Supporting Information

Elemental Analysis

Salt **1** $(NH_4^+)_{0.88}$([15]crown-5)[Ni(dmit)$_2$]$_2$ ($C_{22}H_{24}N_{0.88}O_5S_{20}Ni_2$ for found. C: 23.28, H: 2.41, N: 1.20 %, calc: C: 23.19, H: 2.11, N: 1.09 %).

Salt **2** $(NH_4^+)_{0.7}$([18]crown-6)[Ni(dmit)$_2$]$_2$ ($C_{24}H_{27}N_{0.7}O_6S_{20}Ni_2$ for found. C: 24.13, H: 2.30, N: 1.01 %, calc: C: 24.43, H: 2.29, N: 0.83 %).

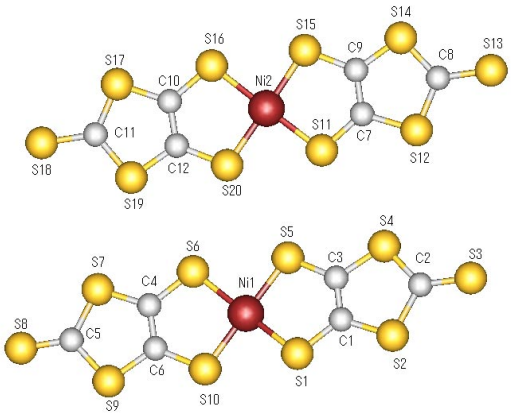
Salt **3** $(NH_2\text{-}NH_3^+)$([12]crown-4)$_2$[Ni(dmit)$_2$]$_4$ ($C_{40}H_{37}N_2O_8S_{40}Ni_4$ for found. C: 21.81, H: 1.69, N: 1.32 %, calc: C: 21.93, H: 1.70, N: 1.28 %).

Salt **4** $(NH_2\text{-}NH_3^+)_2$([15]crown-5)$_3$[Ni(dmit)$_2$]$_6$ ($C_{66}H_{70}N_4O_{15}S_{60}Ni_6$ for found. C: 22.91, H: 2.01, N: 1.30 %, calc: C: 23.07, H: 2.05, N: 1.63 %).

Salt **5** $(NH_2\text{-}NH_3^+)_{0.8}$([18]crown-6)[Ni(dmit)$_2$]$_2$ ($C_{24}H_{28}N_{1.6}O_6S_{20}Ni_2$ for found. C: 23.79, H: 2.27, N: 1.99 %, calc: C: 24.15, H: 2.35, N: 1.88 %).

Salt **7** $(NH_2\text{-}NH_3^+)$([18]crown-6)[Ni(dmit)$_2$] ($C_{18}H_{29}N_2O_6S_{10}Ni$ for found. C: 29.01, H: 3.88, N: 3.86 %, calc: C: 28.87, H: 3.90, N: 3.74 %).

Crystal data (1)



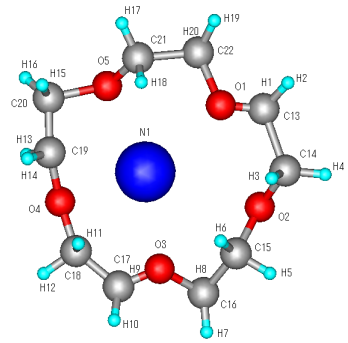


Table S1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Ni(1)	1.0660(4)	0.1658(1)	0.21560(7)	3.82(3)	
S(1)	1.209(1)	0.1079(2)	0.2919(2)	5.08(9)	
S(2)	1.601(1)	0.1328(2)	0.4080(2)	5.7(1)	
S(3)	1.989(1)	0.2142(3)	0.4903(2)	8.1(1)	
S(4)	1.6903(9)	0.2607(2)	0.3736(2)	5.90(9)	
S(10)	0.8548(9)	0.0867(2)	0.1744(2)	5.04(9)	
S(7)	0.4951(9)	0.2014(2)	0.0275(2)	5.25(8)	
S(6)	0.8928(9)	0.2262(2)	0.1427(2)	5.22(8)	
S(5)	1.3022(9)	0.2450(2)	0.2545(2)	5.18(8)	
S(9)	0.4693(9)	0.0705(2)	0.0546(2)	4.76(8)	
S(8)	0.1406(9)	0.1182(2)	-0.0583(2)	5.7(1)	

C(5)	0.348(3)	0.1295(7)	0.0028(6)	4.9(3)	
C(4)	0.689(3)	0.1781(5)	0.0939(5)	3.6(2)	
C(6)	0.683(3)	0.1167(7)	0.1071(6)	4.3(3)	
C(3)	1.460(3)	0.2158(8)	0.3213(7)	5.0(3)	
C(1)	1.427(3)	0.1564(6)	0.3378(6)	3.7(3)	
C(2)	1.782(3)	0.2051(8)	0.4286(6)	5.3(3)	
Ni(2)	0.9827(3)	0.4561(1)	0.27471(7)	3.55(3)	
S(16)	0.7569(9)	0.5174(2)	0.2082(2)	4.93(8)	
S(11)	1.2286(8)	0.3963(2)	0.3386(2)	4.59(7)	
S(13)	1.9014(9)	0.5084(2)	0.5499(2)	6.1(1)	
S(15)	1.1198(9)	0.5384(2)	0.3262(2)	4.70(8)	
S(17)	0.3753(9)	0.4919(2)	0.0916(2)	5.43(9)	
S(12)	1.6119(9)	0.4243(2)	0.4556(2)	5.05(8)	
S(20)	0.8238(9)	0.3757(2)	0.2263(2)	5.10(8)	
S(18)	0.054(1)	0.4089(3)	0.0017(2)	7.3(1)	
S(14)	1.5136(9)	0.5552(2)	0.4435(2)	5.09(9)	
S(19)	0.4299(9)	0.3591(2)	0.1092(2)	5.77(9)	
C(10)	0.591(3)	0.4672(8)	0.1556(6)	4.4(3)	
C(12)	0.614(3)	0.4040(6)	0.1651(5)	3.6(2)	
C(11)	0.282(3)	0.4205(8)	0.0658(6)	5.0(3)	
C(8)	1.679(3)	0.4980(7)	0.4862(5)	4.0(3)	
C(7)	1.381(3)	0.4475(7)	0.3906(5)	3.9(3)	
C(9)	1.342(3)	0.5101(6)	0.3862(6)	3.8(3)	
O(1)	1.465(8)	0.883(2)	0.332(2)	25.0(2)	
O(2)	1.664(5)	0.768(1)	0.365(1)	15.2(7)	
O(5)	1.547(4)	0.910(1)	0.2033(9)	12.6(5)	
O(4)	1.453(7)	0.785(2)	0.147(1)	20.0(1)	
O(3)	1.442(8)	0.706(2)	0.255(2)	26.3(2)	
C(15)	1.508(7)	0.719(1)	0.340(1)	16.8(1)	
C(16)	1.604(5)	0.677(1)	0.2984(9)	11.0(7)	
C(22)	1.546(4)	0.9421(9)	0.3074(8)	7.8(4)	
C(19)	1.359(8)	0.840(2)	0.140(1)	19.8(2)	
C(18)	1.404(6)	0.730(1)	0.163(1)	12.0(8)	
C(21)	1.420(5)	0.939(1)	0.2430(9)	10.1(6)	
C(20)	1.423(5)	0.900(1)	0.1403(9)	8.7(5)	
C(13)	1.569(6)	0.876(1)	0.377(1)	12.4(8)	
C(17)	1.429(6)	0.689(1)	0.208(1)	11.9(8)	
C(14)	1.517(5)	0.8072(8)	0.400(1)	8.4(5)	
N(1)	0.983(4)	0.814(1)	0.2565(9)	6.4(4)	0.85(3)
H(1)	1.784(6)	0.880(1)	0.376(1)	0.02(8)	
H(2)	1.499(6)	0.904(1)	0.408(1)	0.02(8)	
H(3)	1.308(5)	0.7995(8)	0.390(1)	0.02(8)	
H(4)	1.557(5)	0.8007(8)	0.443(1)	0.02(8)	
H(5)	1.502(7)	0.695(1)	0.377(1)	0.03(8)	
H(6)	1.309(7)	0.733(1)	0.329(1)	0.02(8)	
H(7)	1.565(5)	0.634(1)	0.3010(9)	0.02(8)	
H(8)	1.810(5)	0.683(1)	0.2883(9)	0.01(8)	
H(9)	1.635(6)	0.680(1)	0.200(1)	0.02(8)	
H(10)	1.312(6)	0.652(1)	0.205(1)	0.02(8)	
H(11)	1.198(6)	0.738(1)	0.172(1)	-0.00(8)	
H(12)	1.412(6)	0.707(1)	0.125(1)	0.02(8)	
H(13)	1.510(8)	0.839(2)	0.110(1)	-0.02(8)	
H(14)	1.164(8)	0.834(2)	0.120(1)	0.03(8)	
H(15)	1.220(5)	0.915(1)	0.1392(9)	0.01(8)	
H(16)	1.538(5)	0.923(1)	0.1122(9)	0.02(8)	
H(17)	1.346(5)	0.978(1)	0.2289(9)	0.03(8)	

H(18)	1.254(5)	0.913(1)	0.2498(9)	0.01(8)
H(19)	1.470(4)	0.9763(9)	0.3296(8)	0.02(8)
H(20)	1.760(4)	0.9465(9)	0.3041(8)	0.01(8)

Table S2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	0.0551(8)	0.0484(9)	0.0413(8)	-0.0008(7)	0.0004(7)	-0.0007(7)
S(1)	0.084(2)	0.054(2)	0.055(2)	0.002(2)	-0.010(2)	0.003(2)
S(2)	0.086(3)	0.081(3)	0.050(2)	0.016(2)	-0.008(2)	0.002(2)
S(3)	0.080(3)	0.164(6)	0.059(3)	0.022(3)	-0.026(2)	-0.029(3)
S(4)	0.077(2)	0.076(3)	0.069(2)	-0.007(2)	-0.022(2)	-0.010(2)
S(10)	0.083(2)	0.050(2)	0.057(2)	-0.015(2)	-0.013(2)	0.008(2)
S(7)	0.091(3)	0.057(2)	0.050(2)	-0.003(2)	-0.018(2)	0.001(2)
S(6)	0.096(3)	0.044(2)	0.057(2)	-0.009(2)	-0.021(2)	0.001(1)
S(5)	0.086(2)	0.056(2)	0.053(2)	-0.013(2)	-0.015(2)	-0.000(2)
S(9)	0.075(2)	0.057(2)	0.048(2)	-0.015(2)	-0.011(2)	-0.002(2)
S(8)	0.071(2)	0.085(3)	0.060(2)	-0.009(2)	-0.020(2)	-0.006(2)
C(5)	0.068(8)	0.063(8)	0.056(8)	0.004(7)	0.002(6)	0.015(7)
C(4)	0.055(6)	0.035(6)	0.048(6)	-0.001(5)	0.001(5)	-0.005(5)
C(6)	0.058(7)	0.061(9)	0.044(7)	-0.002(6)	0.003(6)	-0.007(6)
C(3)	0.047(6)	0.08(1)	0.057(8)	0.007(7)	-0.000(6)	-0.002(7)
C(1)	0.053(6)	0.043(8)	0.045(6)	0.006(5)	-0.002(5)	0.011(5)
C(2)	0.052(7)	0.10(1)	0.046(7)	0.015(7)	0.003(6)	-0.018(8)
Ni(2)	0.0532(8)	0.0434(8)	0.0380(7)	-0.0013(7)	-0.0028(6)	-0.0003(7)
S(16)	0.086(2)	0.048(2)	0.051(2)	0.008(2)	-0.018(2)	-0.002(2)
S(11)	0.076(2)	0.045(2)	0.052(2)	0.003(1)	-0.017(2)	-0.002(1)
S(13)	0.079(2)	0.088(3)	0.064(2)	-0.023(2)	-0.020(2)	0.007(2)
S(15)	0.083(2)	0.045(2)	0.049(2)	0.001(2)	-0.011(2)	-0.002(2)
S(17)	0.075(2)	0.082(3)	0.048(2)	0.016(2)	-0.014(2)	0.004(2)
S(12)	0.075(2)	0.060(2)	0.055(2)	0.002(2)	-0.015(2)	0.002(2)
S(20)	0.091(2)	0.043(2)	0.058(2)	-0.003(2)	-0.023(2)	0.002(1)
S(18)	0.076(3)	0.140(5)	0.061(2)	-0.008(3)	-0.020(2)	-0.019(3)
S(14)	0.085(2)	0.051(2)	0.057(2)	-0.015(2)	-0.008(2)	-0.002(2)
S(19)	0.087(3)	0.069(2)	0.060(2)	-0.017(2)	-0.020(2)	-0.011(2)
C(10)	0.047(6)	0.08(1)	0.041(6)	0.008(6)	-0.007(5)	-0.005(7)
C(12)	0.062(7)	0.046(6)	0.030(5)	-0.023(5)	-0.001(5)	-0.010(5)
C(11)	0.041(6)	0.10(1)	0.047(7)	-0.001(7)	-0.002(6)	-0.003(8)
C(8)	0.052(6)	0.073(9)	0.027(5)	-0.018(6)	-0.005(5)	-0.009(5)
C(7)	0.054(6)	0.057(8)	0.038(6)	-0.007(6)	-0.001(5)	0.009(6)
C(9)	0.055(7)	0.047(8)	0.042(6)	-0.001(5)	-0.004(6)	-0.007(5)
N(1)	0.09(1)	0.085(9)	0.07(1)	-0.005(7)	0.001(7)	0.010(7)

