Supporting Information

The Sensing of Sulfur Dioxide by Base Metal Thiolates: Structures and Properties of Molecular NiN_2S_2/SO_2 Adducts

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Figure SI-1. Thermogravimetric analysis plot for **Ni-1'**•SO_2.

Figure SI-2. Thermogravimetric analysis plot for **Ni-1**•$2SO_2$.

Figure SI-3. Packing Diagram showing the extended chain interaction zigzagging between dimers containing the short interaction.

Table SI-1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for mdmgm. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table SI-2. Bond lengths [Å] and angles [°] for mdmgm, **Ni-1**•$2SO_2$.

Table SI-3. Anisotropic displacement parameters (Å^{2}x 10^3) for mdmgm, **Ni-1**•$2SO_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table SI-4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for mdmgm, **Ni-1**•$2SO_2$.

Figure SI-1. Thermogravimetric analysis plot for **Ni-1'**•SO_2.

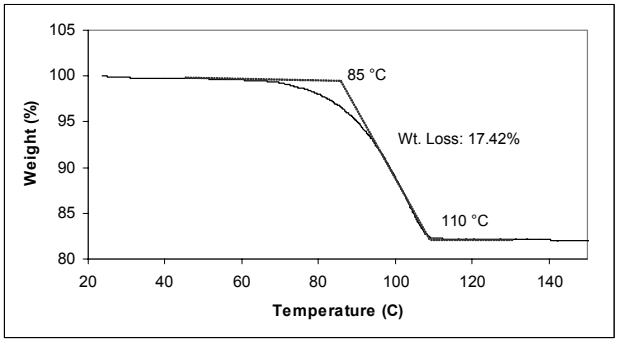

Figure SI-2. Thermogravimetric analysis plot for **Ni-1**•$2SO_2$.

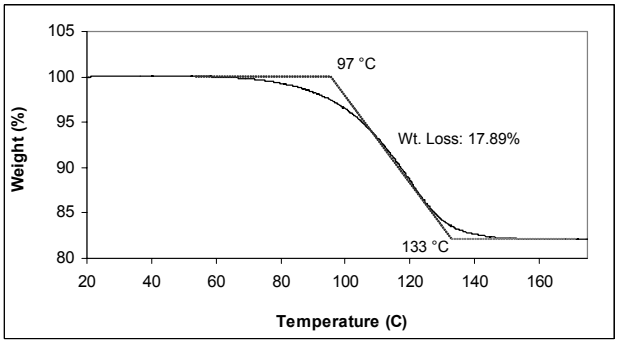

Figure SI-3. Packing Diagram showing the extended chain interaction zigzagging between dimers containing the short interaction.

