# Anionic compounds of hexaazatriphenylene-based ligands: synthesis, structure and properties


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ИФТТ РАН
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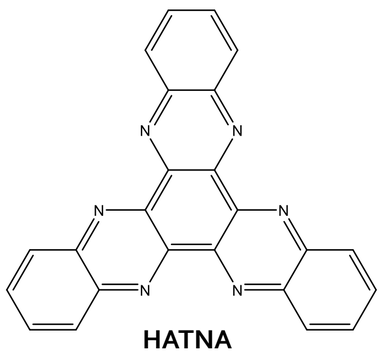
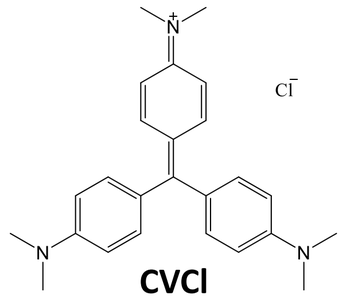


**HATNA**
**Hexaazatrinaphthylene**

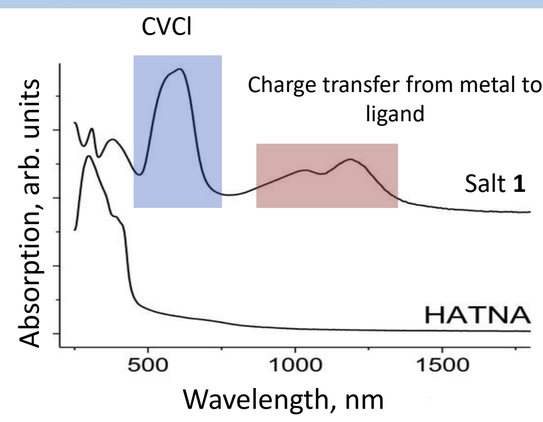


**CVCl**

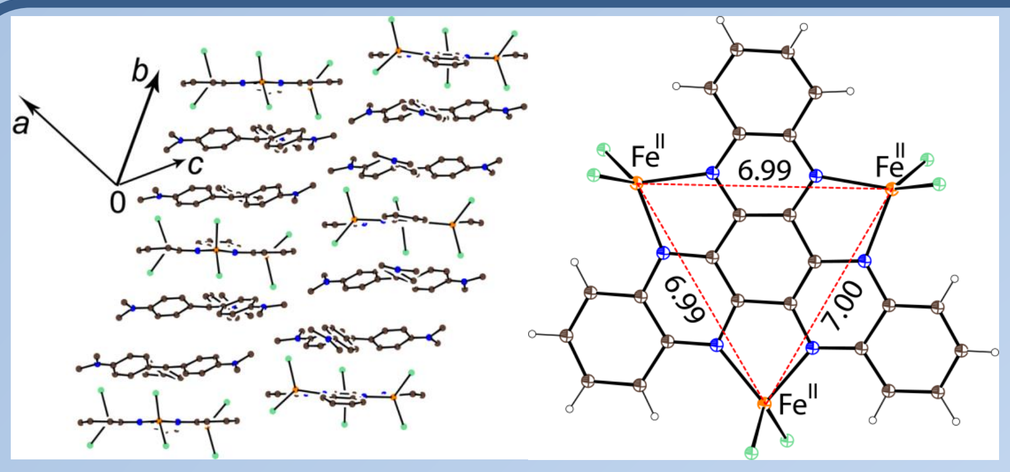
$$HATNA + 2CVCl + Fe(0) \xrightarrow[C_6H_4Cl_2]{} \{CV^+\}_2\{(Fe^{II}Cl_2)_3HATNA\}^{2-}\cdot 3C_6H_4Cl_2\ (1)$$

Fe(0) – powedered iron or $Fe_3(CO)_{12}$

*D.V. Konarev, S.S. Khasanov, **M.V. Mikhailenko**, M.S. Batov, A. Otsuka, H. Yamochi, H. Kitagawa, R.N. Lyubovskaya, Eur. J. Inorg. Chem., 2021, N.1, 86-92.*