The general temperature factor expression:$\exp(-2p^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S3. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ni(1)	S(1)	2.135(4)	Ni(1)	S(10)	2.122(4)
Ni(1)	S(6)	2.154(4)	Ni(1)	S(5)	2.154(4)
S(1)	C(1)	1.71(1)	S(2)	C(1)	1.74(1)
S(2)	C(2)	1.80(2)	S(3)	C(2)	1.59(2)
S(4)	C(3)	1.77(2)	S(4)	C(2)	1.72(2)
S(10)	C(6)	1.73(1)	S(7)	C(5)	1.76(2)
S(7)	C(4)	1.71(1)	S(6)	C(4)	1.70(1)
S(5)	C(3)	1.69(2)	S(9)	C(5)	1.76(1)
S(9)	C(6)	1.75(1)	S(8)	C(5)	1.59(2)

C(4)	C(6)	1.36(2)	C(3)	C(1)	1.34(2)
Ni(2)	S(16)	2.159(4)	Ni(2)	S(11)	2.144(4)
Ni(2)	S(15)	2.166(4)	Ni(2)	S(20)	2.128(4)
S(16)	C(10)	1.71(2)	S(11)	C(7)	1.69(1)
S(13)	C(8)	1.66(1)	S(15)	C(9)	1.70(1)
S(17)	C(10)	1.72(1)	S(17)	C(11)	1.68(2)
S(12)	C(8)	1.75(1)	S(12)	C(7)	1.77(1)
S(20)	C(12)	1.69(1)	S(18)	C(11)	1.69(1)
S(14)	C(8)	1.69(1)	S(14)	C(9)	1.72(1)
S(19)	C(12)	1.72(1)	S(19)	C(11)	1.73(2)
C(10)	C(12)	1.38(2)	C(7)	C(9)	1.37(2)
O(1)	C(22)	1.44(5)	O(1)	C(13)	1.07(4)
O(2)	C(15)	1.38(3)	O(2)	C(14)	1.31(3)
O(5)	C(21)	1.22(2)	O(5)	C(20)	1.45(3)
O(4)	C(19)	1.26(4)	O(4)	C(18)	1.27(4)
O(3)	C(16)	1.31(4)	O(3)	C(17)	1.07(4)
C(15)	C(16)	1.35(3)	C(22)	C(21)	1.47(2)
C(19)	C(20)	1.33(4)	C(18)	C(17)	1.32(3)
C(13)	C(14)	1.59(3)			
C(15)	H(5)	0.95(3)	C(15)	H(6)	0.95(3)
C(16)	H(7)	0.95(3)	C(16)	H(8)	0.95(3)
C(22)	H(19)	0.95(2)	C(22)	H(20)	0.95(2)
C(19)	H(13)	0.95(4)	C(19)	H(14)	0.95(4)
C(18)	H(11)	0.95(3)	C(18)	H(12)	0.95(3)
C(21)	H(17)	0.95(3)	C(21)	H(18)	0.95(3)
C(20)	H(15)	0.95(3)	C(20)	H(16)	0.95(3)
C(13)	H(1)	0.95(3)	C(13)	H(2)	0.95(3)
C(17)	H(9)	0.95(3)	C(17)	H(10)	0.95(3)
C(14)	H(3)	0.95(3)	C(14)	H(4)	0.95(3)

Crystal data (2)

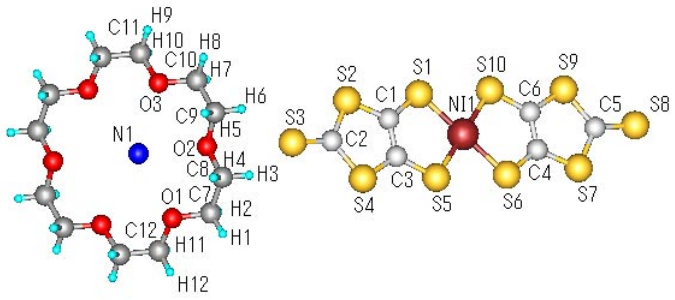


Table S4. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
N(I1)	0.2027(2)	0.02013(6)	0.77899(2)	2.82(1)	
S(1)	0.0919(4)	0.1528(1)	0.74478(3)	3.53(3)	
S(2)	-0.3050(4)	0.1472(1)	0.68681(4)	3.97(4)	
S(3)	-0.7152(4)	0.0273(2)	0.64203(4)	5.82(5)	
S(4)	-0.4611(4)	-0.0976(1)	0.69745(4)	4.06(4)	
S(5)	-0.0797(3)	-0.1088(1)	0.75646(3)	3.39(3)	
S(6)	0.3160(4)	-0.1135(1)	0.81296(3)	3.73(3)	
S(7)	0.7128(4)	-0.1066(1)	0.87084(4)	4.31(4)	
S(8)	1.1049(5)	0.0152(2)	0.91744(4)	6.15(5)	
S(9)	0.8609(4)	0.1388(1)	0.86108(4)	4.13(4)	

S(10)	0.4815(3)	0.1508(1)	0.80162(3)	3.41(3)	
O(1)	0.856(2)	-0.2054(5)	0.5328(1)	8.4(2)	
O(2)	0.907(1)	0.0133(5)	0.5641(1)	7.8(2)	
O(3)	0.911(2)	0.2180(5)	0.5268(1)	8.6(2)	
N(1)	1.248(4)	-0.003(1)	0.5059(3)	14.2(6)	0.70(2)
C(1)	-0.141(1)	0.0821(4)	0.7198(1)	3.1(1)	
C(2)	-0.507(1)	0.0251(5)	0.6735(1)	3.9(1)	
C(3)	-0.221(1)	-0.0356(4)	0.7251(1)	2.8(1)	
C(4)	0.547(1)	-0.0417(4)	0.8381(1)	3.0(1)	
C(5)	0.903(1)	0.0155(6)	0.8851(1)	4.2(1)	
C(6)	0.622(1)	0.0757(5)	0.8333(1)	3.2(1)	
C(7)	0.891(2)	-0.1955(8)	0.5646(2)	8.1(3)	
C(8)	0.770(2)	-0.0841(8)	0.5762(2)	7.7(3)	
C(9)	0.787(2)	0.1188(8)	0.5725(2)	7.4(3)	
C(10)	0.920(2)	0.2206(8)	0.5583(2)	8.2(3)	
C(11)	1.051(3)	0.3121(8)	0.5122(2)	10.8(4)	
C(12)	0.978(3)	-0.3063(8)	0.5200(2)	9.9(4)	
H(1)	0.802(2)	-0.2613(8)	0.5743(2)	9.8(3)	
H(2)	1.095(2)	-0.1948(8)	0.5698(2)	9.8(3)	
H(3)	0.788(2)	-0.0819(8)	0.5983(2)	9.3(3)	
H(4)	0.568(2)	-0.0827(8)	0.5698(2)	9.3(3)	
H(5)	0.588(2)	0.1196(8)	0.5652(2)	9.0(3)	
H(6)	0.795(2)	0.1255(8)	0.5947(2)	9.0(3)	
H(7)	1.120(2)	0.2196(8)	0.5655(2)	9.9(3)	
H(8)	0.830(2)	0.2913(8)	0.5651(2)	9.9(3)	
H(9)	0.970(3)	0.3839(8)	0.5195(2)	13.0(5)	
H(10)	1.255(3)	0.3097(8)	0.5177(2)	13.0(5)	
H(11)	1.182(3)	-0.3060(8)	0.5251(2)	11.9(4)	
H(12)	0.890(3)	-0.3742(8)	0.5288(2)	11.9(4)	

$B_{eq} = 8/3\ p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

Table S5. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(I1)	0.0444(4)	0.0275(3)	0.0355(3)	0.0003(3)	0.0022(3)	0.0002(3)
S(1)	0.0595(9)	0.0302(7)	0.0440(8)	-0.0047(6)	-0.0061(7)	0.0046(6)
S(2)	0.059(1)	0.0457(8)	0.0457(8)	0.0070(7)	-0.0039(8)	0.0076(7)
S(3)	0.069(1)	0.103(1)	0.0476(9)	0.008(1)	-0.0134(8)	-0.002(1)
S(4)	0.0545(9)	0.0456(8)	0.0535(9)	-0.0024(7)	-0.0053(8)	-0.0044(7)
S(5)	0.0540(9)	0.0306(7)	0.0438(8)	-0.0053(6)	-0.0040(7)	0.0021(6)
S(6)	0.067(1)	0.0320(7)	0.0424(8)	-0.0057(7)	-0.0050(7)	0.0039(6)
S(7)	0.078(1)	0.0466(8)	0.0391(8)	0.0038(8)	-0.0057(8)	0.0035(7)
S(8)	0.092(1)	0.084(1)	0.055(1)	0.014(1)	-0.026(1)	-0.009(1)
S(9)	0.061(1)	0.0473(9)	0.0474(9)	-0.0031(7)	-0.0080(8)	-0.0072(7)
S(10)	0.0549(9)	0.0309(7)	0.0436(8)	-0.0039(6)	-0.0035(7)	0.0026(6)
O(1)	0.193(7)	0.066(3)	0.063(4)	-0.001(4)	0.017(4)	0.006(3)
O(2)	0.139(5)	0.074(4)	0.086(4)	-0.006(4)	0.042(4)	-0.009(3)
O(3)	0.188(7)	0.065(4)	0.075(4)	0.001(4)	0.036(4)	-0.008(3)
N(1)	0.38(2)	0.088(9)	0.077(9)	-0.01(1)	0.03(1)	-0.005(6)
C(1)	0.043(3)	0.037(3)	0.035(3)	0.004(2)	0.002(3)	-0.002(2)
C(2)	0.051(4)	0.059(3)	0.040(3)	0.006(3)	0.007(3)	-0.005(3)
C(3)	0.038(3)	0.033(3)	0.037(3)	0.001(2)	0.005(2)	-0.001(2)
C(4)	0.050(3)	0.034(3)	0.030(3)	0.003(2)	0.003(2)	0.000(2)
C(5)	0.061(4)	0.056(4)	0.044(3)	0.012(3)	0.003(3)	-0.005(3)
C(6)	0.047(3)	0.037(3)	0.036(3)	0.005(2)	0.003(3)	-0.004(2)
C(7)	0.140(9)	0.084(6)	0.086(6)	-0.034(6)	0.027(6)	0.009(5)

