

High-Temperature Cooperative Spin Crossover Transitions and Single-Crystal Reflection Spectra of $[\text{Fe}^{\text{III}}(\text{qsal})_2](\text{CH}_3\text{OSO}_3)$ and Related Compounds

Kazuyuki Takahashi ^{1,*}, Kaoru Yamamoto ², Takashi Yamamoto ³, Yasuaki Einaga ³, Yoshihito Shiota ⁴, Kazunari Yoshizawa ⁴ and Hatsumi Mori ⁵

¹ Department of Chemistry, Graduate School of Science, Kobe University, 1-1 Rokkodai, Nada-ku, Kobe, Hyogo 657-8501, Japan

² Department of Applied Physics, Okayama University of Science, 1-1 Ridaicho, Kita-ku, Okayama, Okayama 700-0005, Japan; yamamoto@dap.ous.ac.jp

³ Department of Chemistry, Graduate School of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Kanagawa 223-8522, Japan; takyama@chem.keio.ac.jp (T.Y.); einaga@chem.keio.ac.jp (Y.E.)

⁴ Institute for Materials Chemistry and Engineering, Kyushu University, 744 Motoooka, Nishi-ku, Fukuoka 819-0395, Japan; shiota@ms.ifoc.kyushu-u.ac.jp (Y.S.); kazunari@ms.ifoc.kyushu-u.ac.jp (K.Y.)

⁵ Institute for Solid State Physics, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan; hmori@issp.u-tokyo.ac.jp

* Correspondence: ktaka@crystal.kobe-u.ac.jp; Tel.: +81-78-803-5691

Contents

Table S1. Cartesian coordinates of the LS $[\text{Fe}(\text{qsal})_2]$ cation.	S2
Table S2. Cartesian coordinates of the HS $[\text{Fe}(\text{qsal})_2]$ cation.	S4

Table S1. Cartesian coordinates of the LS [Fe(qsal)₂] cation.

C	-2.14240900	0.18146300	1.97273400
C	2.18121300	4.70016600	-0.40891100
C	2.90118000	4.08049100	-1.41633000
C	2.64995200	2.71466400	-1.72119700
C	1.65451700	2.01609500	-0.97896200
C	3.33868000	1.99119800	-2.73380300
C	3.02643000	0.66269900	-2.95471800
C	2.03014300	0.04657300	-2.15951000
C	-2.14249800	-0.18151100	-1.97268700
C	-3.16931800	0.46028700	-2.71999500
C	-4.05199800	-0.27261600	-3.49973800
C	-3.16908700	-0.46039200	2.72018600
C	-3.95865900	-1.68600400	-3.58896600
C	-2.96111500	-2.33448400	-2.88699600
C	-2.03429700	-1.61475900	-2.07375400
C	-1.00883000	-2.35650400	-1.42230200
C	0.89961200	-2.67259200	-0.03850700
C	1.18523400	-4.00463500	-0.32252400
C	2.18130000	-4.70011200	0.40892500
C	2.90120700	-4.08042900	1.41638200
C	2.64993900	-2.71460600	1.72123800
C	1.65457200	-2.01604000	0.97891000
C	-4.05183700	0.27248400	3.49987600
C	3.33851700	-1.99115800	2.73396200
C	3.02617800	-0.66268800	2.95491000
C	2.02999800	-0.04655000	2.15957400
C	-3.95870800	1.68589700	3.58890700
C	-2.96129300	2.33443400	2.88680400
C	-2.03440100	1.61473600	2.07362700
C	-1.00901300	2.35653300	1.42209800
C	0.89951300	2.67263500	0.03842800
C	1.18512700	4.00466800	0.32249200
Fe	-0.07885900	0.00000500	-0.00002300
N	-0.07295900	1.85426000	0.65046400
N	1.37284500	0.69464000	-1.20710700
N	-0.07285500	-1.85422300	-0.65056700
N	1.37288000	-0.69458600	1.20702900
O	-1.34670700	-0.56882800	1.25289500
O	-1.34683100	0.56880600	-1.25284200
H	2.37578400	5.74155200	-0.16464800

