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

ELECTRONIC SUPPLEMENTARY INFORMATION

Halogen-Bonded Haloamine Trimers – Modelling the X_3 Synthon

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Table S1. Cartesian coordinates (in Å) and ADF total bonding energy (in kcal mol^{-1}) for stationary points of haloamine trimers computed at ZORA-BLYP-D3(BJ)/TZ2P level.

Chloroamine trimer, E_{bond}= -1114.99 kcal/mol

Cl	0.909989	1.546627	0.103965
N	0.662491	3.333687	0.149673
H	1.207561	3.657158	-0.657982
H	1.208762	3.615692	0.971925
Cl	0.883381	-1.776958	-0.004126
N	2.558413	-2.448375	0.007272
H	2.566339	-3.047963	-0.826078
H	2.535995	-3.096209	0.803412
Cl	-1.984789	-0.091385	-0.014161
N	-3.405524	-1.201929	-0.083421
H	-3.919312	-0.859385	-0.903615
H	-3.963297	-0.904661	0.725622

Bromoamine trimer, E_{bond}= -1096.00 kcal/mol

Br	-0.761471	-1.738022	-0.018576
N	-2.531879	-2.603136	-0.018689
H	-2.465595	-3.226210	0.795089
H	-2.465576	-3.226035	-0.832600
Br	1.887214	0.205776	-0.018447
N	3.522740	-0.892927	-0.018488
H	4.028755	-0.523269	0.795257
H	4.028597	-0.523445	-0.832410
Br	-1.124270	1.530704	-0.018403
N	-0.990832	3.496611	-0.018312
H	-1.563691	3.749930	0.795648
H	-1.563993	3.750025	-0.832030

Iodoamine trimer, E_{bond}= -1083.17 kcal/mol

I	0.584729	1.926391	0.014221
N	2.407989	3.074148	0.010250
H	2.296441	3.689635	0.824923
H	2.291888	3.691250	-0.802561
I	-1.957749	-0.473458	0.019105
N	-3.862974	0.532036	0.024732
H	-4.338004	0.124368	0.839041
H	-4.341680	0.126438	-0.788461
I	1.394833	-1.474106	0.008794
N	1.484697	-3.626720	0.006292
H	2.078108	-3.834913	0.818374
H	2.074203	-3.833172	-0.809071

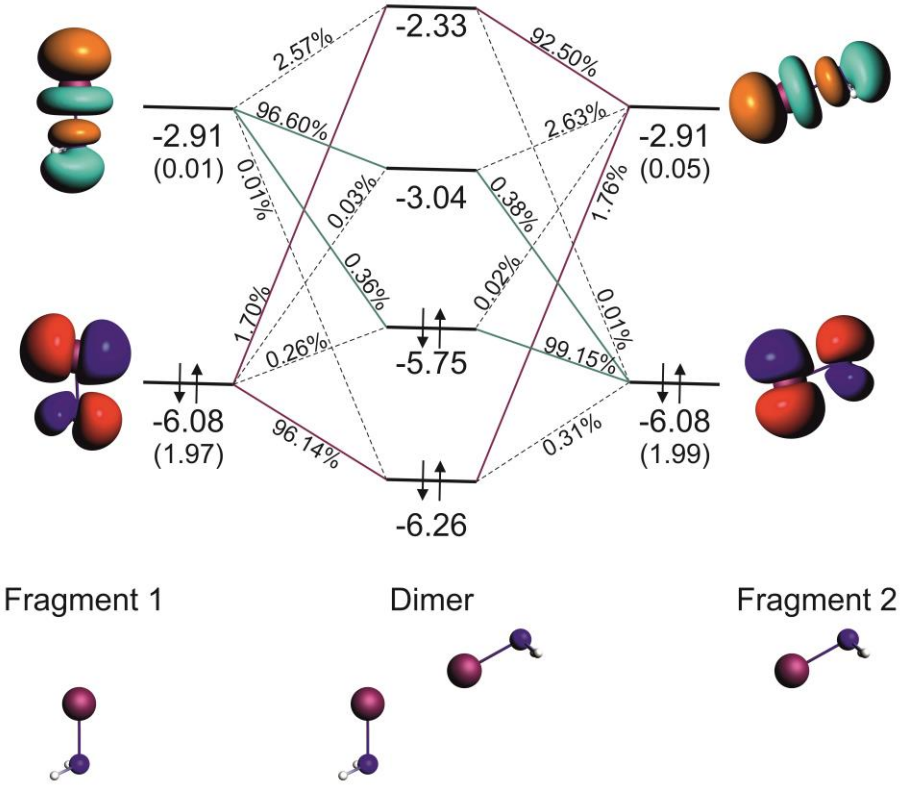

Figure S1. Orbital diagram in A' symmetry for bromoamine dimer (of C_s symmetry) with the geometry of the corresponding trimer; solid lines: σ-donation – cherry; π-back donation – green, orbital energies (in eV) and their contributions, in parentheses: orbital populations (in electrons).