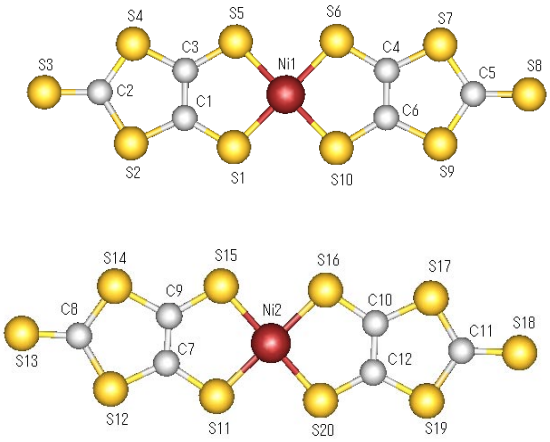
C(8)	0.123(8)	0.098(7)	0.072(6)	-0.023(6)	0.034(6)	0.006(5)
C(9)	0.117(8)	0.091(6)	0.077(6)	0.015(6)	0.025(5)	-0.010(5)
C(10)	0.134(9)	0.081(6)	0.097(7)	0.020(6)	0.039(7)	-0.016(5)
C(11)	0.26(2)	0.054(5)	0.096(7)	-0.007(7)	0.023(9)	0.001(5)
C(12)	0.22(1)	0.062(6)	0.092(7)	-0.003(7)	0.021(8)	0.004(5)

The general temperature factor expression:exp(-2p^2(a*^{2}U$_{11}$h^2 + b*^{2}U$_{22}$k^2 + c*^{2}U$_{33}$l^2 + 2a*b*U$_{12}$hk + 2a*c*U$_{13}$hl + 2b*c*U$_{23}$kl))

Table S6. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ni(1)	S(1)	2.146(2)	Ni(1)	S(5)	2.150(2)
Ni(1)	S(6)	2.149(2)	Ni(1)	S(10)	2.156(2)
S(1)	C(1)	1.681(5)	S(2)	C(1)	1.739(5)
S(2)	C(2)	1.744(6)	S(3)	C(2)	1.620(6)
S(4)	C(2)	1.735(6)	S(4)	C(3)	1.731(5)
S(5)	C(3)	1.687(5)	S(6)	C(4)	1.687(5)
S(7)	C(4)	1.731(5)	S(7)	C(5)	1.730(6)
S(8)	C(5)	1.633(6)	S(9)	C(5)	1.741(6)
S(9)	C(6)	1.736(6)	S(10)	C(6)	1.706(5)
O(1)	C(7)	1.368(9)	O(1)	C(12)	1.39(1)
O(2)	C(8)	1.377(9)	O(2)	C(9)	1.367(9)
O(3)	C(10)	1.347(9)	O(3)	C(11)	1.40(1)
C(1)	C(3)	1.401(7)	C(4)	C(6)	1.390(7)
C(7)	C(8)	1.47(1)	C(9)	C(10)	1.45(1)
C(7)	H(1)	0.95	C(7)	H(2)	0.95
C(8)	H(3)	0.95	C(8)	H(4)	0.95
C(9)	H(5)	0.95	C(9)	H(6)	0.95
C(10)	H(7)	0.95	C(10)	H(8)	0.95
C(11)	H(9)	0.95	C(11)	H(10)	0.95
C(12)	H(11)	0.95	C(12)	H(12)	0.95

Crystal data (3)



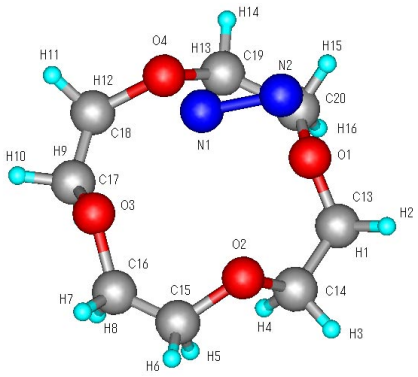


Table S7. Atomic coordinates and B$_{iso}$/B$_{eq}$ and occupancy

atom	x	y	z	B$_{eq}$	occ
Ni(1)	-0.0095(1)	0.21986(3)	0.9314(1)	3.94(3)	
Ni(2)	-0.0147(1)	0.26191(3)	1.3521(2)	3.51(2)	

S(1)	-0.1366(3)	0.25738(6)	0.9312(4)	4.48(6)	
S(2)	-0.1290(3)	0.32502(6)	0.8015(4)	4.84(7)	
S(3)	-0.0094(4)	0.37896(6)	0.6310(4)	6.88(9)	
S(4)	0.1090(3)	0.31758(6)	0.6896(4)	4.76(7)	
S(5)	0.1168(3)	0.24975(6)	0.8116(4)	4.39(6)	
S(6)	0.1198(3)	0.18286(6)	0.9313(4)	4.49(6)	
S(7)	0.1095(3)	0.11375(6)	1.0394(4)	4.97(7)	
S(8)	-0.0153(4)	0.05601(6)	1.1568(5)	6.94(9)	
S(9)	-0.1321(3)	0.11872(7)	1.1302(4)	5.21(7)	
S(10)	-0.1399(3)	0.18876(6)	1.0364(3)	4.40(6)	
S(11)	-0.1466(2)	0.29791(5)	1.3562(3)	3.88(6)	
S(12)	-0.1496(3)	0.36562(6)	1.2282(4)	4.60(7)	
S(13)	-0.0446(4)	0.41985(7)	1.0423(5)	7.3(1)	
S(14)	0.0901(3)	0.36134(6)	1.1175(4)	4.91(7)	
S(15)	0.1109(3)	0.29334(5)	1.2393(3)	3.94(6)	
S(16)	0.1162(2)	0.22553(5)	1.3463(4)	4.17(6)	
S(17)	0.1132(3)	0.15717(6)	1.4619(4)	4.29(6)	
S(18)	0.0009(4)	0.10105(6)	1.6170(4)	6.29(8)	
S(19)	-0.1243(3)	0.16207(5)	1.5788(4)	4.38(6)	
S(20)	-0.1391(2)	0.23083(5)	1.4703(3)	4.05(6)	
O(1)	-0.252(2)	0.0200(4)	0.768(2)	15.0(6)	
O(2)	-0.275(1)	-0.0391(4)	0.625(2)	12.6(6)	
O(3)	-0.360(1)	-0.0102(3)	0.330(2)	10.9(4)	
O(4)	-0.368(1)	0.0504(2)	0.496(2)	8.9(3)	
N(1)	-0.5000	0.0000	0.639(2)	7.5(4)	1/2
N(2)	-0.5000	0.0000	0.818(2)	6.4(4)	1/2
C(1)	-0.068(1)	0.2882(2)	0.838(1)	4.2(3)	
C(2)	-0.007(1)	0.3425(2)	0.701(1)	5.3(3)	
C(3)	0.0467(9)	0.2848(2)	0.784(1)	3.8(2)	
C(4)	0.048(1)	0.1509(2)	1.012(1)	4.2(3)	
C(5)	-0.011(1)	0.0939(2)	1.112(1)	5.1(3)	
C(6)	-0.0665(9)	0.1538(2)	1.057(1)	3.9(2)	
C(7)	-0.0786(9)	0.3296(2)	1.263(1)	3.4(2)	
C(8)	-0.034(1)	0.3845(2)	1.125(1)	4.7(3)	
C(9)	0.032(1)	0.3272(2)	1.215(1)	3.8(2)	
C(10)	0.0470(8)	0.1939(2)	1.436(1)	2.9(2)	
C(11)	-0.003(1)	0.1385(2)	1.554(1)	4.6(2)	
C(12)	-0.0669(9)	0.1962(2)	1.490(1)	3.5(2)	
C(13)	-0.172(2)	0.0002(7)	0.792(3)	15.2(9)	
C(14)	-0.171(2)	-0.0272(4)	0.695(4)	15.3(9)	
C(15)	-0.254(3)	-0.0504(7)	0.467(4)	16.8(1)	
C(16)	-0.289(2)	-0.0364(7)	0.342(4)	16.0(1)	
C(17)	-0.318(3)	0.0168(6)	0.265(3)	16.0(1)	
C(18)	-0.342(2)	0.0447(5)	0.322(2)	12.0(7)	
C(19)	-0.284(2)	0.0643(5)	0.589(5)	16.1(1)	
C(20)	-0.236(2)	0.0495(6)	0.735(3)	13.4(8)	
H(1)	-0.099(2)	0.0104(7)	0.779(3)	18.2(1)	
H(2)	-0.181(2)	-0.0068(7)	0.906(3)	18.2(1)	
H(3)	-0.140(2)	-0.0441(4)	0.760(4)	18.4(1)	
H(4)	-0.121(2)	-0.0227(4)	0.602(4)	18.4(1)	
H(5)	-0.173(3)	-0.0482(7)	0.458(4)	20.1(2)	
H(6)	-0.274(3)	-0.0723(7)	0.462(4)	20.1(2)	
H(7)	-0.333(2)	-0.0527(7)	0.289(4)	19.2(1)	
H(8)	-0.224(2)	-0.0315(7)	0.272(4)	19.2(1)	
H(9)	-0.237(3)	0.0151(6)	0.249(3)	19.2(1)	
H(10)	-0.355(3)	0.0177(6)	0.157(3)	19.2(1)	

H(11)	-0.403(2)	0.0543(5)	0.260(2)	14.4(9)
H(12)	-0.273(2)	0.0563(5)	0.304(2)	14.4(9)
H(13)	-0.220(2)	0.0645(5)	0.513(5)	19.3(1)
H(14)	-0.308(2)	0.0856(5)	0.611(5)	19.3(1)
H(15)	-0.278(2)	0.0598(6)	0.822(3)	16.1(1)
H(16)	-0.157(2)	0.0549(6)	0.744(3)	16.1(1)