*Synthesis of dianionic salt of HATNA (**1**) and its electron spectrum.*

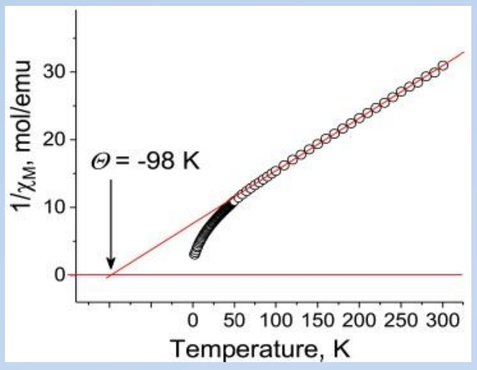



*Crystal structure and magnetic properties of salt **1**.*

d(N-Fe) = **2.05 - 2.14 Å**

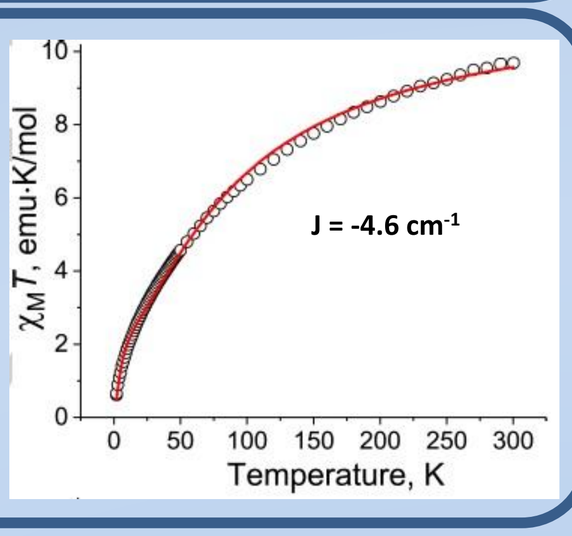
Bond length N-Fe in complex $[HAT\{Fe_3Cl_5(CH_3OH)_4(H_2O)\}]Cl$ is ***2.210 - 2.267 Å (*)***

* M. Shatruk, A. Chouai, A. Prosvirin, K. Dunbar, *Dalton Trans.*, 2005, 1897-1902




Fe(II) spin **S** = **2**

For complex (*****) J = **-2.4 см$^{-1}$**



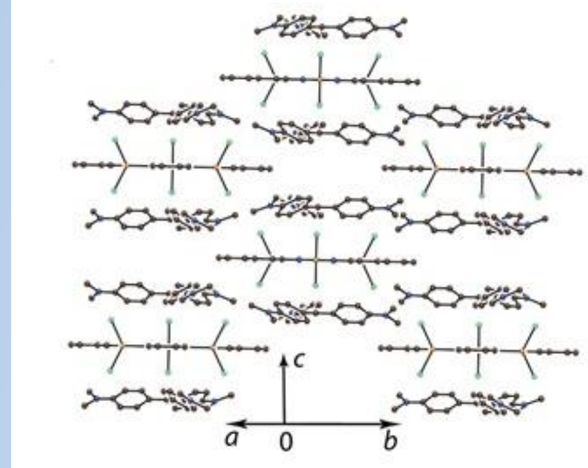

**HATA**

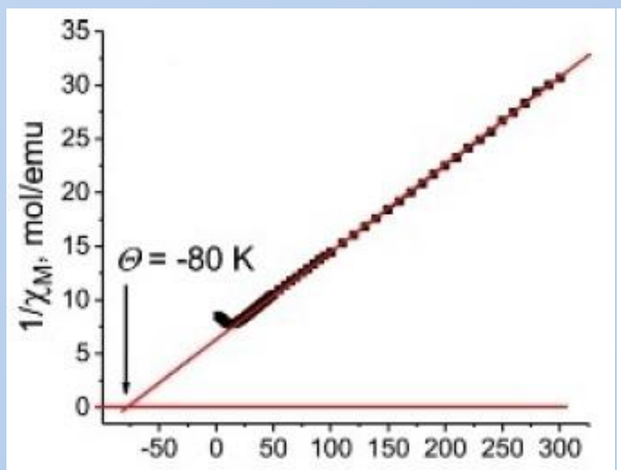
**Hexaazatrianthracene**

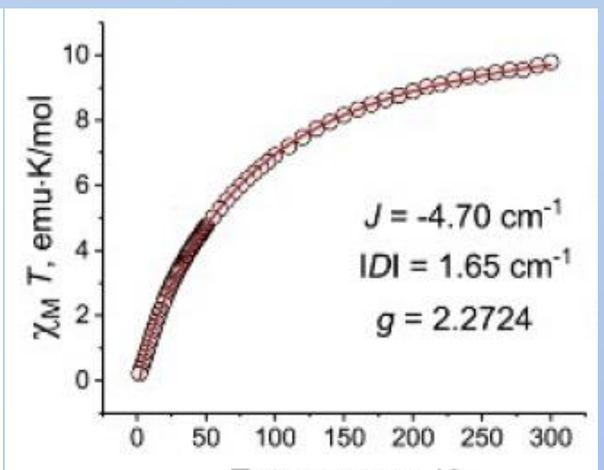
Average bond length d(N-Fe) = **2.106(4) Å**

$$HATA + 3CVCl + Fe(0) \xrightarrow[C_6H_4Cl_2]{} \{CV^+\}_2\{(Fe^{II}Cl_2)_3HATA\}^{2-}\cdot 3C_6H_4Cl_2\ (2)$$

