Anisotropic superexchange in $Mn^{III}_6Os^{III}$ single-molecule magnets

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Possible Sources of anisotropy

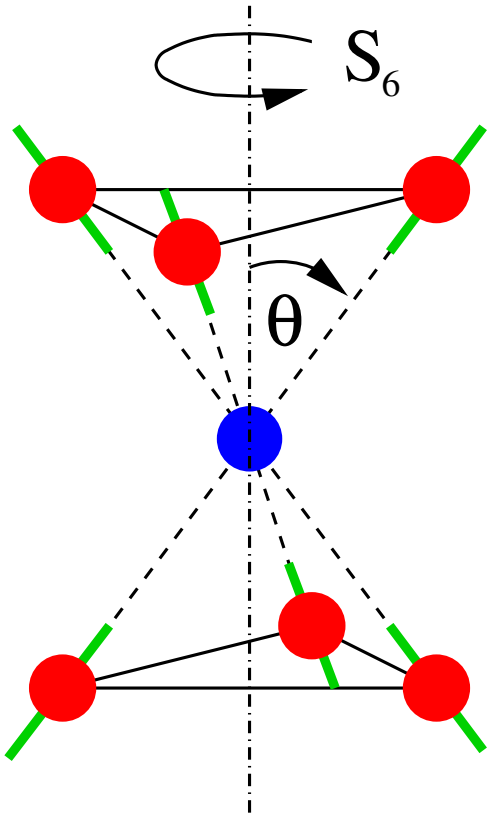
$$\underset{\sim}{H} = -\sum_{i,j} \vec{\underset{\sim}{s}}_i \cdot \mathbf{J}_{ij} \cdot \vec{\underset{\sim}{s}}_j + \sum_i \vec{\underset{\sim}{s}}_i \cdot \mathbf{D}_i \cdot \vec{\underset{\sim}{s}}_i + \mu_B \vec{B} \cdot \sum_i^N \mathbf{g}_i \cdot \vec{\underset{\sim}{s}}_i$$

exchange single-ion Zeeman

Can anisotropic exchange improve SMM properties?

Enhancing the Blocking Temperature in Single-Molecule Magnets by Incorporating 3d-5d Exchange Interactions:
K. S. Pedersen *et al.*, Chem. Eur. J. **16**, 13458 (2010).

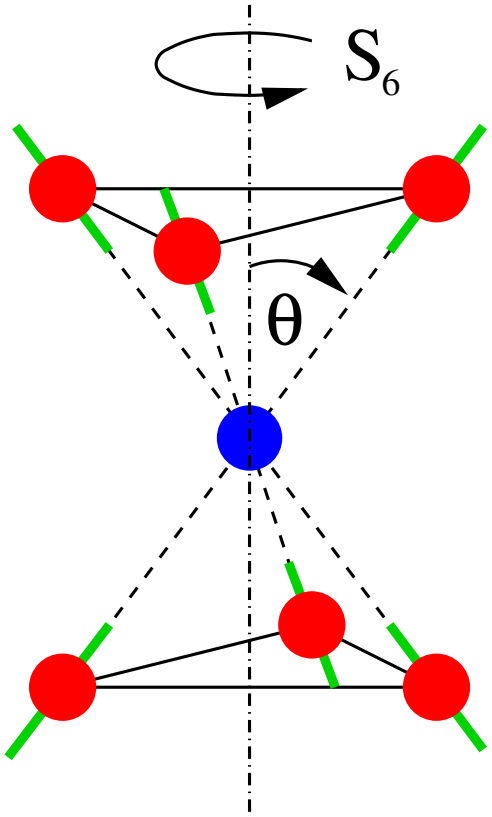
$Mn_6^{III}Os^{III}$



- 6 Mn^{III} with $s = 2$;
- Dominant D terms along Jahn-Teller axes of the Mn^{III};
- Os^{III} effective $s = 1/2$ doublet;
- anisotropic Mn^{III}–Os^{III} exchange.

