Experimental details

*Synthesis of Cu(1,1,3,6,6,8-Hexamethyl-decahydro-3a,5a,8a,10a-tetra-azapyrene)Cl₂*

(Cu₂Cl₂): 0.170 g (0.001 mol) CuCl₂·2H₂O in 10ml of MeOH was added to 0.31g (0.001 mol) of 2 (tetA synthesized according to a literature procedure; R. W. Hay and G. A. Lawrence. *J. Chem. Soc., Perkin 1* 1975, 591.) in 20ml of MeOH with stirring. The solution was then heated at reflux for 16 hours. During the reaction, the solution's colour changed from the initial dark green color to pale red and finally to a yellow-green upon cooling. This reaction yielded light green, needle-like crystals upon cooling. Yield: 0.278 g (63%).

Anal. Cald for CuC₁₉H₃₄N₄Cl₂·0.5 H₂O: C, 48.05; H, 7.84; N, 12.45. Found: C, 48.04; H, 7.64; N, 12.33. \( \lambda_{\text{max}}/\text{nm}, (\varepsilon/ \text{M}^{-1}\text{cm}^{-1}) \): 285(2400), 389(900). FAB\(^+\) mass spectrum (NBA), m/z = 442 (Cu₂Cl₂\(^+\)).
Crystallographic details for Cu$_2$Cl$_2$

ORTEP (50% probability ellipsoids)
Table 1. Crystal data and structure refinement for Cu2Cl2.

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<tr>
<th>Parameter</th>
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<td>Wavelength</td>
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<tr>
<td></td>
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<td>Largest diff. peak and hole</td>
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Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for sj68. $U(eq)$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

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Table 3. Bond lengths [Å] and angles [°] for sja68.

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Table 4. Anisotropic displacement parameters (Å² x 10³) for sja68. The anisotropic displacement factor exponent takes the form: -2π² [ h²a²U₁₁ + ... + 2hκa*b*U₁₂ ]

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</table>
**Computational details**

Table 5. Comparison of observed (solid state, 150K) and calculated bond lengths [Å] for \( \text{CuCl}_2 \) and \( \text{CuCl}_2^2 \). (The bond lengths for \( \text{CuCl}_2 \) are taken from T. J. Hubin, N. W. Alcock, L. L. Seib and D. H. Busch, *Inorg. Chem.*, 2002, **41**, 7006.)

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<tr>
<th></th>
<th>Observed</th>
<th>Calculated</th>
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<tr>
<td><strong>( \text{CuCl}_2 )</strong></td>
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<td>Cu-Cl(1)</td>
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<td><strong>( \text{CuCl}_2^2 )</strong></td>
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<td>Cu-N(4)</td>
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Energy analysis:

The bonding has been analysed by decomposing the molecular bonding or atomization energy ($E_B$) as,

$$E_B = E_O + E_P + E_E$$

where $E_O$, $E_P$ and $E_E$ represent orbital mixing, Pauli repulsion and electrostatic interaction terms respectively. Descriptions of the physical significance of these properties have been given by Landrum, Goldberg and Hoffmann\(^1\) and Baerends and co-workers\(^2,^3\). Both $E_O$ and $E_P$ arise from orbital interaction effects with the former stabilizing and the latter destabilizing. $E_O$ represents the effect of charge transfer, orbital mixing and polarization when filled and empty atomic orbitals overlap.

Cyclam + CuCl\(_2\) --> complex

For \(1\) (all chair), $\Delta E = -311$ kJmol\(^{-1}\).
For \(1\) (two twist boat), $\Delta E = -298$ kJmol\(^{-1}\).
For \(2\) (all chair), $\Delta E = -287$ kJmol\(^{-1}\).
For \(2\) (two twist boat), $\Delta E = -306$ kJmol\(^{-1}\)

Geometry optimizations and energy analyses were performed at the unrestricted UBP86/TZP level with ZORA relativistic effects and frozen (n-1) cores using ADF 2002.02.\(^2,^3,^4\) Relative energies were also determined at the unrestricted UB3LYP/LanL2DZ level using Gaussian 98.\(^5\)