$B_{eq} = 8/3\ p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

Table S8. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	0.0386(8)	0.0579(7)	0.0532(7)	0.0029(6)	0.0006(7)	-0.0028(6)
Ni(2)	0.0361(7)	0.0439(6)	0.0532(6)	-0.0014(5)	-0.0016(6)	-0.0003(5)
S(1)	0.037(2)	0.067(2)	0.066(2)	0.005(1)	0.005(1)	-0.002(1)
S(2)	0.055(2)	0.064(2)	0.065(2)	0.014(1)	-0.007(2)	-0.005(1)
S(3)	0.122(3)	0.060(2)	0.079(2)	0.006(2)	-0.016(3)	0.006(1)
S(4)	0.054(2)	0.064(2)	0.063(2)	-0.001(1)	0.001(2)	0.002(1)
S(5)	0.039(2)	0.060(2)	0.067(2)	0.005(1)	0.006(1)	0.001(1)
S(6)	0.042(2)	0.056(1)	0.073(2)	0.003(1)	0.009(2)	0.000(1)
S(7)	0.055(2)	0.058(1)	0.076(2)	0.005(1)	0.005(2)	0.001(1)
S(8)	0.086(3)	0.064(2)	0.114(2)	-0.006(2)	0.003(3)	0.016(2)
S(9)	0.048(2)	0.071(2)	0.079(2)	-0.006(1)	0.005(2)	0.012(1)
S(10)	0.041(2)	0.067(2)	0.060(2)	0.002(1)	0.002(1)	-0.000(1)
S(11)	0.042(2)	0.044(1)	0.062(1)	-0.001(1)	0.001(1)	0.002(1)
S(12)	0.060(2)	0.047(1)	0.068(2)	0.006(1)	-0.005(2)	0.001(1)
S(13)	0.117(4)	0.054(2)	0.106(2)	0.001(2)	0.003(3)	0.021(2)
S(14)	0.064(2)	0.052(1)	0.070(2)	-0.014(1)	0.005(2)	0.005(1)
S(15)	0.039(2)	0.052(1)	0.059(1)	-0.003(1)	0.006(1)	0.001(1)
S(16)	0.038(2)	0.049(1)	0.071(2)	-0.000(1)	0.007(2)	0.000(1)
S(17)	0.044(2)	0.051(1)	0.068(2)	0.006(1)	0.002(2)	0.001(1)
S(18)	0.079(2)	0.049(1)	0.111(2)	0.002(2)	-0.003(2)	0.016(1)
S(19)	0.047(2)	0.051(1)	0.069(2)	-0.004(1)	0.003(2)	0.006(1)
S(20)	0.037(2)	0.050(1)	0.067(2)	0.001(1)	0.004(1)	0.004(1)
O(1)	0.19(2)	0.15(1)	0.23(2)	-0.01(1)	-0.10(2)	-0.01(1)
O(2)	0.13(1)	0.14(1)	0.20(2)	0.04(1)	0.01(1)	0.01(1)
O(3)	0.15(1)	0.114(9)	0.15(1)	-0.014(9)	0.02(1)	-0.012(7)
O(4)	0.076(8)	0.085(6)	0.18(1)	-0.007(6)	0.017(8)	0.023(7)
N(1)	0.08(1)	0.16(1)	0.049(7)	-0.03(1)	0.0000	0.0000
N(2)	0.07(1)	0.089(9)	0.079(9)	-0.004(9)	0.0000	0.0000
C(1)	0.035(7)	0.067(6)	0.057(6)	0.001(5)	-0.007(5)	-0.012(5)
C(2)	0.09(1)	0.062(6)	0.053(5)	-0.003(7)	-0.008(7)	-0.011(5)
C(3)	0.042(8)	0.056(5)	0.048(5)	-0.008(4)	-0.004(5)	-0.003(4)
C(4)	0.038(7)	0.051(6)	0.070(7)	-0.001(5)	-0.001(5)	-0.004(5)
C(5)	0.068(9)	0.072(6)	0.053(6)	0.008(6)	0.003(6)	0.005(5)
C(6)	0.038(7)	0.054(5)	0.056(6)	-0.004(5)	0.006(5)	-0.002(5)
C(7)	0.038(7)	0.038(5)	0.054(5)	0.000(4)	-0.006(5)	0.002(4)
C(8)	0.08(1)	0.054(5)	0.045(5)	-0.011(5)	0.001(6)	0.006(4)
C(9)	0.047(8)	0.050(5)	0.046(5)	-0.009(5)	-0.001(5)	-0.005(4)
C(10)	0.026(5)	0.040(4)	0.045(5)	-0.001(4)	0.002(4)	0.002(4)
C(11)	0.060(8)	0.049(5)	0.065(6)	0.007(5)	-0.026(7)	-0.005(4)
C(12)	0.037(7)	0.047(5)	0.050(5)	0.002(4)	0.000(5)	0.005(4)
C(13)	0.18(3)	0.26(3)	0.13(2)	0.15(2)	-0.02(2)	-0.03(2)
C(14)	0.05(1)	0.12(1)	0.42(4)	0.030(9)	-0.02(2)	-0.07(2)
C(15)	0.22(4)	0.16(2)	0.26(4)	0.10(2)	-0.10(3)	-0.06(2)
C(16)	0.14(2)	0.22(3)	0.24(3)	0.12(2)	-0.07(2)	-0.11(3)
C(17)	0.28(4)	0.19(2)	0.14(2)	-0.11(2)	0.09(2)	-0.06(2)
C(18)	0.19(3)	0.16(2)	0.11(1)	0.07(2)	0.07(2)	0.06(1)
C(19)	0.13(2)	0.11(2)	0.37(4)	-0.03(1)	-0.08(3)	-0.05(2)

C(20)	0.21(3)	0.16(2)	0.14(2)	-0.13(2)	-0.02(2)	0.03(2)

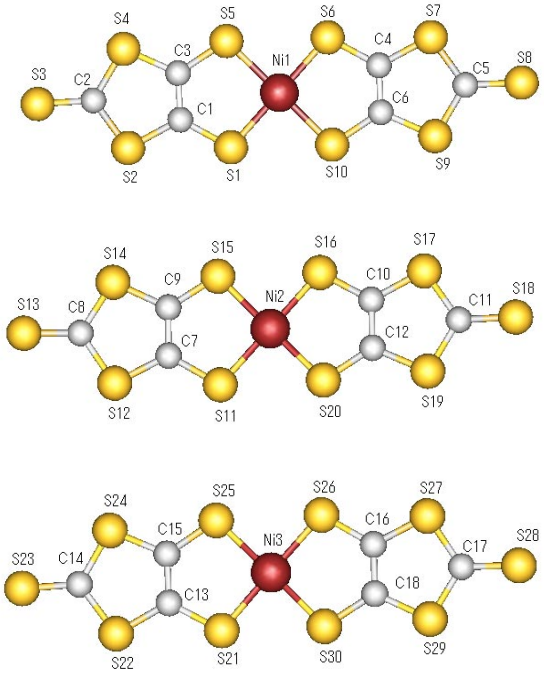
The general temperature factor expression:exp(-2p^2(a*^{2}U$_{11}$h^2 + b*^{2}U$_{22}$k^2 + c*^{2}U$_{33}$l^2 + 2a*b*U$_{12}$hk + 2a*c*U$_{13}$hl + 2b*c*U$_{23}$kl))

Table S9. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ni(1)	S(1)	2.157(3)	Ni(1)	S(5)	2.146(3)
Ni(1)	S(6)	2.158(3)	Ni(1)	S(10)	2.162(3)
Ni(2)	S(11)	2.149(3)	Ni(2)	S(15)	2.156(3)
Ni(2)	S(16)	2.153(3)	Ni(2)	S(20)	2.155(3)
S(1)	C(1)	1.69(1)	S(2)	C(1)	1.73(1)
S(2)	C(2)	1.77(1)	S(3)	C(2)	1.63(1)
S(4)	C(2)	1.71(1)	S(4)	C(3)	1.72(1)
S(5)	C(3)	1.70(1)	S(6)	C(4)	1.70(1)
S(7)	C(4)	1.73(1)	S(7)	C(5)	1.73(1)
S(8)	C(5)	1.63(1)	S(9)	C(5)	1.75(1)
S(9)	C(6)	1.75(1)	S(10)	C(6)	1.70(1)
S(11)	C(7)	1.71(1)	S(12)	C(7)	1.744(9)
S(12)	C(8)	1.75(1)	S(13)	C(8)	1.625(9)
S(14)	C(8)	1.74(1)	S(14)	C(9)	1.76(1)
S(15)	C(9)	1.70(1)	S(16)	C(10)	1.704(8)
S(17)	C(10)	1.733(8)	S(17)	C(11)	1.72(1)
S(18)	C(11)	1.646(9)	S(19)	C(11)	1.73(1)
S(19)	C(12)	1.726(9)	S(20)	C(12)	1.685(9)
O(1)	C(13)	1.26(2)	O(1)	C(14)	2.27(2)
O(1)	C(19)	2.36(3)	O(1)	C(20)	1.28(2)
O(2)	C(13)	2.42(3)	O(2)	C(14)	1.42(2)
O(2)	C(15)	1.35(3)	O(2)	C(16)	2.24(3)
O(3)	C(15)	2.35(3)	O(3)	C(16)	1.38(2)
O(3)	C(17)	1.34(2)	O(3)	C(18)	2.31(2)
O(4)	C(17)	2.37(2)	O(4)	C(18)	1.42(2)
O(4)	C(19)	1.36(2)	O(4)	C(20)	2.43(3)
N(1)	N(2)	1.40(2)	C(1)	C(3)	1.40(1)
C(2)	C(3)	2.58(1)	C(4)	C(6)	1.38(1)
C(7)	C(8)	2.60(1)	C(7)	C(9)	1.34(1)
C(10)	C(11)	2.57(1)	C(10)	C(12)	1.39(1)
C(11)	C(12)	2.58(1)	C(13)	C(14)	1.38(3)
C(13)	C(20)	2.24(3)	C(14)	C(15)	2.25(4)
C(15)	C(16)	1.22(3)	C(16)	C(17)	2.34(4)
C(17)	C(18)	1.28(2)	C(18)	C(19)	2.35(4)
C(19)	C(20)	1.42(3)			
O(1)	H(1)	1.82(2)	O(1)	H(2)	1.77(2)
O(1)	H(15)	1.75(3)	O(1)	H(16)	1.85(2)
O(2)	H(3)	1.91(3)	O(2)	H(4)	1.92(2)
O(2)	H(5)	1.81(4)	O(2)	H(6)	1.90(3)
O(3)	H(7)	1.84(2)	O(3)	H(8)	1.87(2)
O(3)	H(9)	1.89(2)	O(3)	H(10)	1.79(2)
O(4)	H(11)	1.90(2)	O(4)	H(12)	1.89(2)
O(4)	H(13)	1.82(2)	O(4)	H(14)	1.87(2)
C(13)	H(1)	0.95	C(13)	H(2)	0.95
C(13)	H(3)	1.91(3)	C(13)	H(4)	1.87(3)
C(13)	H(16)	2.33(3)	C(14)	H(1)	1.90(3)

C(14)	H(2)	1.88(3)	C(14)	H(3)	0.95(3)
C(14)	H(4)	0.95(3)	C(14)	H(5)	2.06(4)
C(15)	H(4)	2.20(4)	C(15)	H(5)	0.95
C(15)	H(6)	0.95	C(15)	H(7)	1.67(4)
C(15)	H(8)	1.76(5)	C(16)	H(5)	1.70(3)
C(16)	H(6)	1.79(4)	C(16)	H(7)	0.95(4)
C(16)	H(8)	0.95(4)	C(16)	H(9)	2.36(4)
C(17)	H(8)	2.30(3)	C(17)	H(9)	0.95
C(17)	H(10)	0.95	C(17)	H(11)	1.86(3)
C(17)	H(12)	1.76(3)	C(18)	H(9)	1.83(3)
C(18)	H(10)	1.73(3)	C(18)	H(11)	0.95(3)
C(18)	H(12)	0.95	C(18)	H(13)	2.22(4)
C(19)	H(12)	2.27(4)	C(19)	H(13)	0.95(4)
C(19)	H(14)	0.95	C(19)	H(15)	1.84(4)
C(19)	H(16)	1.96(3)	C(20)	H(1)	2.31(3)
C(20)	H(13)	1.86(4)	C(20)	H(14)	1.98(3)
C(20)	H(15)	0.95(3)	C(20)	H(16)	0.95
H(1)	H(2)	1.55	H(1)	H(3)	2.34(3)
H(1)	H(4)	1.98(3)	H(1)	H(16)	2.00(3)
H(2)	H(3)	2.00(3)	H(2)	H(4)	2.58(4)
H(3)	H(4)	1.55	H(3)	H(5)	2.42(4)
H(4)	H(5)	1.67(4)	H(5)	H(6)	1.55
H(5)	H(7)	2.29(4)	H(5)	H(8)	1.73(3)
H(6)	H(7)	1.73(3)	H(6)	H(8)	2.35(5)
H(7)	H(8)	1.55	H(8)	H(9)	1.97(3)
H(9)	H(10)	1.55	H(9)	H(11)	2.53(4)
H(9)	H(12)	1.83(3)	H(10)	H(11)	1.82(2)
H(10)	H(12)	2.21(3)	H(11)	H(12)	1.55
H(12)	H(13)	1.79(4)	H(13)	H(14)	1.55
H(13)	H(15)	2.53(4)	H(13)	H(16)	2.00(3)
H(14)	H(15)	2.00(3)	H(14)	H(16)	2.41(3)
H(15)	H(16)	1.55			

Crystal data (4)