V. Hoeke *et al.*, Inorg. Chem. **53**, 257 (2014).

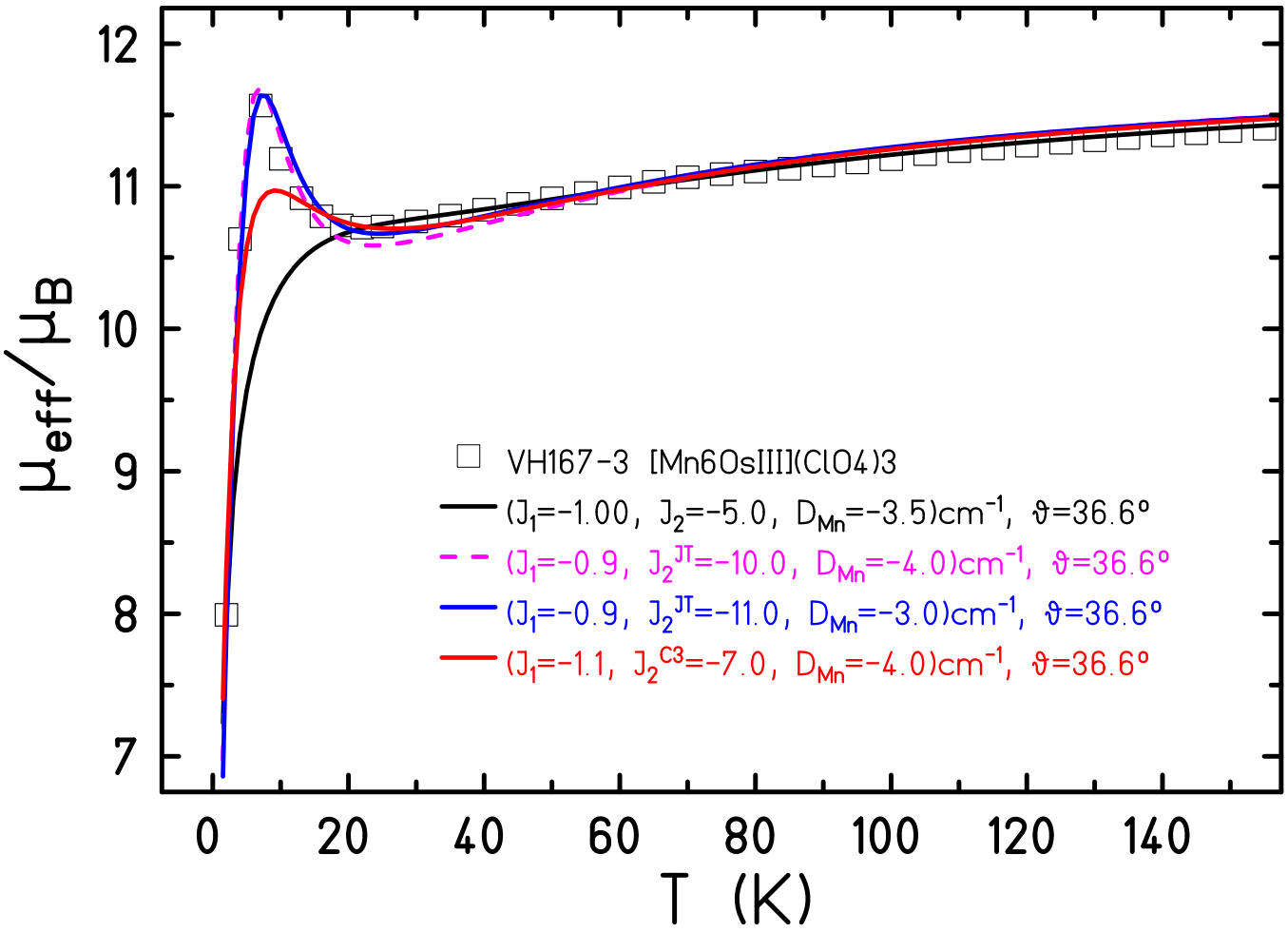
Anisotropic exchange



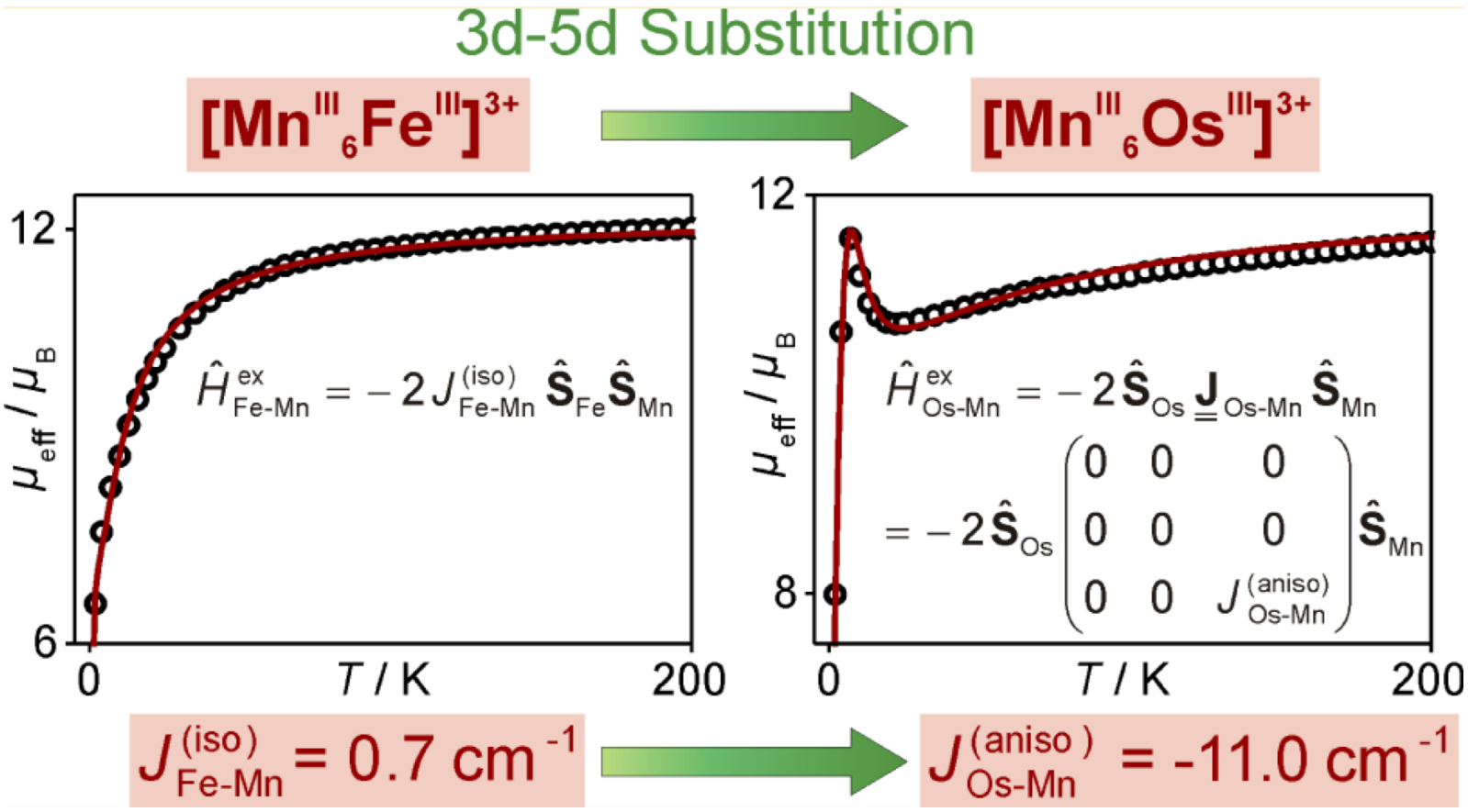
- Mn^{III}–Mn^{III} exchange isotropic;
- Mn^{III}–Os^{III} exchange assumed Ising-like;
- $\underset{\sim}{H}_{\text{ani}} = -2 \sum_{i=1}^{6} \vec{\underset{\sim}{s}}_i \cdot \vec{e}^{\,3}_{i7} \; J^{33}_{i7} \; \vec{e}^{\,3}_{i7} \cdot \vec{\underset{\sim}{s}}_7$;
- Investigate J^{33}_{i7} along several directions, e.g. C3 and JT.

