

: 05.23.05 /
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21.05.08

539.193:544.18

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 , .

(II, III)

(III)

LANL2DZ

DFT/B3LYP

(III)

(II,III).

(III)

(II,III) c

By quantum-chemical method of density functional theory DFT/B3LYP with use of basis LANL2DZ the calculations of binuclear aqua-complexes molecular structures of chrome (III), manganese (II,III) are carried out. A stabilizing model of binuclear aqua-complexes through a sulfate bridge ligand is offered. Vibration frequencies have been calculated to evaluate of stability of the state of binuclear aqua-complexes of chrome (III), manganese (II,III) with sulfate bridge ligand.

p

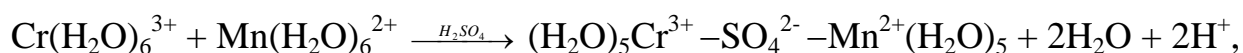
(), (), () [1, 2]. ,

(III) [3]. (III)

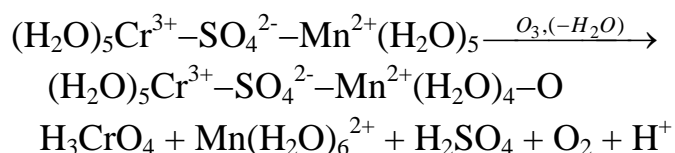
[4]. $\text{Cr}(\text{H}_2\text{O})_6^{3+}$ (III)

[4] (II) [3]. (III) (II)

:



(III) (V):



(III)

(DFT)
B3LYP [5, 6]

(), (,)

DFT

[7].

LANL2

[8].

()

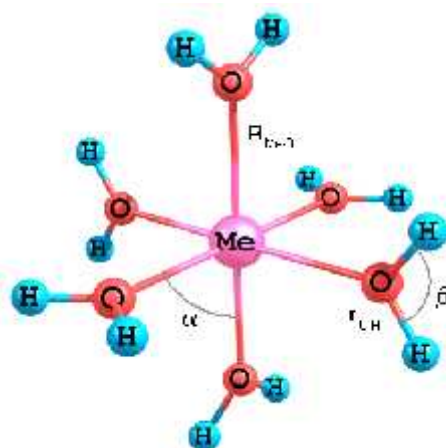
double-DZ.
B3LYP/LANL2DZ
[8].

GAUSSIAN-92 [9].

. 1.,

. 1.

. 2.,



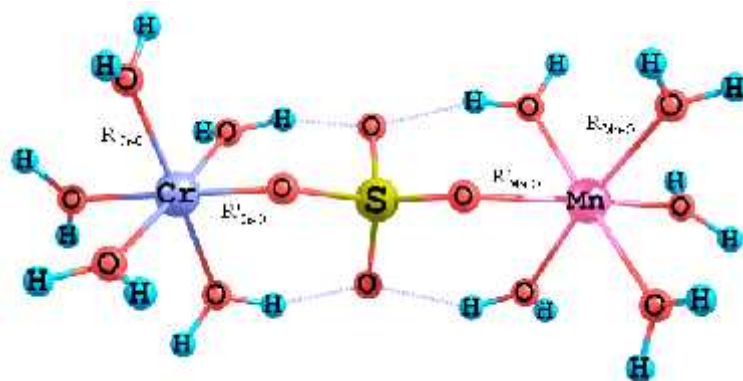
. 1.

Cr (III)

Mn (II,III)

. 2.

	E_{total} (a.u.)	$R_{\text{Me-O}}$ (Å)	$r_{\text{Mn-O}}$ (Å)	θ (°)	ϕ (°)
$[\text{Cr}(\text{H}_2\text{O})_6]^{3+}$	-543,914836	2,00	0,99	90,0	110,3
$[\text{Mn}(\text{H}_2\text{O})_6]^{2+}$	-562,110725	2,19	0,98	90,0	110,5
$[\text{Mn}(\text{H}_2\text{O})_6]^{3+}$	-561,476922	2,03	0,99	90,0	110,3



. 2.

[10].

2

	E_{total} (a.u.)	$R_{\text{Cr-O}}$ (Å)	$R'_{\text{Cr-O}}$ (Å)	$R_{\text{Mn-O}}$ (Å)	$R'_{\text{Mn-O}}$ (Å)
$[(\text{H}_2\text{O})_5\text{Cr}^{\text{III}} - \text{SO}_4 - \text{Cr}^{\text{III}}(\text{H}_2\text{O})_5]^{4+}$	-1246,569317	2,01	1,97	-	-
$[(\text{H}_2\text{O})_5\text{Cr}^{\text{III}} - \text{SO}_4 - \text{Mn}^{\text{II}}(\text{H}_2\text{O})_5]^{3+}$	-1264,764189	2,02	1,89	2,19	2,26
$[(\text{H}_2\text{O})_5\text{Cr}^{\text{III}} - \text{SO}_4 - \text{Mn}^{\text{I}}(\text{H}_2\text{O})_5]^{4+}$	-1264,138959	2,01	1,96	2,06*	1,89

*

DFT/B3LYP

Cr (III) Mn (II,III)

DFT/B3LYP

Mn (II) Mn (III) Cr (III)

Cr (III)

1. ... (...) : 05.17.05. / ... , 1987. – 360 . 2. / ... , 1981. – . 446 – 452.
3. ... // – 1977. – . 42. – 6. – . 628 – 632. 4. / ... , 1975. – 272 . 5. Becke A.D. Density-functional exchange-energy approximation with correct asymptotic behavior // Phys. Rev. – 1988. – A. 38. – P. 3098 – 3100. 6. Lee C., Yang W., Parr R.G. Development of the Colle-Salvetti correlation-energy formula into a function of the electron density // Phys. Rev. – 1988. – B. 37. – P. 785 – 789. 7. Becke A. D. Density-functional thermochemistry. III. The role of exact exchange // J. Chem. Phys. – 1993. – Vol. 98. – . 5648 – 5652. 8. Hay P.J., Wadt W.R. Ab initio effective core potential for molecular calculations // J. Chem. Phys. – 1985. – Vol. 82. – P. 270 – 310. 9. Frisch M.J., Trucks G.W., Schlegel H.B. et al. Gaussian 92/DFT, Revision G.2 / Gaussian Inc. – Pittsburgh: PA, 1993. 10. “GAUSSIAN”: [...] /] . – : . . - . , 2003. – 88 .

03.05.08

666.6.

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A generalised task on making multilayer diffusion silicide coatings is formulated. The equations to calculate parameters of phase formation and redistribution are given, e.g. co-ordinates of interphase boundaries and speed of these boundaries' dislocation. The boundary conditions for these equations are found.