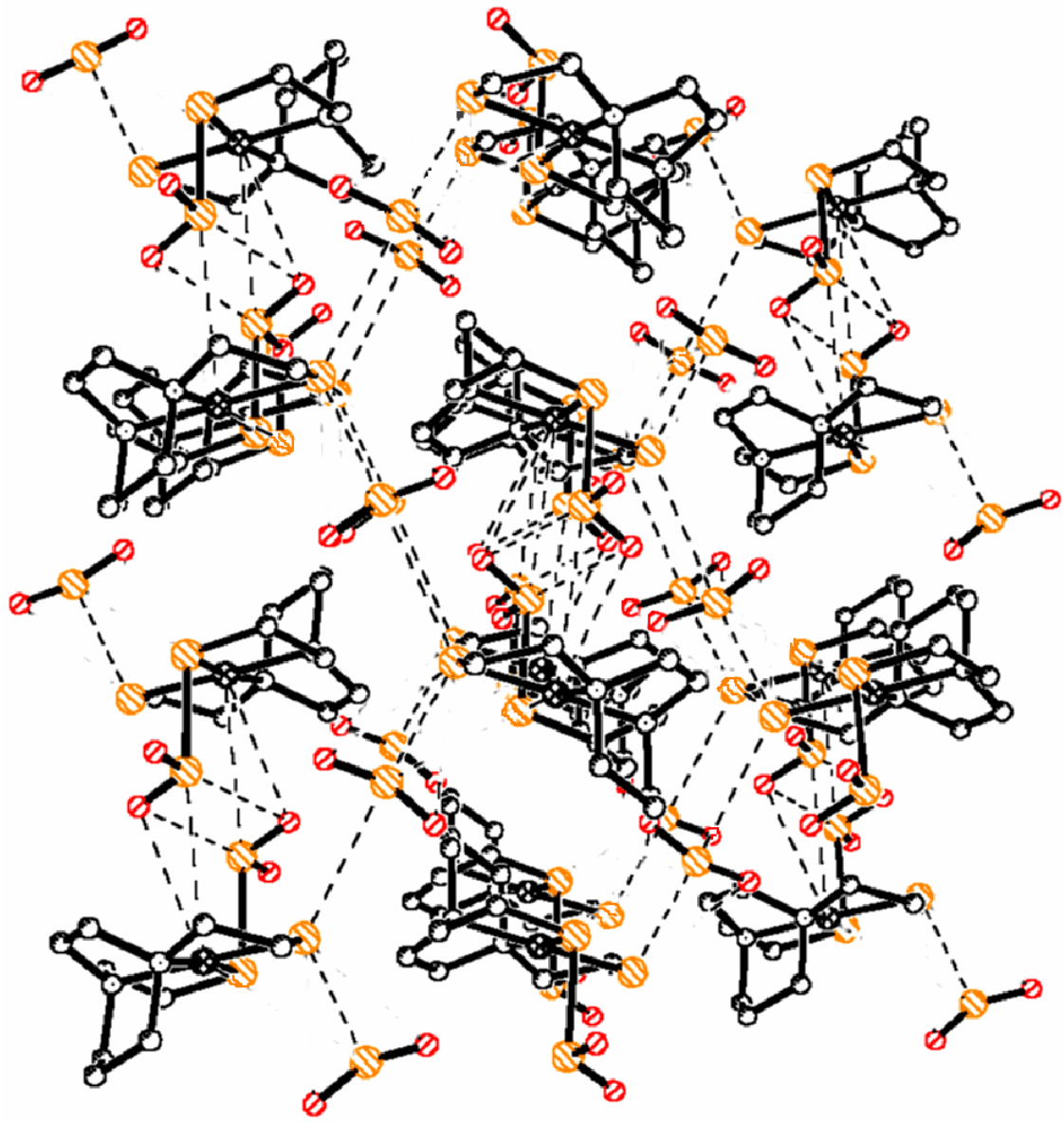

Table SI-1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mdmgm, **Ni-1**•$2SO_2$.. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	8193(1)	5019(1)	2495(1)	12(1)
N(1)	6479(2)	5550(1)	2671(2)	13(1)
N(2)	8564(2)	6367(1)	1989(2)	14(1)
S(1)	7571(1)	3542(1)	3036(1)	15(1)
S(2)	10128(1)	4540(1)	2063(1)	15(1)
S(3)	11439(1)	4634(1)	4105(1)	18(1)
S(4)	7346(1)	2591(1)	881(1)	19(1)
O(1)	12676(1)	4259(1)	3688(1)	23(1)
O(2)	10744(2)	3905(1)	4835(1)	25(1)
O(3)	6516(2)	3301(1)	225(2)	33(1)
O(4)	6681(2)	1712(1)	1308(2)	34(1)
C(1)	5838(2)	3807(2)	3087(2)	17(1)
C(2)	5660(2)	4892(2)	3445(2)	18(1)
C(3)	5909(2)	5623(2)	1379(2)	17(1)
C(4)	6561(2)	6438(2)	627(2)	19(1)
C(5)	8033(2)	6439(2)	691(2)	18(1)
C(6)	6606(2)	6576(2)	3229(2)	18(1)
C(7)	7851(2)	7069(2)	2805(2)	17(1)
C(8)	9987(2)	6584(2)	2049(2)	18(1)
C(9)	10732(2)	5738(2)	1481(2)	18(1)

Table SI-2. Bond lengths [Å] and angles [°] for mdmgm, **Ni-1**•$2SO_2$..

Ni(1)-N(1)	1.9190(18)
Ni(1)-N(2)	1.9216(18)
Ni(1)-S(1)	2.1585(9)
Ni(1)-S(2)	2.1607(9)
N(1)-C(6)	1.500(3)
N(1)-C(2)	1.496(3)
N(1)-C(3)	1.503(3)
N(2)-C(8)	1.494(3)
N(2)-C(5)	1.496(3)
N(2)-C(7)	1.498(3)
S(1)-C(1)	1.824(2)
S(2)-C(9)	1.834(2)
S(2)-S(3)	2.5567(11)
S(3)-O(2)	1.4566(17)
S(3)-O(1)	1.4564(17)
S(4)-O(4)	1.4412(17)
S(4)-O(3)	1.4463(16)
C(1)-C(2)	1.510(3)
C(3)-C(4)	1.528(3)
C(4)-C(5)	1.516(3)
C(6)-C(7)	1.527(3)
C(8)-C(9)	1.509(3)
N(1)-Ni(1)-N(2)	82.87(7)
N(1)-Ni(1)-S(1)	91.54(6)
N(2)-Ni(1)-S(1)	174.20(5)
N(1)-Ni(1)-S(2)	172.06(5)
N(2)-Ni(1)-S(2)	91.16(6)
S(1)-Ni(1)-S(2)	94.25(3)
C(6)-N(1)-C(2)	110.63(17)
C(6)-N(1)-C(3)	110.05(16)
C(2)-N(1)-C(3)	110.52(16)
C(6)-N(1)-Ni(1)	108.00(13)
C(2)-N(1)-Ni(1)	112.24(13)