H	3.66030300	4.62352000	-1.97395200
H	4.10257000	2.49081600	-3.32601000
H	3.52585900	0.07937200	-3.72243200
H	1.76594000	-0.99541500	-2.31467600
H	-3.24334300	1.54224800	-2.64867300
H	-4.83271200	0.24804700	-4.05118700
H	-3.24296000	-1.54237200	2.64900500
H	-4.66021200	-2.24424500	-4.20242100
H	-2.86791000	-3.41810600	-2.94709900
H	-1.02208700	-3.43475700	-1.59227200
H	0.65635300	-4.53605700	-1.10832500
H	2.37588800	-5.74150000	0.16468100
H	3.66030000	-4.62344800	1.97405200
H	-4.83244500	-0.24821900	4.05143700
H	4.10234900	-2.49077900	3.32624200
H	3.52545700	-0.07938600	3.72274100
H	1.76576400	0.99543200	2.31473300
H	-4.66031500	2.24411400	4.20232300
H	-2.86823600	3.41807600	2.94676300
H	-1.02241500	3.43481100	1.59191200
H	0.65624500	4.53605300	1.10831700

Table S2. Cartesian coordinates of the HS [Fe(qsal)₂] cation.

C	2.37473500	0.88825900	1.92032700
C	-1.97780100	4.73729000	-1.38431200
C	-2.78178100	3.94107800	-2.18021700
C	-2.60150900	2.53062300	-2.17176700
C	-1.58069600	1.96144200	-1.35147800
C	-3.39767400	1.63950300	-2.94247800
C	-3.16988600	0.27808400	-2.86468700
C	-2.15330000	-0.19484100	-1.99989900
C	-2.37430800	-0.88846300	1.92074700
C	-3.44064100	-0.47773700	2.76349600
C	-4.42091600	-1.37975000	3.15955400
C	3.44119600	0.47743100	2.76288100
C	-4.38833700	-2.73329500	2.74087400
C	-3.35502800	-3.15922400	1.92432300
C	-2.33207000	-2.26420500	1.49517200
C	-1.28664000	-2.79138200	0.67575100
C	0.72471800	-2.80240100	-0.56925400
C	0.95793300	-4.17470600	-0.57607900
C	1.97838000	-4.73712300	-1.38374400
C	2.78189900	-3.94098100	-2.18019700
C	2.60125800	-2.53057100	-2.17222400
C	1.58052500	-1.96134600	-1.35187000
C	4.42116000	1.37954500	3.15945000
C	3.39699500	-1.63951900	-2.94346800
C	3.16891100	-0.27813100	-2.86605800
C	2.15246900	0.19484400	-2.00110800
C	4.38816300	2.73330400	2.74147300
C	3.35476900	3.15931300	1.92508500
C	2.33210200	2.26419100	1.49542500
C	1.28664500	2.79145000	0.67611000
C	-0.72447600	2.80253600	-0.56932800
C	-0.95729100	4.17490600	-0.57669900
Fe	-0.00001400	0.00002500	0.33926200
H	3.46219700	-0.55973500	3.08715200
H	-3.75774800	-0.43329900	-3.43712200
H	-1.97144500	-1.26275100	-1.90043100
H	-3.46133000	0.55926500	3.08831500
H	-5.22727500	-1.03886700	3.80620200
H	-5.16139600	-3.42508900	3.06341500
H	-3.30969900	-4.19847900	1.60094200

H	-1.37379700	-3.85858700	0.45196000
H	0.37515500	-4.84059200	0.05372100
H	2.12673700	-5.81401600	-1.36478600
H	3.56000500	-4.37797900	-2.80154900
H	5.22760700	1.03858500	3.80595000
H	4.18016700	-2.03940700	-3.58435600
H	3.75644300	0.43320700	-3.43888700
H	1.97045100	1.26276000	-1.90188400
H	5.16098400	3.42517700	3.06441300
H	3.30914000	4.19870900	1.60220300
H	1.37361100	3.85877000	0.45283000
H	-0.37413300	4.84095100	0.05257500
H	-2.12581300	5.81423900	-1.36575700
H	-3.55994400	4.37805400	-2.80151100
H	-4.18093500	2.03935700	-3.58327700
N	0.27023600	2.12736400	0.17220600
N	-1.38893400	0.60923500	-1.27316900
N	-0.27002200	-2.12730100	0.17227700
N	1.38848000	-0.60915500	-1.27391900
O	1.46313200	0.02242400	1.56157900
O	-1.46237600	-0.02275800	1.56248500



© 2019 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).