic cluster size *x* = 4 at 1 % SORI Power.

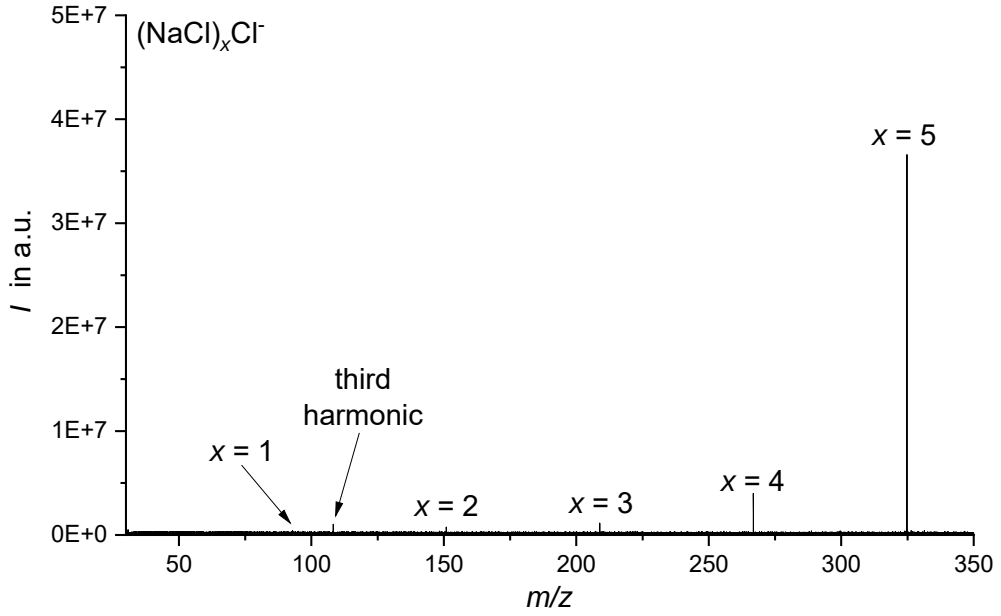

Figure S30: Mass spectrum of the anionic cluster size *x* = 5 at 1 % SORI Power.

6. Quantum Chemical Calculations

In the following chapters 5.1-5.6, the structures of the cationic clusters (chapter 5.1: B3LYP-D3/aug-cc-pVDZ; chapter 5.2: ωB97XD/aug-cc-pVDZ), the anionic clusters (chapter 5.3: B3LYP-D3/aug-cc-pVDZ; chapter 5.4: ωB97XD/aug-cc-pVDZ) and the neutral clusters (chapter 5.5: B3LYP-D3/aug-cc-pVDZ; chapter 5.6: ωB97XD/aug-cc-pVDZ) are listed.

6.1 Structures Cationic Clusters: B3LYP-D3/aug-cc-pVDZ

C1a
Na 0.000000 -0.000000 2.493268
Cl 0.000000 0.000000 0.000000
Na 0.000000 0.000000 -2.493268

C2a
Cl 0.000000 0.000000 1.747963
Na -0.000000 2.036912 -0.000000
Na -1.764017 -1.018456 -0.000000
Na 1.764017 -1.018456 -0.000000
Cl 0.000000 0.000000 -1.747963

C2b
Cl -0.000000 -2.552744 -0.000117
Na -0.000000 0.000000 0.001367
Cl 0.000000 2.552744 -0.000117
Na -0.859986 4.859979 -0.000503
Na 0.859986 -4.859979 -0.000503

C2c
Na -0.000000 1.782555 0.861439
Cl 0.000000 0.000000 2.623818
Na -0.000000 -1.782555 0.861439
Cl 0.000000 -0.000000 -1.284478
Na 0.000000 -0.000000 -3.792767

C3a
Cl 0.000000 2.274767 0.147216
Na 0.000000 0.000000 1.653838
Na 0.000000 -2.578971 -0.778796
Cl -1.970006 -1.137383 0.147216
Na -2.233454 1.289486 -0.778796
Na 2.233454 1.289486 -0.778796
Cl 1.970006 -1.137383 0.147216

C3c
Na -0.000000 1.729401 2.991697
Cl -0.000000 0.000000 4.823544
Na -0.000000 -1.729401 2.991697
Cl -0.000000 0.000000 0.906709
Na 0.000000 -0.000000 -1.661599
Cl 0.000000 -0.000000 -4.207422
Na 0.000000 -0.000000 -6.675260

