# Supporting Information

## A "Green" High-initiation-power Primary Explosive: Synthesis, 3D Structure and Energetic Properties of Potassium 3,4-Bis(3-dinitromethylfurazan-4-oxy)furazan

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Table of Contents



## 1 X-ray crystallography

Band angles and dihedral of the data collection and refinement are given in Table S1.

Table S1. Selected bond lengths and bond angles for the compound $K_2$BDFOF

| | | | |
|---|---|---|---|
| K(1)-O(1) | 2.695(2) | O(1)-K(1)-O(2)#1 | 132.10(7) |
| K(1)-O(2)#1 | 2.711(2) | O(1)-K(1)-O(1)#2 | 87.87(6) |
| K(1)-O(1)#2 | 2.812(2) | O(2)#1-K(1)-O(1)#2 | 135.15(6) |
| K(1)-O(3) | 2.867(2) | O(1)-K(1)-O(3) | 55.19(5) |
| K(1)-O(3)#3 | 2.8944(19) | O(2)#1-K(1)-O(3) | 87.55(6) |
| K(1)-O(4)#3 | 2.963(2) | O(1)#2-K(1)-O(3) | 137.23(6) |
| K(1)-O(4)#4 | 3.021(2) | O(1)-K(1)-O(3)#3 | 110.87(6) |
| K(1)-N(3)#4 | 3.059(2) | O(2)#1-K(1)-O(3)#3 | 69.31(6) |
| K(1)-N(3)#5 | 3.235(3) | O(1)#2-K(1)-O(3)#3 | 120.72(6) |
| K(1)-N(1)#3 | 3.275(2) | O(3)-K(1)-O(3)#3 | 64.74(6) |
| N(1)-O(4) | 1.241(3) | O(1)-K(1)-O(4)#3 | 144.26(6) |
| N(1)-O(3) | 1.247(3) | O(2)#1-K(1)-O(4)#3 | 69.62(6) |
| N(1)-C(1) | 1.390(3) | O(1)#2-K(1)-O(4)#3 | 89.28(6) |
| N(2)-O(1) | 1.239(3) | O(3)-K(1)-O(4)#3 | 107.99(5) |
| N(2)-O(2) | 1.253(2) | O(3)#3-K(1)-O(4)#3 | 43.24(5) |
| N(2)-C(1) | 1.379(3) | O(1)-K(1)-O(4)#4 | 119.00(6) |
| N(3)-C(2) | 1.300(3) | O(2)#1-K(1)-O(4)#4 | 66.79(6) |
| N(3)-O(5) | 1.391(3) | O(1)#2-K(1)-O(4)#4 | 76.62(6) |
| N(3)-K(1)#6 | 3.059(2) | O(3)-K(1)-O(4)#4 | 137.25(6) |
| N(4)-C(3) | 1.284(3) | O(3)#3-K(1)-O(4)#4 | 127.90(6) |
| N(4)-O(5) | 1.373(3) | O(4)#3-K(1)-O(4)#4 | 94.82(6) |
| N(5)-C(4) | 1.290(4) | O(1)-K(1)-N(3)#4 | 65.67(6) |
| N(5)-O(7) | 1.390(3) | O(2)#1-K(1)-N(3)#4 | 110.44(7) |
| O(1)-K(1)#2 | 2.812(2) | O(1)#2-K(1)-N(3)#4 | 62.92(6) |
| O(2)-K(1)#7 | 2.711(2) | O(3)-K(1)-N(3)#4 | 110.70(6) |
| O(2)-K(1)#2 | 3.421(2) | O(3)#3-K(1)-N(3)#4 | 175.38(6) |
| O(6)-C(4) | 1.348(3) | O(4)#3-K(1)-N(3)#4 | 141.29(6) |
| O(6)-C(3) | 1.368(3) | O(4)#4-K(1)-N(3)#4 | 54.63(6) |
| O(7)-N(5)#8 | 1.390(3) | O(1)-K(1)-N(3)#5 | 61.60(6) |
| C(1)-C(2) | 1.457(3) | O(2)#1-K(1)-N(3)#5 | 147.62(6) |
| C(2)-C(3) | 1.421(3) | O(1)#2-K(1)-N(3)#5 | 61.98(6) |
| C(4)-C(4)#8 | 1.415(5) | O(3)-K(1)-N(3)#5 | 80.12(6) |

Symmetry transformations used to generate equivalent atoms: #1 x,y+1,z; #2 -x+2,-y+2,-z+1; #3 -x+3/2,-y+5/2,-z+1; #4 x+1/2,y+1/2,z; #5 -x+3/2,-y+3/2,-z+1; #6 x-1/2,y-1/2,z; #7 x,y-1,z; #8 -x+2,y,-z+3/2.