***M.V. Mikhailenko**, S.S. Khasanov, A.F. Shestakov, A.V. Kuzmin, A. Otsuka, H. Yamochi, H. Kitagawa, D. Konarev, Chem. Eur. J., 2022, 28, e202104165.*

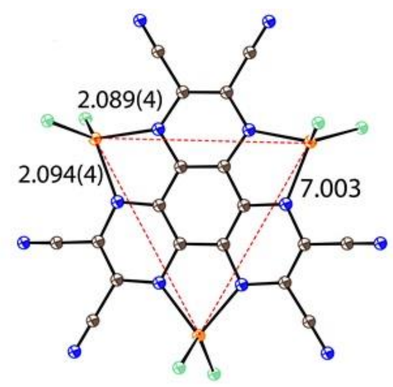


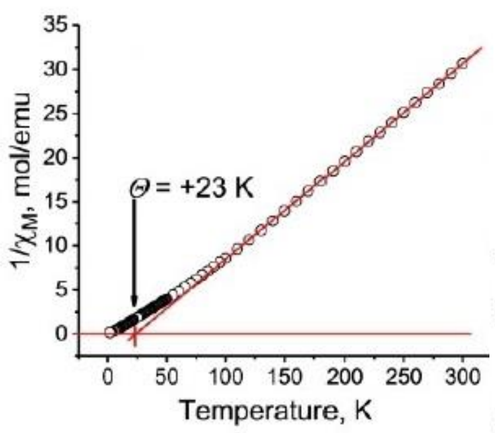




*Synthesis, crystal structure and magnetic properties of dianionic salt of HATA (**2**).*

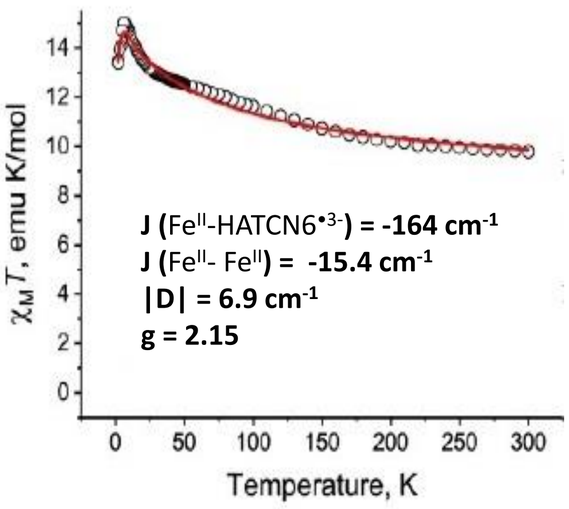
**HATCN6**




Average bond length d(N-Fe) = **2.092(4) Å**

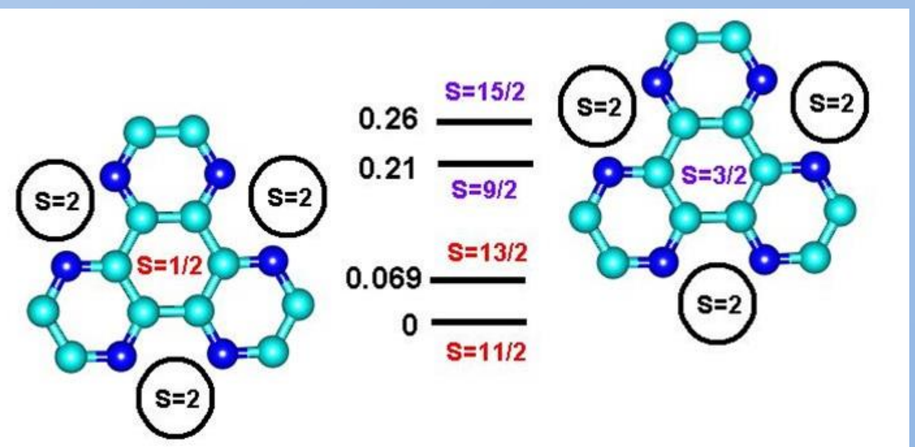



Parallel alignment of Fe$^{II}$ spins forms high-spin system with **S = 11/2**




**J** (Fe$^{II}$-HATCN6$^{\bullet 3-}$) = **-164 cm$^{-1}$**
**J** (Fe$^{II}$- Fe$^{II}$) = **-15.4 cm$^{-1}$**
**|D| = 6.9 cm$^{-1}$**
**g = 2.15**

$$HATCN6 + 3CVCl + Fe \xrightarrow[C_6H_4Cl_2]{} \{CV^+\}_3\{(Fe^{II}Cl_2)_3HATCN6\}^{3-}\cdot 0{,}5(CVCl)\cdot 2{,}5C_6H_4Cl_2\ (3)$$




*Synthesis, crystal structure and magnetic properties of trianionic salt of HATCN6 (**3**).*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