C3d
Na -0.000000 7.307436 0.080484
Cl -0.000021 4.920715 -0.493598
Na 0.000022 2.418960 0.078272
Cl -0.000000 -0.000000 0.781747
Na -0.000022 -2.418960 0.078272
Cl 0.000021 -4.920715 -0.493598
Na 0.000000 -7.307436 0.080484

C4a
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Na -2.504504 -2.571625 -0.134536
Cl -0.000000 -2.772899 0.505198
Na 2.504504 -2.571625 -0.134536
Cl 2.693266 -0.000000 -0.419586
Na 2.504504 2.571625 -0.134536

C4b
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Na -1.956013 -2.784312 -0.000000
Cl -0.427501 -1.856514 -1.894294
Na -0.427501 0.747500 -1.811302
Cl -1.167425 2.595860 0.000000
Na 1.554331 -1.779157 -0.000000
Na 1.330772 3.437509 0.000000
Cl 1.974490 0.878378 -0.000000

C4c
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Na -0.000000 3.458145 0.243044
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Na -0.000000 -0.000000 2.635742
Cl -1.540640 -1.655316 1.393180
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Na 1.630167 0.506011 -1.136765
Cl 0.682809 -1.889685 -1.667630

C4d
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Na -1.925183 -1.111505 0.101213
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Na 0.000000 0.000000 -2.657164
Cl 0.000000 0.000000 2.134512
Na 0.000000 0.000000 4.630863

C4g
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Cl 0.000000 0.000000 -2.561760
Na 1.738880 -0.000000 -4.658142
Cl 0.000000 0.000000 6.475113
Na -0.000000 -1.738880 4.658142
Cl 0.000000 0.000000 -6.475113
Na -1.738880 0.000000 -4.658142

C4h
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Na 0.000000 2.032623 -1.389267
Cl -0.000000 -2.260235 -3.867923
Na -0.000000 -2.032623 -1.389267
Cl 0.000000 0.000000 0.331537
Na 0.000000 0.000000 2.916339
Cl 0.000000 0.000000 5.455030
Na 0.000000 0.000000 7.926314

C4i
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Na 4.765452 0.492299 0.000000
Cl 2.311966 1.027021 0.000000
Na -0.000000 -0.009801 -0.000000
Cl -2.313993 -1.040780 -0.000000
Na -4.764626 -0.492975 -0.000000
Na 9.551378 1.214821 0.000000
Cl -7.316506 -0.190605 -0.000000
Na -9.553283 -1.197116 -0.000000

C5a
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Cl 2.416282 -1.520286 -0.000000
Na 1.404071 0.876555 -0.000000
Cl -0.644266 0.256020 -2.053868
Na -0.644266 2.845682 -2.251560
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Na 0.635348 -2.357166 -1.796154
Cl -1.151113 -3.170861 -0.000000

C5b
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Na 1.736104 1.002340 1.802050
Na -1.736104 1.002340 -1.802050
Na 1.736104 1.002340 -1.802050
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Na -0.000000 -2.004680 1.802050
Cl 0.000000 -0.000000 -3.463214
Na -0.000000 -2.004680 -1.802050
Cl -1.942160 -1.121307 0.000000
Cl 1.942160 -1.121307 0.000000

C5c
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Cl 1.941215 2.566541 -0.394166
Na 0.000000 3.213383 -1.985329
Cl -1.941215 2.566541 -0.394166
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Na 0.000000 -2.649420 1.509858
Cl 0.000000 0.000000 1.969281
Na 0.000000 2.649420 1.509858
Cl 1.941215 -2.566541 -0.394166
Na -0.000000 -3.213383 -1.985329

C5d
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Cl -0.835077 -2.188513 -1.240374
Na -1.348816 0.300448 -1.977722

C5e
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Cl -1.939762 -1.417825 0.675263
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C5f
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Cl 0.259363 -2.192360 1.164032
Na 2.741828 -1.437021 0.953074
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Na 3.619945 1.594042 -1.178283

C5g
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Na -1.874732 -1.082377 -1.354174
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Na 0.000000 0.000000 3.112315
Cl 0.000000 0.000000 5.658445
Na 0.000000 0.000000 8.126536
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Cl -0.000000 -2.315740 -2.723446

C5h
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C5i
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Cl -4.870780 -0.206809 -0.610273
Na -7.106024 -0.167822 0.376308

C5j
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Cl -6.376377 -0.590415 0.068436
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Na -0.560812 -0.162791 -0.063834
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Na 0.337636 3.318663 0.039449
Cl 1.844627 1.146811 0.012370
Na 4.249256 0.254089 0.020875
Cl 6.644355 -0.610959 0.017278
Na 8.764241 -1.871184 0.003271

