

***Electronic Supplementary Information (ESI)***

**An unusually water-poor 5,5'-azobistetrazolate of dysprosium: stabilization of a nitrogen-rich heterocycle by a minimum of hydrogen bonds**

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**Submitted to New Journal of Chemistry**

## Vibrational spectroscopy

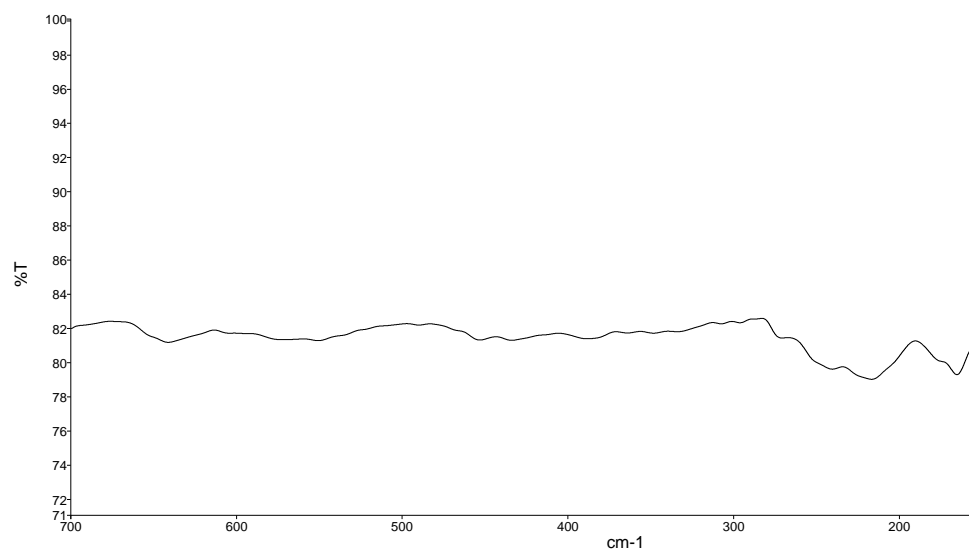
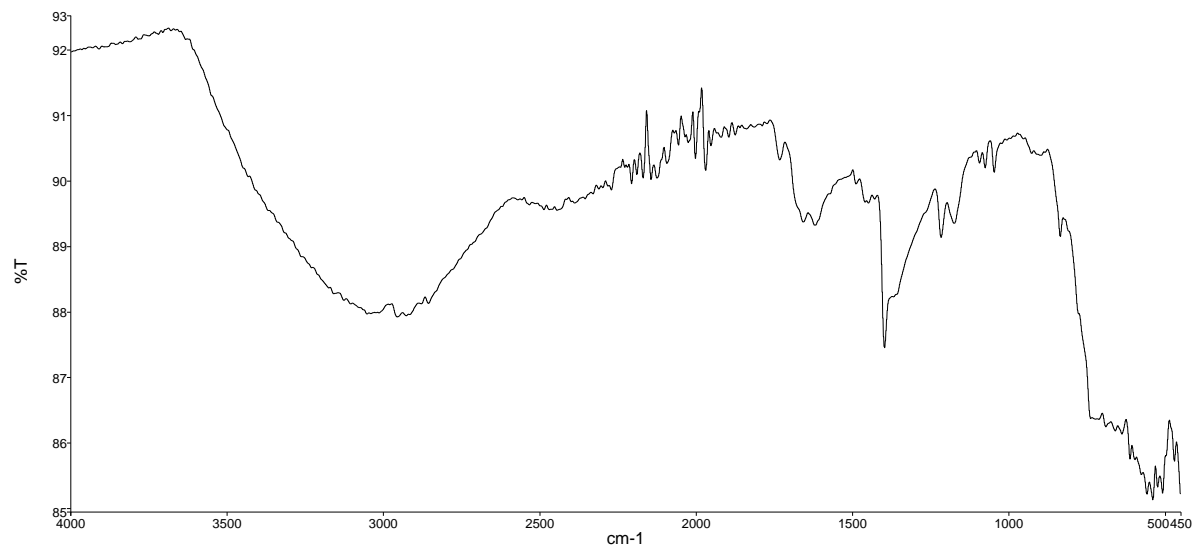
### Raman measurement settings

Due to the strong intensity differences of the Raman peaks 3 measurements using different settings A, B and C have been performed. These settings represent changes of the number of spectra accumulated; used filter, acquisition time and slit width (see Table S1).