C(3)-N(1)-Ni(1)	105.23(13)
C(8)-N(2)-C(5)	110.85(16)
C(8)-N(2)-C(7)	110.67(16)
C(5)-N(2)-C(7)	110.16(16)
C(8)-N(2)-Ni(1)	111.92(13)
C(5)-N(2)-Ni(1)	105.02(12)
C(7)-N(2)-Ni(1)	108.04(13)
C(1)-S(1)-Ni(1)	97.55(7)
C(9)-S(2)-Ni(1)	98.30(8)
C(9)-S(2)-S(3)	94.56(7)
Ni(1)-S(2)-S(3)	105.21(3)
O(2)-S(3)-O(1)	113.04(9)
O(2)-S(3)-S(2)	100.53(7)
O(1)-S(3)-S(2)	99.04(7)
O(4)-S(4)-O(3)	114.22(11)
C(2)-C(1)-S(1)	108.75(15)
N(1)-C(2)-C(1)	109.98(18)
N(1)-C(3)-C(4)	112.21(17)
C(5)-C(4)-C(3)	115.73(18)
N(2)-C(5)-C(4)	112.10(17)
N(1)-C(6)-C(7)	109.51(18)
N(2)-C(7)-C(6)	110.05(17)
N(2)-C(8)-C(9)	110.50(17)
C(8)-C(9)-S(2)	109.06(15)

Symmetry transformations used to generate equivalent atoms:

Table SI-3. Anisotropic displacement parameters ($Å^2$x 10^3) for mdmgm **Ni-1**•$2SO_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	10(1)	11(1)	14(1)	1(1)	1(1)	0(1)
N(1)	13(1)	14(1)	14(1)	0(1)	0(1)	1(1)
N(2)	14(1)	14(1)	13(1)	0(1)	0(1)	-1(1)
S(1)	13(1)	13(1)	19(1)	3(1)	0(1)	-1(1)
S(2)	12(1)	18(1)	16(1)	0(1)	2(1)	0(1)
S(3)	16(1)	18(1)	19(1)	-3(1)	-3(1)	3(1)
S(4)	15(1)	17(1)	23(1)	-1(1)	0(1)	1(1)
O(1)	14(1)	24(1)	31(1)	-6(1)	-3(1)	1(1)
O(2)	26(1)	29(1)	20(1)	7(1)	1(1)	5(1)
O(3)	41(1)	30(1)	26(1)	-8(1)	-14(1)	18(1)
O(4)	44(1)	23(1)	36(1)	-7(1)	12(1)	-14(1)
C(1)	11(1)	20(1)	21(1)	3(1)	0(1)	-2(1)
C(2)	14(1)	22(1)	18(1)	1(1)	3(1)	-1(1)
C(3)	14(1)	20(1)	17(1)	0(1)	-3(1)	1(1)
C(4)	21(1)	21(1)	13(1)	1(1)	-3(1)	2(1)
C(5)	25(1)	16(1)	12(1)	0(1)	-1(1)	-2(1)
C(6)	21(1)	17(1)	16(1)	-3(1)	0(1)	5(1)
C(7)	22(1)	14(1)	16(1)	-2(1)	-1(1)	1(1)
C(8)	20(1)	17(1)	17(1)	1(1)	-1(1)	-6(1)
C(9)	13(1)	23(1)	18(1)	4(1)	2(1)	-3(1)

Table SI-4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for mdmgm, **Ni-1**•$2SO_2$.

	x	y	z	U(eq)
H(1A)	5424	3683	2284	21
H(1B)	5440	3373	3685	21
H(2A)	4754	5078	3329	21
H(2B)	5905	4981	4310	21
H(3A)	4989	5767	1414	21
H(3B)	6005	4982	969	21
H(4A)	6275	6364	-230	22
H(4B)	6260	7085	907	22
H(5A)	8349	5877	218	21
H(5B)	8346	7051	319	21
H(6A)	6629	6526	4122	21
H(6B)	5863	6983	2975	21
H(7A)	7641	7681	2357	21
H(7B)	8400	7243	3518	21
H(8A)	10276	6670	2903	22
H(8B)	10155	7203	1612	22
H(9A)	11650	5806	1693	22
H(9B)	10621	5760	589	22