Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

S1. IR spectra

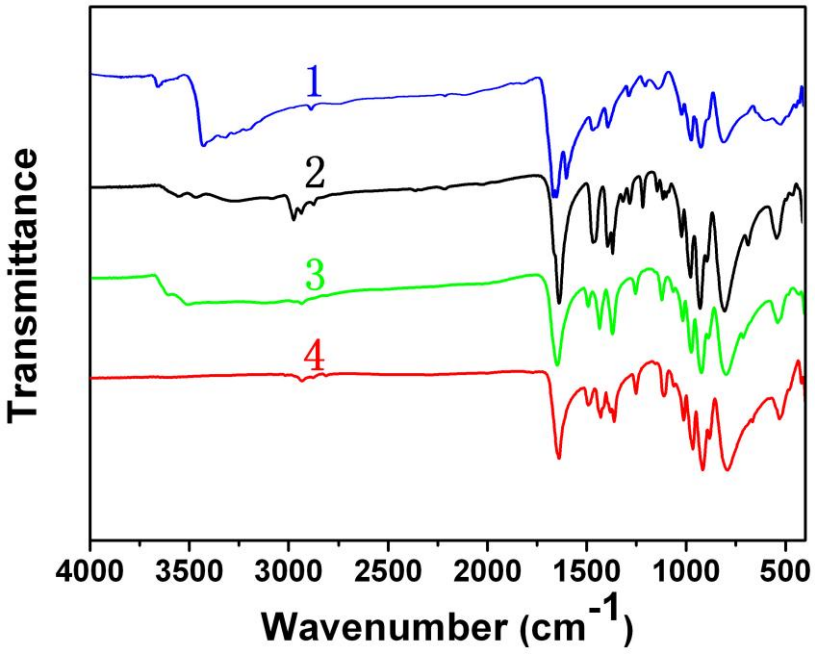

Figure S1. IR spectra of **1**-**4**.

S2. Thermogravimetry (TG) curve

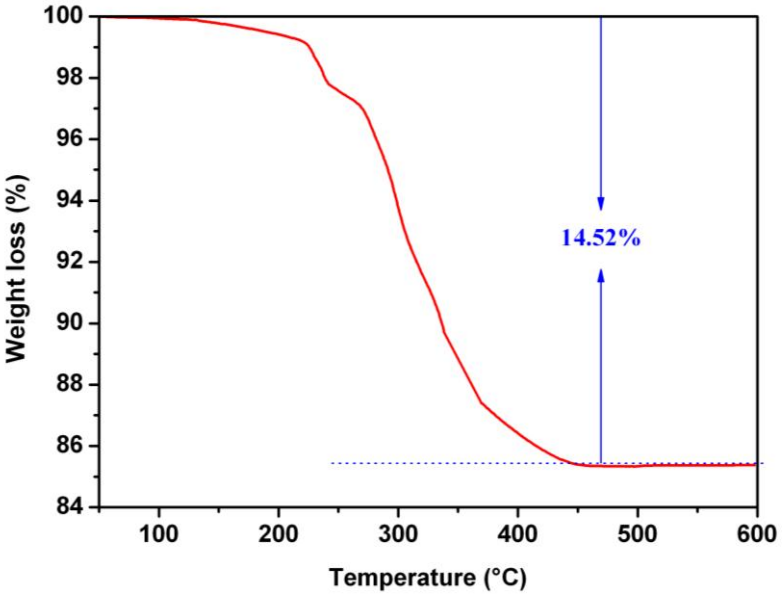

Figure S2-1. Thermogravimetry (TG) curve of **1**.

