

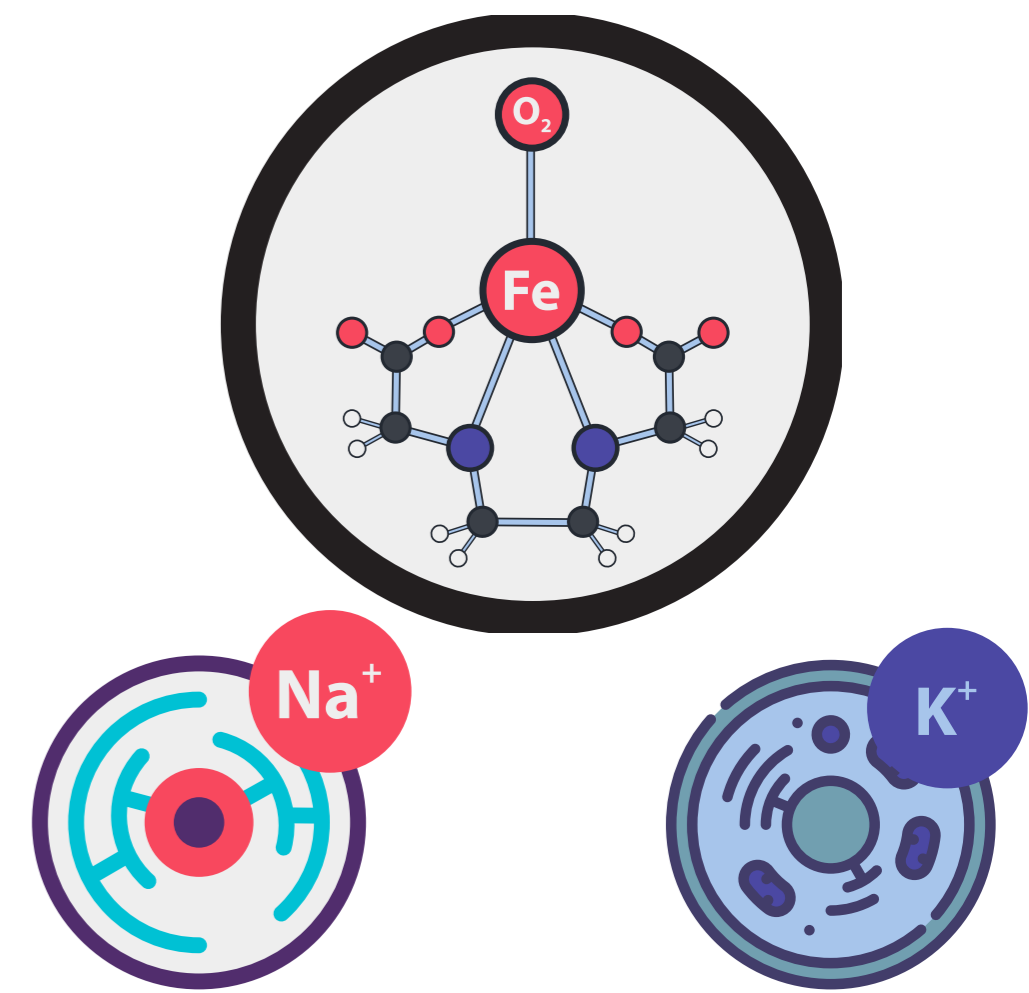
# HETEROMETALLIC $\{Fe^{III}_4Na_2\}$ PIVALATE CLUSTER SYNTHESIS AND STRUCTURE CHARACTERISATION

