

## Supporting Information

Sulfur-Bridged Ta–M (M = Mo, Cr) Multinuclear Complexes Bearing a Four-Electron-Reduced Dinitrogen Ligand

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## Experimental

**General Procedures.** All manipulations were performed using a glove box under an atmosphere of oxygen-free dry argon or standard Schlenk techniques under argon. Dried solvents were purchased from Nacalai Tesque, Inc. or Kanto Chemical Co., Inc., and were purified by passing through a column of activated alumina under an inert atmosphere in a glove box. The compounds [Cp\*TaCl<sub>4</sub>] and KC<sub>8</sub> were prepared according to literature procedures.<sup>1,2</sup> NMR spectra were recorded on a JEOL Lambda 300, a JEOL Lambda 400, or a Bruker AVANCE 300 FT-NMR spectrometer at room temperature. IR spectra were recorded on a JASCO FT/IR-6200 spectrometer with an attenuated total reflection (ATR) accessory. Elemental analyses were performed by the Analytical Research Service Center at Osaka City University on J-SCIENCE LAB JM10 or FISOONS Instrument EA1108 elemental analyzers. Photolysis was carried out using an Ushio UM-452 450W high-pressure Hg lamp placed in a water-cooled quartz jacket.

**Synthesis of [Cp\*Ta(SC<sub>6</sub>H<sub>4</sub>Me)<sub>2</sub>]<sub>2</sub>(μ-η<sup>1</sup>:η<sup>1</sup>-N<sub>2</sub>) (1).** [Cp\*TaCl<sub>4</sub>] (183 mg, 0.400 mmol), di-*p*-tolyl disulfide (99 mg, 0.40 mmol), and KC<sub>8</sub> (270 mg, 2.00 mmol) were placed in a glass tube with a Teflon valve, and then THF (10 mL) was added via vacuum transfer at -196 °C. The glass tube was filled with dinitrogen at -196 °C, and sealed. The sample was allowed to warm to -78 °C, and stirred for 2 h. The reaction mixture was allowed to warm to 0 °C and stirred overnight at 0 °C. The resulting dark brown suspension was warmed to room temperature and filtered through Celite, followed by removal of the solvent to yield a brown oil. A small amount of hexane was added to the brown oil to cause precipitation of a red powder. The powder was washed with hexane, and then recrystallized from THF/hexane to afford red crystals of **1** (83 mg, 18%). Anal. Calcd for C<sub>48</sub>H<sub>58</sub>N<sub>2</sub>S<sub>4</sub>Ta<sub>2</sub>: C, 49.99; H, 5.07; N, 2.43. Found: C, 50.32; H, 5.17; N, 2.42. <sup>1</sup>H NMR (300 MHz, C<sub>6</sub>D<sub>6</sub>): δ 1.99 (s, 30H, C<sub>5</sub>Me<sub>5</sub>), 2.14 (s, 12H, SC<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>), 6.97 (d, 8H, *J* = 8.0 Hz, SC<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>), 7.75 (d, 8H, *J* = 8.0 Hz, SC<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>). IR (ATR, cm<sup>-1</sup>): 2910 (m), 1485 (s), 1377 (m), 1082 (m), 1016 (m), 876 (s), 804 (s). The <sup>1</sup>H NMR and IR spectra of **1** are shown in Figures S1 and S3, respectively.

**Synthesis of [Cp\*Ta(μ-SC<sub>6</sub>H<sub>4</sub>Me)<sub>2</sub>Mo(CO)<sub>4</sub>]<sub>2</sub>(μ-η<sup>1</sup>:η<sup>1</sup>-N<sub>2</sub>)·C<sub>6</sub>H<sub>6</sub> (2).** A glass tube with a Teflon valve was charged with **1** (17 mg, 0.015 mmol), [Mo(CO)<sub>6</sub>] (8 mg, 0.030 mmol), and benzene (7 mL). The tube was sealed, and then the red suspension was irradiated with a high-pressure Hg lamp for 3 h, during which time red-brown crystals appeared. The red-brown crystals were collected and washed several times with THF to give red crystals of **2** (10 mg, 42%). Anal. Calcd for C<sub>62</sub>H<sub>64</sub>Mo<sub>2</sub>N<sub>2</sub>O<sub>8</sub>S<sub>4</sub>Ta<sub>2</sub>: C, 45.21; H, 3.92; N, 1.70; Found: C, 45.74; H, 3.89; N, 1.69. Benzene as a solvent of crystallization was removed under high vacuum. Anal. Calcd for C<sub>56</sub>H<sub>58</sub>Mo<sub>2</sub>N<sub>2</sub>O<sub>8</sub>S<sub>4</sub>Ta<sub>2</sub>: C, 42.87; H, 3.73; N, 1.79; Found: C, 43.59; H, 3.67; N, 1.71. IR (ATR, cm<sup>-1</sup>): 2910 (m), 2019 (s, ν<sub>CO</sub>), 1936 (m, ν<sub>CO</sub>), 1890 (s, ν<sub>CO</sub>), 1487 (m), 1375 (m), 1016 (m), 843 (s), 806 (s), 599 (s), 573 (s). The IR spectrum of **2** is shown in Figure S3.

**NMR Experiments for the Reaction of 1 with [Mo(CO)<sub>6</sub>].** An NMR tube with a Teflon valve was charged with **1** (7 mg, 0.006 mmol), [Mo(CO)<sub>6</sub>] (3 mg, 0.01 mmol), and benzene-*d*<sub>6</sub> (0.5 mL). The red suspension was irradiated with a high-pressure Hg lamp, and <sup>1</sup>H NMR measurements were performed. The <sup>1</sup>H NMR spectra are shown in Figure 4. The new species was assigned to the Ta<sub>2</sub>Mo trinuclear complex [Cp\*Ta(μ-SC<sub>6</sub>H<sub>4</sub>Me)<sub>2</sub>Mo(CO)<sub>4</sub>](μ-η<sup>1</sup>:η<sup>1</sup>-N<sub>2</sub>)[Cp\*Ta(SC<sub>6</sub>H<sub>4</sub>Me)<sub>2</sub>] (**4**). <sup>1</sup>H NMR (300 MHz, C<sub>6</sub>D<sub>6</sub>): δ 1.61 (s, 15H, C<sub>5</sub>Me<sub>5</sub>), 1.90 (s, 15H, C<sub>5</sub>Me<sub>5</sub>), 2.07 (s, 12H, SC<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>),

6.81 (4H, d,  $J = 8.0$  Hz,  $SC_6H_4CH_3$ ), 7.11 (4H, d,  $J = 8.0$  Hz,  $SC_6H_4CH_3$ ) 7.76 (4H, d,  $J = 8.0$  Hz,  $SC_6H_4CH_3$ ), 7.88 (4H, d,  $J = 8.0$  Hz,  $SC_6H_4CH_3$ ).