C5k
Na -2.699772 -2.140847 -0.000000
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Cl -5.530980 -1.776378 -0.000000
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Cl 7.350319 2.268138 0.000000
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C5l
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C6a
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Na 2.483365 -1.433771 -1.396197
Cl 2.155586 -1.244528 1.387921
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Cl -0.000000 -2.489056 -1.387921
Na 0.000000 0.000000 0.000000
Cl -2.155586 -1.244528 1.387921
Na -2.483365 -1.433771 -1.396197

C6b
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Na 2.092183 1.207922 -1.507070
Cl -0.000000 2.771113 -1.678898
Na -2.092183 1.207922 -1.507070
Cl -2.399854 -1.385556 -1.678898
Na -0.000000 -2.415845 -1.507070
Cl -0.000000 -2.347729 1.472455
Na -0.000000 2.977109 0.923571
Cl -2.033193 1.173864 1.472455
Na -2.578252 -1.488554 0.923571
Cl 2.399854 -1.385556 -1.678898
Na 2.578252 -1.488554 0.923571

C6c
Na 2.120491 1.815451 0.324573
Cl 0.000000 3.220740 -0.320350
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Na 0.000000 1.776975 -2.506751
Cl 1.966167 -0.000000 -1.845121
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C6f
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Cl -1.939115 0.080807 0.000000
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Na 0.692569 0.817298 -2.005826
Cl 0.093039 -1.298964 -3.469053
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Cl 2.155632 -0.583170 -0.000000
Cl -0.417980 -3.500331 -0.000000
Na 1.267733 4.527353 0.000000
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C7o
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Cl -1.780244 -2.444866 -1.998261
Na -2.551724 -0.881449 0.000000
Cl -1.876188 1.689748 0.000000
Na -2.378279 4.312340 0.000000
Cl 0.213244 4.537879 0.000000
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Na 3.056557 -0.396682 0.000000
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Na 0.361031 2.465539 -1.716049
Cl -1.780244 -2.444866 1.998261
Na -0.889248 -3.968885 0.000000

C7p
Na 2.461219 -1.737087 -0.638249
Cl 2.963295 0.410696 0.982775
Na 1.749576 1.743155 2.930947
Cl 0.000000 2.536131 0.096159
Na 2.340365 1.984002 -1.089246
Cl 2.305361 -0.075585 -2.766545
Cl -2.305361 0.075585 -2.766545
Na -2.461219 1.737087 -0.638249
Cl -2.963295 -0.410696 0.982775
Na -1.749576 -1.743155 2.930947
Cl -0.000000 -2.536131 0.096159
Na -2.340365 -1.984002 -1.089246
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Na 0.000000 0.000000 -3.841343
Cl -0.000000 -0.000000 3.673957

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C7s
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C7t
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Cl -0.335947 1.203804 -1.424155
Cl 0.538646 -2.808639 -0.696177
Na 1.611098 0.192792 0.566341
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Cl -0.359761 -0.193513 2.290733
Na -2.036887 1.312450 0.875843
Cl -3.221005 -1.720492 -0.360897
Na 3.067493 -3.195201 -0.525680
Cl 4.132729 -1.021573 0.318010
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C7u
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Na -1.845858 -0.152642 0.084121
Cl 0.228367 -0.829863 1.726361
Cl 5.025971 -1.532188 0.616959
Na 5.402724 0.905596 0.193088

C7v
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Na 1.223981 -3.211524 0.000000
Cl -3.194772 0.232294 0.000000
Na -1.583510 -0.788573 -2.007749
Cl 0.103493 -2.771447 -2.312478
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Na -5.614368 0.894900 0.000000
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C7w
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Cl -6.339466 -2.802347 0.000000
Na -4.006940 -3.863829 0.000000
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Cl -0.452175 4.078601 0.000000
Na -2.259839 5.806545 0.000000
Cl -3.898646 7.790644 0.000000
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C7y
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C8b
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Cl -2.003430 0.203627 -3.830174

C8c
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C8d
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Cl 0.482281 1.836047 3.257248
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C8e
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C8h
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Cl 0.019556 1.868505 -2.676755

C8i
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C8j
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C8k
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C8l

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C8m
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C8n
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Cl 1.215370 2.276715 2.075354
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Cl -1.415516 -0.507614 2.139690
Na -1.501984 2.123912 -2.046980
Cl -1.415516 -0.507614 -2.139690
Na -0.129765 -3.159359 -2.051738
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C8o
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C8p
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Na -1.645097 2.071039 2.069506
Cl 1.027397 2.511622 2.026891
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Na 1.351939 0.282414 3.518197
Cl 2.330239 -1.608400 2.065502