V. Hoeke *et al.*, Inorg. Chem. **53**, 257 (2014).

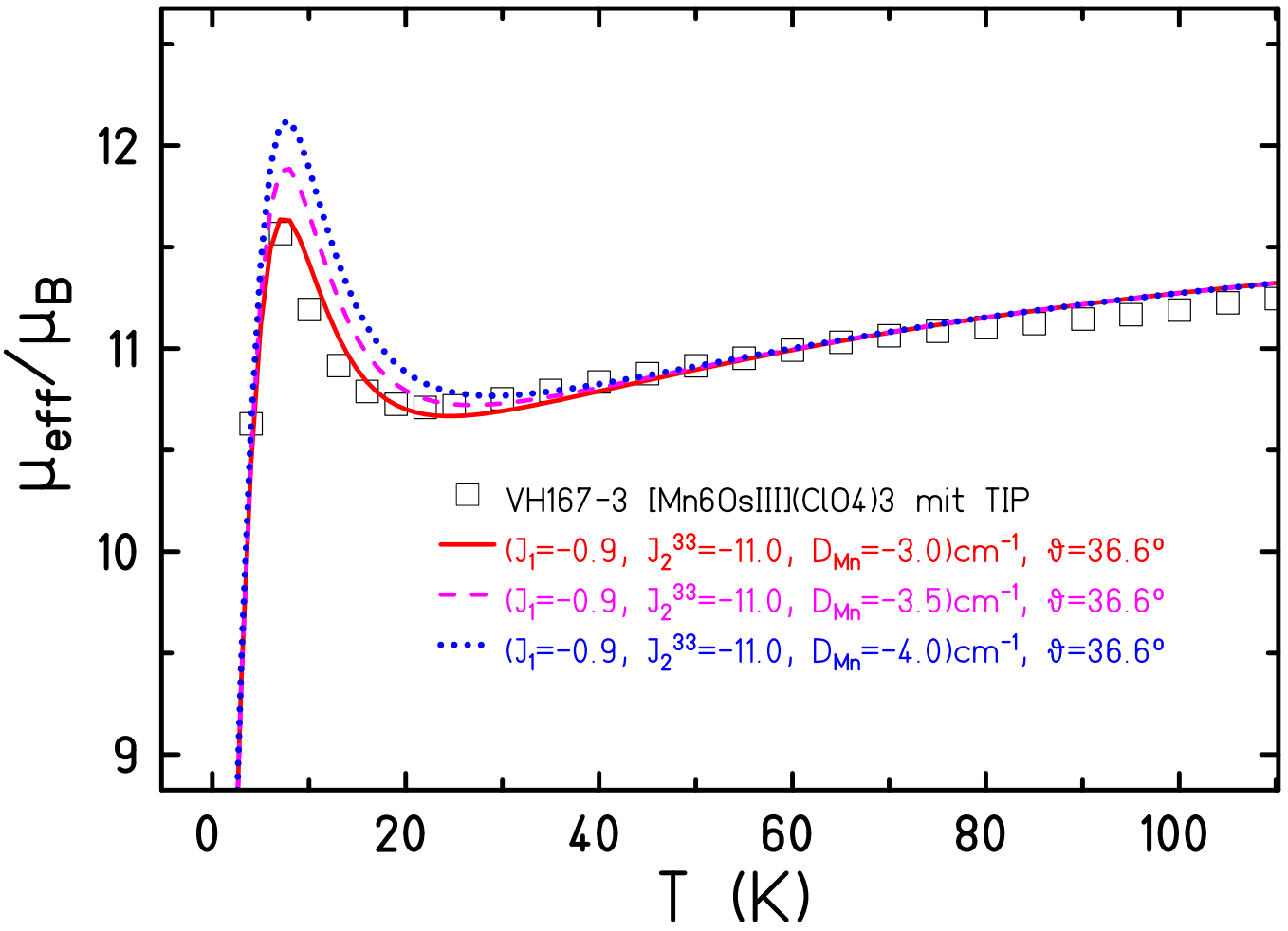
Effective magnetic moment



Effective magnetic moment compared to Fe^{III} l.s.