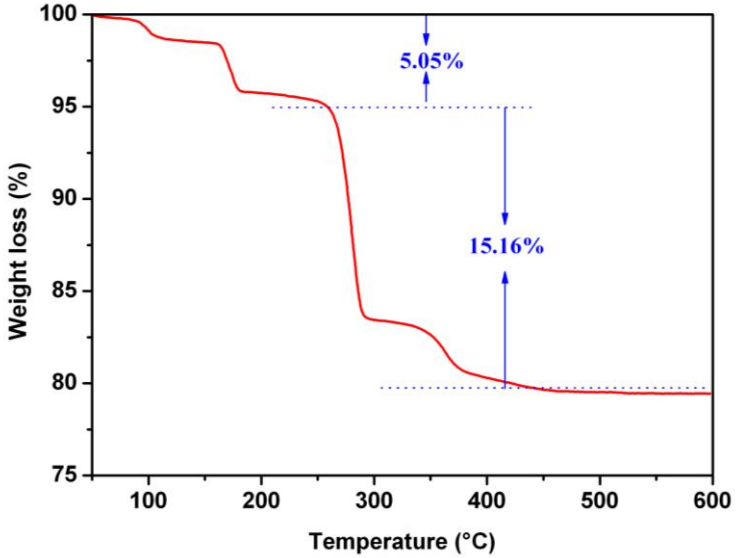

Figure S2-2. Thermogravimetry (TG) curve of **2**.

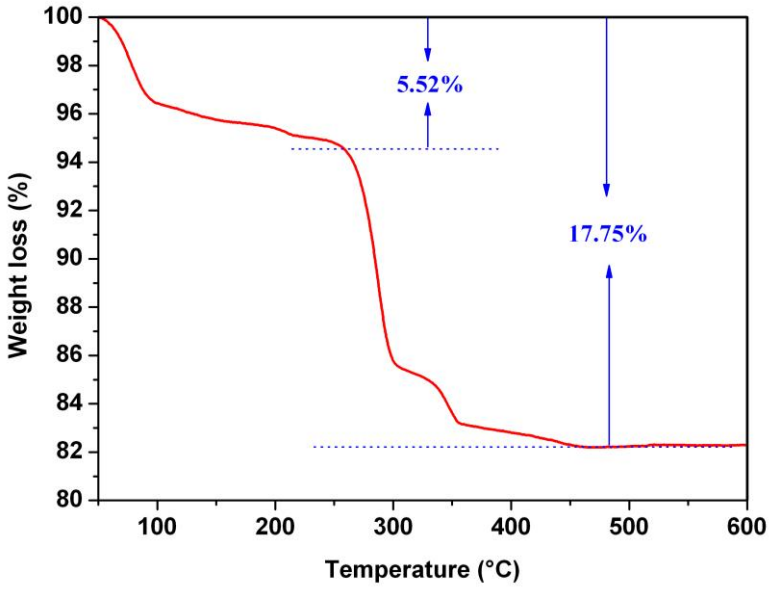

Figure S2-3. Thermogravimetry (TG) curve of **3**.

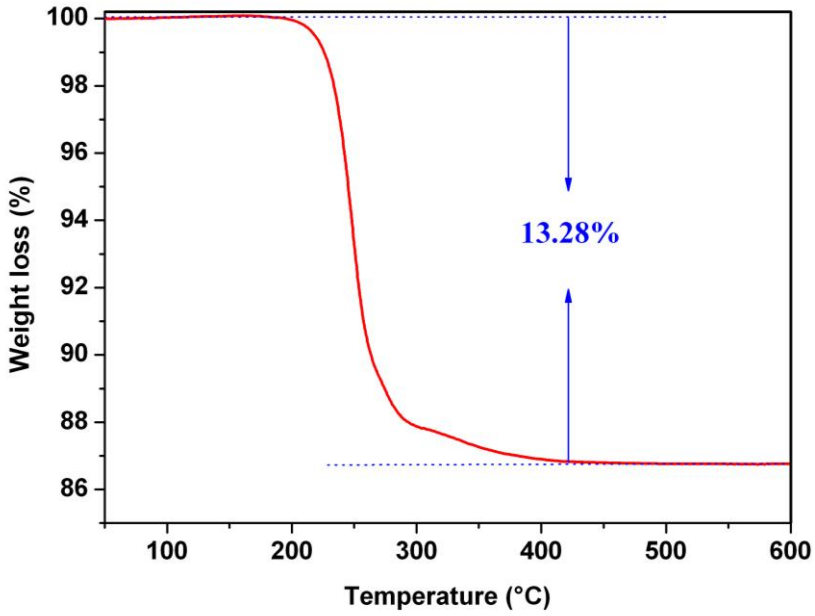

Figure S2-4. Thermogravimetry (TG) curve of **4**.

