

## 3,4-二乙氧基苯甲酸与 2,2'-联吡啶三元稀土配合物的合成、 晶体结构及热化学性质

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## Synthesis, Crystal Structures and Thermochemical Properties of Ternary Rare Earth Complexes Based on 3,4-Diethoxybenzoic Acid and 2,2'-Bipyridine

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表 S1 配合物 1 的舒平摩尔热容和热力学函数值

Table S1 Smoothed values of  $C_{p,m}$  and thermodynamic functions of complex 1

| $T/K$  | $C_{p,m}/(\text{J mol}^{-1} \text{K}^{-1})$ | $(H_T-H_{298.15\text{K}})/(\text{kJ mol}^{-1})$ | $(S_T-S_{298.15\text{K}})/(\text{J mol}^{-1} \text{K}^{-1})$ | $(G_T-G_{298.15\text{K}})/(\text{kJ mol}^{-1})$ |
|--------|---|---|--|---|
| 258.15 | 2295.84                                     | -96.63  | -347.58  | -6.90   |
| 261.15 | 2314.28                                     | -89.71  | -320.94  | -5.90   |
| 264.15 | 2331.78                                     | -82.74  | -294.41  | -4.98   |
| 267.15 | 2348.98                                     | -75.72  | -267.98  | -4.13   |
| 270.15 | 2366.26                                     | -68.65  | -241.65  | -3.37   |
| 273.15 | 2383.77                                     | -61.52  | -215.42  | -2.68   |
| 276.15 | 2401.59                                     | -54.35  | -189.29  | -2.08   |
| 279.15 | 2419.67                                     | -47.11  | -163.24  | -1.55   |
| 282.15 | 2437.99                                     | -39.83  | -137.28  | -1.10   |
| 285.15 | 2456.48                                     | -32.49  | -111.39  | -0.72   |
| 288.15 | 2475.10                                     | -25.09  | -85.59   | -0.43   |
| 291.15 | 2493.82                                     | -17.64  | -59.85   | -0.21   |
| 294.15 | 2512.65                                     | -10.13  | -34.19   | -0.07   |
| 297.15 | 2531.60                                     | -2.56   | -8.60  | 0.004   |
| 300.15 | 2550.67                                     | 5.11  | 17.10  | -0.02   |
| 303.15 | 2569.90                                     | 12.80   | 42.56  | -0.11   |
| 306.15 | 2589.28                                     | 20.53   | 67.96  | -0.27   |
| 309.15 | 2608.78                                     | 28.33   | 93.30  | -0.51   |
| 312.15 | 2628.38                                     | 36.19   | 118.59   | -0.83   |
| 315.15 | 2647.97                                     | 44.10   | 143.83   | -1.23   |
| 318.15 | 2667.44                                     | 52.08   | 169.00   | -1.69   |
| 321.15 | 2686.66                                     | 60.11   | 194.13   | -2.24   |
| 324.15 | 2705.47                                     | 68.19   | 219.20   | -2.86   |
| 327.15 | 2723.73                                     | 76.34   | 244.21   | -3.55   |
| 330.15 | 2741.34                                     | 84.54   | 269.15   | -4.32   |
| 333.15 | 2758.26                                     | 92.79   | 294.02   | -5.17   |
| 336.15 | 2774.60                                     | 101.09  | 318.82   | -6.09   |
| 339.15 | 2790.64                                     | 109.43  | 343.55   | -7.08   |
| 342.15 | 2806.92                                     | 117.83  | 368.20   | -8.15   |

表 S2 配合物 2 的舒平摩尔热容和热力学函数值

Table S2 Smoothed values of  $C_{p,m}$  and thermodynamic functions of complex 2

| $T/K$  | $C_{p,m}/(\text{J mol}^{-1} \text{K}^{-1})$ | $(H_T-H_{298.15\text{K}})/(\text{kJ mol}^{-1})$ | $(S_T-S_{298.15\text{K}})/(\text{J mol}^{-1} \text{K}^{-1})$ | $(G_T-G_{298.15\text{K}})/(\text{kJ mol}^{-1})$ |
|--------|---|---|--|---|
| 258.15 | 2213.79                                     | -94.02  | -338.13  | -6.73   |
| 261.15 | 2237.97                                     | -87.34  | -312.41  | -5.75   |
| 264.15 | 2258.50                                     | -80.59  | -286.73  | -4.85   |
| 267.15 | 2277.62                                     | -73.79  | -261.11  | -4.03   |
| 270.15 | 2296.53                                     | -66.93  | -235.57  | -3.29   |
| 273.15 | 2315.80                                     | -60.01  | -210.11  | -2.62   |

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|--------|---------|--------|---------|-------|
| 276.15 | 2335.56 | -53.03 | -184.70 | -2.03 |
| 279.15 | 2355.72 | -46.00 | -159.36 | -1.51 |
| 282.15 | 2376.08 | -38.90 | -134.07 | -1.07 |
| 285.15 | 2396.45 | -31.74 | -108.83 | -0.71 |
| 288.15 | 2416.64 | -24.52 | -83.64  | -0.42 |
| 291.15 | 2436.56 | -17.24 | -58.51  | -0.21 |
| 294.15 | 2456.13 | -9.90  | -33.43  | -0.07 |
| 297.15 | 2475.37 | -2.50  | -8.41   | 0.00  |
| 300.15 | 2494.30 | 5.00   | 16.72   | -0.02 |
| 303.15 | 2512.97 | 12.51  | 41.62   | -0.10 |
| 306.15 | 2531.42 | 20.08  | 66.45   | -0.27 |
| 309.15 | 2549.69 | 27.70  | 91.23   | -0.50 |
| 312.15 | 2567.80 | 35.38  | 115.94  | -0.81 |
| 315.15 | 2585.74 | 43.11  | 140.58  | -1.20 |
| 318.15 | 2603.50 | 50.89  | 165.17  | -1.66 |
| 321.15 | 2621.08 | 58.73  | 189.68  | -2.19 |
| 324.15 | 2638.50 | 66.62  | 214.14  | -2.79 |
| 327.15 | 2655.79 | 74.56  | 238.52  | -3.47 |
| 330.15 | 2673.05 | 82.55  | 262.84  | -4.23 |
| 333.15 | 2690.41 | 90.60  | 287.10  | -5.05 |
| 336.15 | 2708.02 | 98.70  | 311.30  | -5.95 |
| 339.15 | 2726.04 | 106.85 | 335.44  | -6.92 |
| 342.15 | 2744.51 | 115.05 | 359.53  | -7.96 |

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