6.2 Structures Cationic Clusters: ωB97XD/aug-cc-pVDZ

C1a
Na 0.000000 -0.000000 2.523338
Cl 0.000000 0.000000 0.000000
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C2a
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Cl 0.000000 0.000000 -1.757538

C2b
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C2c
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C3b
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C3d
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C4b
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C4d
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C5a
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C5c
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C5f
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C5g
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C5j
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C5k
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C6e
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C6l
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C6n
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C6p
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C6t
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C6u
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C7a
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Cl 4.991968 0.923941 -1.682940
Na 5.440227 -0.968681 -0.089593

C8m
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Cl -0.017945 -1.130454 2.102596
Na -0.017945 -3.744162 1.868836
Cl -1.799837 -4.078141 0.000000
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Na 1.653052 -0.848209 0.000000
Cl 1.773190 1.793824 0.000000
Na -0.355350 1.668387 -1.864644
Cl -2.385285 1.306430 0.000000
Na -1.955859 -1.332136 0.000000
Cl -0.649471 4.311960 2.024239
Na -2.369429 4.042640 0.000000
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Na 1.068084 4.448256 0.000000
Cl 2.267914 -3.753098 0.000000
Na 4.636237 -4.681225 0.000000

C8o
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Cl 0.205441 3.691115 0.000000
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Na -1.217545 -2.149745 1.805067
Cl -3.097366 -2.440722 0.000000
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Na 3.880881 -1.501361 0.000000
Cl 3.238380 1.062248 0.000000
Na 2.844542 3.617371 0.000000
Cl -1.217545 0.498670 -2.058568
Na -1.821549 3.121627 -1.791488
Cl -3.732141 2.899446 0.000000
Na -3.249041 0.262685 0.000000
Cl 4.706319 -3.916464 0.000000
Na 2.365433 -4.791346 0.000000

6.3 Structures Anionic Clusters: B3LYP-D3/aug-cc-pVDZ

A1a
Cl 0.000000 -0.000000 2.522373
Na 0.000000 0.000000 0.000000
XX 0.000000 0.000000 -2.522373

A2a
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Cl 0.000000 -4.629091 -0.751003
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Cl 0.000000 4.629091 -0.751003

A2b
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A2c
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Cl -0.000000 -0.000000 3.385742

A3a
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Na 0.000000 1.918691 0.131225
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Cl -0.000000 -2.798247 -0.774518
Na 1.661635 -0.959345 0.131225
Cl 0.000000 0.000000 2.068823

A3b
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Cl 0.369623 -2.531921 -0.000000
Na 2.199485 -0.552061 -0.000000
Cl 4.664667 -0.005344 -0.000000

A3c
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Na 2.721246 3.133037 0.000000
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Na -1.647473 -2.840351 0.000000
Cl -1.680430 -5.332509 0.000000

A3d
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A4b
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Na 0.528122 -1.760764 -1.488818

A4c
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A4d
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Cl 0.000000 0.000000 -3.242874
Na 0.000000 0.000000 2.002441
Cl 0.000000 0.000000 4.520359

A4e
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Na 1.807071 4.594333 0.000000
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Na -0.000000 -6.808773 -0.225150
Cl -0.000000 -8.991661 0.921948

A5a
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A5b
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Na 1.631124 -2.358406 -0.376733
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A5e
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Na -2.750147 -0.982600 0.032829
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A5g
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Na 0.000000 0.000000 4.505604

Cl 0.000000 0.000000 6.958224

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Cl 2.307767 -1.769892 -0.000000

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A6g
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A6h
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A6m
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A6n
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A8c
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6.4 Structures Anionic Clusters: ωB97XD/aug-cc-pVDZ

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Cl	3.428404	-0.267491	2.049643
Cl	-1.551819	-1.448836	-2.869546
Na	0.898052	-1.105112	-2.029285

A8k

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Cl -0.000000 3.598358 1.692404
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Na -1.596012 -1.926070 0.059777
Cl 0.000000 -2.130339 -2.059047
Na 1.596012 -1.926070 0.059777
Cl 3.258081 -0.000000 -0.865244
Na -0.000000 -1.785101 3.590962
Cl -0.000000 -0.000000 5.492171
Na -1.541203 0.000000 -3.119823
Cl 0.000000 2.130339 -2.059047
Na 1.596012 1.926070 0.059777
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Cl 0.000000 0.000000 -5.295155
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A8l