Daniel PODGORNII, Svetlana G. BACA, Victor Ch. Kravtsov

Institute of Applied Physics, Chisinau, Academiei 5, Republic of Moldova

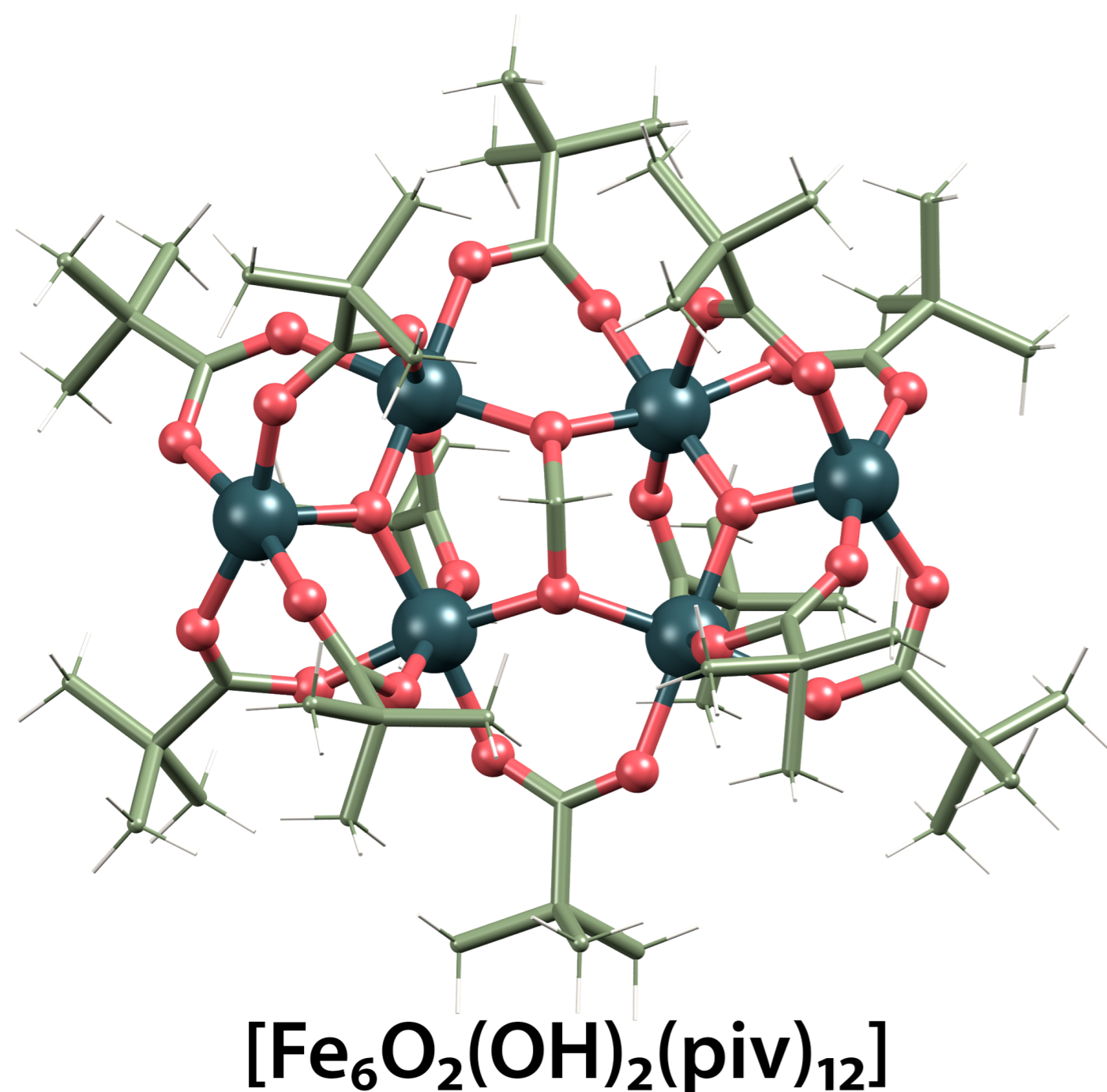
## WHY DOES THIS RESEARCH MATTER?

Coordination compounds with biological active ions and molecules are of great interest in biotechnology and biomedicine. Coordination compounds such as iron containing enzymes, siderophores, and others are known for their essential role in life processes as oxygen carriers. Coordination chemistry of lithium, sodium and potassium has colossal value due to their remarkable role in different biological mechanisms, especially for cell biology and natural fluids biochemistry some of them being responsible for maintenance of the ionic equilibrium in living bodies and for electrochemical gradients across cell membranes which affect transmission of nerve impulse and regulation of cell functions



## SYNTHESIS

$[Fe_4Na_2O_2(piv)_{10}(MeCN)_2]$  (1) synthesized by refluxing the mixture of hexanuclear iron (III) pivalate,  $[Fe_6O_2(OH)_2(piv)_{12}]$  (Hpiv = pivalic acid) and sodium azide  $NaN_3$  in MeCN.



