Supporting Information

Synthesis, Characterization, and Calculated Electronic Structure of the Crystalline Metal-Organic Polymers $[Hg(SC_6H_4S)(en)]_n$ and $[Pb(SC_6H_4S)(dien)]_n$

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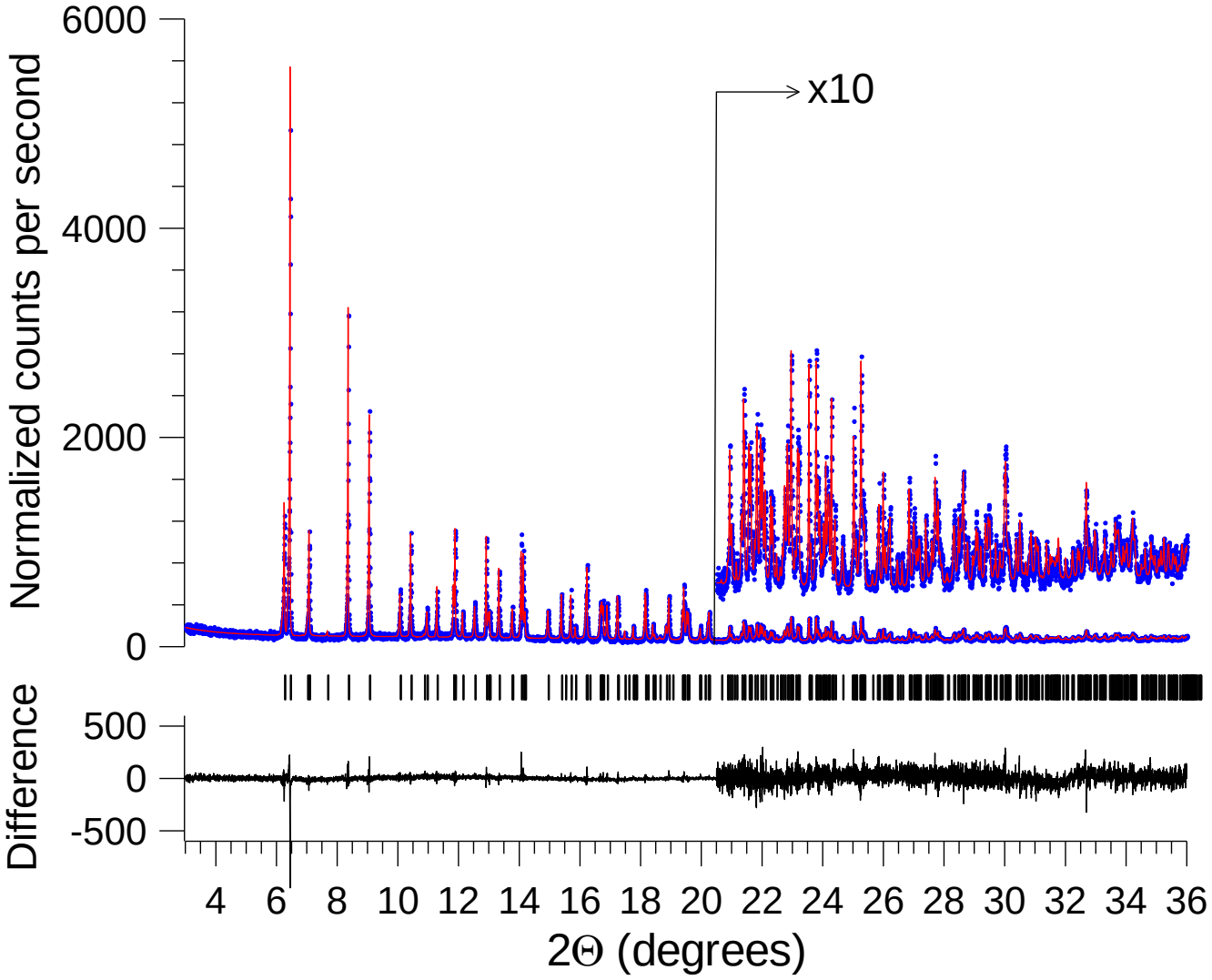

Figure S1. Rietveld refinement fit for $[Hg(SC_6H_4S)(en)]_n$. Experimental data is blue dots, calculated pattern is red line, and black difference plot is shown below.

