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

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

Andre Nicolai Petelski,[a] Silvana Carina Pamies,[a] Agustín Gabriel Sejas,[a] Nélida María Peruchena,*[b,c] and Gladis Laura Sosa*[a,c]

[a.] *Grupo de Investigación en Química Teórica y Experimental (QuiTEx), Departamento de Ingeniería Química, Facultad Regional Resistencia, Universidad Tecnológica Nacional, French 414 (H3500CHJ), Resistencia, Chaco, Argentina.*
[b.] *Laboratorio de Estructura Molecular y Propiedades, Facultad de Ciencias Exactas y Naturales y Agrimensura, Universidad Nacional del Nordeste, Avenida Libertad 5460, 3400 Corrientes, Argentina.*
[c.] *Instituto de Química Básica y Aplicada del Nordeste Argentino, IQUIBA-NEA, UNNE-CONICET, Avenida Libertad 5460, 3400 Corrientes, Argentina.*

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

Figure S2. LMOEDA energy components as a function of ***r*** dinstance [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.

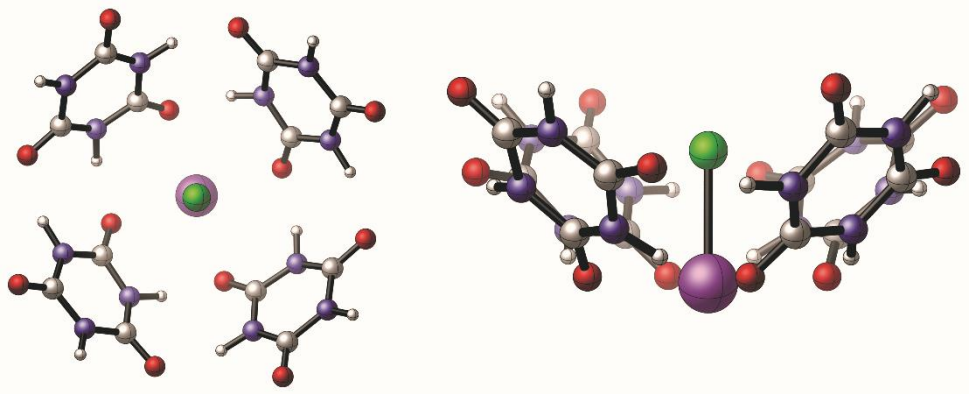
Figure S4. Correlations between LMOEDA parameters (BLYP-D3/6-311++G**) and some topological properties of QTAIM (ω-B97XD/6-311++G**) for the CA···Cl– complex. The molecular graph of the equilibrium geometry is presented.

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.: $\Delta\rho = \rho_{cage@A} - \rho_{cage}$; A = Na^+, Cl^-, Ar).



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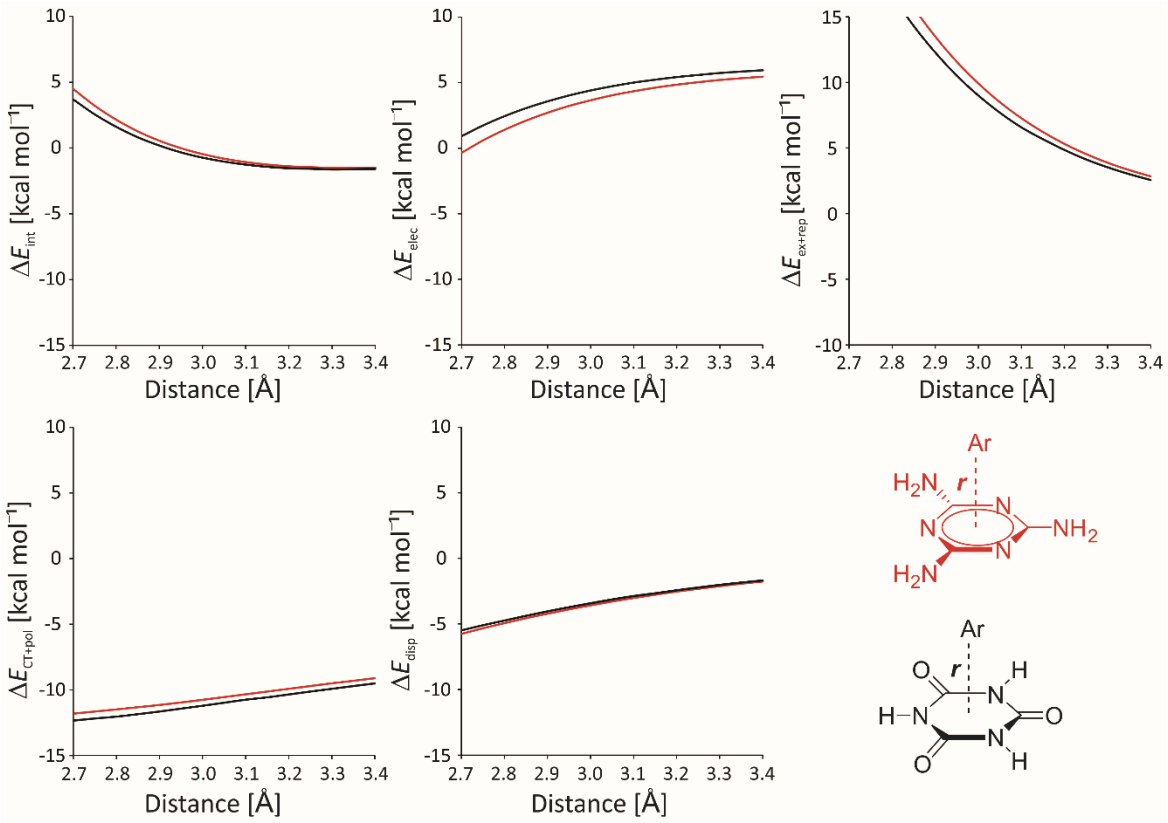