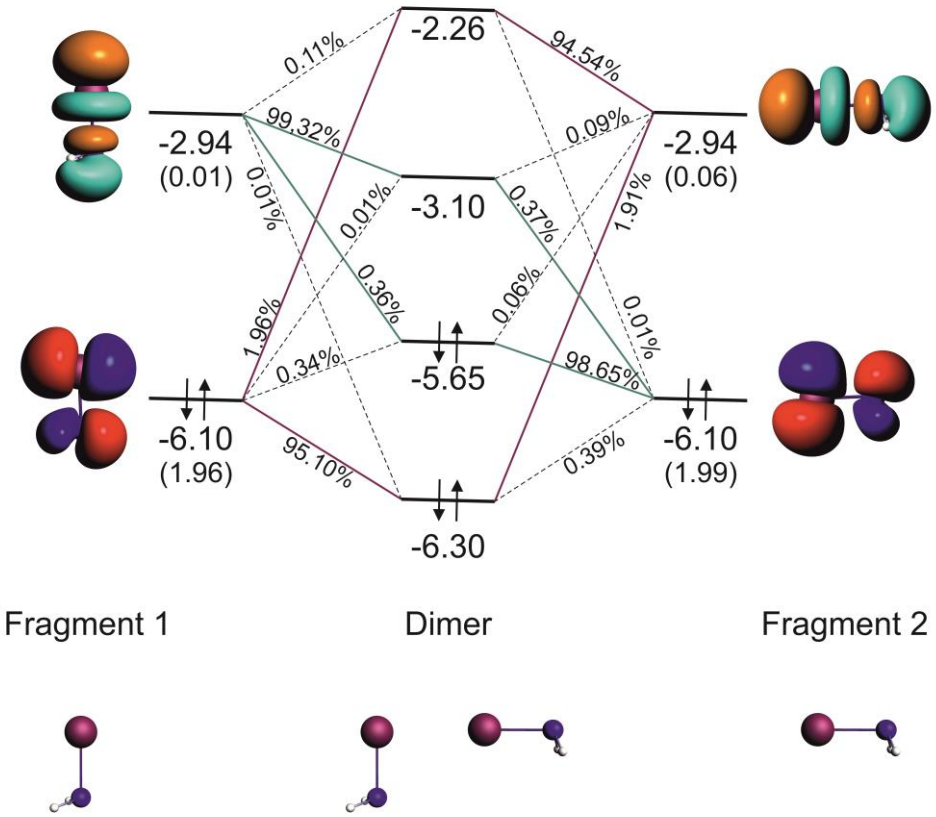

Figure S2. Orbital diagram in A' symmetry for bromoamine dimer (of C_s symmetry) with the geometry of the corresponding tetramer; solid lines: σ-donation – violet; π-back donation – green, orbital energies (in eV) and their contributions, in parentheses: orbital populations (in electrons).

