البحث السادس (بحث رقم 2 فى قائمة الأبحاثمحل تقييم اللجنة الموقرة)

Title	Geometrical control of the magnetic anisotropyin six coordinate cobalt complexes
	التحكم الهندسى في التباين المغناطيسى لمتراكبات الكوبلت السداسية
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Abstract:

The geometry of cobalt(II) ions in the axially distorted octahedralcation in [Co(MeCN)6](BF4)2 (**1**) was compared to the trigonal prismaticcation in [CoTppy]PF6 (**2**) which revealed significant differencesin magnetic anisotropy. Combined experimental and ab initioCASSCF/NEVPT2 calculations support the observed zero field SMMbehaviour for **2**, with easy axis anisotropy(B_0^2= -150.5 cm^{-1}) with minimal transverseanisotropy component, attributed to the rigidityof the trigonal prismatic ligand. Strong transverse anisotropy (B_0^2= +148.9 cm^{-1}, B_2^2= 44.5 cm^{-1})for **1**leads to significant quantum tunneling processesdue to the non-rigidMeCN ligands in the distorted octahedral coordinationenvironment.