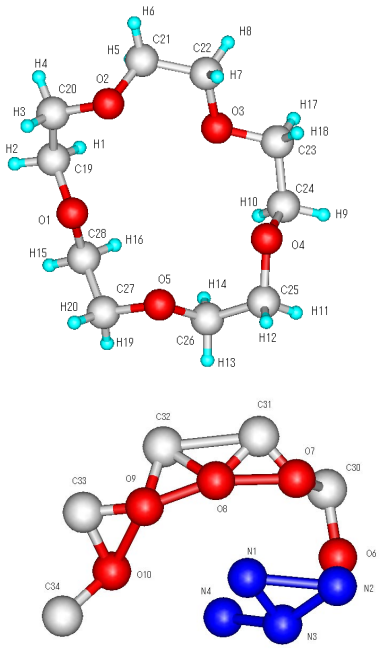


Table S10. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Ni(1)	0.28676(7)	0.00080(3)	0.03707(3)	1.20(1)	
Ni(2)	0.85897(7)	0.33292(3)	-0.00931(3)	1.18(1)	
Ni(3)	0.42980(7)	0.33431(3)	0.06182(3)	1.27(1)	
S(1)	0.3423(1)	-0.08894(7)	-0.03314(5)	1.42(2)	
S(2)	0.2261(1)	-0.09445(7)	-0.16112(5)	1.58(2)	
S(3)	0.0300(2)	-0.02841(9)	-0.26473(6)	2.35(3)	
S(4)	0.0264(1)	0.06557(7)	-0.14976(5)	1.65(2)	
S(5)	0.1309(1)	0.08325(7)	-0.02094(5)	1.43(2)	
S(6)	0.2329(1)	0.09208(6)	0.10666(5)	1.38(2)	
S(7)	0.3474(1)	0.09643(7)	0.23540(5)	1.51(2)	
S(8)	0.5362(2)	0.02615(9)	0.34120(6)	2.27(3)	
S(9)	0.5356(1)	-0.06533(7)	0.22568(6)	1.69(2)	
S(10)	0.4360(1)	-0.08354(7)	0.09590(5)	1.41(2)	
S(11)	0.7734(1)	0.24424(7)	-0.06364(5)	1.44(2)	
S(12)	0.6419(1)	0.25478(7)	-0.19082(6)	1.79(2)	
S(13)	0.5373(2)	0.34493(9)	-0.30324(7)	2.92(3)	
S(14)	0.6934(1)	0.41962(7)	-0.20524(5)	1.63(2)	
S(15)	0.8298(1)	0.42155(7)	-0.08036(5)	1.35(2)	
S(16)	0.9490(1)	0.42110(7)	0.04364(5)	1.43(2)	
S(17)	1.0623(1)	0.41778(7)	0.17205(5)	1.56(2)	
S(18)	1.1276(2)	0.33827(8)	0.29178(6)	2.19(3)	
S(19)	0.9958(1)	0.25559(7)	0.19167(5)	1.53(2)	
S(20)	0.8818(1)	0.24676(7)	0.06371(5)	1.45(2)	
S(21)	0.3363(1)	0.24565(7)	0.01051(5)	1.47(2)	
S(22)	0.2116(1)	0.24674(7)	-0.11595(5)	1.54(2)	
S(23)	0.1217(2)	0.32504(8)	-0.23361(6)	2.13(3)	
S(24)	0.2693(1)	0.40983(7)	-0.13770(5)	1.49(2)	
S(25)	0.4035(1)	0.41880(7)	-0.01241(5)	1.42(2)	
S(26)	0.5183(1)	0.42312(7)	0.11573(5)	1.42(2)	
S(27)	0.6237(1)	0.41840(7)	0.24663(6)	1.71(2)	
S(28)	0.6855(2)	0.33762(9)	0.36620(6)	2.63(3)	
S(29)	0.5645(1)	0.25535(7)	0.26347(6)	1.74(2)	
S(30)	0.4496(1)	0.24783(7)	0.13508(5)	1.50(2)	
O(1)	-0.2898(7)	-0.2190(3)	0.4782(2)	4.4(1)	
O(2)	-0.0980(6)	-0.2254(3)	0.5821(2)	3.7(1)	
O(3)	0.0568(5)	-0.1085(3)	0.5214(2)	4.0(1)	
O(4)	0.1881(6)	-0.1527(4)	0.4013(2)	5.1(1)	
O(5)	-0.0870(8)	-0.2224(3)	0.3653(2)	4.5(1)	
O(6)	0.283(1)	-0.5052(7)	0.4595(4)	3.8(2)	1/2
O(7)	0.180(2)	-0.4486(7)	0.392(1)	8.2(4)	1/2
O(8)	-0.008(1)	-0.4228(5)	0.3963(4)	2.5(2)	1/2
O(9)	-0.172(2)	-0.4255(7)	0.4227(4)	5.1(3)	1/2
O(10)	-0.241(1)	-0.4700(7)	0.4820(5)	5.4(3)	1/2
N(1)	0.0508(9)	-0.2925(4)	0.4689(3)	3.1(1)	0.700
N(2)	0.258(1)	-0.2992(7)	0.4711(5)	6.9(3)	0.700
N(3)	0.137(2)	-0.3396(9)	0.5093(7)	2.4(3)	0.300
N(4)	0.008(2)	-0.403(1)	0.5106(7)	2.6(3)	0.300
C(1)	0.2307(5)	-0.0463(3)	-0.0915(2)	1.31(9)	
C(2)	0.0919(6)	-0.0190(3)	-0.1958(2)	1.59(9)	
C(3)	0.1374(6)	0.0291(3)	-0.0863(2)	1.42(9)	
C(4)	0.3417(6)	0.0486(3)	0.1663(2)	1.40(9)	

C(5)	0.4748(6)	0.0195(3)	0.2711(2)	1.68(9)
C(6)	0.4311(6)	-0.0283(3)	0.1614(2)	1.34(9)
C(7)	0.7251(6)	0.2957(3)	-0.1296(2)	1.44(9)
C(8)	0.6206(6)	0.3397(3)	-0.2373(2)	1.7(1)
C(9)	0.7514(6)	0.3742(3)	-0.1360(2)	1.42(9)
C(10)	0.9852(5)	0.3742(3)	0.1112(2)	1.32(9)
C(11)	1.0660(6)	0.3370(3)	0.2221(2)	1.66(9)
C(12)	0.9546(5)	0.2963(3)	0.1197(2)	1.37(9)
C(13)	0.2954(6)	0.2916(3)	-0.0573(2)	1.47(9)
C(14)	0.1973(6)	0.3274(3)	-0.1665(2)	1.61(9)
C(15)	0.3243(5)	0.3689(3)	-0.0668(2)	1.25(8)
C(16)	0.5518(6)	0.3751(3)	0.1838(2)	1.44(9)
C(17)	0.6283(6)	0.3370(3)	0.2953(2)	1.9(1)
C(18)	0.5226(6)	0.2974(3)	0.1925(2)	1.56(9)
C(19)	-0.358(1)	-0.1821(5)	0.5339(3)	4.2(2)
C(20)	-0.2680(9)	-0.2273(4)	0.5854(3)	4.0(2)
C(21)	-0.0536(9)	-0.1599(5)	0.6125(3)	3.8(2)
C(22)	0.0961(9)	-0.1343(5)	0.5819(3)	4.6(2)
C(23)	0.1865(9)	-0.0770(7)	0.4905(3)	5.8(2)
C(24)	0.156(1)	-0.0731(6)	0.4232(3)	4.9(2)
C(25)	0.1455(9)	-0.1604(5)	0.3384(3)	5.0(2)
C(26)	-0.0398(9)	-0.1567(4)	0.3335(3)	3.5(1)
C(27)	-0.266(1)	-0.2184(5)	0.3699(3)	5.5(2)
C(28)	-0.3442(9)	-0.1752(5)	0.4259(3)	4.3(2)
C(30)	0.259(1)	-0.5263(5)	0.4038(3)	5.0(2)
C(31)	0.094(3)	-0.451(1)	0.3581(5)	10.9(5)
C(32)	-0.1247(9)	-0.4654(4)	0.3734(3)	3.7(2)
C(33)	-0.311(2)	-0.4400(5)	0.4319(5)	6.4(3)
C(34)	-0.359(1)	-0.4330(7)	0.5207(6)	7.0(3)
H(1)	-0.344(1)	-0.1277(5)	0.5346(3)	5.0(2)
H(2)	-0.474(1)	-0.1847(5)	0.5383(3)	5.0(2)
H(3)	-0.2817(9)	-0.2817(4)	0.5834(3)	4.7(2)
H(4)	-0.3150(9)	-0.2049(4)	0.6233(3)	4.7(2)
H(5)	-0.1444(9)	-0.1162(5)	0.6120(3)	4.5(2)
H(6)	-0.0319(9)	-0.1746(5)	0.6536(3)	4.5(2)
H(7)	0.1857(9)	-0.1787(5)	0.5803(3)	5.4(2)
H(8)	0.1267(9)	-0.0920(5)	0.6045(3)	5.4(2)
H(9)	0.230(1)	-0.0431(6)	0.4023(3)	5.9(2)
H(10)	0.043(1)	-0.0494(6)	0.4166(3)	5.9(2)
H(11)	0.1779(9)	-0.1171(5)	0.3158(3)	5.3(2)
H(12)	0.2047(9)	-0.2096(5)	0.3220(3)	5.3(2)
H(13)	-0.0642(9)	-0.1597(4)	0.2918(3)	4.1(2)
H(14)	-0.1001(9)	-0.1083(4)	0.3508(3)	4.1(2)
H(15)	-0.4628(9)	-0.1674(5)	0.4253(3)	5.4(2)
H(16)	-0.3094(9)	-0.1246(5)	0.4269(3)	5.4(2)
H(17)	0.1814(9)	-0.0240(7)	0.5051(3)	7.2(3)
H(18)	0.2929(9)	-0.1079(7)	0.4977(3)	7.2(3)
H(19)	-0.312(1)	-0.1914(5)	0.3349(3)	7.1(3)
H(20)	-0.290(1)	-0.2712(5)	0.3711(3)	7.1(3)

$B_{eq} = 8/3\ p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

Table S11. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	0.0185(3)	0.0121(3)	0.0144(3)	-0.0013(2)	-0.0013(2)	0.0016(2)
Ni(2)	0.0181(3)	0.0118(3)	0.0147(3)	-0.0014(2)	-0.0017(2)	0.0017(2)