**Synthesis of  $[Cp^*Ta(\mu-SC_6H_4Me)_2Cr(CO)_4]_2(\mu-\eta^1:\eta^1-N_2)\cdot C_6H_6$  (**3**).** A glass tube with a Teflon valve was charged with **1** (17 mg, 0.015 mmol),  $[Cr(CO)_6]$  (7 mg, 0.03 mmol), and benzene (7 mL). The tube was sealed, and then the red suspension was irradiated with a high-pressure Hg lamp for 15 h, during which time red-brown crystals appeared. The red-brown crystals were collected and washed several times with toluene to give red crystals of **3** (10 mg, 45%). Elemental analysis of the sample, which was dried under high vacuum, showed the presence of cocrystallized  $[Cr(CO)_6]$ . Anal. Calcd for  $C_{56}H_{58}Cr_2N_2O_8S_4Ta_2 \cdot 0.4Cr(CO)_6$ : C, 44.70; H, 3.73; N, 1.79; Found: C, 44.40; H, 3.86; N, 1.85. IR (ATR,  $cm^{-1}$ ): 2910 (m), 2010 (s,  $\nu_{CO}$ ), 1930 (m,  $\nu_{CO}$ ), 1886 (s,  $\nu_{CO}$ ), 1488 (m), 1375 (m), 1016 (m), 843 (s), 807 (s), 676 (m), 655 (s), 623 (s). The IR spectrum of **3** is shown in Figure S3.

The residue obtained from the mother liquid and washings was recrystallized from toluene–hexane to afford a small amount of red crystals of  $[Cp^*Ta(\mu-SC_6H_4Me)_2Cr(CO)_4](\mu-\eta^1:\eta^1-N_2)[Cp^*Ta(SC_6H_4Me)_2]$  (**5**).

**NMR Experiments for the Reaction of **1** with  $[Cr(CO)_6]$ .** An NMR tube with a Teflon valve was charged with **1** (5 mg, 0.004 mmol),  $[Cr(CO)_6]$  (2 mg, 0.009 mmol), and benzene- $d_6$  (0.5 mL). The red suspension was irradiated with a high-pressure Hg lamp, and  $^1H$  NMR measurements were performed. The  $^1H$  NMR spectrum after irradiation for 30 min is shown in Figure S2. The new species was assigned to the  $Ta_2Cr$  trinuclear complex  $[Cp^*Ta(\mu-SC_6H_4Me)_2Cr(CO)_4](\mu-\eta^1:\eta^1-N_2)-[Cp^*Ta(SC_6H_4Me)_2]$  (**5**).  $^1H$  NMR (300 MHz,  $C_6D_6$ ):  $\delta$  1.68 (s, 15H,  $C_5Me_5$ ), 1.89 (s, 15H,  $C_5Me_5$ ), 2.04 (s, 6H,  $SC_6H_4CH_3$ ), 2.06 (s, 6H,  $SC_6H_4CH_3$ ), 6.77 (d, 4H,  $J = 8.0$  Hz,  $SC_6H_4CH_3$ ), 7.14 (d, 4H,  $J = 8.0$  Hz,  $SC_6H_4CH_3$ ) 7.75 (d, 4H,  $J = 8.0$  Hz,  $SC_6H_4CH_3$ ), 7.93 (d, 4H,  $J = 8.0$  Hz,  $SC_6H_4CH_3$ ).

**X-Ray Crystal Structure Determination of **1**, **2**, **3**, and **5**.** A single crystal of **1**, **2**, **3**, or **5** was mounted on a glass fiber. The diffraction data were collected on an AFC7/CCD Mercury diffractometer using the rotation method with  $0.5^\circ$  frame width and with 10 s exposure time per frame. The data were processed and corrected for Lorentz and polarization effects using CrystalClear software.<sup>3</sup> The analyses were carried out using the CrystalStructure 3.8 crystallographic software package.<sup>4</sup> Absorption corrections were applied using the Multi Scan method. The structures were solved using direct methods (SIR92<sup>5</sup> for **1** and **3**, SHELXS97<sup>6</sup> for **2**, SIR97<sup>7</sup> for **5**)

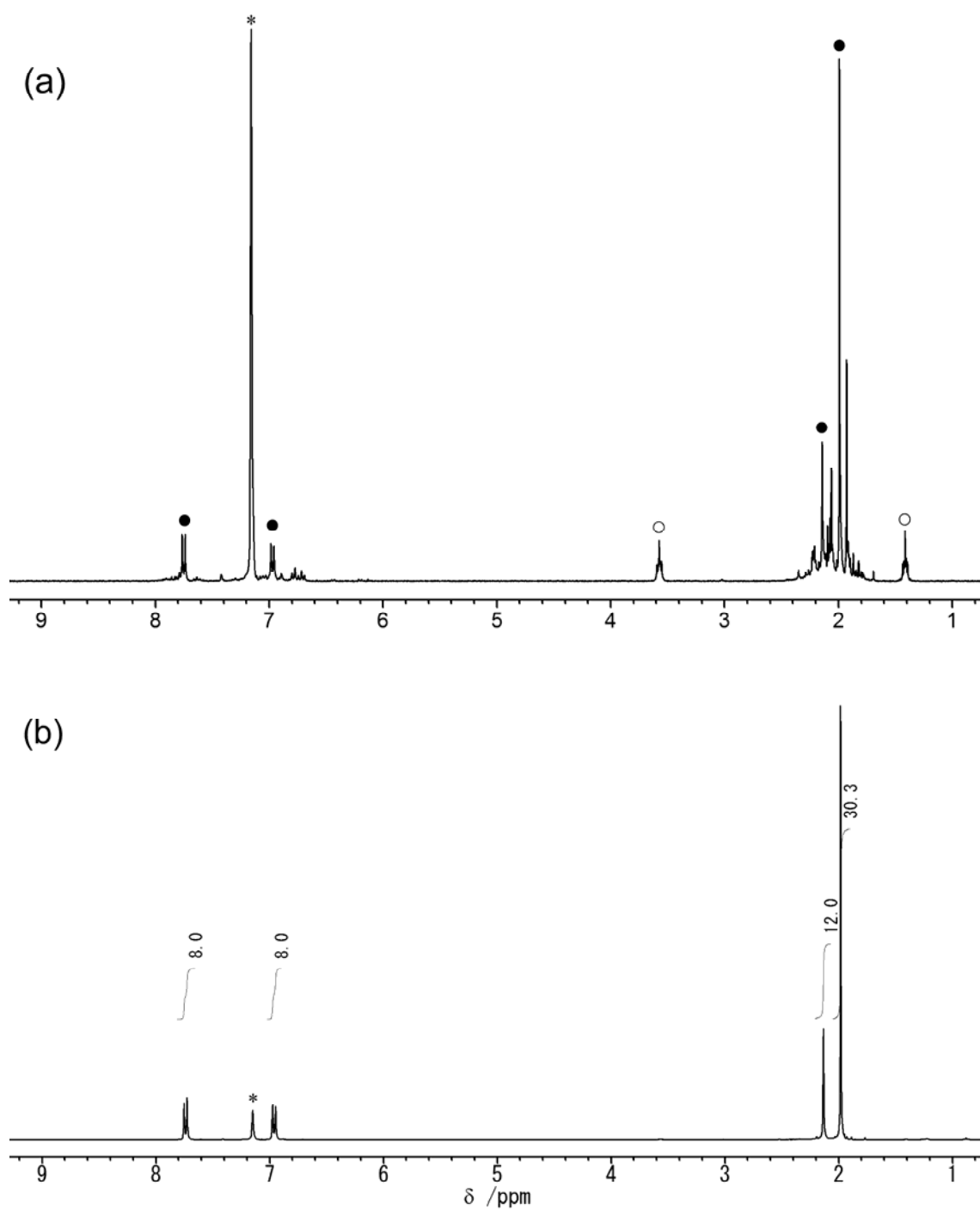
and refined by full-matrix least-squares on  $F^2$  using SHELXL.<sup>6</sup> Crystallographic data are summarized in Table S1. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were located on calculated positions with C–H(aromatic) = 0.95 Å and C–H(methyl) = 0.98 Å, and were refined using a riding model with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