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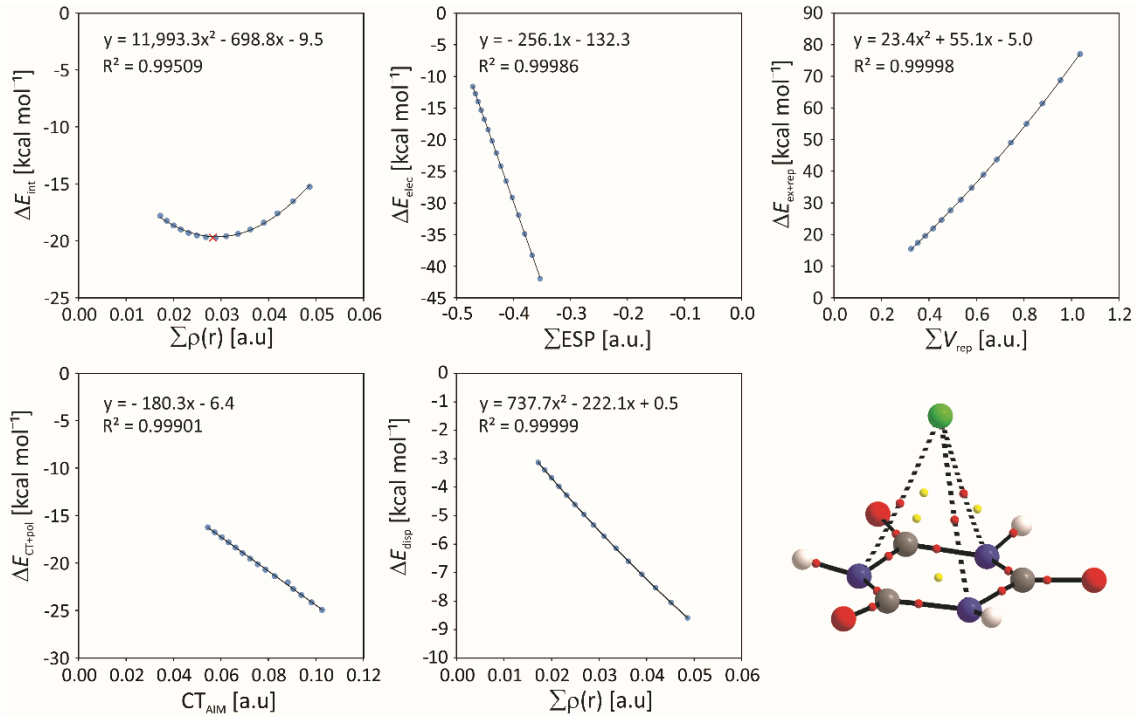
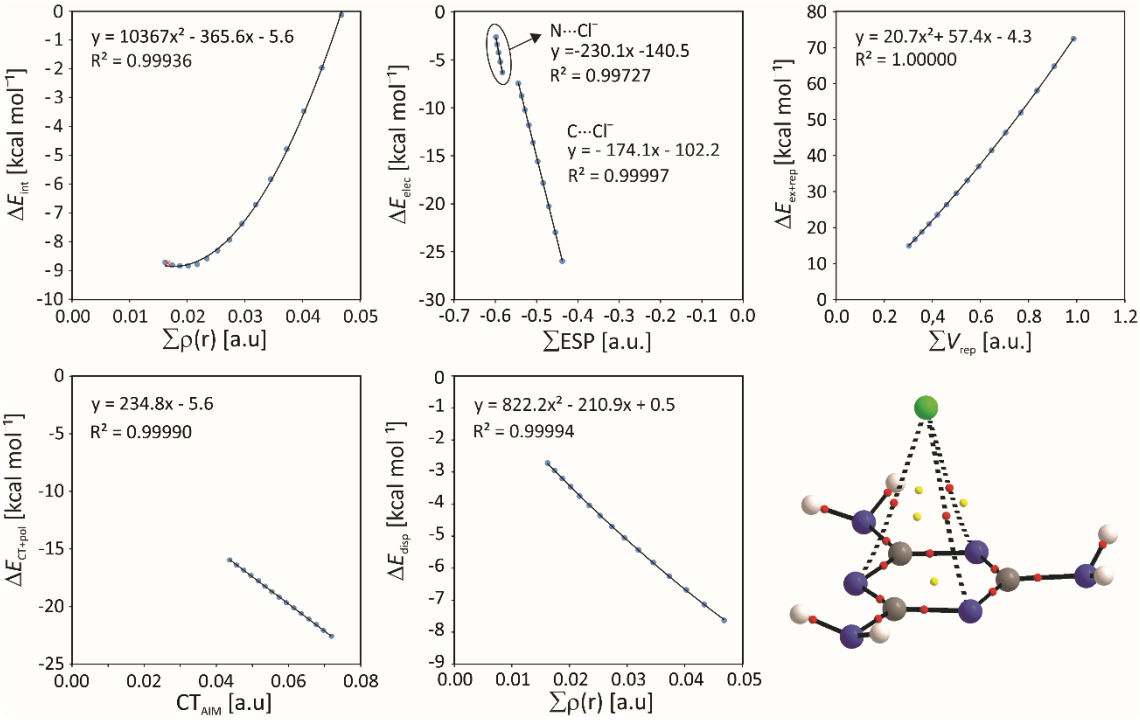