Ni(3)	0.0200(3)	0.0132(3)	0.0145(3)	-0.0013(2)	-0.0007(2)	0.0013(2)
S(1)	0.0215(6)	0.0140(5)	0.0174(6)	0.0003(4)	-0.0024(5)	0.0006(4)
S(2)	0.0239(6)	0.0196(6)	0.0165(6)	-0.0040(5)	0.0002(5)	-0.0013(4)
S(3)	0.0328(7)	0.0417(8)	0.0173(6)	-0.0121(6)	-0.0046(5)	0.0017(6)
S(4)	0.0221(6)	0.0219(6)	0.0190(6)	-0.0034(5)	-0.0045(5)	0.0050(5)
S(5)	0.0216(6)	0.0147(5)	0.0171(6)	0.0003(4)	-0.0032(5)	0.0014(4)
S(6)	0.0229(6)	0.0125(5)	0.0159(6)	0.0002(4)	-0.0022(5)	0.0013(4)
S(7)	0.0234(6)	0.0185(6)	0.0151(6)	-0.0021(5)	-0.0017(5)	0.0001(4)
S(8)	0.0342(7)	0.0338(7)	0.0177(6)	-0.0026(6)	-0.0062(5)	0.0021(5)
S(9)	0.0252(6)	0.0194(6)	0.0191(6)	-0.0011(5)	-0.0053(5)	0.0046(5)
S(10)	0.0213(6)	0.0135(5)	0.0181(6)	-0.0009(4)	-0.0030(5)	0.0009(4)
S(11)	0.0228(6)	0.0150(5)	0.0172(6)	-0.0039(4)	-0.0025(5)	0.0009(4)
S(12)	0.0261(6)	0.0202(6)	0.0219(6)	-0.0034(5)	-0.0058(5)	-0.0036(5)
S(13)	0.0440(8)	0.0372(8)	0.0275(7)	0.0042(6)	-0.0195(6)	-0.0041(6)
S(14)	0.0223(6)	0.0218(6)	0.0171(6)	-0.0007(5)	-0.0037(5)	0.0023(5)
S(15)	0.0199(5)	0.0144(5)	0.0165(6)	-0.0013(4)	-0.0016(5)	0.0015(4)
S(16)	0.0230(6)	0.0147(5)	0.0173(6)	-0.0045(4)	-0.0032(5)	0.0034(4)
S(17)	0.0228(6)	0.0193(6)	0.0178(6)	-0.0050(5)	-0.0036(5)	0.0018(5)
S(18)	0.0320(7)	0.0322(7)	0.0186(6)	-0.0031(6)	-0.0066(5)	0.0034(5)
S(19)	0.0225(6)	0.0174(5)	0.0175(6)	-0.0011(4)	-0.0024(5)	0.0050(4)
S(20)	0.0235(6)	0.0135(5)	0.0181(6)	-0.0029(4)	-0.0023(5)	0.0025(4)
S(21)	0.0261(6)	0.0130(5)	0.0170(6)	-0.0042(4)	-0.0017(5)	0.0019(4)
S(22)	0.0225(6)	0.0167(5)	0.0197(6)	-0.0046(5)	-0.0020(5)	0.0001(4)
S(23)	0.0303(7)	0.0314(7)	0.0197(6)	-0.0045(5)	-0.0074(5)	0.0000(5)
S(24)	0.0219(6)	0.0169(5)	0.0170(6)	-0.0014(4)	-0.0011(5)	0.0037(4)
S(25)	0.0238(6)	0.0128(5)	0.0176(6)	-0.0043(4)	-0.0007(5)	0.0015(4)
S(26)	0.0220(6)	0.0131(5)	0.0181(6)	-0.0013(4)	-0.0019(5)	0.0018(4)
S(27)	0.0244(6)	0.0183(6)	0.0216(6)	-0.0013(5)	-0.0042(5)	0.0013(5)
S(28)	0.0448(8)	0.0333(8)	0.0204(7)	-0.0012(6)	-0.0083(6)	0.0024(6)
S(29)	0.0270(6)	0.0205(6)	0.0179(6)	-0.0026(5)	-0.0006(5)	0.0048(5)
S(30)	0.0266(6)	0.0156(5)	0.0153(6)	-0.0054(5)	-0.0015(5)	0.0027(4)
O(1)	0.100(4)	0.039(3)	0.028(2)	-0.014(3)	-0.013(2)	0.009(2)
O(2)	0.058(3)	0.049(3)	0.025(2)	0.013(2)	-0.003(2)	0.004(2)
O(3)	0.035(2)	0.083(4)	0.030(2)	-0.006(2)	-0.005(2)	0.017(2)
O(4)	0.034(2)	0.106(5)	0.038(3)	0.023(3)	0.006(2)	0.020(3)
O(5)	0.117(5)	0.026(2)	0.024(2)	-0.002(3)	-0.003(3)	0.000(2)
O(6)	0.041(5)	0.075(7)	0.026(5)	0.000(5)	0.005(4)	-0.012(5)
O(7)	0.069(9)	0.036(6)	0.20(2)	-0.013(6)	0.07(1)	-0.00(1)
O(8)	0.036(4)	0.030(4)	0.030(4)	-0.009(3)	-0.001(3)	0.008(3)
O(9)	0.078(8)	0.068(8)	0.031(5)	0.033(6)	0.006(5)	0.011(5)
O(10)	0.081(8)	0.068(7)	0.044(6)	0.008(6)	0.029(6)	0.013(5)
N(1)	0.047(4)	0.036(4)	0.021(3)	0.029(3)	0.001(3)	0.001(3)
N(2)	0.078(7)	0.106(9)	0.047(6)	0.065(6)	0.001(5)	0.005(6)
N(3)	0.033(8)	0.025(7)	0.028(8)	0.018(6)	-0.027(7)	-0.019(6)
N(4)	0.037(8)	0.042(9)	0.021(8)	-0.007(7)	-0.001(7)	0.010(7)
C(1)	0.014(2)	0.019(2)	0.018(2)	-0.006(2)	-0.003(2)	-0.001(2)
C(2)	0.020(2)	0.028(3)	0.013(2)	-0.008(2)	0.000(2)	0.004(2)
C(3)	0.022(2)	0.020(2)	0.013(2)	-0.007(2)	-0.004(2)	0.002(2)
C(4)	0.019(2)	0.019(2)	0.015(2)	-0.004(2)	-0.000(2)	0.001(2)
C(5)	0.020(2)	0.024(2)	0.019(2)	-0.004(2)	0.004(2)	-0.000(2)
C(6)	0.020(2)	0.021(2)	0.011(2)	-0.006(2)	-0.003(2)	0.005(2)
C(7)	0.021(2)	0.015(2)	0.017(2)	0.002(2)	0.001(2)	-0.001(2)
C(8)	0.020(2)	0.022(2)	0.023(3)	0.003(2)	-0.004(2)	-0.003(2)
C(9)	0.024(2)	0.019(2)	0.009(2)	0.001(2)	-0.002(2)	0.003(2)
C(10)	0.016(2)	0.017(2)	0.016(2)	-0.000(2)	-0.001(2)	0.001(2)
C(11)	0.017(2)	0.021(2)	0.024(3)	0.000(2)	-0.004(2)	0.003(2)

C(12)	0.015(2)	0.019(2)	0.017(2)	0.001(2)	-0.003(2)	0.006(2)
C(13)	0.015(2)	0.020(2)	0.020(2)	-0.003(2)	-0.005(2)	0.004(2)
C(14)	0.017(2)	0.025(3)	0.017(2)	0.002(2)	0.001(2)	-0.004(2)
C(15)	0.009(2)	0.021(2)	0.015(2)	0.002(2)	-0.002(2)	-0.002(2)
C(16)	0.017(2)	0.014(2)	0.023(2)	0.001(2)	-0.002(2)	-0.000(2)
C(17)	0.021(2)	0.020(2)	0.029(3)	0.001(2)	0.000(2)	0.003(2)
C(18)	0.024(2)	0.016(2)	0.017(2)	0.003(2)	0.002(2)	0.001(2)
C(19)	0.069(5)	0.064(5)	0.026(3)	-0.007(4)	-0.012(3)	0.015(3)
C(20)	0.071(5)	0.047(4)	0.032(3)	-0.004(3)	-0.009(3)	0.017(3)
C(21)	0.049(4)	0.065(5)	0.027(3)	-0.003(3)	0.006(3)	0.008(3)
C(22)	0.052(4)	0.084(6)	0.034(4)	0.002(4)	-0.003(3)	0.014(4)
C(23)	0.042(4)	0.15(1)	0.035(4)	-0.039(5)	-0.005(3)	0.024(5)
C(24)	0.055(4)	0.100(7)	0.032(4)	-0.021(5)	0.001(3)	0.015(4)
C(25)	0.054(4)	0.090(6)	0.026(3)	0.035(4)	0.012(3)	0.008(4)
C(26)	0.070(4)	0.033(3)	0.027(3)	0.004(3)	-0.013(3)	0.002(2)
C(27)	0.128(8)	0.060(5)	0.035(4)	-0.055(5)	-0.022(4)	0.018(3)
C(28)	0.059(4)	0.078(5)	0.032(4)	-0.028(4)	-0.017(3)	0.024(3)
C(30)	0.101(6)	0.047(4)	0.032(4)	0.005(4)	0.020(4)	0.000(3)
C(31)	0.23(2)	0.16(1)	0.026(5)	-0.03(1)	0.001(8)	-0.011(7)
C(32)	0.052(4)	0.049(4)	0.038(4)	0.001(3)	-0.010(3)	0.007(3)
C(33)	0.119(9)	0.049(5)	0.072(7)	0.005(5)	-0.054(6)	0.003(4)
C(34)	0.047(5)	0.103(8)	0.112(9)	-0.003(5)	0.016(5)	-0.055(7)

The general temperature factor expression:$\exp(-2p^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S12. Bond lengths (Å)

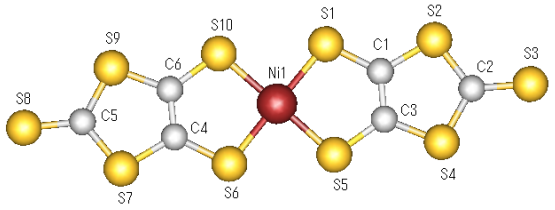
atom	atom	distance	atom	atom	distance
Ni(1)	S(1)	2.147(1)	Ni(1)	S(5)	2.168(1)
Ni(1)	S(6)	2.155(1)	Ni(1)	S(10)	2.170(1)
Ni(2)	S(11)	2.157(1)	Ni(2)	S(15)	2.149(1)
Ni(2)	S(16)	2.151(1)	Ni(2)	S(20)	2.152(1)
Ni(3)	S(21)	2.151(1)	Ni(3)	S(25)	2.154(1)
Ni(3)	S(26)	2.165(1)	Ni(3)	S(30)	2.159(1)
S(1)	C(1)	1.691(5)	S(1)	C(3)	2.672(5)
S(2)	C(1)	1.743(5)	S(2)	C(2)	1.728(5)
S(2)	C(3)	2.645(5)	S(3)	C(2)	1.635(5)
S(4)	C(1)	2.659(5)	S(4)	C(2)	1.749(5)
S(4)	C(3)	1.748(5)	S(5)	C(1)	2.678(5)
S(5)	C(3)	1.702(5)	S(6)	C(4)	1.707(5)
S(6)	C(6)	2.685(5)	S(7)	C(4)	1.732(5)
S(7)	C(5)	1.726(5)	S(7)	C(6)	2.645(5)
S(8)	C(5)	1.653(5)	S(9)	C(4)	2.649(5)
S(9)	C(5)	1.739(5)	S(9)	C(6)	1.741(5)
S(10)	C(4)	2.703(5)	S(10)	C(6)	1.716(5)
S(11)	C(7)	1.711(5)	S(11)	C(9)	2.690(5)
S(12)	C(7)	1.737(5)	S(12)	C(8)	1.746(5)
S(12)	C(9)	2.670(5)	S(13)	C(8)	1.624(5)
S(14)	C(7)	2.651(5)	S(14)	C(8)	1.739(5)
S(14)	C(9)	1.747(5)	S(15)	C(7)	2.687(5)
S(15)	C(9)	1.679(5)	S(16)	C(10)	1.690(5)
S(16)	C(12)	2.679(5)	S(17)	C(10)	1.730(5)
S(17)	C(11)	1.746(5)	S(17)	C(12)	2.666(5)
S(18)	C(11)	1.634(5)	S(19)	C(10)	2.658(5)
S(19)	C(11)	1.735(5)	S(19)	C(12)	1.743(5)
S(20)	C(10)	2.689(5)	S(20)	C(12)	1.684(5)