**Computational details.** Structures of complexes **1**, **2**, and **5** were optimized using the Gaussian 03 program package.<sup>8</sup> The B3LYP density functional method and the LANL2DZ basis set were used for the calculations. The initial models were obtained from the crystal structures determined in this work. The optimized structures of **1**, **2**, and **5** are shown in Figures S8, S10, and S12, respectively, and the molecular coordinates are listed in Tables S6, S7, and S8. Molecular orbitals for the optimized structures are depicted in Figures S9, S11, and S13.

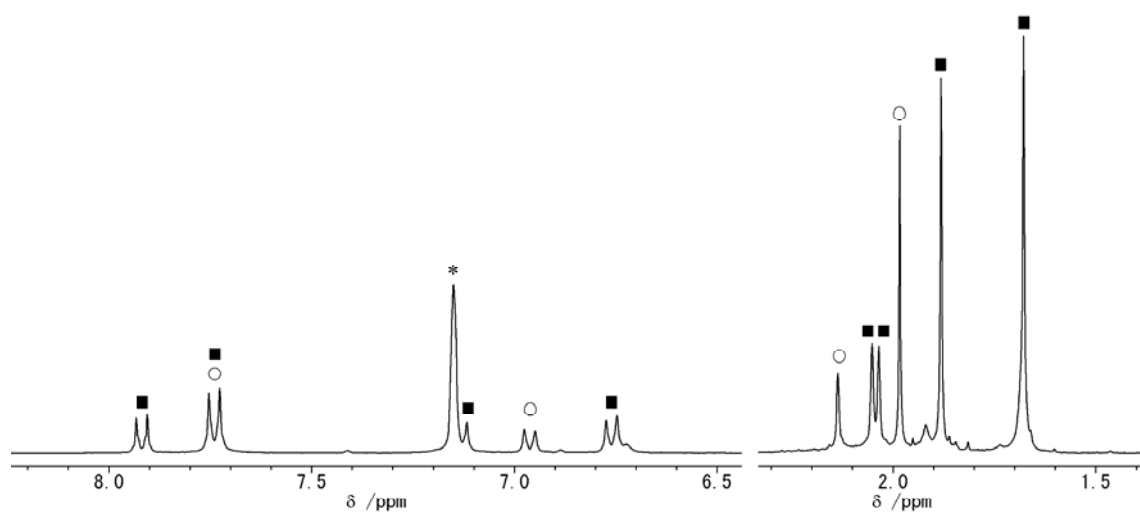
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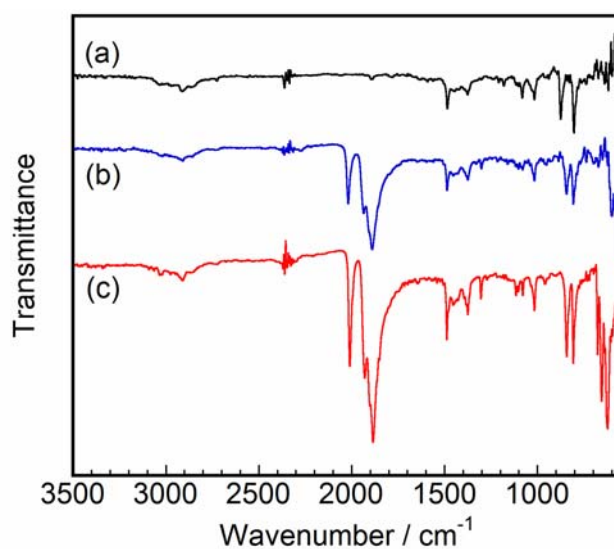
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**Figure S1.** <sup>1</sup>H NMR spectra (300 MHz) of (a) the crude reaction mixture of complex **1** and (b) isolated **1** in  $C_6D_6$ . Solid and open circles in (a) denote signals of **1** and THF, respectively. A residual solvent signal is marked with an asterisk.



**Figure S2.**  $^1\text{H}$  NMR spectrum of the photochemical reaction of **1** with  $[\text{Cr}(\text{CO})_6]$  in  $\text{C}_6\text{D}_6$  after irradiation for 30 min. Signals for complex **1** are denoted by  $\circ$ , those for complex **5** by  $\blacksquare$ , and those for residual solvent signals by  $*$ .