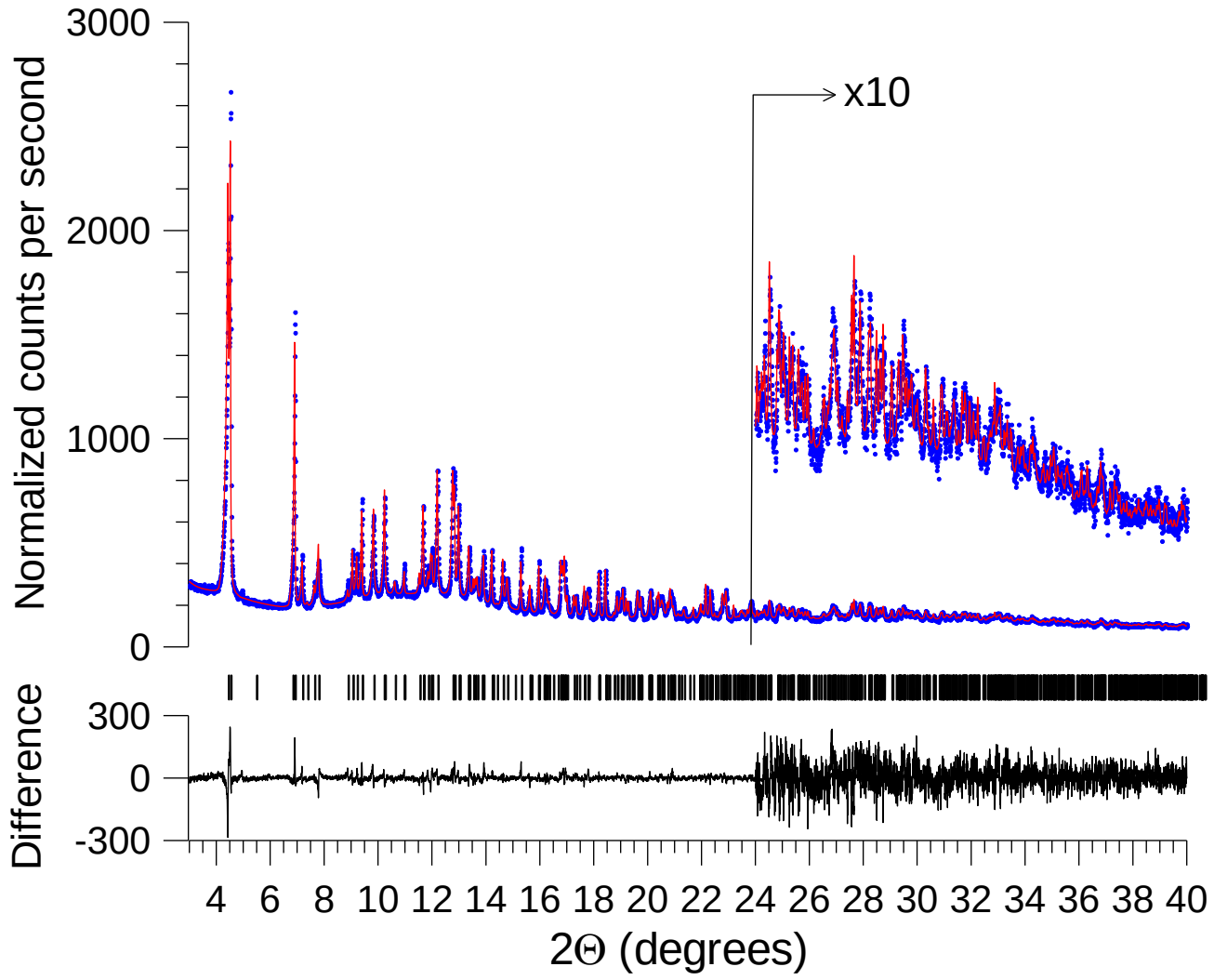

Figure S2. Rietveld refinement fit for $[Pb(SC_6H_4S)(dien)]_n$. Experimental data is blue dots, calculated pattern is red line, and black difference plot is shown below.

The two DFT-calculated structures are below in CIF format. Simply copy all of the text below the line of pound signs, save it as a plain text (ASCII) file, and then re-name the extension to .cif to open in a program such as Mercury.

