

Impact of Confinement in Multimolecular Inclusion Compounds of Melamine and Cyanuric Acid

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Figure S1. Top (left) and side (right) views of CA4-2@NaCl complex

Figure S2. LMOEDA energy components as a function of r distance [Å]. Chemical structures of the scanned systems are shown, where r is the scanned distance.

Figure S3. Correlations between LMOEDA parameters (BLYP-D3/6-311++G**) and some topological properties of QTAIM (ω -B97XD/6-311++G**) for the CA...Cl⁻ complex. The molecular graph of the equilibrium geometry is presented.

Figure S4. Correlations between LMOEDA parameters (BLYP-D3/6-311++G**) and some topological properties of QTAIM (ω -B97XD/6-311++G**) for the CA...Cl⁻ complex. The molecular graph of the equilibrium geometry is presented.

Figure S5. Correlations between LMOEDA parameters (BLYP-D3/6-311++G**) and some topological properties of QTAIM (ω -B97XD/6-311++G**) for the CA...Ar complex. The molecular graph of the equilibrium geometry is presented.

Figure S6. Correlations between LMOEDA parameters (BLYP-D3/6-311++G**) and some topological properties of QTAIM (ω -B97XD/6-311++G**) for the M...Ar complex. The molecular graph of the equilibrium geometry is presented.

Table S1. Topological parameters (in a.u.) at bond critical points of encapsulation interactions.

Table S2. Changes in local topological properties (in a.u.) at H...N and H...O bond critical points. (e.g.: $\Delta\rho = \rho_{\text{cage}@A} - \rho_{\text{cage}}$; A = Na⁺, Cl⁻, Ar).