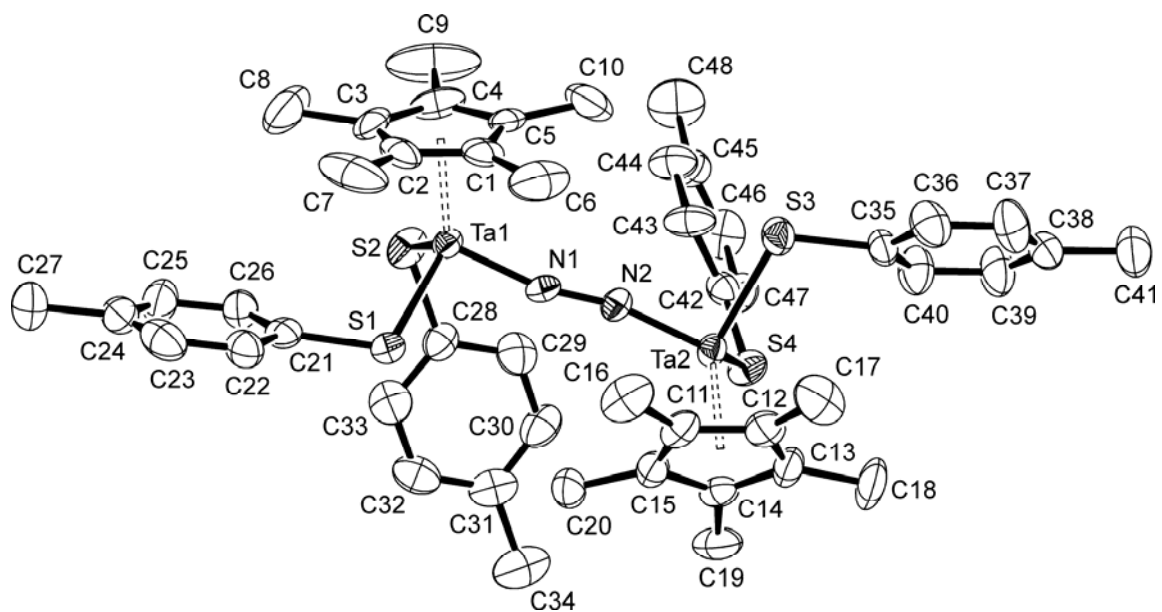


**Figure S3.** IR spectra of complexes (a) **1** (black spectrum), (b) **2** (blue spectrum), and (c) **3** (red spectrum).

**Table S1.** Crystallographic data for **1**, **2**, **3**, and **5**

	<b>1</b>	<b>2</b>	<b>3</b>	<b>5</b>
Empirical formula	C <sub>48</sub> H <sub>58</sub> N <sub>2</sub> S <sub>4</sub> Ta <sub>2</sub>	C <sub>62</sub> H <sub>64</sub> Mo <sub>2</sub> N <sub>2</sub> O <sub>8</sub> S <sub>4</sub> Ta <sub>2</sub>	C <sub>62</sub> H <sub>64</sub> Cr <sub>2</sub> N <sub>2</sub> O <sub>8</sub> S <sub>4</sub> Ta <sub>2</sub>	C <sub>52</sub> H <sub>58</sub> CrN <sub>2</sub> O <sub>4</sub> S <sub>4</sub> Ta <sub>2</sub>
Formula weight	1153.14	1647.21	1559.32	1317.17
Temperature/K	193	193	193	193
Wavelength/Å	0.71070	0.71075	0.71075	0.71075
Crystal system	monoclinic	triclinic	triclinic	monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>a</i>	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>a</i> /Å	14.647(2)	12.085(2)	12.0474(10)	15.1344(9)
<i>b</i> /Å	16.757(2)	12.083(2)	12.0476(10)	21.6161(10)
<i>c</i> /Å	19.581(3)	13.180(2)	13.1510(11)	16.7735(9)
$\alpha$ /°	90	109.8845(18)	112.9333(10)	90
$\beta$ /°	90.797(4)	112.865(2)	110.0577(7)	109.6084(14)
$\gamma$ /°	90	101.8279(17)	101.5447(13)	90
<i>V</i> /Å <sup>3</sup>	4805.6(12)	1536.2(5)	1523.4(2)	5169.2(5)
<i>Z</i>	4	1	1	4
<i>D</i> <sub>calcd</sub> /Mg·m <sup>-3</sup>	1.594	1.780	1.700	1.692
$\mu$ (Mo K $\alpha$ )/mm <sup>-1</sup>	4.751	4.133	4.113	4.630
<i>F</i> (000)	2280	808	772	2600
Crystal size/mm <sup>3</sup>	0.16 × 0.07 × 0.06	0.17 × 0.07 × 0.04	0.20 × 0.14 × 0.09	0.15 × 0.13 × 0.04
Reflections collected	46301	14746	14657	48958
Independent reflections	10782 ( <i>R</i> <sub>int</sub> = 0.066)	6568 ( <i>R</i> <sub>int</sub> = 0.045)	6467 ( <i>R</i> <sub>int</sub> = 0.021)	11632 ( <i>R</i> <sub>int</sub> = 0.041)
Completeness to $\theta$	97.8% ( $\theta$ = 27.48°)	95.0% ( $\theta$ = 25.0°)	94.4% ( $\theta$ = 25.0°)	98.1% ( $\theta$ = 27.48°)
Max. and min. transmission	0.7634 and 0.5165	0.8519 and 0.5397	0.7082 and 0.4930	0.8363 and 0.5431
No. of data/restraints/params	10782/0/506	6568/0/362	6467/0/362	11632/0/587
Goodness of fit on <i>F</i> <sup>2</sup>	1.145	1.045	1.056	1.119
Final <i>R</i> indices [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	<i>R</i> 1 = 0.0605	<i>R</i> 1 = 0.0472	<i>R</i> 1 = 0.0267	<i>R</i> 1 = 0.0411
<i>R</i> indices (all data)	w <i>R</i> 2 = 0.1027	w <i>R</i> 2 = 0.0936	w <i>R</i> 2 = 0.0581	w <i>R</i> 2 = 0.1011
Largest diff. peak and hole (e <sup>-</sup> ·Å <sup>-3</sup> )	0.94 and -0.81	2.11 and -1.31	1.43 and -0.84	2.50 and -1.77

