

金属串配合物 $(n, m)[Cr_3(PhPyF)_4Cl_2]$ ($n=2, 3, 4; m=2, 1, 0$)的 配位结构及其与电场的关系

丁丹丹¹ 许旋^{1,2,3,4,5,*} 吴子文¹ 周沃华¹ 陈蓉¹
徐志广^{1,2,5}

(¹华南师范大学化学与环境学院, 广州 510006; ²教育部环境理论化学重点实验室, 广州 510006; ³广东省高校电化学储能与发电技术重点实验室, 广州 510006; ⁴电化学储能材料与技术教育部工程研究中心, 广州 510006; ⁵广州市能源转化与储能材料重点实验室, 广州 510006)

Coordination Structures of Metal String Complexes $(n, m)[Cr_3(PhPyF)_4Cl_2]$ ($n=2, 3, 4; m=2, 1, 0$) and Relationship with External Electric Field

DING Dan-Dan¹ XU Xuan^{1,2,3,4,5,*} WU Zi-Wen¹ ZHOU Wo-Hua¹
CHEN Rong¹ XU Zhi-Guang^{1,2,5}

(¹School of Chemistry & Environment, South China Normal University, Guangzhou 510006, P. R. China; ²Key Laboratory of Theoretical Chemistry of Environment, Ministry of Education, Guangzhou 510006, P. R. China; ³Key Laboratory of Electrochemical Technology on Energy Storage and Power Generation in Guangdong Universities, Guangzhou 510006, P. R. China; ⁴Engineering Research Center of Materials and Technology for Electrochemical Energy Storage, Ministry of Education of China, Guangzhou 510006, P. R. China; ⁵Key Laboratory of Materials for Energy Conversion and Storage of Guangzhou, Guangzhou 510006, P. R. China)

*Corresponding author. Email: xuxuan@scnu.edu.cn; Tel: +86-13560091753.

表 S1 配合物优化的能量(kJ·mol⁻¹)

Table S1 Optimized molecular energy for complexes (kJ·mol⁻¹)

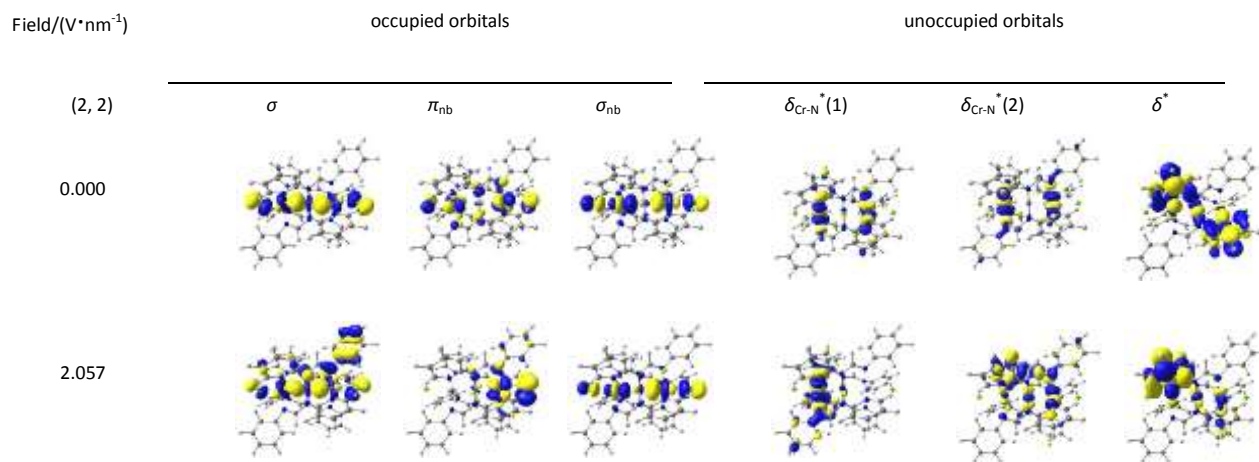
	BP86/ LANL2DZ	BP86/ SDD	B3LYP/ LANL2DZ	B3LYP/ SDD	BP86/LANL2DZ	
		(2, 2)			(3, 1)	(4, 0)
Triplet	-9688666	-9694160	-9687649	-9688042	-9688668	-9688682
Quintet	-9688752	-9694239	-9688121	-9693635	-9688750	-9688749
Septuplet	-9688651	-9694160	-9687990	-9693504	-9688664	-9688671

6-31G* for H, C, N; 6-311G* for Cl; LANL2DZ and SDD basis set for Cr

表 S2 配合物(2, 2)的部分键长(nm)

Table S2 Some bond lengths (nm) of complexes (2, 2)

Bond length	BP86/LANL2DZ	BP86/SDD	B3LYP/ LANL2DZ	B3LYP/SDD	Exp. ³
$d_{Cr1-Cr2}$	0.2466	0.2472	0.2568	0.2558	0.2438
$d_{Cr3-Cr2}$	0.2464	0.2471	0.2568	0.2557	0.2460
$d_{Cr1-Cl4}$	0.2528	0.2497	0.2551	0.2519	0.2485
$d_{Cr3-Cl5}$	0.2526	0.2497	0.2549	0.2518	0.2473
d_{Cr1-N1}	0.2151	0.2150	0.2198	0.2046	0.2131
d_{Cr2-N2}	0.2025	0.2025	0.2051	0.2197	0.2025
d_{Cr3-N3}	0.2151	0.2151	0.2199	0.2197	0.2137



5.142

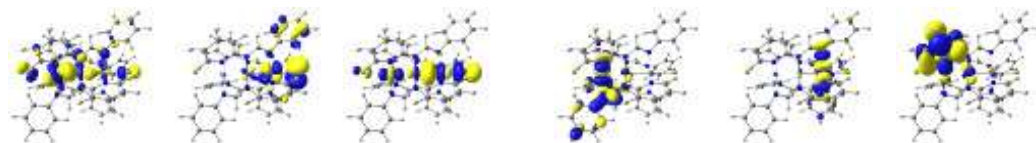


图 S1 电场作用下配合物(2, 2)分子轨道空间分布的变化

Fig.S1 Variation of spatial distribution of molecular orbital under electric field for complex (2, 2)