##

```
data_Hg(SC6H4S)(en)-DFT
_audit_creation_method 'Created with Endeavour Version 1.7c'
_audit_creation_date          2011-08-04
_audit_update_record          2011-08-04
_chemical_formula_sum     'C32 H48 Hg4 N8 S8'
_chemical_formula_weight 1603.673
_cell_length_a         13.0777
_cell_length_b          7.1213
_cell_length_c         11.6166
_cell_angle_alpha    90.000
_cell_angle_beta     101.570
_cell_angle_gamma 90.000
_cell_volume           1059.9(0)
_symmetry_int_tables_number       15
_symmetry_space_group_name_H-M       'C 1 2/c 1'
_symmetry_space_group_name_Hall       '-C_2yc'

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,0.500-z
3 -x,-y,-z
4 x,-y,0.500+z
5 0.500+x,0.500+y,z
6 0.500-x,0.500+y,0.500-z
7 0.500-x,0.500-y,-z
8 0.500+x,0.500-y,0.500+z
```

```
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_atom_type_symbol
_atom_type_oxidation_number
_atom_type_radius_bond
C     ?       1.200
H     ?       1.200
Hg    ?       1.200
N     ?       1.200
S     ?       1.200


loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_attached_hydrogens
_atom_site_calc_flag
_atom_site_thermal_displace_type
_atom_site_u_iso_or_equiv
C1A C  0.7968  0.0798  0.5479  1.000 8 f ? d ? ?
C2A C  0.7338  0.1860  0.6079  1.000 8 f ? d ? ?
C3A C  0.6884  0.3530  0.5610  1.000 8 f ? d ? ?
C7A C  0.9981  0.4265  0.8150  1.000 8 f ? d ? ?
H1A H  0.0508  0.7573  0.0661  1.000 8 f ? d ? ?
H1B H  0.8606  0.2835  0.8150  1.000 8 f ? d ? ?
H2A H  0.2798  0.8621  0.3067  1.000 8 f ? d ? ?
H7A H  0.4645  0.0617  0.8367  1.000 8 f ? d ? ?
H7B H  0.9217  0.5812  0.1321  1.000 8 f ? d ? ?
H3A H  0.8602  0.9330  0.8899  1.000 8 f ? d ? ?
```

```
Hg1 Hg  0.0000  0.9823  0.7500  1.000 4 e ? d ? ?
N1A N  0.9394  0.2646  0.8447  1.000 8 f ? d ? ?
S1A S  0.1467  0.8656  0.8951  1.000 8 f ? d ? ?

#===END

data_Pb(SC6H4S)(dien)-DFT
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_cell_length_b         10.2934
_cell_length_c         10.2881
_cell_angle_alpha    61.180
_cell_angle_beta      86.280
_cell_angle_gamma 85.840
_cell_volume          674.4
_symmetry_int_tables_number      2
_symmetry_space_group_name_H-M       'P -1'
_symmetry_space_group_name_Hall       '-P_1'

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_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z

loop_
_atom_type_symbol
_atom_type_oxidation_number
_atom_type_radius_bond
C      ?          1.200
```

H ? 1.200

N ? 1.200

Pb ? 1.200

S ? 1.200

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_occupancy

_atom_site_symmetry_multiplicity

_atom_site_Wyckoff_symbol

_atom_site_attached_hydrogens

_atom_site_calc_flag

_atom_site_thermal_displace_type

_atom_site_u_iso_or_equiv

C1B C 0.9372 0.8903 0.4665 1.000 2 i ? d ? ?

C7A C 0.0167 0.7126 0.0712 1.000 2 i ? d ? ?

C1 C 0.4663 0.4697 0.8816 1.000 2 i ? d ? ?

C3B C 0.0503 0.8512 0.5870 1.000 2 i ? d ? ?

C3 C 0.4103 0.3743 0.0298 1.000 2 i ? d ? ?

C2B C 0.1121 0.9575 0.6186 1.000 2 i ? d ? ?

C2 C 0.5572 0.5968 0.8549 1.000 2 i ? d ? ?

C10A C 0.6335 0.0487 0.7184 1.000 2 i ? d ? ?

C9A C 0.6574 0.0639 0.8557 1.000 2 i ? d ? ?

C8A C 0.1702 0.8170 0.0388 1.000 2 i ? d ? ?

H3B H 0.0917 0.7339 0.6569 1.000 2 i ? d ? ?

H3 H 0.3401 0.2740 0.0543 1.000 2 i ? d ? ?

H2B H 0.7996 0.0776 0.2867 1.000 2 i ? d ? ?

H2 H 0.6025 0.6745 0.7409 1.000 2 i ? d ? ?

HC7B H 0.8860 0.7595 0.0953 1.000 2 i ? d ? ?

HC7A H 0.0031 0.2982 0.0290 1.000 2 i ? d ? ?

HC10B H 0.2393 0.0007 0.3078 1.000 2 i ? d ? ?

HC10A H 0.4771 0.0291 0.2571 1.000 2 i ? d ? ?

HC9A H 0.5301 0.1154 0.8792 1.000 2 i ? d ? ?

HC9B H 0.6805 0.9523 0.9530 1.000 2 i ? d ? ?

HC8A H 0.1395 0.9241 0.9376 1.000 2 i ? d ? ?

HC8B H 0.6984 0.2299 0.9849 1.000 2 i ? d ? ?

HN3B H 0.3630 0.8051 0.5063 1.000 2 i ? d ? ?

HN3A H 0.5469 0.7794 0.4145 1.000 2 i ? d ? ?

HN2A H 0.9280 0.1296 0.7985 1.000 2 i ? d ? ?

HN1B H 0.0713 0.4779 0.7490 1.000 2 i ? d ? ?

HN1A H 0.8670 0.5026 0.8215 1.000 2 i ? d ? ?

N3A N 0.5937 0.1940 0.5909 1.000 2 i ? d ? ?

N2A N 0.1954 0.8389 0.1661 1.000 2 i ? d ? ?

N1A N 0.0521 0.5694 0.2027 1.000 2 i ? d ? ?

Pb1 Pb 0.2340 0.5969 0.4006 1.000 2 i ? d ? ?

S1B S 0.8674 0.7597 0.4188 1.000 2 i ? d ? ?

S1 S 0.4217 0.4270 0.7411 1.000 2 i ? d ? ?

#===END