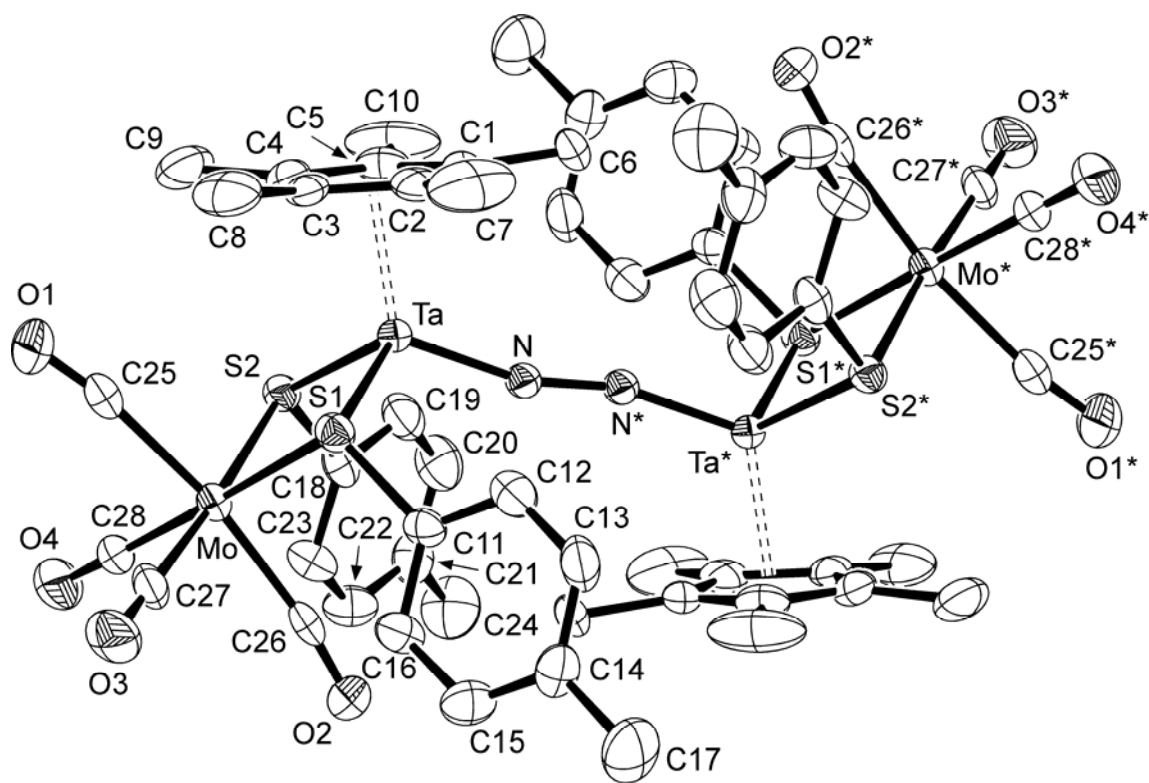




**Figure S4.** ORTEP drawing of **1** with thermal ellipsoids at the 50% probability level. Hydrogen atoms are omitted for clarity.

**Table S2.** Selected bond lengths/Å and angles/° for **1**

Ta(1)–S(1)	2.3916(18)	Ta(2)–S(3)	2.393(2)
Ta(1)–S(2)	2.401(2)	Ta(2)–S(4)	2.4007(18)
Ta(1)–N(1)	1.813(5)	Ta(2)–N(2)	1.814(5)
Ta(1)–C(1)	2.337(7)	Ta(2)–C(11)	2.362(7)
Ta(1)–C(2)	2.438(7)	Ta(2)–C(12)	2.439(7)
Ta(1)–C(3)	2.479(7)	Ta(2)–C(13)	2.479(7)
Ta(1)–C(4)	2.437(8)	Ta(2)–C(14)	2.441(7)
Ta(1)–C(5)	2.380(7)	Ta(2)–C(15)	2.395(7)
S(1)–C(21)	1.788(7)	S(3)–C(35)	1.799(6)
S(2)–C(28)	1.790(7)	S(4)–C(42)	1.774(7)
N(1)–N(2)	1.281(7)		
Ta(1)···Ta(2)	4.8793(3)		
S(1)–Ta(1)–S(2)	110.07(6)	S(3)–Ta(2)–S(4)	107.35(6)
S(1)–Ta(1)–N(1)	94.75(17)	S(3)–Ta(2)–N(2)	94.28(18)
S(2)–Ta(1)–N(1)	101.97(17)	S(4)–Ta(2)–N(2)	105.54(17)
Ta(1)–S(1)–C(21)	109.9(2)	Ta(2)–S(3)–C(35)	110.8(2)
Ta(1)–S(2)–C(28)	98.7(2)	Ta(2)–S(4)–C(42)	112.7(2)
Ta(1)–N(1)–N(2)	166.9(4)	Ta(2)–N(2)–N(1)	165.8(4)



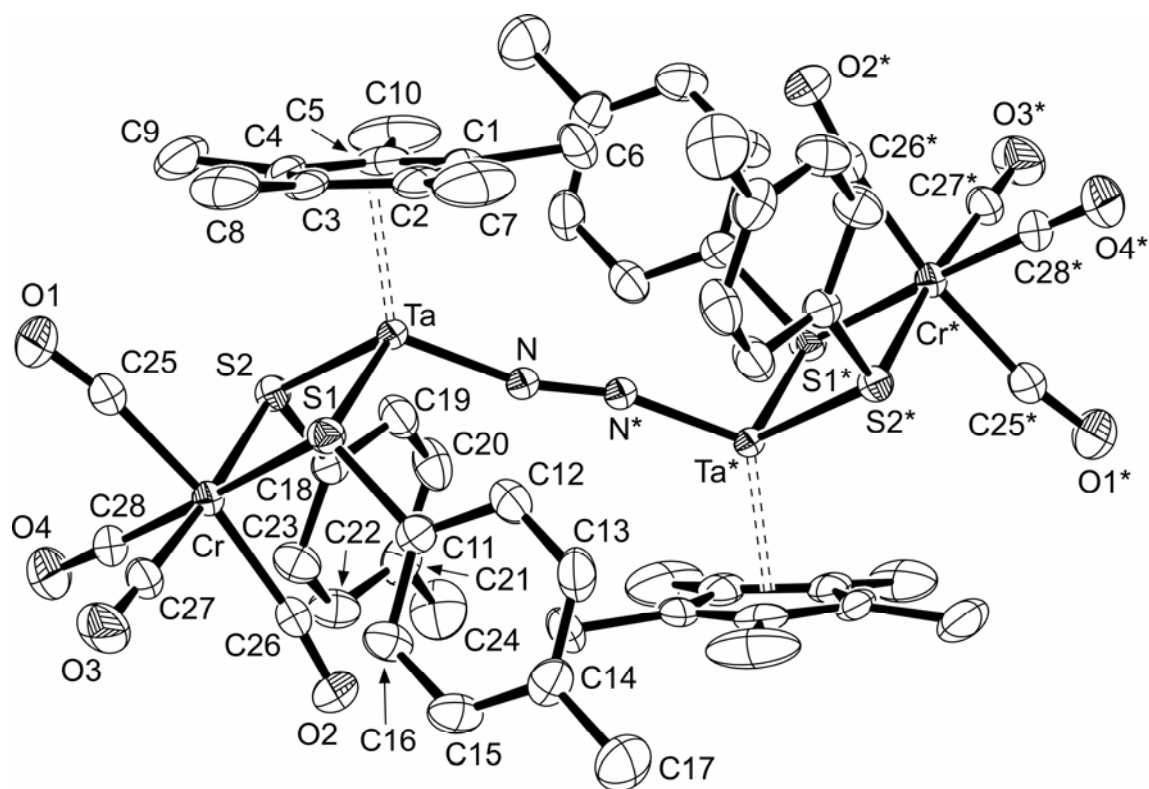
**Figure S5.** ORTEP drawing of **2** with thermal ellipsoids at the 50% probability level. Hydrogen atoms are omitted for clarity.