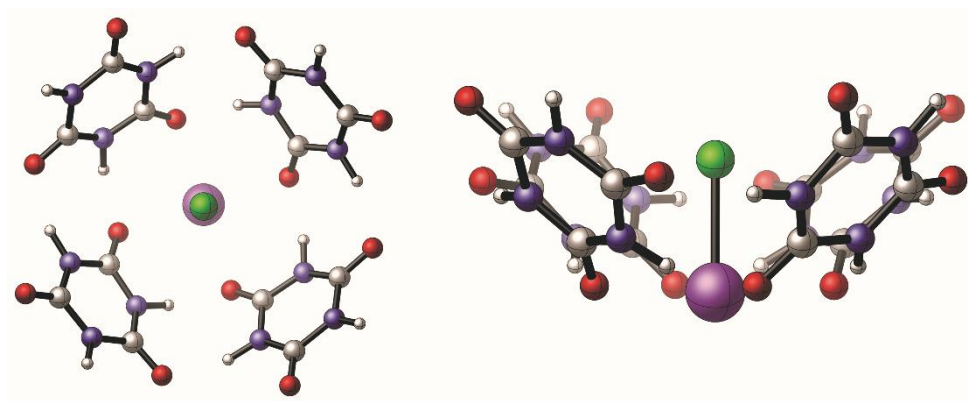


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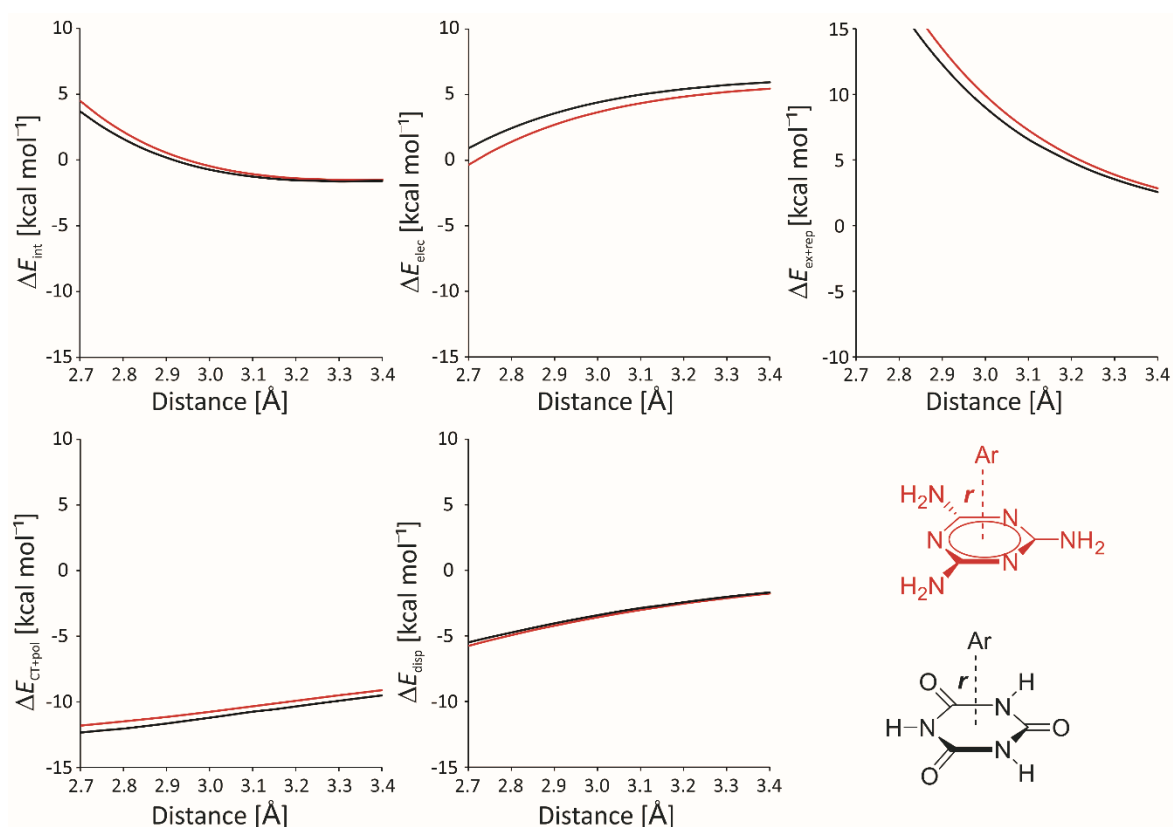


Figure S2. LMOEDA energy components as a function of r distance [Å]. Chemical structures of the scanned systems are shown, where r is the scanned distance.

