Supplementary Material

X-ray Crystallographic Data Collection and Refinement of the Structure

An orange colored transparent parallelepiped of 0.28x0.06x0.06 mm^3 was coated with perfluoropolyether, picked up with a glass fiber and immediately mounted in the nitrogen cold stream (100 K) of the diffractometer to prevent loss of solvent. A Nonius Kappa-CCD diffractometer equipped with a Mo-target rotating-anode X-ray source and a graphite monochromator (Mo-Kα , λ=0.71073Å) was used. Final cell constants were obtained from least squares fits of all measured reflections. Indices of crystal faces were determined and the Gaussian-type absorption correction routine embedded in XPREP[1] was applied. The Siemens ShelXTL[1] software package was used for solution and artwork of the structure, ShelXL97[2] was used for the refinement. The structures were readily solved by direct methods and subsequent difference Fourier techniques. Crystallographic data of the compounds are listed in Table S1. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms attached to carbon atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters. Hydrogen atoms of OH and OH2 fragments in the complex were located from the difference map and refined with a constrained O-H distance. Localization of H-atoms of the water molecules of crystallization was not possible in all cases due to disorder problems. Most of the perchlorate anions were found to be disordered. There are five crystallographic anion sites of which two are on special positions. Perchlorate containing Cl(3) is disordered on a two-fold axis by rotation with O(301) and Cl(3) lying on that axis. The anion containing Cl(4) is disordered by inversion. Anions with Cl(2) and Cl(5) are disordered and were split on two sites. Perchlorate with Cl(1) is not disordered. Cl-O and O-O distances in disordered perchlorate anions were restrained to be equal within errors (SADI instruction) and equal thermal displacement parameters were given for split atoms (EADP instruction).

(1) ShelXTL V.5, Siemens Analytical X-Ray Instruments, Inc., Madison, Wisconsin, USA 1994

(2) ShelXL97, G. M. Sheldrick, University of Göttingen 1997

Table S1. Crystallographic data for **1** · 12 H_2O

	1 · 12 H_2O
Chem formula	$C_{60}H_{94}Cl_4N_{20}Ni_9O_{50}$
Fw	2565.74
space group	*C2/c , No. 15*
a, Å	24.704(2)
b, Å	31.015(3)
c, Å	26.032(2)
α, deg	90
β, deg	100.13(2)
γ, deg	90
V, Å	19635(3)
Z	8
T, K	100(2)
ρ calcd, g cm^{-3}	1.736
refl. collected / $2\Theta_{max}$	103240 / 45.00
unique refl. / I>2σ(I)	12807 / 10268
no. of params	930
λ, Å / μ(Kα), cm^{-1}	0.71073 / 18.99
R1 [a] / goodness of fit [b]	0.0717 / 1.111
wR2 [c] (I>2σ(I))	0.1593
residual density, e$Å^{-3}$	+1.65 / -0.84

a) Observation criterion: $I > 2\sigma(I)$. $R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, b) $GooF = [\Sigma[w(F_o^2-F_c^2)^2]/(n-p)]^{1/2}$

c) $wR2 = [\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$ where $w = 1/\sigma^2(F_o^2)+(aP)^2+bP$, $P = (F_o^2+2F_c^2)/3$