Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

A silver coordination cage assembled from $[Ag_2(bis(isoxazolyl)_3]$: DFT approach of the binding forces within the host-guest interactions

R. Guajardo-Maturana[*ac], Ximena Zarate*[*b], Francisca Claveria-Cadiz[c], Eduardo Schott[a]*

[a]Departamento de Química Inorgánica, Facultad de Química, Pontificia Universidad Católica de Chile, Vicuña Mackenna 4860, Macul, Santiago.

[b]Instituto de Ciencias Químicas Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile. Avenida Pedro de Valdivia 641, Santiago, Chile.

[c]Doctorado en Fisicoquímica Molecular, Universidad Andrés Bello, República 275, Santiago, Chile.

*rhguajar@uc.cl

Table S1. Selected calculated distances (Å) and Angles (degrees) for [Ag_2($bisox_3$)] (Cage) and cage-gas systems.

Bond length(Å)/Angles°	Cage	Cage [N_2]	Cage[CO_2]	Cage[C_2H_6]	Cage [exp]
Ag-N_1	2.29	2.25	2.24	2.23	2.23
Ag-N_2	2.29	2.27	2.26	2.24	2.23
Ag-N_3	2.29	2.29	2.29	2.32	2.23
N-O	1.41	1.41	1.41	1.41	1.35
N-C	1.32	1.32	1.32	1.32	1.30
O-C	1.36	1.36	1.36	1.36	1.35
Ag-N_1-N_2	119.8	122.9	125.7	114.7	119.6
Ag-N_1-N_2	119.0	120.4	117.6	131.3	119.6
Ag-N_1-N_2	120.4	115.8	116.3	112.9	119.6
C-C_1-C_2	113.1	112.5	111.5	112.2	111.9
Ag-N_1-O	118.7	120.3	118.18	119.17	114.3

Table S2. Energy decomposition analysis (EDA kcal.mol^{-1}) denoting the interaction cage and several storage gases.

EDA (kcal/mol)	$[Ag_2(bisox)_3][N_2]_4$	$[Ag_2(bisox)_3][CH_4]_4$	$[Ag_2(bisox)_3][CO_2]_4$	$[Ag_2(bisox)_3][H_2O]_4$	$[Ag_2(bisox)_3][C_2H_6]_3$
ΔE_{Pauli}	9.09	13.72	19.83	27.82	18.51
ΔE_{orb}	-7.06(23.5%)	-6.47(17.4%)	-8.01(17.21%)	-18.73(31.1%)	-8.05(17.4%)
ΔE_{elstat}	-6.00(19.9%)	-8.17(22.0%)	-14.42(30.98%)	-24.84(41.3%)	-10.88(23.4%)
ΔE_{Disp}	-17.04(56.6%)	-22.50(60.6%)	-24.12(51.8%)	-16.57(27.6%)	-27.33(59.2%)
ΔE_{int}	-21.01	-23.43	-26.73	-32.33	-27.75