## 2 $^{1}$H and $^{13}$C NMR spectra

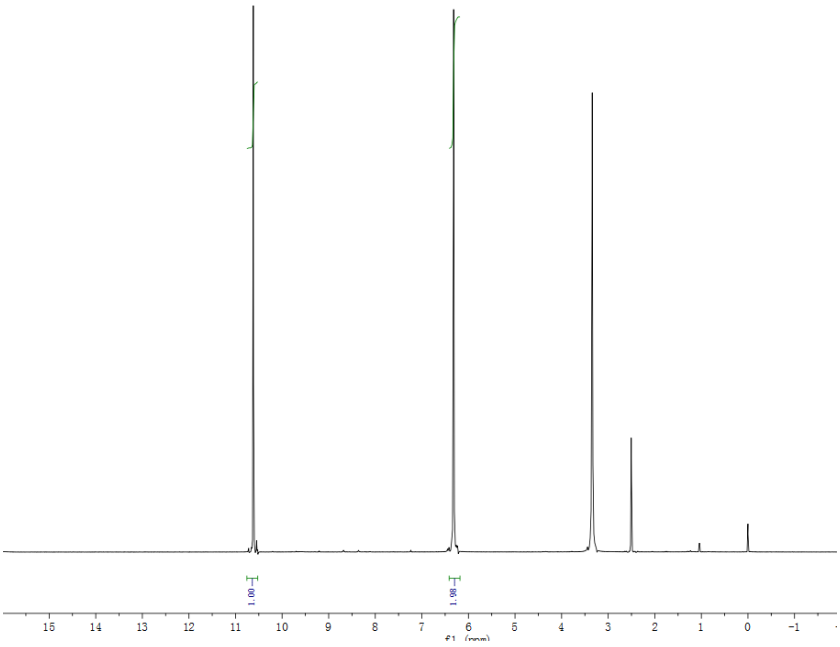


**Fig. S1** $^{1}$H NMR spectrum of **2** in DMSO-*d*6

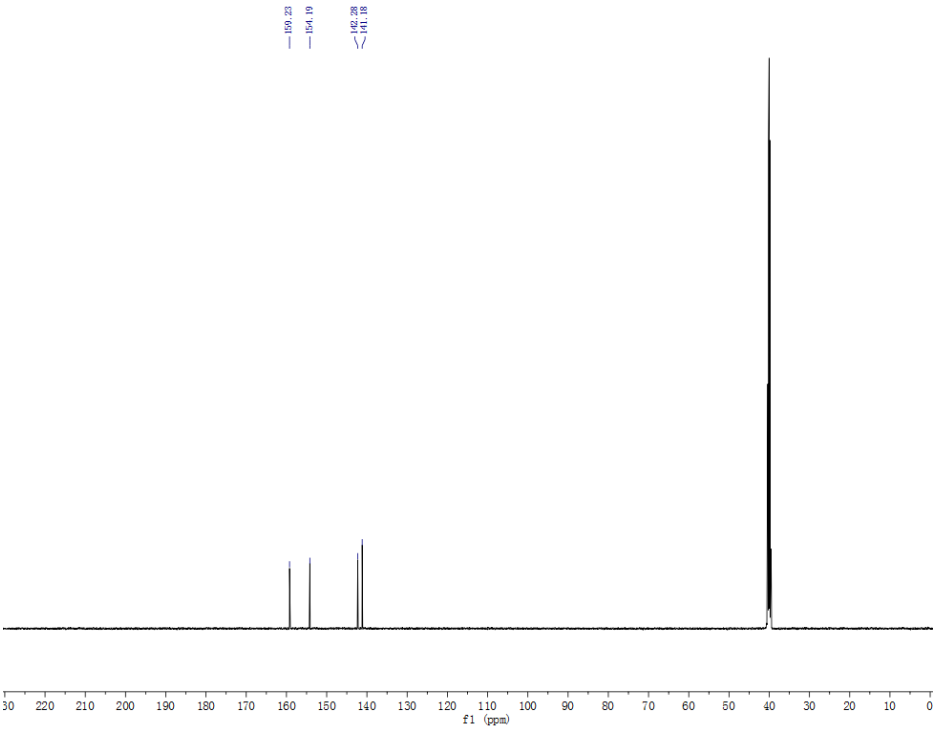


**Fig. S2** $^{13}$C NMR spectrum