**Table S3.** Selected bond lengths/Å and angles/° for **2**

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Ta(1)–S(1)	2.438(2)	Mo(1)–S(1)	2.5494(16)
Ta(1)–S(2)	2.4363(15)	Mo(1)–S(2)	2.551(2)
Ta(1)–N(1)	1.826(6)	Mo(1)–C(25)	2.033(10)
Ta(1)–C(1)	2.359(6)	Mo(1)–C(26)	2.054(7)
Ta(1)–C(2)	2.396(5)	Mo(1)–C(27)	1.981(9)
Ta(1)–C(3)	2.481(7)	Mo(1)–C(28)	1.976(7)
Ta(1)–C(4)	2.497(8)	O(1)–C(25)	1.143(13)
Ta(1)–C(5)	2.392(9)	O(2)–C(26)	1.146(9)
S(1)–C(11)	1.799(9)	O(3)–C(27)	1.142(12)
S(2)–C(18)	1.793(6)	O(4)–C(28)	1.155(9)
N(1)–N(1)*	1.308(9)		
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Ta(1)···Ta(1)*	4.9245(4)	Ta(1)···Mo(1)	3.2018(6)
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S(1)–Ta(1)–S(2)	103.24(6)	S(2)–Mo(1)–C(27)	176.3(2)
S(1)–Ta(1)–N(1)	107.5(2)	S(2)–Mo(1)–C(28)	85.7(2)
S(2)–Ta(1)–N(1)	107.41(14)	C(25)–Mo(1)–C(26)	171.3(3)
Ta(1)–S(1)–C(11)	116.1(2)	C(25)–Mo(1)–C(27)	85.7(4)
Ta(1)–S(2)–C(18)	115.8(2)	C(25)–Mo(1)–C(28)	85.9(3)
Ta(1)–N(1)–N(1)*	164.6(4)	C(26)–Mo(1)–C(27)	88.2(3)
S(1)–Mo(1)–S(2)	97.03(6)	C(26)–Mo(1)–C(28)	88.0(3)
S(1)–Mo(1)–C(25)	91.9(2)	C(27)–Mo(1)–C(28)	91.5(3)
S(1)–Mo(1)–C(26)	93.91(18)	Ta(1)–S(1)–Mo(1)	79.85(6)
S(1)–Mo(1)–C(27)	85.70(19)	Mo(1)–S(1)–C(11)	114.19(17)
S(1)–Mo(1)–C(28)	176.6(2)	Ta(1)–S(2)–Mo(1)	79.85(6)
S(2)–Mo(1)–C(25)	91.7(3)	Mo(1)–S(2)–C(18)	114.0(3)
S(2)–Mo(1)–C(26)	94.1(2)		

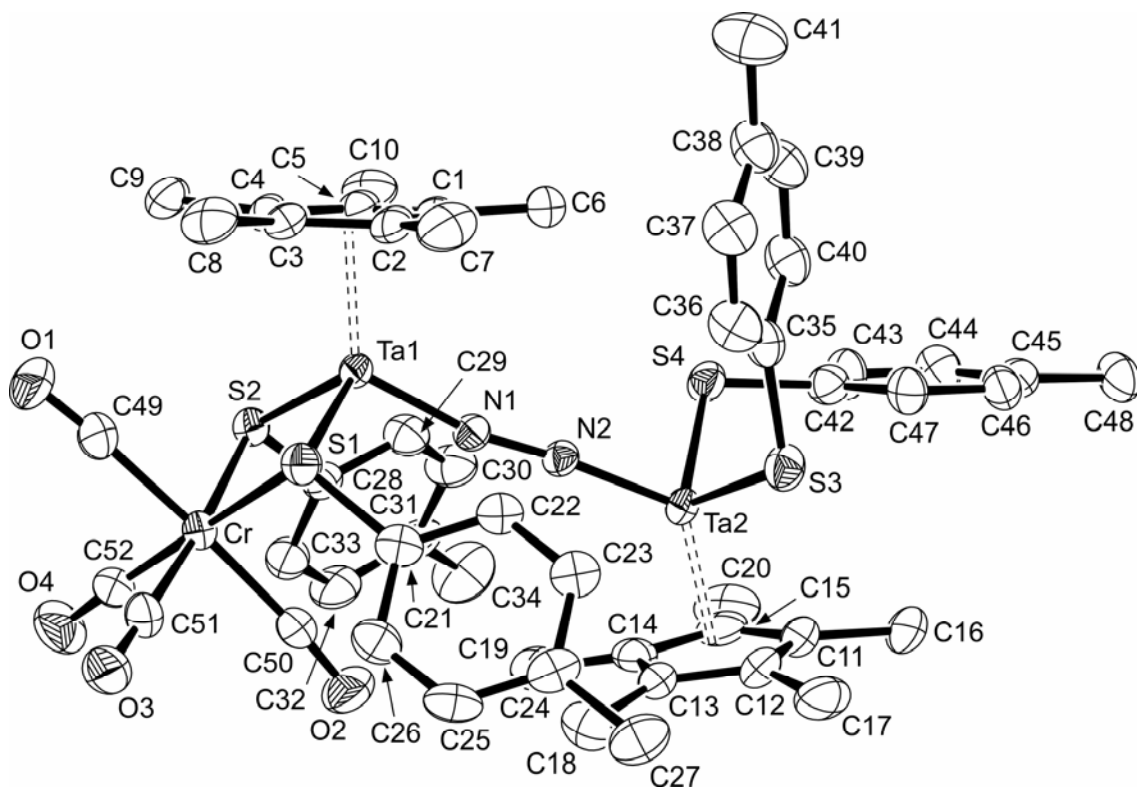
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**Figure S6.** ORTEP drawing of **3** with thermal ellipsoids at the 50% probability level. Hydrogen atoms are omitted for clarity.

**Table S4.** Selected bond lengths/Å and angles/° for **3**

Ta(1)–S(1)	2.4279(6)	Cr(1)–S(1)	2.4388(13)
Ta(1)–S(2)	2.4288(11)	Cr(1)–S(2)	2.4385(8)
Ta(1)–N(1)	1.833(3)	Cr(1)–C(25)	1.891(4)
Ta(1)–C(1)	2.373(3)	Cr(1)–C(26)	1.921(3)
Ta(1)–C(2)	2.394(4)	Cr(1)–C(27)	1.856(3)
Ta(1)–C(3)	2.497(4)	Cr(1)–C(28)	1.854(5)
Ta(1)–C(4)	2.501(3)	O(1)–C(25)	1.147(6)
Ta(1)–C(5)	2.390(2)	O(2)–C(26)	1.138(4)
S(1)–C(11)	1.792(3)	O(3)–C(27)	1.153(3)
S(2)–C(18)	1.794(4)	O(4)–C(28)	1.150(6)
N(1)–N(1)*	1.295(4)		
Ta(1)···Ta(1)*	4.9303(2)	Ta(1)···Cr(1)	3.1483(5)
S(1)–Ta(1)–S(2)	99.66(2)	S(2)–Cr(1)–C(27)	174.46(15)
S(1)–Ta(1)–N(1)	108.10(6)	S(2)–Cr(1)–C(28)	85.25(10)
S(2)–Ta(1)–N(1)	108.02(11)	C(25)–Cr(1)–C(26)	171.90(16)
Ta(1)–S(1)–C(11)	115.30(11)	C(25)–Cr(1)–C(27)	85.42(16)
Ta(1)–S(2)–C(18)	115.40(14)	C(25)–Cr(1)–C(28)	85.6(2)
Ta(1)–N(1)–N(1)*	165.6(2)	C(26)–Cr(1)–C(27)	88.93(15)
S(1)–Cr(1)–S(2)	99.09(3)	C(26)–Cr(1)–C(28)	88.65(19)
S(1)–Cr(1)–C(25)	91.14(16)	C(27)–Cr(1)–C(28)	90.21(18)
S(1)–Cr(1)–C(26)	94.17(14)	Ta(1)–S(1)–Cr(1)	80.62(3)
S(1)–Cr(1)–C(27)	85.27(15)	Cr(1)–S(1)–C(11)	114.80(14)
S(1)–Cr(1)–C(28)	174.63(13)	Ta(1)–S(2)–Cr(1)	80.60(3)
S(2)–Cr(1)–C(25)	91.04(10)	Cr(1)–S(2)–C(18)	114.80(8)
S(2)–Cr(1)–C(26)	94.14(8)		