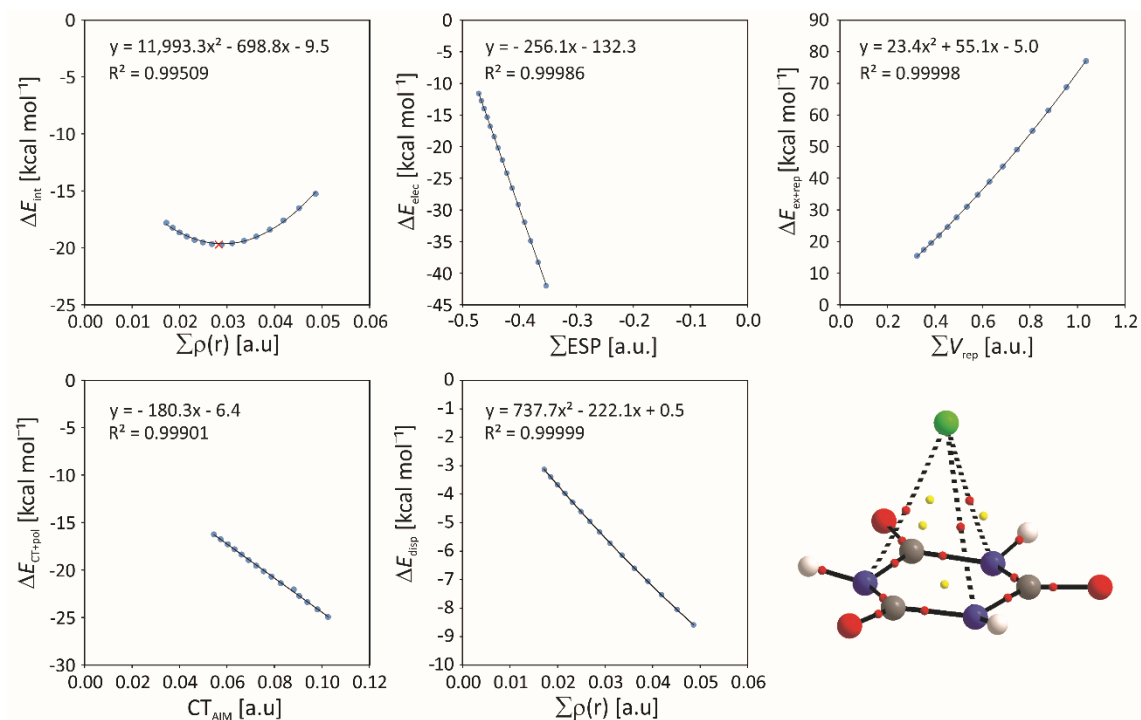


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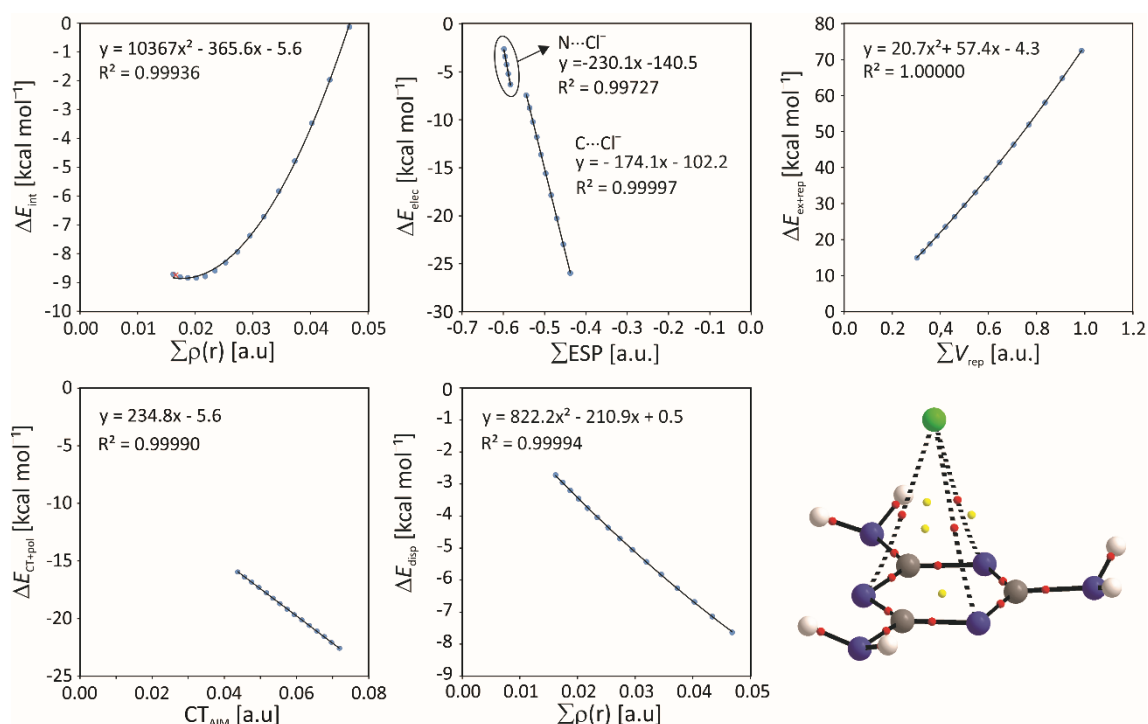


Figure S4. Correlations between LMOEDA parameters (BLYP-D3/6-311++G**) and some topological properties of QTAIM (ω -B97XD/6-311++G**) for the M...Cl⁻ complex. The molecular graph of the equilibrium geometry is presented.

