- Supporting Material -

A new synthetic approach to force bond formation between a transition metal complex and a thiostannate anion: solvothermal synthesis and crystal structure of [Co$_2$(cyclam)$_2$Sn$_2$S$_6$]·2H$_2$O

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Experimental Details

Single crystal X-ray analysis

Datacollection was performed using an Imaging Plate Diffracxtion System (IPDS-1) from STOE & CIE using Kα_1-radiation. The structure was solved with direct methods using SHELXS-97 and structure refinements were performed against F^2 using SHELXL-97. Numerical absorption correction was applied using X-RED and X-SHAPE of the program package X-Area. All non hydrogen atoms were refined with anisotropic displacement parameters. All C-H hydrogen atoms were positioned with idealized geometry and were refined isotropic with $U_{iso}(H) = -1.2\ U_{eq}(C)$ using a riding model. The O-H hydrogen atoms were located in difference map, their bond lengths set to ideal values and afterwards they were refined isotropic with $U_{iso}(H) = -1.5\ U_{eq}(O)$ using a riding model.

CCDC ?????? contain the supplementary crystallographic data for this paper. These data can be obtained free charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif.

Raman spectroscopy

The Raman spectrum was measured in the region from 100 to 3500 cm^{-1} with a Bruker IFS 66 Fourier Transform Raman spectrometer (wavelength: 541.5 nm).

UV/Vis spectroscopy

UV/Vis spectroscopic investigation was conducted at room temperature using a UV-VIS-NIR two-channel spectrometer Cary 5 from Varian Techtron Pty., Darmstadt. The absorption data were calculated with the Kubelka-Munk relation for diffuse reflectance data. BaSO$_4$ powder was used as reference material.

Table S1.   Bond lengths and angles in Å and °. Symmetry codes to generate equivalent atoms: A: -x+1,-y+2,-z+2; B: -x+1,-y+2,-z+1; C: #3 -x,-y+1,-z+1

Sn1-S2	2.336(1)	Sn1-S3	2.447(1)
Sn1-S1	2.339(1)	Sn1-S3A	2.456(1)
S2-Sn1-S1	113.92(3)	S2-Sn1-S3A	112.63(3)
S2-Sn1-S3	112.29(3)	S1-Sn1-S3A	110.82(3)
S1-Sn1-S3	112.25(2)	S3-Sn1-S3A	93.21(2)
Sn1-S1-Co1	124.34(3)	Sn1-S2-Co2	116.91(3)
Sn1-S3-Sn1A	86.79(2)	Co1-S1B	2.715(1)
Co1-S1	2.715(1)	Co1-N1	1.982(2)
Co1-N2	1.986(2)	Co1-N2B	1.986(2)
Co1-N1B	1.982(2)	N2B-Co1-S1B	93.65(7)
N1B-Co1-N2B	86.31(11)	N2-Co1-S1B	86.35(7)
N1-Co1-N2B	93.69(11)	N1B-Co1-S1	88.68(7)
N1B-Co1-N2	93.69(11)	N1-Co1-S1	91.32(7)
N1-Co1-N2	86.31(11)	N2B-Co1-S1	86.35(7)
N1B-Co1-S1B	91.32(7)	N2-Co1-S1	93.65(7)
N1-Co1-S1B	88.68(7)	S1B-Co1-S1	180.0
N1B-Co1-N1	180.0	N2B-Co1-N2	180.0
Co-S2	2.806(1)	Co2-S2C	2.806(1)
Co2-N12	1.985(2)	Co2-N11	1.977(2)
Co2-N12C	1.985(2)	Co2-N11C	1.977(2)
N11-Co2-N12	86.00(10)	N11-Co2-S2	92.30(7)
N11C-Co2-N12	94.00(10)	N11C-Co2-S2	87.70(7)
N11-Co2-N12C	94.00(10)	N12-Co2-S2	94.57(7)
N11C-Co2-N12C	86.00(10)	N12C-Co2-S2	85.43(7)
N11-Co2-S2C	87.70(7)	N11-Co2-N11C	180.0)
N11C-Co2-S2C	92.30(7)	N12-Co2-N12C	180.0
N12-Co2-S2C	85.43(7)	S2C-Co2-S2	180.0
N12C-Co2-S2C	94.57(7)		

Table S2: Hydrogen bonding in Å and °. Symmetry codes to generate equivalent atoms: A = -x+1, -y+2, -z+2; B = -x, -y+1, -z+1; C: -x, -y+2, -z+1.