Figure S3. Correlations between LMOEDA parameters (BLYP-D3/6-311++G**) and some topological properties of QTAIM (ω-B97XD/6-311++G**) for the CA···Cl^- complex. The molecular graph of the equilibrium geometry is presented.



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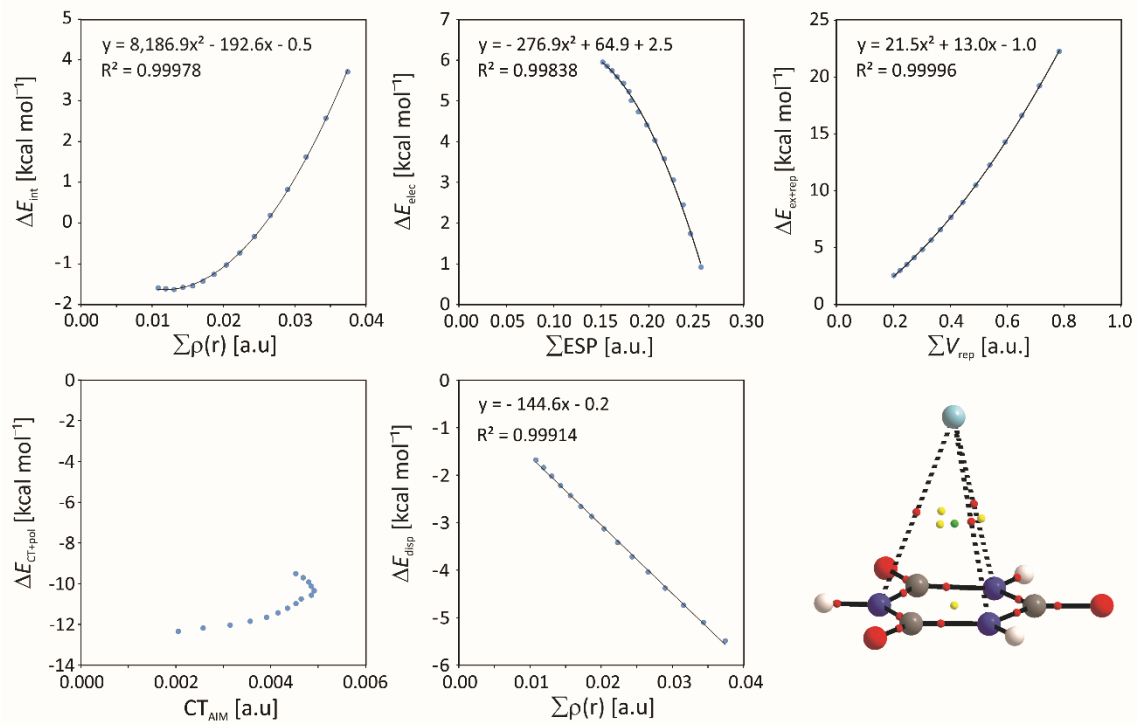