S3. X-ray powder diffraction

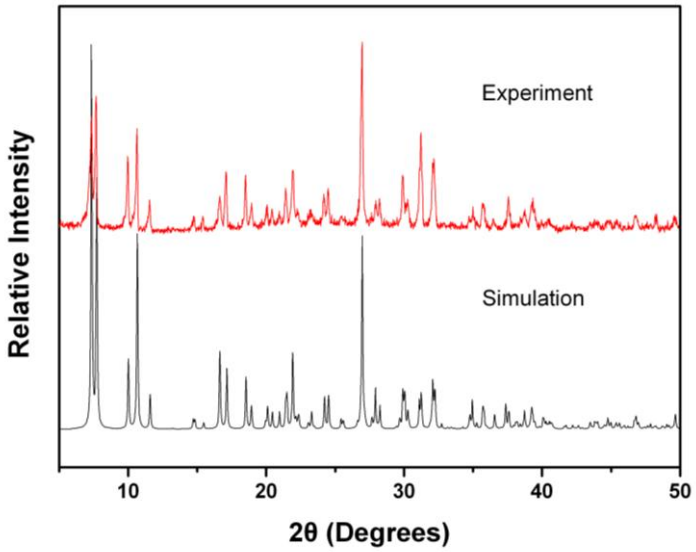

Figure S3-1. XRD patterns of compound **1**.

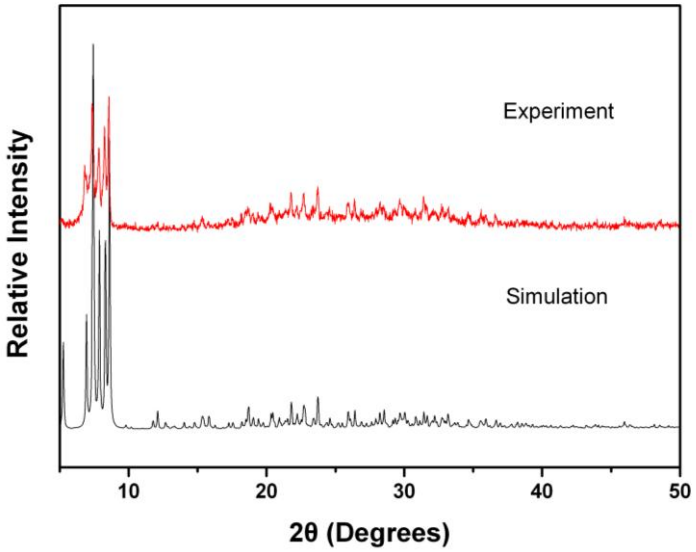

Figure S3-2. XRD patterns of compound **2**.

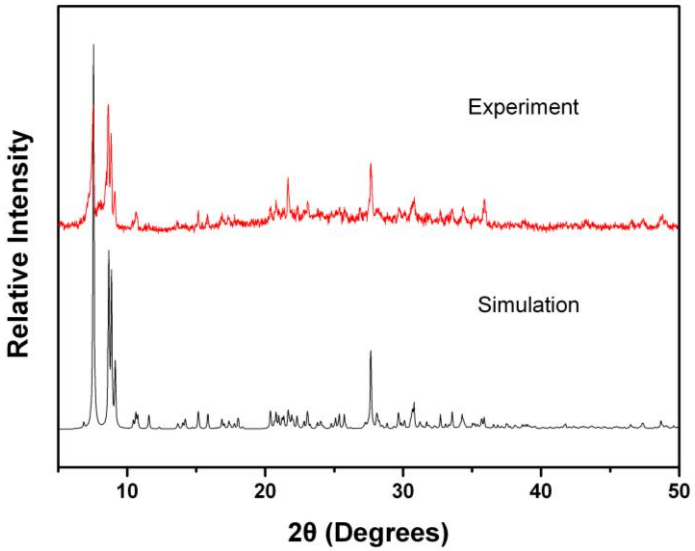

Figure S3-3. XRD patterns of compound **3**.