$[Fe_6O_2(OH)_2(piv)_{12}]$



## CRYSTAL DATA FOR (1)

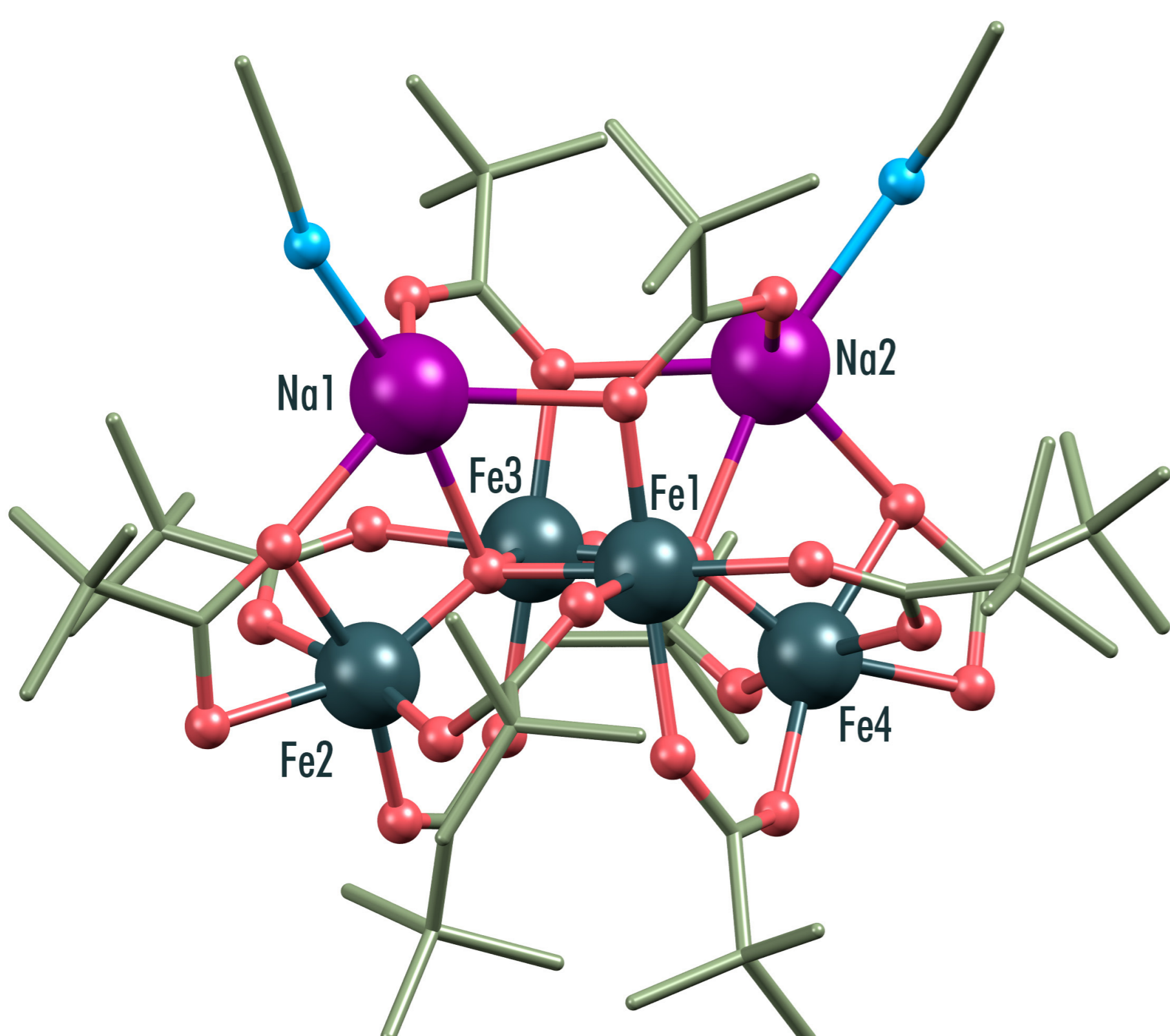
|                    |             |
|--------------------|-------------|
| Crystal system     | monoclinic  |
| Space group        | Cc          |
| $a(\text{\AA})$    | 19.3924(9)  |
| $b(\text{\AA})$    | 19.2415(15) |
| $c(\text{\AA})$    | 20.0436(12) |
| $\alpha(^{\circ})$ | 90          |
| $\beta(^{\circ})$  | 91.136(4)   |
| $\gamma(^{\circ})$ | 90          |
| $V(\text{\AA}^3)$  | 7431        |