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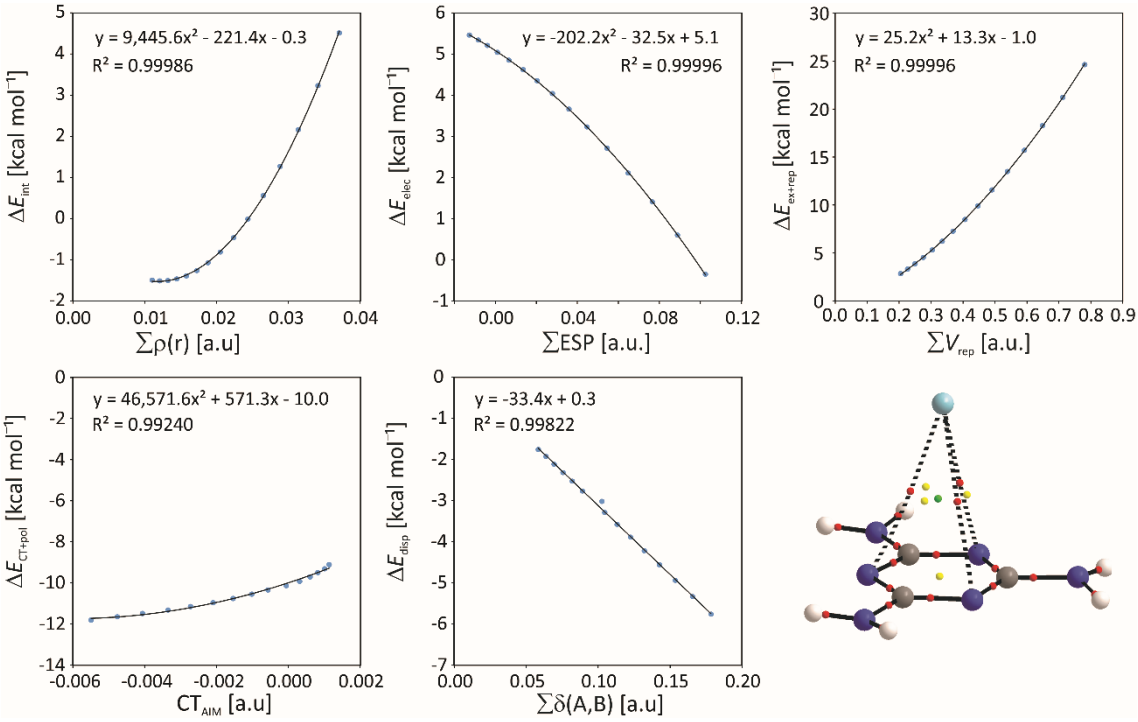

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Table S1. Topological parameters (in a.u.) at bond critical points of encapsulation interactions.

Complex	Atoms	ρ	$\nabla^2\rho$	H	ε	δ(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
	N···Cl^-	0.005	0.013	0.000	0.927	0.031	0.192
(AC4-1)@Ar	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	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	0.566
	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
(AC4-2)@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_2M_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_2M_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.: $\Delta\rho$ = $\rho_{cage@A} - \rho_{cage}$; A = Na^+, Cl^-, Ar).

Complex	Guest	Atoms	$\Delta\rho$	ΔH	$\Delta\varepsilon$	$\Delta\delta$(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_2CA_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