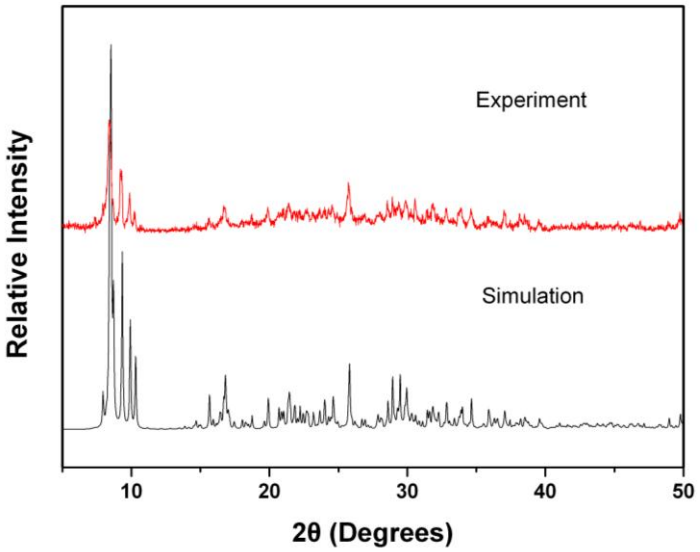

Figure S3-4. XRD patterns of compound **4**.

S4. Electron paramagnetic resonance (ESR) spectra

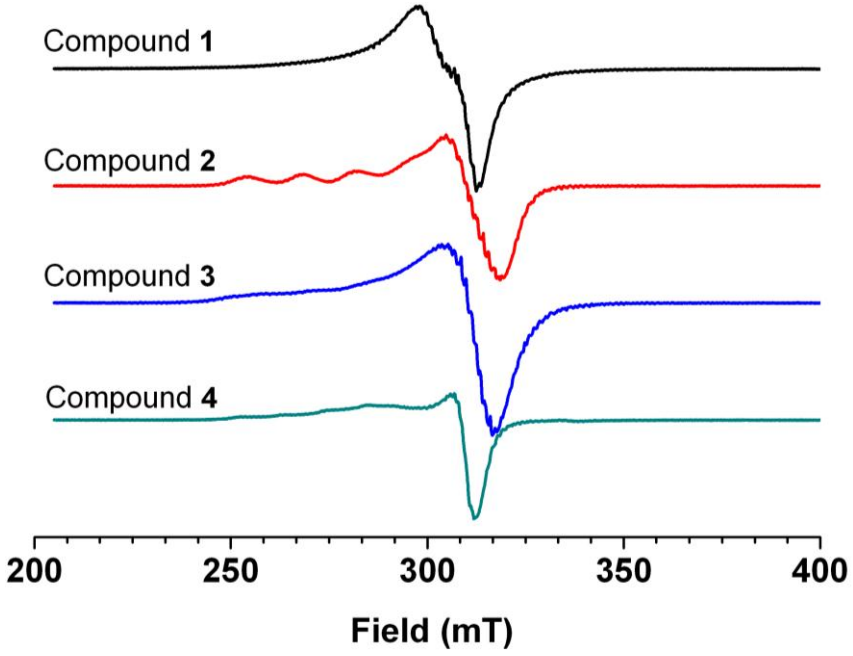

Figure S4.The ESR spectra for powdered samples of **1**-**4**.

S5&S6. UV/Vis spectra stability studies of 1-4.

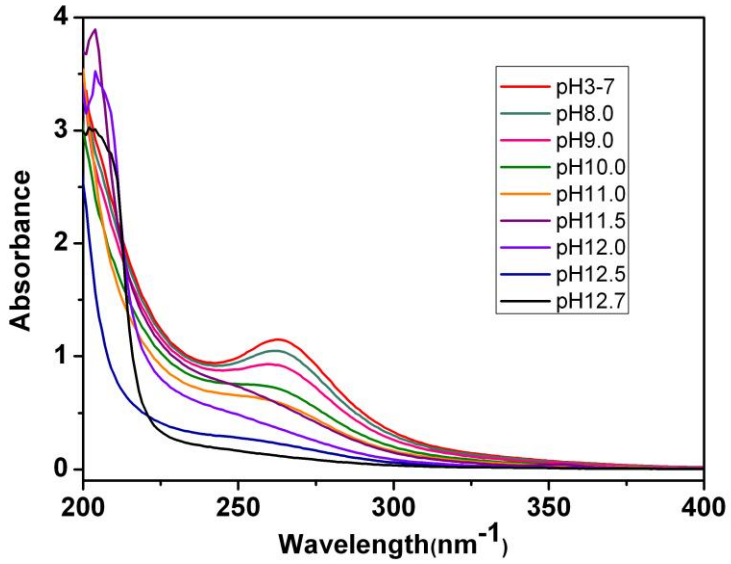

Figure S5-1. UV/Vis spectra of **1** in aqueous solution at different pH.