of **2** in DMSO-*d*6

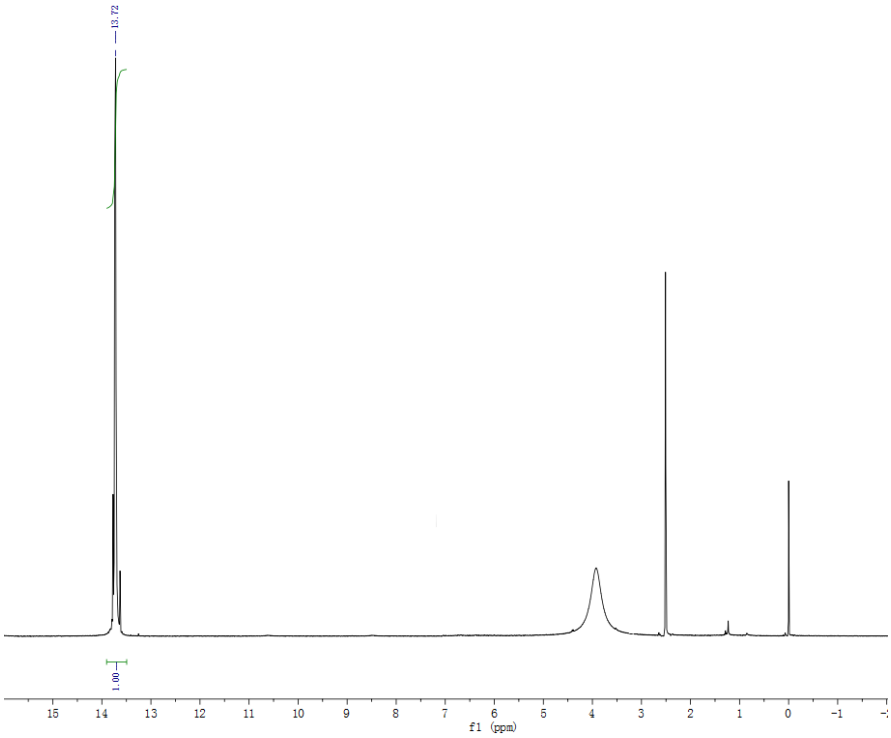


**Fig. S3** $^{1}$H NMR spectrum of **3** in DMSO-*d*6

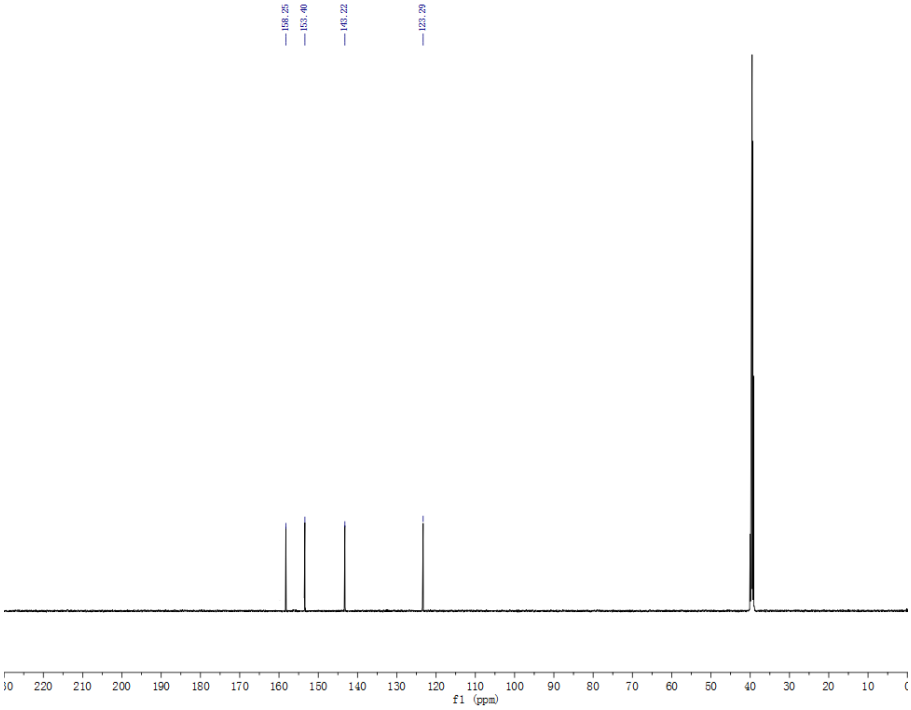


**Fig. S4** $^{13}$C NMR spectrum of **3** in