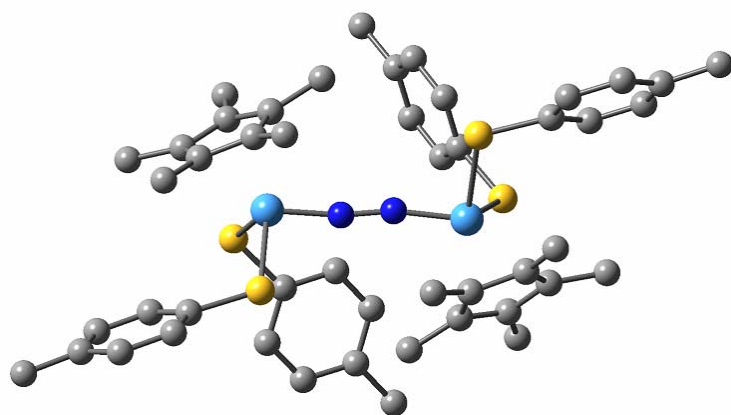


**Figure S7.** ORTEP drawing of **5** with thermal ellipsoids at the 50% probability level. Hydrogen atoms are omitted for clarity.

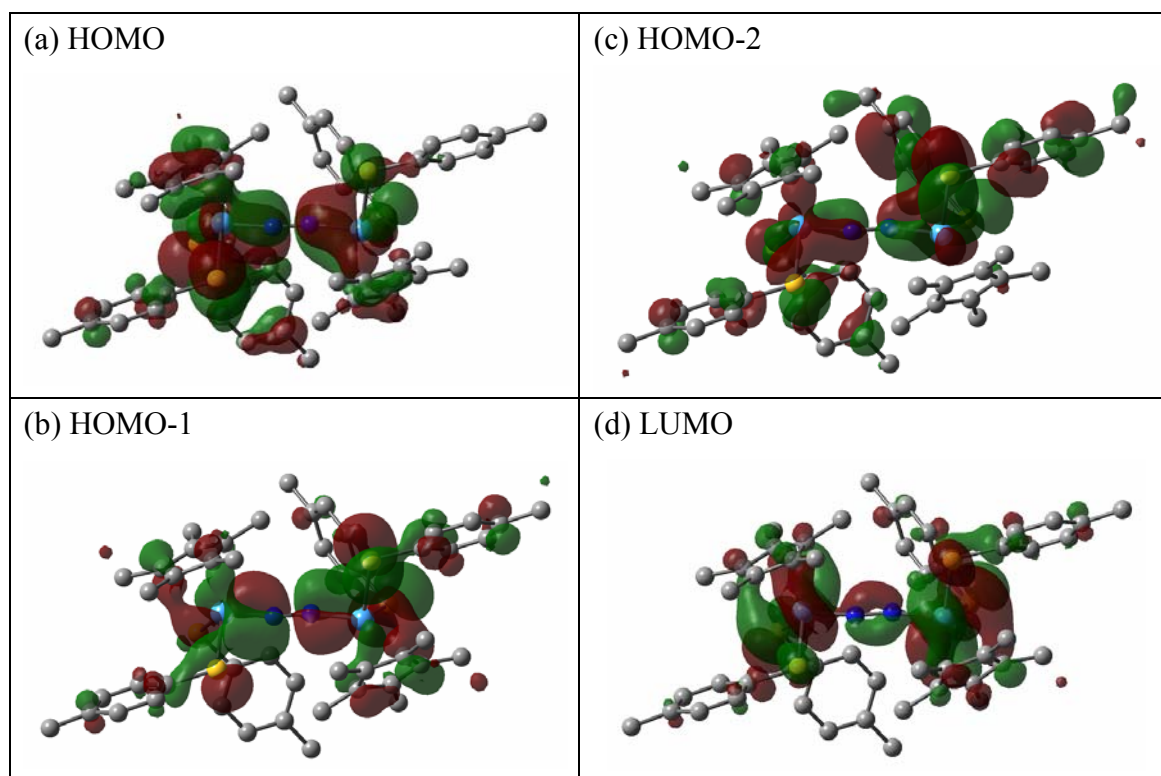
**Table S5.** Selected bond lengths/Å and angles/° for **5**

