# البحث الثانى (بحث رقم 5 فى قائمة الأبحاثمحل تقييم اللجنة الموقرة )

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| **Title** | Titanium(III) Member of the Family of Trigonal Building Blocks withScorpionate and Cyanide Ligands. |
| | **متراكب التيتانيوم الثلاثى للسيانيد والمركبات العقربية المانحة** |
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**Abstract:**

A series of mononuclear titanium complexes; [Et4N][Tp*TiCl3] (**1**) ([Et4N] = tetraethylamonium;Tp* = 3,5-dimethyltrispyrazolylhydroborate), [Tp*TiCl2pz*]pz* (**2**; pz* = 3,5-dimethylpyrazole) and the first example of a trigonal titanium(III)cyanide molecule[Et4N][Tp*Ti(CN)3](**3**)were synthesized and structurally chracterized using spectroscopic (IR, UV) and single crystal Xray measurements which reveals trigonally distorted octahedral coordination geometry. Magneticdata and ab initio calculations of **1** and **3**verified that the molecule isan S = 1/2 paramagnet and that it exhibits significanttemperature-independent paramagnetism.To further understand the magnetic properties of 1 and 3,single-point calculations were performed using crystallographicparameters. The electronic configuration of TiIII is d1, which givesrise, in the ligand field, to five spin doublet states. These wereobtained from a complete active space self-consistent field(CASSCF) calculation, followed by a second-order perturbationcalculation (CASPT2). The computed g values; [Tp TiCl3] : g|| =

1.96, g⊥= 1.71, [Tp Ti(CN)3] : g|| = 1.97, g ⊥= 1.77 are inline with experimental values and the stronger ligand field of CN ligands. This newbuilding block may lead to anisotropy in higher-nuclearitycompounds depending on the degree of distortion imposed byadditional metal spin centers bonded through the nitrogen end ofthe cyanide ligands.