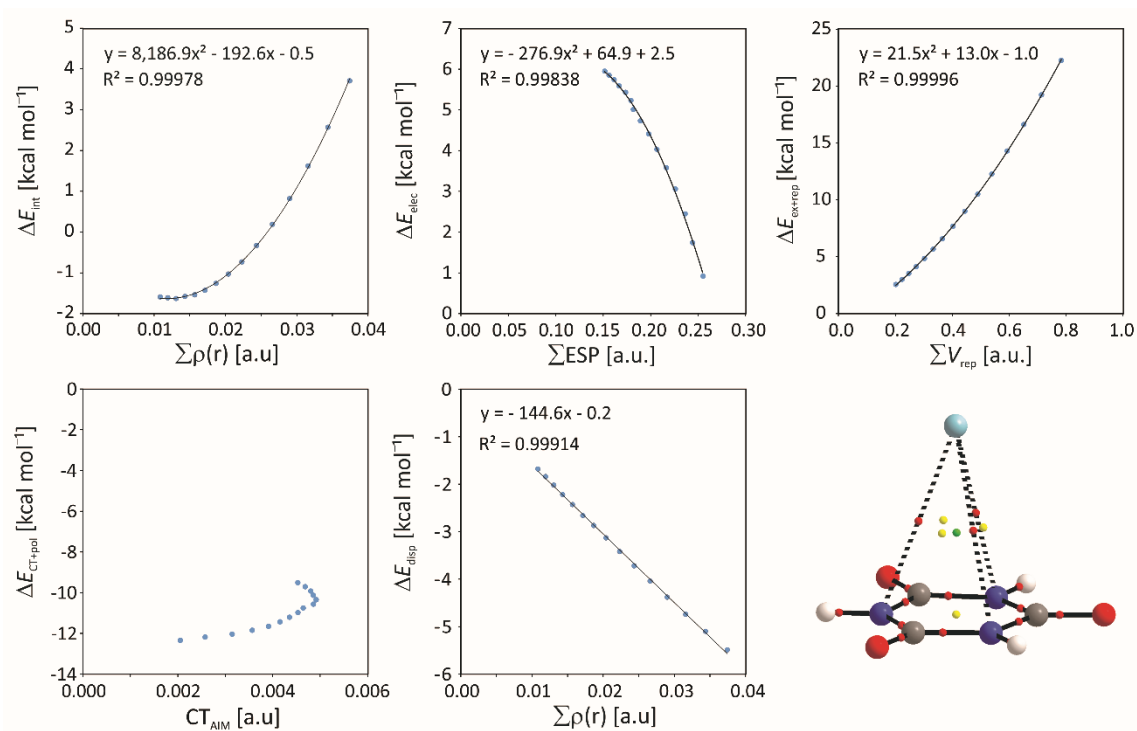


Figure S5. Correlations between LMOEDA parameters (BLYP-D3/6-311++G**) and some topological properties of QTAIM (ω -B97XD/6-311++G**) for the CA...Ar complex. The molecular graph of the equilibrium geometry is presented.