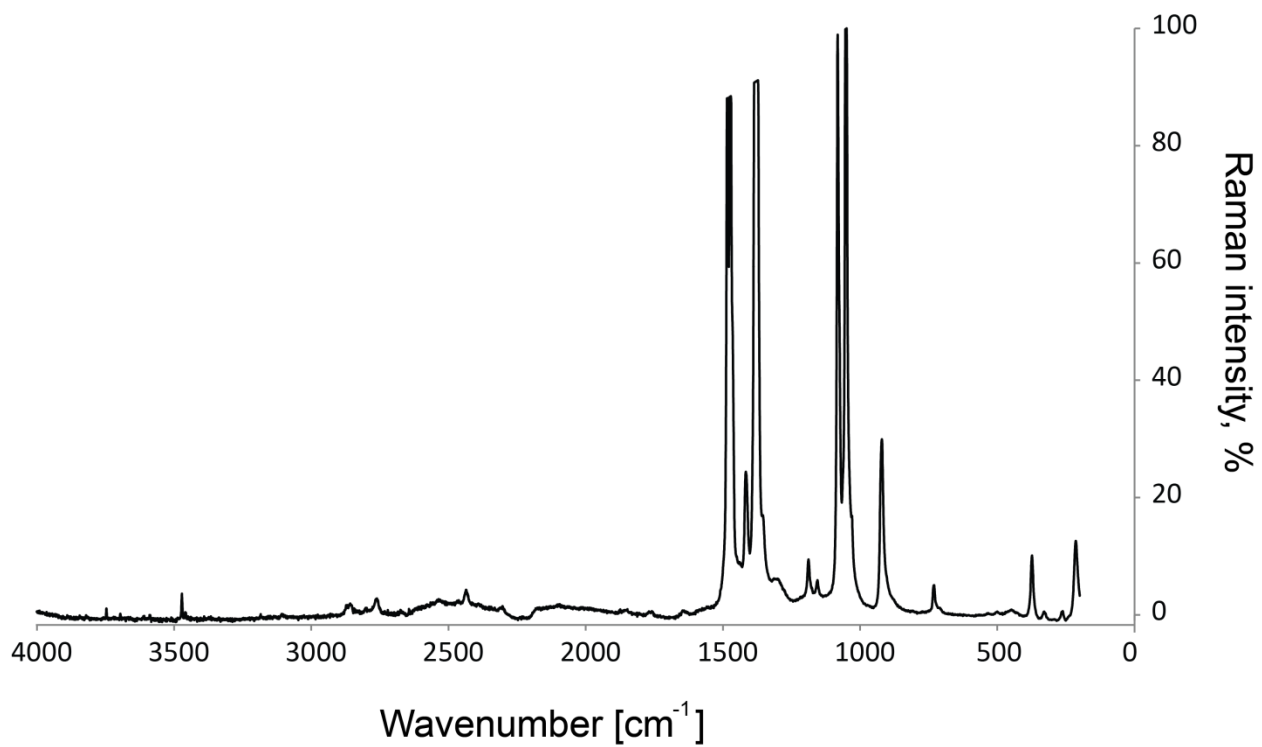
**Table S1:** Settings A, B and C of the Raman measurements

A	Filter D 0.3	1000 $\mu\text{m}$ hole	100 $\mu\text{m}$ slit	5 x 1 s
B	No filter	1000 $\mu\text{m}$ hole	250 $\mu\text{m}$ slit	1 x 10 s
C	No filter	1000 $\mu\text{m}$ hole	500 $\mu\text{m}$ slit	1 x 30 s