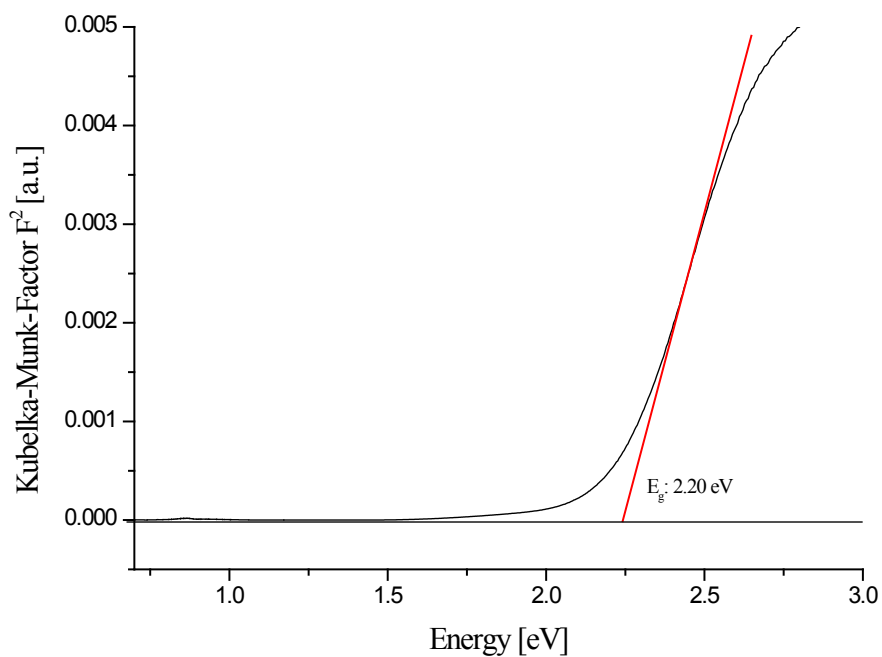|	D-H	d(H..A)	d(D..A)
N1-H1N⋯S3	2.553	154.5	3.397
N11-H11N⋯S1	2.491	155.5	3.341
N12-H12N⋯O1B	2.615	161.8	3.491
O1-H1O⋯S2	2.526	166.1	3.328

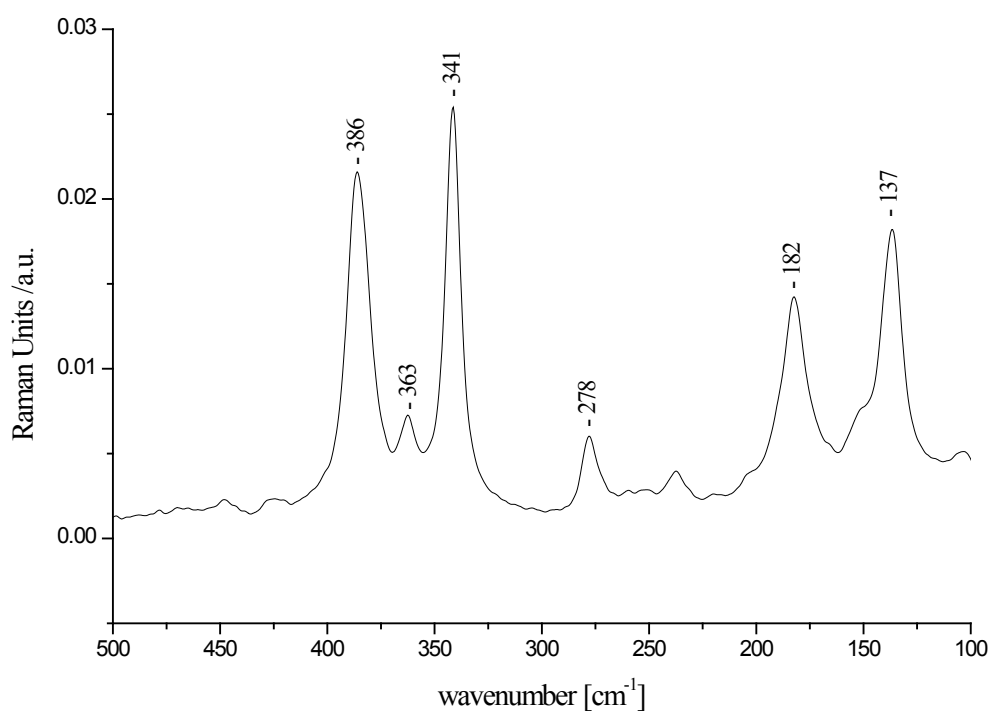Fig. S1: The UV-Vis spectrum of the title compound to determine the optical bandgap.

Fig. S2: The Raman spectrum of the title compound with the wavenumbers of the most prominent bands.