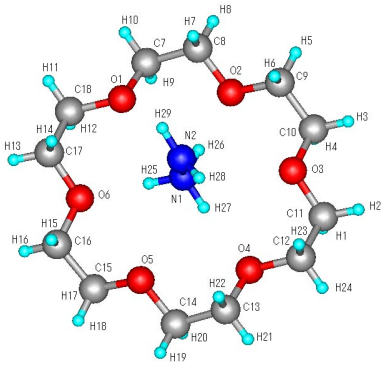
S(21)	C(13)	1.694(5)	S(21)	C(15)	2.672(5)
S(22)	C(13)	1.729(5)	S(22)	C(14)	1.745(5)
S(22)	C(15)	2.666(5)	S(23)	C(14)	1.629(5)
S(24)	C(13)	2.647(5)	S(24)	C(14)	1.743(5)
S(24)	C(15)	1.746(5)	S(25)	C(13)	2.682(5)
S(25)	C(15)	1.686(5)	S(26)	C(16)	1.706(5)
S(26)	C(18)	2.702(5)	S(27)	C(16)	1.741(5)
S(27)	C(17)	1.734(5)	S(27)	C(18)	2.652(5)
S(28)	C(17)	1.647(5)	S(29)	C(16)	2.660(5)
S(29)	C(17)	1.727(5)	S(29)	C(18)	1.732(5)
S(30)	C(16)	2.694(5)	S(30)	C(18)	1.708(5)
O(1)	C(19)	1.418(8)	O(1)	C(20)	2.367(8)
O(1)	C(27)	2.372(9)	O(1)	C(28)	1.410(7)
O(2)	C(19)	2.410(9)	O(2)	C(20)	1.386(9)
O(2)	C(21)	1.410(8)	O(2)	C(22)	2.40(1)
O(3)	C(21)	2.368(7)	O(3)	C(22)	1.428(8)
O(3)	C(23)	1.405(8)	O(3)	C(24)	2.368(8)
O(4)	C(23)	2.35(1)	O(4)	C(24)	1.41(1)
O(4)	C(25)	1.451(9)	O(4)	C(26)	2.447(8)
O(5)	N(1)	2.755(8)	O(5)	C(25)	2.37(1)
O(5)	C(26)	1.407(8)	O(5)	C(27)	1.44(1)
O(5)	C(28)	2.43(1)	O(6)	O(7)	1.92(2)
O(6)	N(4)	2.77(2)	O(6)	C(30)	1.31(1)
O(7)	O(8)	1.51(2)	O(7)	C(30)	1.39(2)
O(7)	C(31)	1.05(2)	O(7)	C(32)	2.59(2)
O(8)	O(9)	1.43(1)	O(8)	N(4)	2.55(2)
O(8)	C(30)	2.55(1)	O(8)	C(31)	1.19(2)
O(8)	C(32)	1.41(1)	O(8)	C(33)	2.61(2)
O(9)	O(10)	1.62(2)	O(9)	N(4)	2.55(2)
O(9)	C(31)	2.49(2)	O(9)	C(32)	1.28(1)
O(9)	C(33)	1.21(2)	O(9)	C(34)	2.58(2)
O(10)	N(4)	2.60(2)	O(10)	C(32)	2.52(1)
O(10)	C(33)	1.32(1)	O(10)	C(34)	1.32(1)
N(1)	N(2)	1.67(1)	N(1)	N(3)	1.33(2)
N(1)	N(4)	2.15(2)	N(2)	N(3)	1.51(2)
N(3)	N(4)	1.62(2)	C(1)	C(2)	2.608(7)
C(1)	C(3)	1.370(6)	C(2)	C(3)	2.609(7)
C(4)	C(5)	2.599(7)	C(4)	C(6)	1.377(7)
C(5)	C(6)	2.607(7)	C(7)	C(8)	2.611(7)
C(7)	C(9)	1.389(6)	C(8)	C(9)	2.628(7)
C(10)	C(11)	2.598(7)	C(10)	C(12)	1.396(6)
C(11)	C(12)	2.609(7)	C(13)	C(14)	2.598(7)
C(13)	C(15)	1.385(6)	C(14)	C(15)	2.620(7)
C(16)	C(17)	2.603(7)	C(16)	C(18)	1.390(6)
C(17)	C(18)	2.591(7)	C(19)	C(20)	1.508(9)
C(19)	C(28)	2.368(9)	C(20)	C(21)	2.35(1)
C(21)	C(22)	1.488(9)	C(22)	C(23)	2.358(9)
C(23)	C(24)	1.51(1)	C(24)	C(25)	2.40(1)
C(25)	C(26)	1.51(1)	C(26)	C(27)	2.37(1)
C(27)	C(28)	1.49(1)	C(30)	C(31)	1.99(2)
C(31)	C(32)	1.84(2)	C(32)	C(33)	1.92(1)
C(33)	C(34)	1.97(2)			
O(1)	H(1)	1.963(9)	O(1)	H(2)	1.952(9)
O(1)	H(3)	2.530(7)	O(1)	H(15)	1.953(8)
O(1)	H(16)	1.937(8)	O(1)	H(20)	2.516(9)
O(2)	H(1)	2.618(8)	O(2)	H(3)	1.908(9)

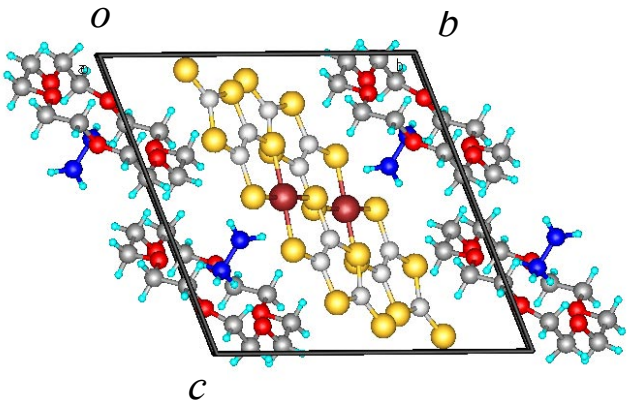
O(2)	H(4)	1.914(8)	O(2)	H(5)	1.936(9)
O(2)	H(6)	1.940(8)	O(2)	H(7)	2.565(9)
O(3)	H(5)	2.521(7)	O(3)	H(7)	1.966(8)
O(3)	H(8)	1.974(9)	O(3)	H(10)	2.499(8)
O(3)	H(17)	1.92(1)	O(3)	H(18)	1.963(8)
O(4)	H(9)	1.95(1)	O(4)	H(10)	1.95(1)
O(4)	H(11)	1.966(8)	O(4)	H(12)	1.982(9)
O(4)	H(14)	2.631(8)	O(4)	H(18)	2.50(1)
O(5)	H(12)	2.550(9)	O(5)	H(13)	1.942(7)
O(5)	H(14)	1.945(8)	O(5)	H(16)	2.56(1)
O(5)	H(19)	1.96(1)	O(5)	H(20)	1.972(9)
C(19)	H(1)	0.950(9)	C(19)	H(2)	0.95
C(19)	H(3)	2.021(9)	C(19)	H(4)	2.032(9)
C(19)	H(15)	2.567(9)	C(19)	H(16)	2.571(9)
C(20)	H(1)	2.037(9)	C(20)	H(2)	2.03(1)
C(20)	H(3)	0.95(1)	C(20)	H(4)	0.95(1)
C(20)	H(5)	2.38(1)	C(20)	H(6)	2.77(1)
C(21)	H(4)	2.38(1)	C(21)	H(5)	0.95
C(21)	H(6)	0.95	C(21)	H(7)	2.005(9)
C(21)	H(8)	2.02(1)	C(22)	H(5)	2.001(9)
C(22)	H(6)	2.020(9)	C(22)	H(7)	0.95
C(22)	H(8)	0.95	C(22)	H(17)	2.66(1)
C(22)	H(18)	2.466(9)	C(23)	H(7)	2.61(1)
C(23)	H(8)	2.540(9)	C(23)	H(9)	2.042(9)
C(23)	H(10)	2.05(1)	C(23)	H(17)	0.95(1)
C(23)	H(18)	0.95	C(24)	H(9)	0.95
C(24)	H(10)	0.95	C(24)	H(11)	2.46(1)
C(24)	H(17)	2.02(1)	C(24)	H(18)	2.05(1)
C(25)	H(9)	2.65(1)	C(25)	H(10)	2.55(1)
C(25)	H(11)	0.95(1)	C(25)	H(12)	0.95(1)
C(25)	H(13)	2.03(1)	C(25)	H(14)	2.040(9)
C(26)	H(10)	2.78(1)	C(26)	H(11)	2.02(1)
C(26)	H(12)	2.034(9)	C(26)	H(13)	0.950(9)
C(26)	H(14)	0.950(9)	C(26)	H(19)	2.38(1)
C(27)	H(13)	2.62(1)	C(27)	H(14)	2.51(1)
C(27)	H(15)	2.02(1)	C(27)	H(16)	2.00(1)
C(27)	H(19)	0.95(1)	C(27)	H(20)	0.95(1)
C(28)	H(1)	2.52(1)	C(28)	H(2)	2.643(9)
C(28)	H(15)	0.95	C(28)	H(16)	0.95
C(28)	H(19)	2.01(1)	C(28)	H(20)	2.00(1)
H(1)	H(2)	1.55	H(1)	H(3)	2.79(1)
H(1)	H(4)	2.335(9)	H(1)	H(5)	2.44(1)
H(1)	H(15)	2.76(1)	H(1)	H(16)	2.364(9)
H(2)	H(3)	2.315(9)	H(2)	H(4)	2.315(9)
H(2)	H(15)	2.491(9)	H(3)	H(4)	1.551(9)
H(4)	H(5)	2.22(1)	H(4)	H(6)	2.57(1)
H(5)	H(6)	1.55	H(5)	H(7)	2.76(1)
H(5)	H(8)	2.31(1)	H(6)	H(7)	2.317(9)
H(6)	H(8)	2.29(1)	H(7)	H(8)	1.55(1)
H(7)	H(18)	2.37(1)	H(8)	H(17)	2.51(1)
H(8)	H(18)	2.63(1)	H(9)	H(10)	1.55
H(9)	H(11)	2.38(1)	H(9)	H(17)	2.28(1)
H(9)	H(18)	2.39(1)	H(10)	H(11)	2.60(1)
H(10)	H(14)	2.25(1)	H(10)	H(17)	2.37(1)
H(11)	H(12)	1.55(1)	H(11)	H(13)	2.30(1)
H(11)	H(14)	2.33(1)	H(12)	H(13)	2.330(9)

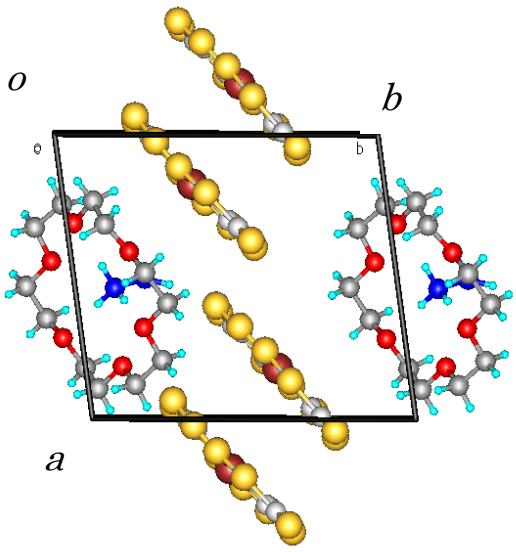
H(12)	H(14)	2.799(9)	H(13)	H(14)	1.551(9)
H(13)	H(19)	2.32(1)	H(14)	H(16)	2.37(1)
H(14)	H(19)	2.45(1)	H(15)	H(16)	1.55
H(15)	H(19)	2.27(1)	H(15)	H(20)	2.34(1)
H(16)	H(19)	2.33(1)	H(16)	H(20)	2.75(1)
H(17)	H(18)	1.55	H(19)	H(20)	1.55

Crystal data (7)









Figures shows the unit cell of salt **7** viewed along the *a*- and *c*-axes, respectively. The $[Ni(dmit)_2]^-$ anions form the π – π dimer structure, which are interacted along the a-axis. The supramolecular cations of $(NH_2\text{-}NH_3^+)$([18]crown-6) are arranged along the *c*-axis.