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Cl -0.792190 -1.944099 -1.070830
Na -3.086769 -1.490524 0.584110
Cl -4.588879 -1.255508 -1.619237
Na 4.094841 -0.948897 0.386549
Cl 3.897126 0.809670 -1.553141
Na 1.568100 -0.785784 -1.600231
Cl 2.853229 -3.105475 -0.317866
Na 0.620572 -2.419961 1.173189
Cl -1.464016 -1.707470 2.784102
Na -0.653712 0.853097 2.089294
Cl 0.454890 3.576700 1.533862
Cl -2.882551 1.397897 0.611675
Na -1.299383 3.222603 -0.339305

A8m

Cl 1.409408 -1.455378 -1.822283
Na 0.000000 -3.658902 -0.759288
Cl -1.721696 -3.843508 -2.732766
Na -1.389747 -1.258527 -2.208268
Cl -1.409408 1.455378 -1.822283
Na -1.347908 1.043296 0.882903
Cl -1.731044 -1.627927 0.581457
Na -0.725957 -2.460626 2.871678
Cl 1.266504 -3.701831 1.690288
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Na 0.725957 2.460626 2.871678
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Na 0.000000 3.658902 -0.759288

A8n

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Cl	2.058690	-2.134208	-0.003226
Na	-0.055649	-1.926156	1.598605
Cl	0.873937	0.000898	3.256417
Na	-3.597615	-1.787648	0.017872
Cl	-5.490990	0.005849	0.008197
Na	3.113905	-0.004646	-1.547966
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Na	-0.056357	1.925138	1.594913
Cl	-1.694752	-3.596749	0.010281
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A8o

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Cl 1.215755 0.417489 -0.719769
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Cl 0.693191 -3.595359 -0.603443
Na -0.491709 -2.935396 1.612567
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Na 0.187355 0.438844 1.807008
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Cl -2.788411 -1.322209 -3.132939
Cl -5.400752 1.431236 0.112156
Na -3.104519 1.751196 1.229091
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Cl 3.276585 3.809032 -1.235342
Na 0.932838 3.142116 -0.379272

A8p

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Na 1.796044 -0.000000 -1.387538
Cl -0.000000 -0.000000 -3.700093

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Cl 0.000000 4.163266 2.506342
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Na -1.796044 0.000000 -1.387538
Cl 2.061025 2.674267 -1.587115
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Cl -0.000000 -4.163266 2.506342

A8q
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Cl 0.504280 -1.368282 3.856151
Na -1.396873 -2.104659 2.315977

A8s
Cl 1.244070 0.645475 0.033909
Na 2.940864 2.771093 -0.184334
Cl 0.987889 4.518092 0.188026
Na -0.684801 2.476719 0.554993
Cl -1.722643 0.857675 2.540387
Na 0.275392 -0.913008 2.020856
Cl -1.323446 -2.518645 0.260489
Na 1.110132 -3.592461 -0.063865
Cl 1.934410 -2.439863 -2.261466
Na 3.452099 -0.929279 -0.314601
Cl 5.034380 1.215480 -0.547680
Na -3.171945 -0.521116 0.759898
Cl -2.213853 1.089757 -1.596935
Na -0.189152 -0.839553 -1.664292
Cl 2.495476 -2.530222 1.871786
Cl -5.770620 -0.450909 -0.017806
Na -4.761340 0.949763 -1.836115

A8t
Na 3.510383 1.070180 0.592431
Cl 5.214262 -0.998881 0.864456
Na 3.107082 -2.440173 0.380579
Cl 1.368720 -0.563642 1.241757
Na -0.366187 1.464116 1.555050
Cl 1.677449 3.269948 1.181683
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Cl 2.993995 1.211097 -2.171691
Na 1.114245 -0.604885 -1.633954
Cl -0.968066 1.204836 -1.328944
Na -4.404756 -0.492692 1.194628
Cl -2.179654 -0.262025 2.585736
Cl -3.376102 -2.145505 -0.691989
Na -0.993463 -1.922248 0.588165
Cl 0.996214 -3.226818 -1.119796
Cl -5.492199 1.337729 -0.343301
Na -3.491673 0.332215 -1.673899

A8u
Cl -1.449246 0.623034 -1.130940
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Cl -0.425050 4.495450 -1.043743
Na 0.843718 2.147821 -1.294804
Cl 1.446781 1.272246 1.374950
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Cl 1.453924 -3.116811 -0.361049
Na -0.030150 -1.533128 -2.052333
Cl -2.493020 -2.940123 -1.539024
Na -0.962858 -3.449297 0.576575
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Na -1.158253 0.541704 1.742274
Cl 2.100013 0.153385 -2.599050
Na 3.868146 1.340854 2.190383
Cl 5.333770 -0.343875 1.058503

