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Title:	Rational design of a room temperature molecular spin switch. The light-driven coordination induced spin state switch (LD-CISSS) approach
Authors:	Venkataramani, Sugumar (/jspui/browse?type=author&value=Venkataramani%2C+Sugumar)
Keywords:	Photochromic Ligand Paramagnetic State Nickel Complex
Issue Date:	2014
Publisher:	Royal Society of Chemistry
Citation:	Dalton Transactions, 43(46), pp.17395-17405.
Abstract:	Extensive use of quantum chemical calculations has been made to rationally design a molecule whose spin state can be switched reversibly using light of two different wavelengths at room temperature in solution. Spin change is induced by changing the coordination number of a nickel complex. The coordination number in turn is switched using a photochromic ligand that binds in one configuration and dissociates in the other. We demonstrate that successful design relies on a precise geometry fit and delicate electronic tuning. Our designer complex exhibits an extremely high long-term switching stability (more than 20 000 cycles) and a high switching efficiency. The high-spin state is extraordinarily stable with a half-life of 400 days at room temperature. Switching between the dia- and paramagnetic state is achieved with visible light (500 and 430 nm). The compound can also be used as a molecular logic gate with light and pH as input and the magnetic state as non-destructive read-out.
Description:	Authors sequences are not necessary in order Only IISERM authors are available in the record.
URI:	<a href="https://pubs.rsc.org/en/content/articlelanding/2014/dt/c4dt03048f#divAbstract">https://pubs.rsc.org/en/content/articlelanding/2014/dt/c4dt03048f#divAbstract</a> ( <a href="https://pubs.rsc.org/en/content/articlelanding/2014/dt/c4dt03048f#divAbstract">https://pubs.rsc.org/en/content/articlelanding/2014/dt/c4dt03048f#divAbstract</a> ) <a href="http://hdl.handle.net/123456789/2753">http://hdl.handle.net/123456789/2753</a> ( <a href="http://hdl.handle.net/123456789/2753">http://hdl.handle.net/123456789/2753</a> )
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