The pH was adjusted in the range of 3-7 by addition of aqueous HCl and 7–12.7 by addition of NaOH

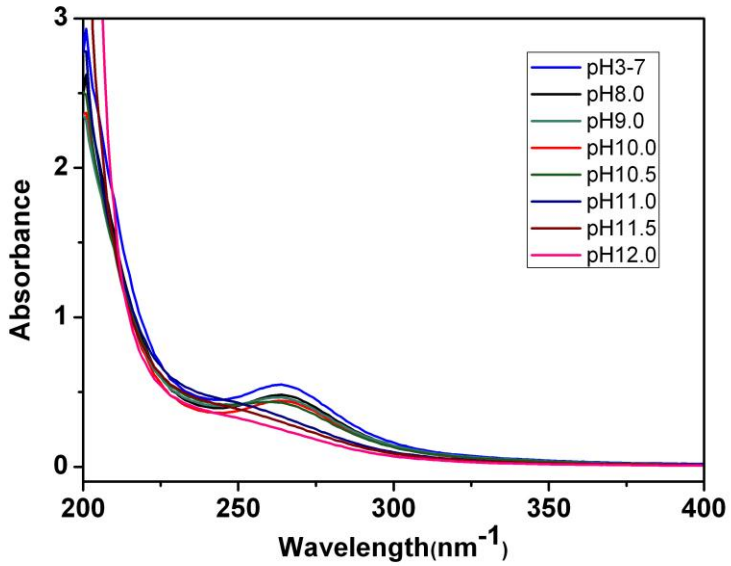

Figure S5-2. UV/Vis spectra of **2** in aqueous solution at different pH.

The pH was adjusted in the range of 3-7 by addition of aqueous HCl and 7–12 by addition of NaOH

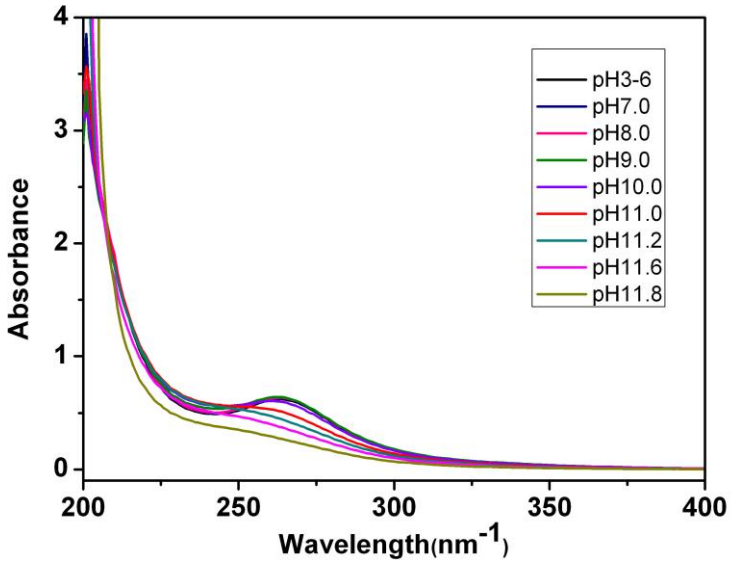

Figure S5-3. UV/Vis spectra of **3** in aqueous solution at different pH.

The pH was adjusted in the range of 3-7 by addition of aqueous HCl and 7–11.8 by addition of NaOH