6.5 Structures Neutral Clusters: B3LYP-D3/aug-cc-pVDZ

N1a
Na 0.000000 0.000000 -1.450473
Cl 0.000000 0.000000 0.938541

N2a
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Cl 0.000000 -0.000000 -2.002027

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N3b
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Na 0.000000 -0.000000 -2.718573
Cl -0.000000 0.000000 2.768297

N4a
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N4b
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Cl -0.064560 -1.791912 -1.823009
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N4e
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Cl 0.000000 -2.523214 -1.855947

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N5b
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Cl -3.019319 0.000000 -0.632331
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N5d
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N6b
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Cl 2.375191 -1.371317 -1.457361

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Cl -3.578423 -0.099968 -0.642400
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Na -1.024668 0.116274 -1.666424
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Cl 1.654739 0.273173 -1.882801

N6e
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N6f
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N6i
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Cl 1.034108 -4.356146 -0.000000
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Cl -1.815633 -0.209186 -0.000000
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Cl -1.591708 3.833845 0.000000
Na -0.000000 1.766802 0.000000
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Na -3.841343 5.075387 0.000000

N6j
Cl 0.000000 0.000000 -0.077569
Na 0.000000 2.288441 -1.397734
Cl 0.940184 4.295083 -2.727365
Na 0.065778 5.603977 -0.752968
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Na 0.722589 -1.681118 2.223533
Cl -0.000000 -0.000000 4.001505

N6k
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Cl 0.878024 -4.638124 -0.000000
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Cl 1.903841 -0.515854 -0.000000
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Na -3.639142 1.682417 0.000000
Na 4.465848 -0.371494 -0.000000
Cl 5.563645 -2.627505 -0.000000

N6l
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Cl 5.714787 0.732562 1.358340
Na 5.319788 -1.705362 0.845081

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N8m
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Na -4.665014 -1.709476 0.490074

N8p
Na 3.461568 0.759705 -1.010163
Cl 4.971985 -1.344994 -0.799246
Na 2.895665 -2.163512 0.449875
Cl 1.112428 -0.886962 -1.441936
Na -0.296287 1.318816 -1.551334
Cl 1.784082 2.981902 -1.467067
Na 1.456842 2.983384 1.118331
Cl 2.755319 0.834428 1.865728
Na 0.446844 -0.333500 1.958556
Cl 0.380260 -2.925455 1.579756
Na -0.842452 -2.446083 -0.710993
Cl -2.778796 -0.715524 -1.423296
Na -3.492874 0.796659 0.880472
Cl -1.082542 1.771572 1.198804
Cl -6.013971 0.310095 0.666256
Na -5.373761 -0.954201 -1.411380

N8q
Na -0.516295 2.504296 -0.860865
Cl 1.188919 4.444674 -0.520702
Na 2.476864 2.496403 0.525285
Cl 1.610218 0.653093 -1.439338
Na -0.140081 -1.301990 -1.608681
Cl -2.206032 0.416774 -1.854629
Na -2.568928 -0.162350 1.392778
Cl -0.634235 1.617274 1.775539
Na 1.077253 -0.303676 1.902068
Cl 3.644683 0.110517 1.600136
Na 3.495604 -1.055073 -0.796732
Cl 2.085790 -3.228004 -1.519266
Na 0.960403 -4.203004 0.536657
Cl -0.621443 -2.284773 1.170071
Cl -5.112667 -0.507238 0.988694
Na -4.715636 0.136357 -1.400384

N8r
Cl -1.542006 1.266698 0.000000
Na -1.324191 3.880086 0.000000
Cl -1.732812 6.467174 0.000000
Na -1.206810 8.986201 0.000000
Cl 1.309901 9.143194 0.000000
Na 1.191961 6.555878 0.000000
Cl 1.406570 3.942890 0.000000
Na 1.206810 1.331437 0.000000
Cl 1.542006 -1.266698 0.000000
Na 1.324191 -3.880086 0.000000
Cl 1.732812 -6.467174 0.000000
Na -1.191961 -6.555878 0.000000
Cl -1.406570 -3.942890 0.000000
Na -1.206810 -1.331437 0.000000
Cl -1.309901 -9.143194 0.000000
Na 1.206810 -8.986201 0.000000

N8s
Cl -0.000000 -0.000000 0.485440
Na -0.812647 -1.673322 2.863524
Cl -0.000000 -0.000000 4.604485
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Cl 1.517858 3.634449 1.272999
Na 0.529678 2.230371 -0.798607
Cl 0.000000 4.190670 -2.430184
Na -1.089634 6.488032 -2.835347
Cl -0.419643 7.920699 -0.872288
Na 0.759181 5.783701 -0.026236
Na -0.529678 -2.230371 -0.798607
Cl -1.517858 -3.634449 1.272999
Na -0.759181 -5.783701 -0.026236
Cl -0.000000 -4.190670 -2.430184
Na 1.089634 -6.488032 -2.835347
Cl 0.419643 -7.920699 -0.872288