DMSO-*d*6

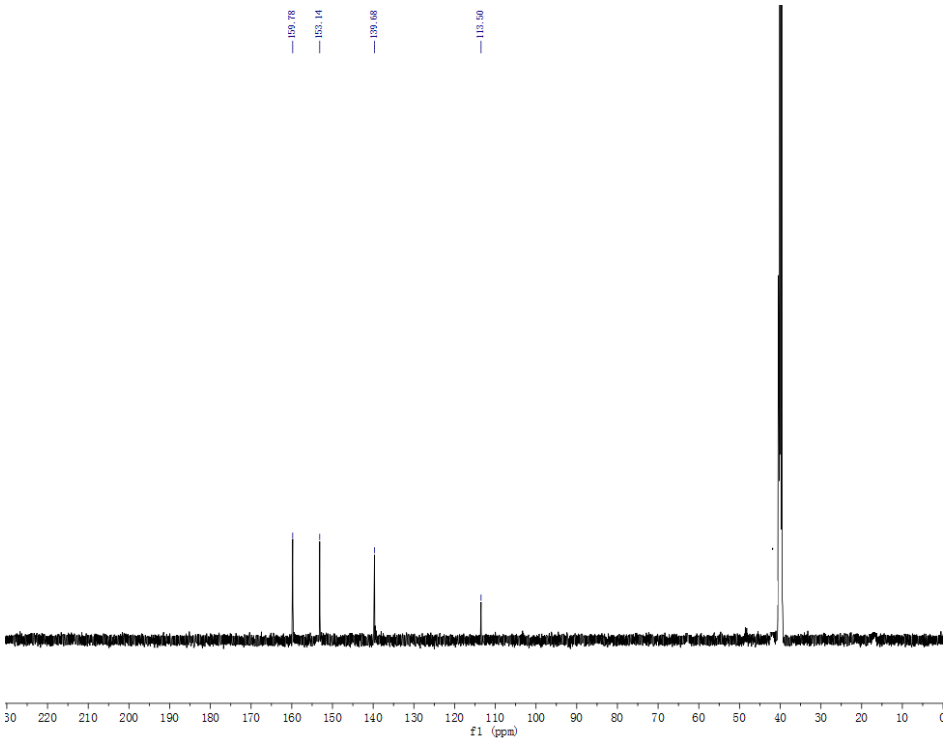


**Fig. S5** $^{13}$C NMR spectrum of **4** in DMSO-*d*6

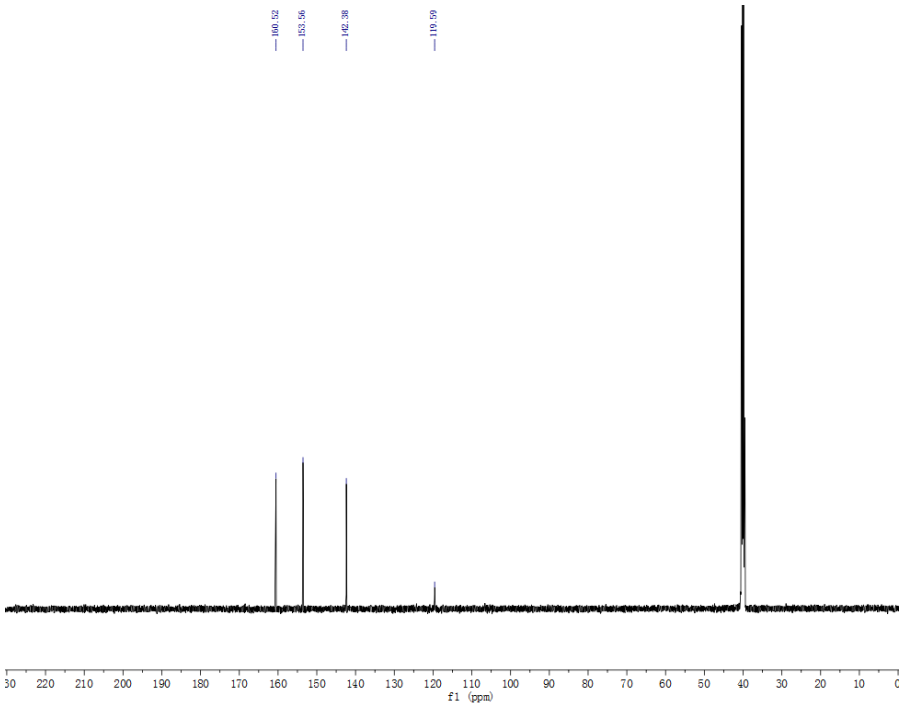


**Fig. S6** $^{13}$C NMR spectrum of $K_2$BDFOF in DMSO-*d*6