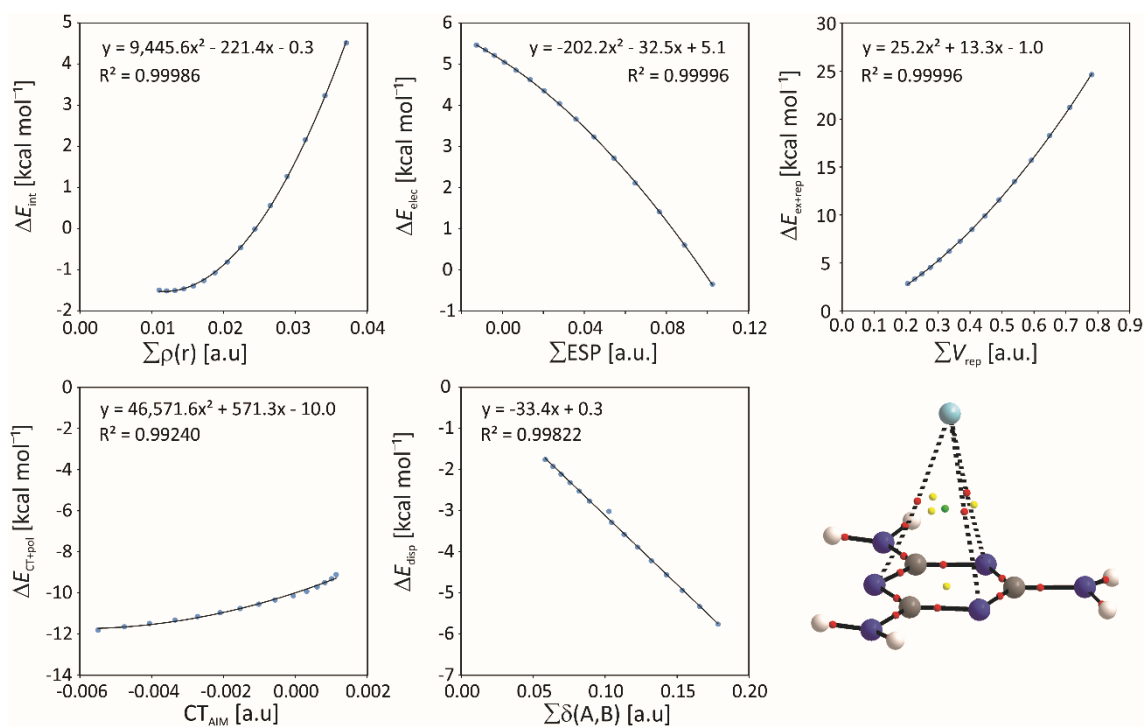


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Table S1. Topological parameters (in a.u.) at bond critical points of encapsulation interactions.

Complex	Atoms	ρ	$\nabla^2\rho$	H	ε	$\delta(A.B)$	V_{rep}
$M_4@Cl^-$	C...Cl ⁻	0.007	0.022	0.001	1.058	0.023	0.267
	C...Cl ⁻	0.007	0.022	0.001	1.006	0.023	0.270
	H...Cl ⁻	0.023	0.063	0.001	0.075	0.104	0.916
	H...Cl ⁻	0.023	0.063	0.001	0.074	0.105	0.920
$M_4@Ar$	N...Ar	0.003	0.012	0.001	0.722	0.017	0.131
	N...Ar	0.003	0.012	0.001	0.914	0.017	0.136
	N...Ar	0.004	0.013	0.001	0.312	0.024	0.154
	N...Ar	0.004	0.014	0.001	0.351	0.025	0.156
$(AC_4-1)@Cl^-$	N...Cl ⁻	0.004	0.010	0.000	3.435	0.023	0.142
	N...Cl ⁻	0.004	0.010	0.000	2.264	0.024	0.148
	N...Cl ⁻	0.004	0.010	0.000	1.533	0.025	0.151
	N...Cl ⁻	0.004	0.012	0.000	1.253	0.028	0.174
	N...Cl ⁻	0.004	0.012	0.000	1.556	0.029	0.181
	N...Cl ⁻	0.005	0.012	0.000	0.745	0.030	0.183
	N...Cl ⁻	0.005	0.012	0.000	1.050	0.030	0.186
	N...Cl ⁻	0.005	0.012	0.000	1.218	0.030	0.187
	N...Cl ⁻	0.005	0.012	0.000	0.836	0.031	0.190
	N...Cl ⁻	0.005	0.012	0.000	0.795	0.031	0.192
$(AC_4-1)@Ar$	N...Ar	0.005	0.013	0.000	0.927	0.031	0.192
	N...Ar	0.003	0.011	0.001	1.903	0.016	0.123
	N...Ar	0.003	0.011	0.001	1.630	0.015	0.124
	N...Ar	0.003	0.012	0.001	2.160	0.016	0.125
	N...Ar	0.003	0.012	0.001	1.876	0.016	0.126
	N...Ar	0.003	0.012	0.001	2.963	0.016	0.127
	N...Ar	0.003	0.012	0.001	1.785	0.016	0.129
	N...Ar	0.003	0.012	0.001	1.505	0.016	0.130
	N...Ar	0.003	0.012	0.001	1.497	0.016	0.130
	$(AC_4-2)@Na^+$	O...Na ⁺	0.015	0.090	0.004	0.035	0.058
O...Na ⁺		0.015	0.090	0.004	0.035	0.058	0.566
O...Na ⁺		0.015	0.090	0.004	0.035	0.058	0.566
O...Na ⁺		0.015	0.090	0.004	0.035	0.058	0.567
$(AC_4-2)@Cl^-$	C...Cl ⁻	0.005	0.016	0.001	2.970	0.017	0.196
	C...Cl ⁻	0.005	0.016	0.001	3.208	0.017	0.197
	N...Cl ⁻	0.006	0.017	0.001	0.918	0.046	0.251
	N...Cl ⁻	0.006	0.017	0.001	1.015	0.046	0.252
$(AC_4-2)@NaCl$	O...Cl ⁻	0,007	0,019	0,001	0,786	0,044	0,307
	O...Cl ⁻	0,007	0,019	0,001	0,784	0,044	0,307
	O...Cl ⁻	0,007	0,019	0,001	0,777	0,044	0,307
	O...Cl ⁻	0,007	0,019	0,001	0,785	0,044	0,307
	O...Na ⁺	0,013	0,076	0,003	0,063	0,050	0,544
	O...Na ⁺	0,013	0,076	0,003	0,063	0,050	0,545
	O...Na ⁺	0,013	0,076	0,003	0,063	0,050	0,545
	O...Na ⁺	0,013	0,076	0,003	0,063	0,050	0,545
$(AC_4-2)@Ar$	N...Ar	0.003	0.010	0.001	1.054	0.015	0.104
	N...Ar	0.003	0.010	0.001	0.998	0.015	0.104
	N...Ar	0.003	0.010	0.001	0.982	0.015	0.104
	N...Ar	0.003	0.010	0.001	1.055	0.015	0.104