6.6 Structures Neutral Clusters: ωB97XD/aug-cc-pVDZ

N1a
Na 0.000000 0.000000 -1.458648
Cl 0.000000 0.000000 0.943831

N2a
Na 0.000000 1.603431 0.000000
Cl -0.000000 -0.000000 2.014710
Na -0.000000 -1.603431 0.000000
Cl 0.000000 -0.000000 -2.014710

N3a
Na 0.000000 2.329987 -0.000000
Cl 2.373080 1.370099 0.000000
Na 2.017828 -1.164993 0.000000
Cl -2.373080 1.370099 -0.000000
Na -2.017828 -1.164993 -0.000000
Cl -0.000000 -2.740197 0.000000

N3b
Na -0.000000 1.463121 0.645222
Cl 1.837539 -0.000000 -0.924305
Na -0.000000 -1.463121 0.645222
Cl -1.837539 0.000000 -0.924305
Na 0.000000 0.000000 -2.698098
Cl -0.000000 -0.000000 2.759446

N4a
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Cl 1.438020 -1.438020 1.438020
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Cl -1.438020 1.438020 1.438020
Na -1.223849 1.223849 -1.223849
Cl -1.438020 -1.438020 -1.438020
Cl 1.438020 1.438020 -1.438020
Na 1.223849 -1.223849 -1.223849

N4b
Cl 2.478677 2.478677 -0.000000
Na 0.000000 3.109557 0.000000
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Cl 2.478677 -2.478677 -0.000000
Na 3.109557 -0.000000 0.000000

N4c
Na -0.144621 -1.830198 1.486917
Cl 0.670311 -3.766265 0.000000
Na -0.144621 -1.830198 -1.486917
Cl -2.204848 -0.828358 0.000000
Na -1.184889 1.587313 0.000000
Cl 1.308761 0.208505 0.000000
Cl -0.144621 3.974631 0.000000
Na 2.046564 2.709017 0.000000

N4d
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Na 0.782587 0.263778 0.000000
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Cl -1.809821 1.545101 0.000000
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Cl -0.082131 -1.790128 -1.842819
Na 0.854721 -3.302241 0.000000

N4e
Na 0.000000 1.623045 0.386156
Cl 0.000000 2.306852 -2.086822
Na 0.000000 -0.000000 -3.182988
Cl -0.000000 -2.306852 -2.086822
Na -0.000000 -1.623045 0.386156
Cl -1.815918 0.000000 1.720875
Cl 1.815918 -0.000000 1.720875
Na 0.000000 0.000000 3.541785

N4g
Cl 0.000000 0.000000 -1.291512
Na -0.000000 2.458494 -2.200677
Cl -0.000000 4.032222 -0.251683
Na -0.000000 1.926360 1.289938
Cl -0.000000 -0.000000 2.973482
Na -0.000000 -1.926360 1.289938
Cl -0.000000 -4.032222 -0.251683
Na -0.000000 -2.458494 -2.200677

N5a
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Cl 1.267452 1.433350 -0.000000
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Cl -0.794991 -0.798395 -2.444940
Na -0.794991 1.760894 -1.773287
Cl -2.729343 1.844788 0.000000
Na -1.966673 -0.789758 0.000000
Cl -0.794991 -0.798395 2.444940
Na 1.743311 -0.896512 1.662386
Cl 3.097189 -2.288942 -0.000000

N5b
Na 1.150849 1.092124 1.708017
Cl -0.536924 2.375201 0.012414
Na 1.155381 1.117714 -1.697142
Cl 0.504296 -1.433830 -2.001205
Na -1.333301 -1.590314 -0.006197
Cl 0.506943 -1.464221 1.985733
Na 2.270100 -1.660986 -0.012472
Cl 3.195161 0.842300 0.006931
Cl -3.798469 -0.724829 -0.000637
Na -3.043678 1.667958 0.002793

N5c
Na 0.000000 0.000000 -1.431204
Cl 0.000000 2.865271 -0.747512
Na -1.832149 -1.832062 0.749479
Cl 0.000000 0.000000 1.980309
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Cl 2.864033 -0.000000 -0.749520
Na 1.832149 -1.832062 0.749479
Cl -2.864033 0.000000 -0.749520
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Cl -0.000000 -2.865271 -0.747512