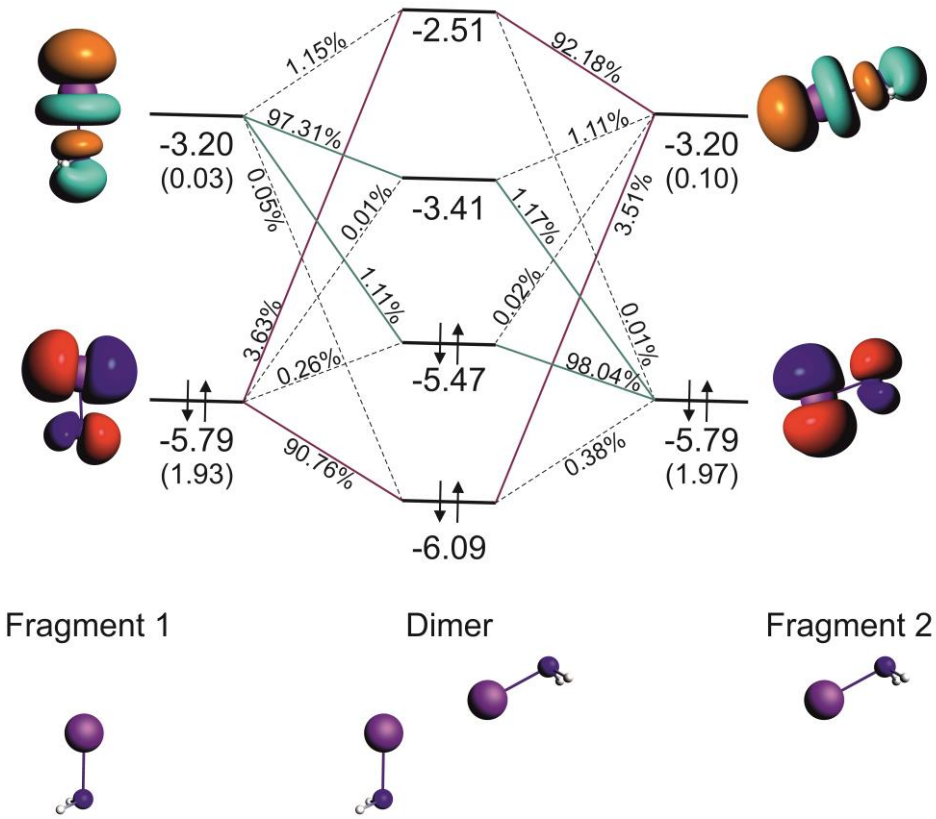

Figure S3. Orbital diagram in A' symmetry for bromoamine dimer (of C_s symmetry) with the geometry of the corresponding trimer; solid lines: σ-donation – violet; π-back donation – green, orbital energies (in eV) and their contributions, in parentheses: orbital populations (in electrons).

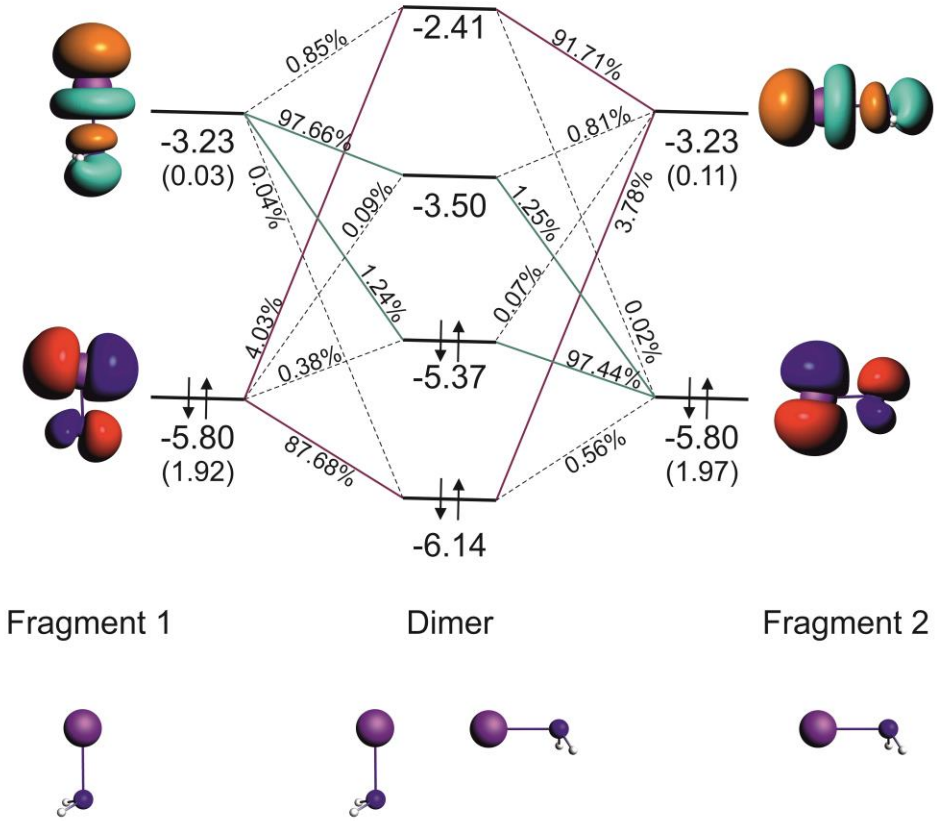

Figure S4. Orbital diagram in A' symmetry for bromoamine dimer (of C_s symmetry) with the geometry of the corresponding tetramer; solid lines: σ-donation – violet; π-back donation – green, orbital energies (in eV) and their contributions, in parentheses: orbital populations (in electrons).