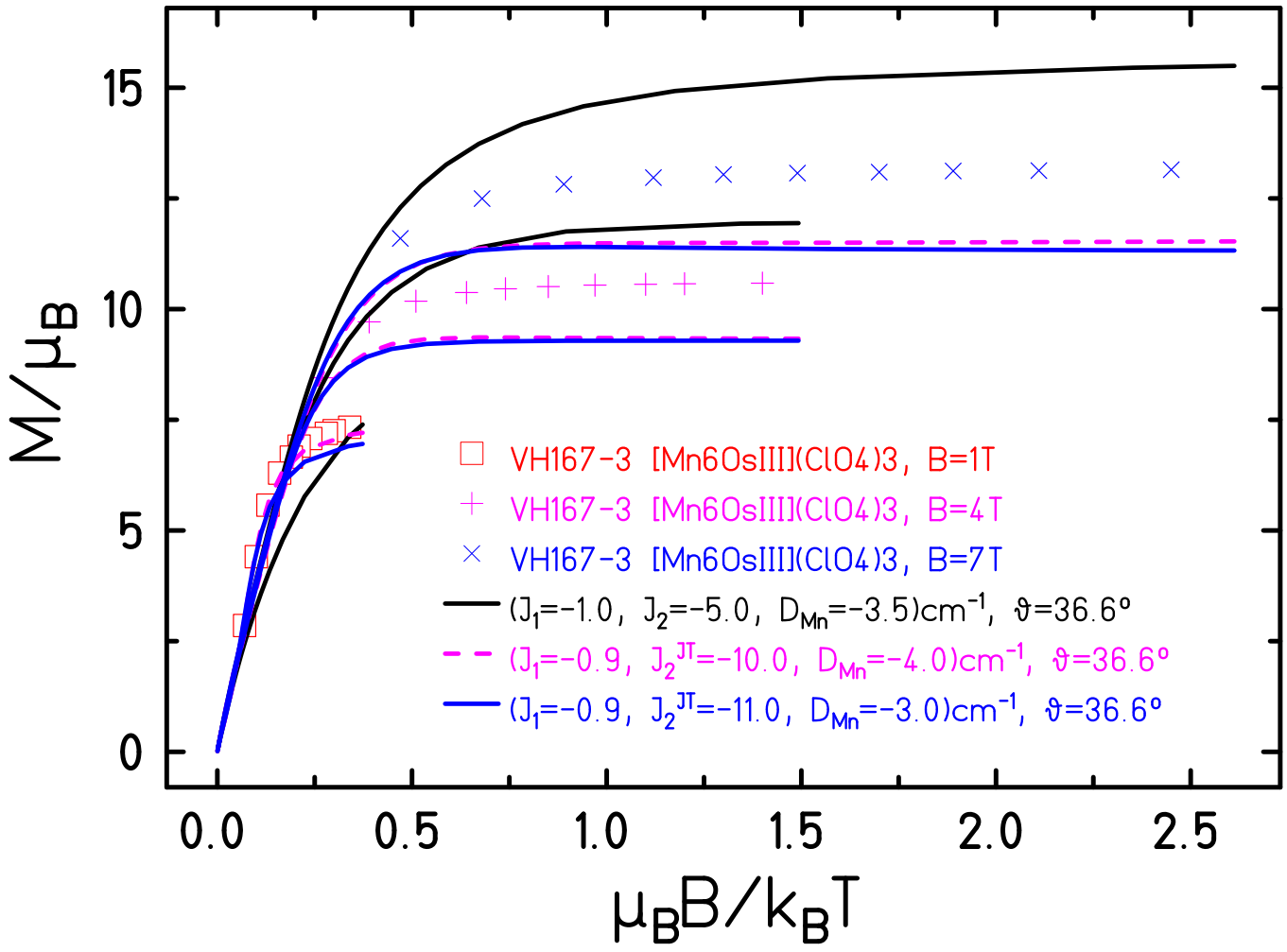


Effective magnetic moment

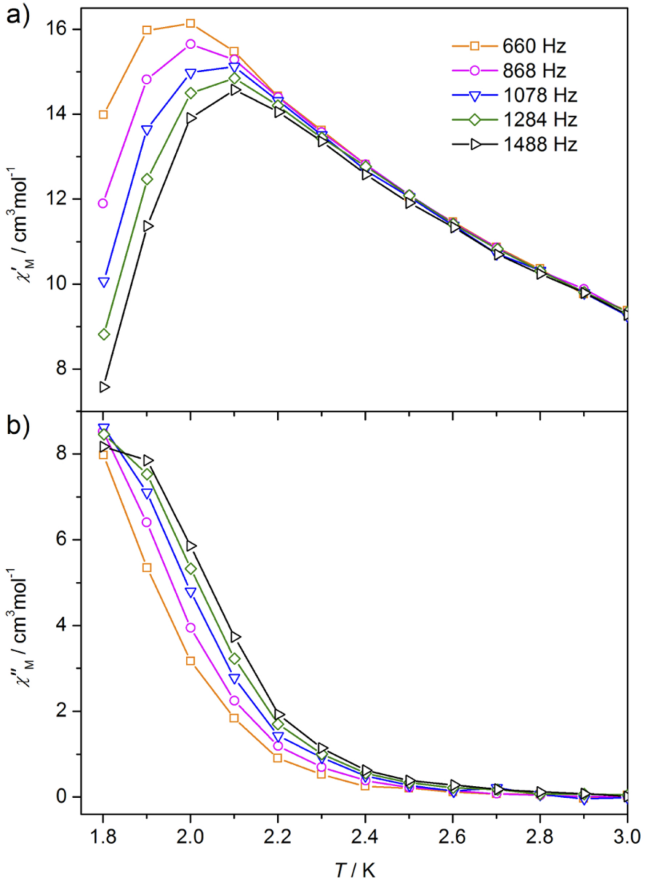


Unusual scaling with D.

Magnetization



Summary



$Mn_6^{III}Os^{III}$: AC susceptibility

- Mn^{III}–Os^{III} exchange is anisotropic;
- Exchange more complicated than Ising-like;
- Enhancement of SMM behavior, but not simple.

S. Piligkos *et al.*, J. Am. Chem. Soc. **129**, 760 (2007);

A. V. Palii *et al.*, J. Phys. Chem. A **113**, 6886 (2009);

K. S. Pedersen *et al.*, Chem. Eur. J. **16**, 13458 (2010);

J. Dreiser *et al.*, Chem. Eur. J **19**, 3693 (2013);

E. M. V. Kessler, S. Schmitt, and C. van Wüllen, J. Chem. Phys. **139**, (2013);

S. K. Singh and G. Rajaraman, Chem. Eur. J. **20**, 113 (2014).

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Thank you very much for your attention.

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