N5d
Na -0.107907 -1.140604 2.644940
Cl -0.249750 -1.361911 -0.000000
Na -0.107907 -1.140604 -2.644940
Cl 0.046226 -1.415528 -5.236533
Na 0.185396 1.106160 -5.161016
Cl 0.046226 1.690940 -2.628401
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Cl 0.046226 1.690940 2.628401
Na 0.185396 1.106160 5.161016
Cl 0.046226 -1.415528 5.236533

N5e
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Cl 2.535341 1.683018 0.000280
Na -0.110126 1.783065 0.000477
Cl -2.705126 2.050264 -0.000694
Na -2.966105 -0.250131 -1.486608
Cl -4.548834 -1.622512 0.000188
Na 4.963093 0.719786 -0.000652
Cl 4.617397 -1.783251 -0.000301

N5f
Cl 2.519767 3.468162 -0.000000
Na -0.000000 3.918055 -0.000000
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Cl -0.000000 -4.286884 -0.000000
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Cl 4.077069 -1.324720 -0.000000
Na 3.726291 1.210745 -0.000000

N6a
Cl 0.000000 -0.000000 2.152625
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Na -2.634441 -0.000000 1.698318

N6b
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Cl -0.000000 2.757172 -1.472012
Na 2.175119 1.255806 -1.226573
Cl 2.387781 1.378586 1.472012
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Cl -0.000000 -2.757172 1.472012
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Cl -2.387781 1.378586 1.472012
Na -2.175119 1.255806 -1.226573
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Cl 2.387781 -1.378586 -1.472012

N6c
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Na 0.026015 1.735063 -2.177696
Cl 0.051187 3.254830 -0.068864
Na 2.149523 1.736311 0.664445
Cl 1.977875 -0.030057 -1.671148
Na -0.026324 -1.735664 -2.177586
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Cl 3.011780 -0.041923 2.281096
Cl -3.011315 0.042471 2.281460
Na -2.149435 -1.736148 0.664992
Na 2.084756 -1.797381 0.675914

N6d
Na -1.287690 -1.580282 0.568139
Cl 0.667473 -2.798957 -0.725168
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Cl 0.621837 -0.001420 1.933115
Cl 3.697110 0.000406 -0.474437
Na 2.425365 1.824169 0.913233
Na 1.082328 0.000906 -1.523384
Cl 0.668670 2.799166 -0.723098
Na -1.284005 1.574470 0.568197
Cl -3.408252 -0.000206 1.479642
Na -4.157052 0.005781 -0.971753
Cl -1.731563 0.000079 -1.790459

N6e
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N6f
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Na 1.273738 6.428573 0.142526

N6h
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Na 2.860406 -1.903253 0.100169

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N6j
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Na -0.000000 -5.702009 -0.853027
Cl -0.900390 -4.351610 -2.799342
Na -0.106869 -2.373330 -1.311585
Na 0.688330 -1.655225 2.215672
Cl 0.000000 -0.000000 4.049020

N6k
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Na 3.085372 -3.713579 -0.000000
Cl 1.903461 -0.699574 -0.000000
Na 0.000000 1.181138 0.000000
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Cl -5.202339 3.880045 0.000000
Na -3.507559 1.903791 0.000000
Na 4.516732 -0.469618 -0.000000
Cl 5.514897 -2.771462 -0.000000

N6l
Na -4.242320 -0.253432 1.477805
Cl -5.796003 -1.644959 -0.022930
Na -4.221586 -0.246627 -1.495409
Cl -3.979716 2.043686 -0.003182
Na -1.379709 1.805556 0.011363
Cl 1.256698 1.656377 0.020658
Na 3.843644 1.000526 0.008511
Cl 3.371861 -1.779556 0.027368
Na 0.834242 -1.020200 0.023045
Cl -1.821856 -0.903121 0.009044
Cl 6.444683 0.851770 -0.034503
Na 5.976060 -1.632307 -0.019836

N6n
Cl -1.464784 1.810424 -0.003002
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Cl -6.103316 0.580012 0.003770
Na -5.100064 -1.781491 0.001657
Cl -2.732645 -2.735140 -0.002258
Na -0.968817 -0.848264 -0.003953
Cl 1.708954 -0.615477 -0.001845
Na 1.213739 2.150451 -0.000180
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Cl 5.643465 -1.751608 0.002294

N6o
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N7b
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N7d
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N7e
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N7h
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N7i
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Cl -0.232810 -3.439519 0.000000
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Na -2.841018 1.194378 -0.000000
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Cl -0.893005 3.147797 -0.000000

N7j
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Cl 1.712916 0.812110 1.918762
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