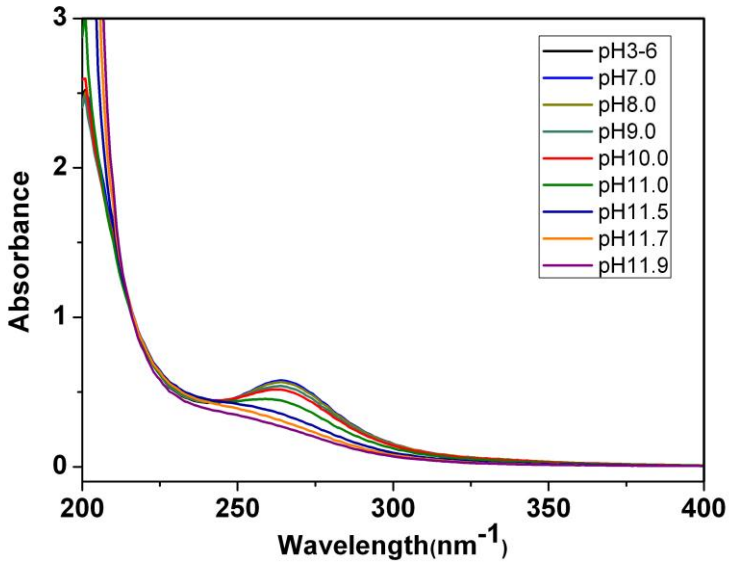

Figure S5-4. UV/Vis spectra of **4** in aqueous solution at different pH.

The pH was adjusted in the range of 3-7 by addition of aqueous HCl and 7–11.9 by addition of NaOH

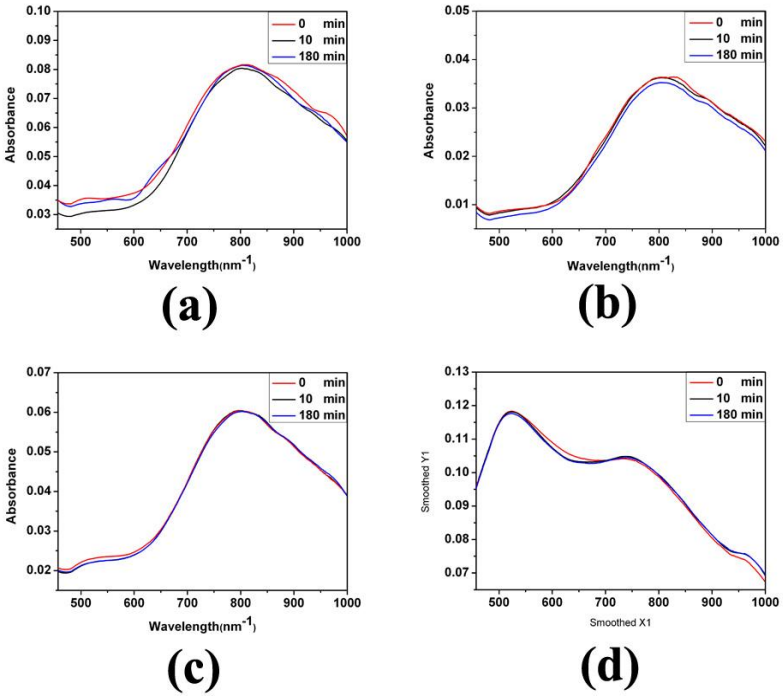

Figure S6. UV/Vis spectra of **1**-**4** in aqueous solution.

Excess of Oxygen were bubbled through the stirred solution and the UV spectrum was detected after 0 min, 10 min and 180 minutes (the characteristic peak is located at 264 nm), respectively.

Figure S7. _platon_squeeze_details

There is a big solvent accessible void present in the structure of 0D, 1D and 2D. QUEEZE has been used; SQUEEZE results were listed as follow:

0D:
loop_
_platon_squeeze_void_nr
_platon_squeeze_void_average_x
_platon_squeeze_void_average_y
_platon_squeeze_void_average_z
_platon_squeeze_void_volume
_platon_squeeze_void_count_electrons
_platon_squeeze_void_content
1 0.000 0.000 0.500 68 3 ' '
2 0.500 0.500 0.500 68 3' '

1D:
loop_
_platon_squeeze_void_nr
_platon_squeeze_void_average_x
_platon_squeeze_void_average_y
_platon_squeeze_void_average_z
_platon_squeeze_void_volume
_platon_squeeze_void_count_electrons
_platon_squeeze_void_content
1 -0.009 0.000 0.000 743 33 ' '
2 -0.007 0.500 0.500 743 33 ' '

2D:
loop_
_platon_squeeze_void_nr
_platon_squeeze_void_average_x
_platon_squeeze_void_average_y
_platon_squeeze_void_average_z
_platon_squeeze_void_volume
_platon_squeeze_void_count_electrons
_platon_squeeze_void_content
1 0.500 0.057 0.500 123 68 ' '
2 0.500 0.324 0.000 111 60 ' '
3 1.000 0.557 0.500 122 68 ' '
4 0.000 0.824 0.000 111 60 ' '