CA ₂ M ₂ @Cl ⁻	N...Cl ⁻	0.005	0.014	0.001	2.413	0.034	0.219
	N...Cl ⁻	0.005	0.015	0.001	2.652	0.034	0.221
	C...Cl ⁻	0.009	0.029	0.001	0.725	0.030	0.373
	C...Cl ⁻	0.009	0.029	0.001	0.693	0.030	0.378
CA ₂ M ₂ @Ar	C...Ar	0.003	0.014	0.001	0.222	0.008	0.133
	C...Ar	0.003	0.015	0.001	0.390	0.009	0.140
	C...Ar	0.004	0.015	0.001	0.271	0.011	0.149
	C...Ar	0.004	0.016	0.001	0.365	0.012	0.156

Table S2. Changes in local topological properties (in a.u.) at H...N and H...O bond critical points. (e.g.: $\Delta\rho = \rho_{\text{cage@A}} - \rho_{\text{cage}}$; A = Na⁺, Cl⁻, Ar).

Complex	Guest	Atoms	$\Delta\rho$	ΔH	$\Delta\varepsilon$	$\Delta\delta(\text{H,N/O})$	ΔV_{rep}
M ₄	Cl ⁻	H...N	-0.168	0.001	-0.008	-0.007	-0.011
	Ar	H...N	0.000	0.000	-0.001	0.000	0.070
CA ₄ -1	Cl ⁻	H...O	0.005	0.000	0.004	0.011	0.221
	Ar	H...O	0.000	0.025	0.042	0.768	-0.598
CA ₄ -2	Na ⁺	H...O	-0.005	0.000	0.008	-0.009	-0.136
		H...O	0.006	-0.002	0.028	0.016	0.325
	Cl ⁻	H...O	0.007	-0.001	-0.019	0.016	-1.768
		H...O	0.000	0.000	0.002	0.002	-2.235
	NaCl	H...O	0.006	-0.001	0.002	0.018	0.316
		H...O	0.002	-0.001	0.023	0.007	0.228
	Ar	H...O	0.001	0.000	-0.001	0.003	0.089
		H...O	-0.001	0.000	0.000	-0.001	0.063
M ₂ CA ₂	Cl ⁻	H...O	-0.002	0.000	-0.007	-0.005	-0.104
		H...O	-0.001	0.000	0.030	-0.007	-0.109
		H...N	-0.002	0.001	0.015	-0.003	-0.163
	Ar	H...O	0.000	0.000	0.001	0.001	0.048
		H...O	0.000	0.000	-0.002	0.001	0.066
		H...N	0.000	0.000	0.000	0.000	0.092