Table S13. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ni(1)	0.17698(2)	0.40599(2)	0.47907(2)	2.687(4)
S(1)	0.32346(5)	0.50665(4)	0.48304(4)	3.37(1)
S(2)	0.39574(5)	0.57151(4)	0.67365(4)	3.62(1)
S(3)	0.37131(6)	0.56383(5)	0.91137(5)	4.80(1)
S(4)	0.20288(5)	0.44482(4)	0.83280(4)	3.52(1)
S(5)	0.11404(5)	0.37099(4)	0.65579(4)	3.61(1)
S(6)	0.02553(5)	0.30969(4)	0.47718(4)	3.26(1)
S(7)	-0.06158(4)	0.25625(4)	0.28595(4)	3.27(1)
S(8)	-0.03869(6)	0.25421(6)	0.05145(5)	5.23(2)
S(9)	0.13546(5)	0.37246(5)	0.12595(4)	4.08(1)
S(10)	0.24015(5)	0.43792(4)	0.30232(4)	3.41(1)
O(1)	0.4475(1)	-0.0623(1)	0.6859(1)	4.20(3)
O(2)	0.7174(1)	-0.0583(1)	0.6560(1)	4.00(3)
O(3)	0.8156(1)	0.1146(1)	0.7016(1)	4.05(3)
O(4)	0.6792(1)	0.1962(1)	0.8650(1)	4.44(3)
O(5)	0.4118(1)	0.1828(1)	0.9089(1)	4.54(3)
O(6)	0.3135(1)	0.0219(1)	0.8477(1)	4.65(3)
N(1)	0.5410(1)	0.1232(1)	0.7215(1)	3.53(3)
N(2)	0.5081(2)	0.2190(2)	0.6209(2)	6.51(6)
C(1)	0.3027(2)	0.5022(1)	0.6207(1)	2.89(4)
C(2)	0.3253(2)	0.5289(2)	0.8111(1)	3.34(4)
C(3)	0.2127(2)	0.4431(1)	0.6960(1)	2.89(3)
C(4)	0.0397(2)	0.3187(1)	0.3384(1)	2.67(3)
C(5)	0.0097(2)	0.2922(2)	0.1489(2)	3.57(4)
C(6)	0.1318(2)	0.3739(1)	0.2628(1)	2.94(4)
C(7)	0.5364(2)	-0.1511(2)	0.6637(2)	5.06(6)
C(8)	0.6497(2)	-0.1008(2)	0.5932(2)	4.59(5)
C(9)	0.8220(2)	-0.0009(2)	0.5907(2)	4.57(5)
C(10)	0.8945(2)	0.0294(2)	0.6661(2)	4.54(5)
C(11)	0.8795(2)	0.1465(2)	0.7749(2)	4.25(5)
C(12)	0.7939(2)	0.2401(2)	0.8031(2)	4.54(5)
C(13)	0.5925(3)	0.2798(2)	0.8976(2)	5.57(6)
C(14)	0.4851(2)	0.2222(2)	0.9723(2)	5.31(6)
C(15)	0.3154(2)	0.1169(2)	0.9769(2)	5.47(6)
C(16)	0.2338(2)	0.0913(2)	0.9032(2)	5.29(5)
C(17)	0.2476(2)	-0.0054(2)	0.7721(2)	5.19(6)
C(18)	0.3292(2)	-0.1008(2)	0.7442(2)	4.95(6)
H(1)	0.8967(2)	0.0820(2)	0.8425(2)	5.08(9)
H(2)	0.9589(2)	0.1729(2)	0.7382(2)	5.06(9)
H(3)	0.9721(2)	0.0578(2)	0.6268(2)	5.4(1)
H(4)	0.9155(2)	-0.0374(2)	0.7308(2)	5.4(1)
H(5)	0.8771(2)	-0.0493(2)	0.5570(2)	5.42(9)
H(6)	0.7884(2)	0.0677(2)	0.5329(2)	5.4(1)
H(7)	0.6205(2)	-0.0391(2)	0.5272(2)	5.8(1)
H(8)	0.7059(2)	-0.1578(2)	0.5715(2)	5.8(1)
H(9)	0.5643(2)	-0.2076(2)	0.7334(2)	6.5(1)
H(10)	0.4951(2)	-0.1859(2)	0.6249(2)	6.5(1)
H(11)	0.2849(2)	-0.1246(2)	0.6977(2)	6.2(1)
H(12)	0.3477(2)	-0.1638(2)	0.8127(2)	6.2(1)
H(13)	0.1661(2)	-0.0282(2)	0.8069(2)	6.0(1)
H(14)	0.2344(2)	0.0599(2)	0.7044(2)	6.0(1)
H(15)	0.1991(2)	0.1616(2)	0.8480(2)	5.7(1)
H(16)	0.1648(2)	0.0519(2)	0.9480(2)	5.7(1)

H(17)	0.3558(2)	0.0462(2)	1.0276(2)	6.3(1)
H(18)	0.2630(2)	0.1584(2)	1.0192(2)	6.3(1)
H(19)	0.4301(2)	0.2747(2)	1.0011(2)	6.7(1)
H(20)	0.5202(2)	0.1579(2)	1.0337(2)	6.7(1)
H(21)	0.6370(3)	0.3119(2)	0.9369(2)	7.2(1)
H(22)	0.5587(3)	0.3392(2)	0.8320(2)	7.2(1)
H(23)	0.7713(2)	0.3019(2)	0.7348(2)	5.7(1)
H(24)	0.8374(2)	0.2669(2)	0.8477(2)	5.7(1)
H(25)	0.4642(1)	0.0931(1)	0.7606(1)	4.50(9)
H(26)	0.5975(1)	0.0654(1)	0.7014(1)	4.50(9)
H(27)	0.5830(1)	0.1471(1)	0.7694(1)	4.49(9)
H(28)	0.5292(2)	0.2925(2)	0.6110(2)	7.7(1)
H(29)	0.4653(2)	0.2095(2)	0.5640(2)	7.7(1)

$B_{eq} = 8/3\ p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

Table S14. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	0.0401(1)	0.0348(1)	0.0303(1)	-0.00904(9)	-0.00172(8)	-0.01377(8)
S(1)	0.0457(3)	0.0570(3)	0.0335(2)	-0.0212(2)	0.0048(2)	-0.0218(2)
S(2)	0.0449(3)	0.0587(3)	0.0462(3)	-0.0176(2)	0.0011(2)	-0.0295(2)
S(3)	0.0826(4)	0.0653(4)	0.0498(3)	-0.0132(3)	-0.0151(3)	-0.0335(3)
S(4)	0.0619(3)	0.0454(3)	0.0298(2)	-0.0143(2)	-0.0008(2)	-0.0150(2)
S(5)	0.0607(3)	0.0505(3)	0.0316(2)	-0.0283(2)	0.0027(2)	-0.0139(2)
S(6)	0.0479(3)	0.0475(3)	0.0324(2)	-0.0183(2)	0.0039(2)	-0.0158(2)
S(7)	0.0414(2)	0.0456(3)	0.0435(2)	-0.0148(2)	-0.0022(2)	-0.0192(2)
S(8)	0.0745(4)	0.0914(5)	0.0539(3)	-0.0315(3)	-0.0060(3)	-0.0409(3)
S(9)	0.0610(3)	0.0698(3)	0.0354(2)	-0.0295(3)	0.0065(2)	-0.0258(2)
S(10)	0.0503(3)	0.0522(3)	0.0359(2)	-0.0257(2)	0.0054(2)	-0.0203(2)
O(1)	0.0508(8)	0.0464(8)	0.0693(9)	-0.0136(6)	-0.0064(7)	-0.0248(7)
O(2)	0.0538(8)	0.0530(8)	0.0501(8)	-0.0103(6)	0.0017(6)	-0.0243(7)
O(3)	0.0445(7)	0.0496(8)	0.0645(9)	-0.0105(6)	-0.0048(6)	-0.0238(7)
O(4)	0.0632(9)	0.0462(8)	0.0686(9)	-0.0054(7)	-0.0080(7)	-0.0313(7)
O(5)	0.0649(9)	0.0611(9)	0.0453(7)	0.0070(7)	-0.0027(7)	-0.0246(7)
O(6)	0.0421(8)	0.0646(9)	0.0650(9)	-0.0012(7)	-0.0036(7)	-0.0200(8)
N(1)	0.0427(8)	0.0487(9)	0.0485(9)	-0.0079(7)	-0.0019(7)	-0.0237(7)
N(2)	0.124(2)	0.057(1)	0.062(1)	-0.007(1)	-0.026(1)	-0.012(1)
C(1)	0.0393(9)	0.0414(9)	0.0335(8)	-0.0075(7)	-0.0024(7)	-0.0176(7)
C(2)	0.051(1)	0.042(1)	0.0385(9)	-0.0001(8)	-0.0095(8)	-0.0205(8)
C(3)	0.044(1)	0.0368(9)	0.0305(8)	-0.0082(7)	-0.0048(7)	-0.0116(7)
C(4)	0.0383(9)	0.0356(9)	0.0327(8)	-0.0079(7)	-0.0031(7)	-0.0165(7)
C(5)	0.049(1)	0.052(1)	0.042(1)	-0.0118(9)	-0.0037(8)	-0.0243(9)
C(6)	0.043(1)	0.0420(9)	0.0312(8)	-0.0140(8)	-0.0008(7)	-0.0155(7)
C(7)	0.071(1)	0.049(1)	0.086(2)	-0.008(1)	-0.017(1)	-0.038(1)
C(8)	0.068(1)	0.058(1)	0.057(1)	0.006(1)	-0.012(1)	-0.035(1)
C(9)	0.056(1)	0.059(1)	0.057(1)	-0.008(1)	0.009(1)	-0.023(1)
C(10)	0.043(1)	0.056(1)	0.073(1)	-0.0093(9)	0.011(1)	-0.026(1)
C(11)	0.045(1)	0.059(1)	0.057(1)	-0.019(1)	-0.0065(9)	-0.014(1)
C(12)	0.069(1)	0.052(1)	0.061(1)	-0.023(1)	-0.014(1)	-0.022(1)
C(13)	0.087(2)	0.062(1)	0.081(2)	0.005(1)	-0.019(1)	-0.048(1)
C(14)	0.082(2)	0.074(2)	0.056(1)	0.022(1)	-0.020(1)	-0.043(1)
C(15)	0.075(2)	0.070(2)	0.053(1)	0.010(1)	0.004(1)	-0.023(1)
C(16)	0.047(1)	0.068(1)	0.067(1)	0.005(1)	0.012(1)	-0.013(1)
C(17)	0.041(1)	0.077(2)	0.071(1)	-0.016(1)	-0.008(1)	-0.013(1)

C(18)	0.059(1)	0.065(1)	0.073(1)	-0.031(1)	-0.011(1)	-0.024(1)

The general temperature factor expression:exp(-2p^2(a*^{2}U$_{11}$h^2 + b*^{2}U$_{22}$k^2 + c*^{2}U$_{33}$l^2 + 2a*b*U$_{12}$hk + 2a*c*U$_{13}$hl + 2b*c*U$_{23}$kl))

Table S15. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ni(1)	S(1)	2.168(1)	Ni(1)	S(5)	2.16(2)
Ni(1)	S(6)	2.164(1)	Ni(1)	S(10)	2.17(1)
S(1)	C(1)	1.717(2)	S(2)	C(1)	1.75(1)
S(2)	C(2)	1.73(2)	S(3)	C(2)	1.64(1)
S(4)	C(2)	1.733(6)	S(4)	C(3)	1.737(2)
S(5)	C(3)	1.719(9)	S(6)	C(4)	1.714(4)
S(7)	C(4)	1.75(1)	S(7)	C(5)	1.73(2)
S(8)	C(5)	1.64(1)	S(9)	C(5)	1.728(6)
S(9)	C(6)	1.743(2)	S(10)	C(6)	1.718(8)
O(1)	C(7)	1.420(8)	O(1)	C(18)	1.425(9)
O(2)	C(8)	1.42(1)	O(2)	C(9)	1.42(1)
O(3)	C(10)	1.42(1)	O(3)	C(11)	1.416(9)
O(4)	C(12)	1.43(1)	O(4)	C(13)	1.42(1)
O(5)	C(14)	1.438(9)	O(5)	C(15)	1.41(2)
O(6)	C(16)	1.42(1)	O(6)	C(17)	1.419(8)
N(1)	N(2)	1.43(4)	C(1)	C(3)	1.36(2)
C(4)	C(6)	1.36(2)	C(7)	C(8)	1.48(1)
C(9)	C(10)	1.482(9)	C(11)	C(12)	1.48(1)
C(13)	C(14)	1.48(2)	C(15)	C(16)	1.494(7)
C(17)	C(18)	1.48(1)			
N(1)	H(25)	0.950(6)	N(1)	H(26)	0.950(6)
N(1)	H(27)	0.950(6)	N(2)	H(28)	0.950(4)
N(2)	H(29)	0.950(3)	C(7)	H(9)	0.95(2)
C(7)	H(10)	0.950(7)	C(8)	H(7)	0.95(2)
C(8)	H(8)	0.950(7)	C(9)	H(5)	0.950(9)
C(9)	H(6)	0.95(2)	C(10)	H(3)	0.950(6)
C(10)	H(4)	0.95(2)	C(11)	H(1)	0.95(2)
C(11)	H(2)	0.950(5)	C(12)	H(23)	0.95(2)
C(12)	H(24)	0.950(7)	C(13)	H(21)	0.950(7)
C(13)	H(22)	0.95(2)	C(14)	H(19)	0.950(8)
C(14)	H(20)	0.95(2)	C(15)	H(17)	0.95(2)
C(15)	H(18)	0.95(1)	C(16)	H(15)	0.95(2)
C(16)	H(16)	0.95(1)	C(17)	H(13)	0.950(4)
C(17)	H(14)	0.95(2)	C(18)	H(11)	0.950(6)
C(18)	H(12)	0.95(2)			