## BOND DISTANCES FOR COORDINATION POLYHERDA OF (1)

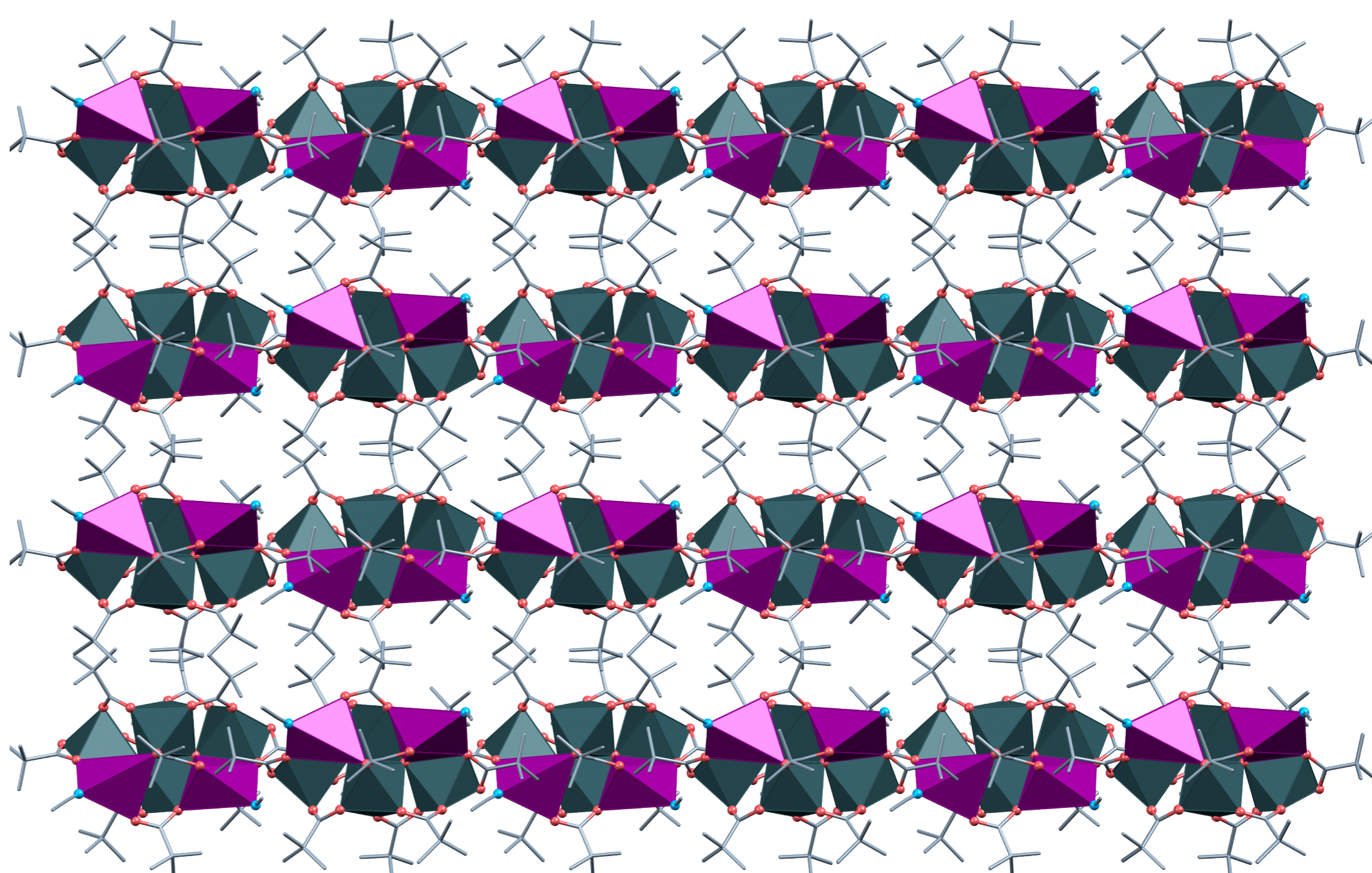
| Bond type | Range (Å)             |
|-----------|-----------------------|
| Fe - O    | 1.847(8) - 2.196(9)   |
| Na - O    | 2.255(14) - 2.486(10) |
| Na - N    | 2.415(16) - 2.549(16) |

## X-RAY CRYSTALLOGRAPHY

The cluster core  $\{Fe_4Na_2\}$  contains two Fe-Fe edge sharing distorted  $Fe_3Na$  tetrahedra with  $\mu_4-O_2^-$  bridges inside each tetrahedron. Coordination spheres of  $Na^+$  ions consist of four O atoms from three pivalate ligands, one  $\mu_4-O_2^-$  moiety and one N atom from capped acetonitrile molecule, resulting in  $NO_4$  distorted trigonal-bipyramidal surrounding. Peripheral ligation of Fe and Na atoms is provided by six bridging in  $\eta^1:\eta^1:\mu_2$  mode and four bridging in  $\eta^1:\eta^2:\mu_3$  pivalate ligands.



Structure of  $[Fe_4Na_2O_2(piv)_{10}(MeCN)_2]$



Packing of (1), view along  $c$  axis

## CONCLUSIONS AND PERSPECTIVE

Using pre-designed  $\mu_3$ -oxo hexanuclear Fe(III) pivalate cluster and sodium azide led to formation of heterometallic  $[Fe_4Na_2O_2(piv)_{10}(MeCN)_2]$  cluster. Work is in progress to investigate its magnetic properties and the possibility to use obtained cluster as precursor for other bigger molecules.

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