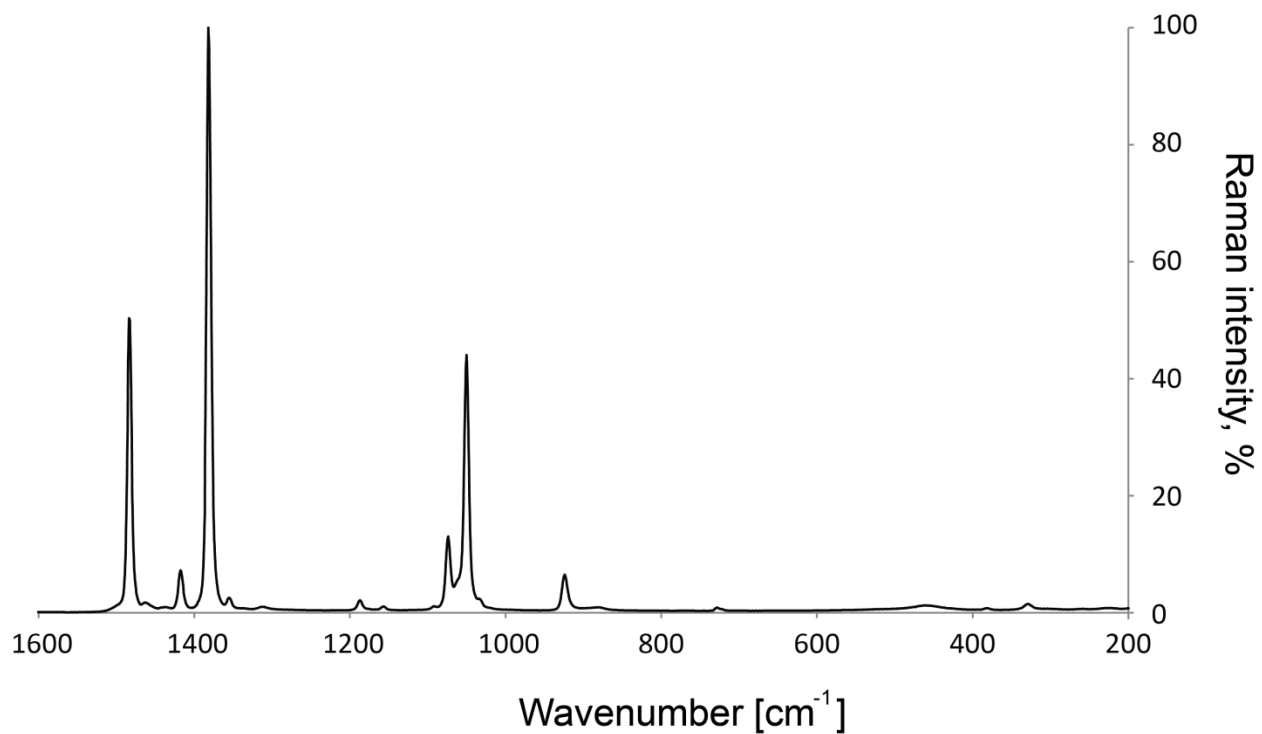
### IR Spectra of 1:



Raman Spectrum of **1**:



Raman Spectrum of **2**:



**Table S1.** Selected bond lengths (Å) and angles (°) of the ZT moiety as calculated and measured.

	B3LYP	Measured (XRD)
<i>Bond lengths</i>		
C1–N7	1.349	1.335(2)
C1–N10	1.349	1.335(2)
N7–N8	1.332	1.340(2)
N8–N9	1.339	1.318(2)
N9–N10	1.331	1.336(2)
N1–C1	1.402	1.410(2)
N1–N2	1.260	1.258(2)
N2–C2	1.402	1.409(2)
C2–N3	1.349	1.336(2)
C2–N6	1.349	1.330(2)
N3–N4	1.332	1.339(2)
N4–N5	1.339	1.322(2)
N5–N6	1.331	1.337(2)
<i>Bond angles</i>		
N7–C1–N10	111.5	112.8(1)
N7–C1–N1	129.4	128.9(1)
C1–N7–N8	104.6	103.7(1)
N7–N8–N9	109.7	109.8(1)
N8–N9–N10	109.3	109.8(1)
N9–N10–C1	104.9	104.0(1)
N10–C1–N1	119.1	118.3(1)
C1–N1–N2	115.7	112.5(1)

**Table S2.** IR and Raman frequencies of **(1)** and **(2)** vs. calculated values for **(2)** (in  $\text{cm}^{-1}$ ).

IR <b>(1)</b>	IR <b>(2)</b>	Calc. IR <b>(2)</b> B3LYP	Raman <b>(1)</b>	Raman <b>(2)</b>	Calc. Raman <b>(2)</b> B3LYP
1734			1479	1483	1538
1657			1475		
1620	1603		1417	1415	1406
	1453	1438	1381	1382	1362
1398	1401	1380		1182	1207
1365			1090	1146	1180
1216			1057	1073	1046
	1195	1206	919	1050	1033
1174	1162	1176		922	910
1093	1075	1042		374	370
1075	1052			324	308
1046	1041	1018			
	881				
	773	792			
	738	743			
	732				
641					
	426	443			
240					
216					
165	164				