Ta(1)–S(1)	2.4163(13)	Ta(2)–S(3)	2.4064(13)
Ta(1)–S(2)	2.4072(10)	Ta(2)–S(4)	2.3901(12)
Ta(1)–N(1)	1.822(4)	Ta(2)–N(2)	1.822(4)
Ta(1)–C(1)	2.380(4)	Ta(2)–C(11)	2.532(#)
Ta(1)–C(2)	2.391(4)	Ta(2)–C(12)	2.480(4)
Ta(1)–C(3)	2.483(5)	Ta(2)–C(13)	2.418(4)
Ta(1)–C(4)	2.469(4)	Ta(2)–C(14)	2.374(5)
Ta(1)–C(5)	2.400(4)	Ta(2)–C(15)	2.465(6)
S(1)–C(21)	1.787(4)	S(3)–C(35)	1.781(5)
S(2)–C(28)	1.792(5)	S(4)–C(42)	1.785(6)
Cr(1)–S(1)	2.4585(15)	O(1)–C(49)	1.141(7)
Cr(1)–S(2)	2.4517(14)	O(2)–C(50)	1.135(6)
Cr(1)–C(49)	1.905(5)	O(3)–C(51)	1.144(7)
Cr(1)–C(50)	1.906(5)	O(4)–C(52)	1.162(6)
Cr(1)–C(51)	1.865(5)	N(1)–N(2)	1.283(6)
Cr(1)–C(52)	1.838(5)		
Ta(1)···Ta(2)	4.9113(2)	Ta(1)···Cr(1)	3.0156(8)
S(1)–Ta(1)–S(2)	104.62(4)	S(3)–Ta(2)–S(4)	107.84(4)
S(1)–Ta(1)–N(1)	101.52(12)	S(3)–Ta(2)–N(2)	104.39(12)
S(2)–Ta(1)–N(1)	101.44(12)	S(4)–Ta(2)–N(2)	91.87(12)
Ta(1)–S(1)–C(21)	110.94(19)	Ta(2)–S(3)–C(35)	112.37(16)
Ta(1)–S(2)–C(28)	110.60(16)	Ta(2)–S(4)–C(42)	110.11(14)
Ta(1)–N(1)–N(2)	168.1(3)	Ta(2)–N(2)–N(1)	174.5(3)
S(1)–Cr(1)–S(2)	102.04(5)	C(49)–Cr(1)–C(51)	89.1(2)
S(1)–Cr(1)–C(49)	90.38(17)	C(49)–Cr(1)–C(52)	87.4(2)
S(1)–Cr(1)–C(50)	92.49(16)	C(50)–Cr(1)–C(51)	90.6(2)
S(1)–Cr(1)–C(51)	85.30(16)	C(50)–Cr(1)–C(52)	89.7(2)
S(1)–Cr(1)–C(52)	171.5(2)	C(51)–Cr(1)–C(52)	86.4(2)
S(2)–Cr(1)–C(49)	88.21(17)	Ta(1)–S(1)–Cr(1)	76.42(4)
S(2)–Cr(1)–C(50)	91.67(17)	Cr(1)–S(1)–C(21)	114.92(17)
S(2)–Cr(1)–C(51)	172.21(16)	Ta(1)–S(2)–Cr(1)	76.72(3)
S(2)–Cr(1)–C(52)	86.12(18)	Cr(1)–S(2)–C(28)	118.58(14)
C(49)–Cr(1)–C(50)	177.1(2)		





**Figure S8.** Molecular structure of **1** optimized by the DFT calculation.



**Figure S9.** (a) HOMO, (b) HOMO-1, (c) HOMO-2, and (d) LUMO of **1** calculated by DFT.

**Table S6.** Molecular coordinates of **1** optimized by the density functional calculation

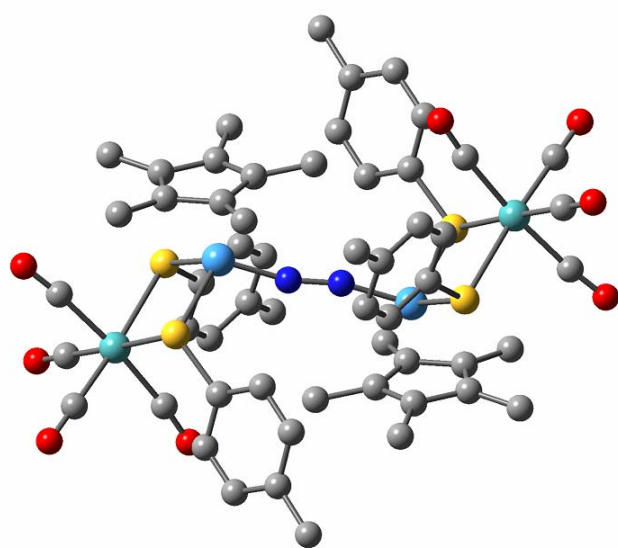
	Atomic number	$x/\text{\AA}$	$y/\text{\AA}$	$z/\text{\AA}$
1	73	2.373716	-0.106668	-0.764398
2	73	-2.305379	-0.311169	0.674298
3	16	3.072151	-1.728926	0.962688
4	16	-3.065010	-1.522684	-1.342707
5	16	3.293700	2.087848	-0.115611
6	16	-3.339048	1.934091	0.597768
7	7	0.655438	-0.081972	-0.189763
8	7	-0.619797	-0.109390	0.037654
9	6	-1.140932	5.360167	-4.096606
10	6	-1.742572	5.014652	-1.641817
11	6	-1.676314	4.508361	-2.959265
12	6	-2.218541	4.223924	-0.580878
13	6	-2.107774	3.181761	-3.178901
14	6	0.444832	4.269083	4.957911
15	6	0.412970	3.532806	2.512848
16	6	1.117351	3.684948	3.727709
17	6	-2.637874	2.899049	-0.817818
18	6	1.040333	3.027132	1.359066
19	6	2.475616	3.298309	3.757268
20	6	-2.581059	2.378469	-2.124216
21	6	3.113816	2.790547	2.610605
22	6	2.397081	2.657498	1.405684
23	6	2.616832	2.127497	-3.564380
24	6	-2.814995	1.218297	3.920625
25	6	-7.190507	-1.048963	-1.012225
26	6	-5.806316	-0.808468	-0.937816
27	6	2.748144	0.696219	-3.107341
28	6	-2.718095	-0.071372	3.146206
29	6	0.267670	-0.064867	-3.538766
30	6	5.352823	0.681023	-2.764854
31	6	-9.195838	-2.514930	-1.597384
32	6	5.797089	-0.857207	0.861734
33	6	-5.293910	-0.446273	2.805013
34	6	7.185464	-1.062021	0.967689
35	6	-0.128895	-0.475246	3.401578

36	6	-7.700145	-2.278223	-1.487395
37	6	1.693246	-0.285820	-3.100353
38	6	3.991198	0.031868	-2.758730
39	6	-4.893663	-1.807276	-1.333493
40	6	-3.845309	-0.842099	2.657518
41	6	-1.514786	-0.835190	2.926156
42	6	4.908659	-1.939830	1.020143
43	6	7.722533	-2.338994	1.243239
44	6	9.219502	-2.545452	1.391060
45	6	-6.772730	-3.266771	-1.885413
46	6	2.275614	-1.552333	-2.709624
47	6	-5.386251	-3.037577	-1.813997
48	6	3.702878	-1.354999	-2.530742
49	6	-3.340351	-2.081206	2.136203
50	6	-1.894373	-2.071970	2.275258
51	6	5.429356	-3.219570	1.302590
52	6	6.818635	-3.412471	1.409046
53	6	1.564887	-2.883714	-2.676147
54	6	-4.153461	-3.266061	1.684572
55	6	4.701082	-2.461990	-2.314761
56	6	-0.975791	-3.231859	1.975692
57	1	3.042372	3.392896	4.682094
58	1	-2.905583	1.360235	-2.319023
59	1	1.611345	2.521162	-3.381081
60	1	-2.083885	2.769301	-4.186306
61	1	0.472673	2.917462	0.440298
62	1	0.655068	5.344668	5.049852
63	1	-0.638060	3.810814	2.460130
64	1	6.085104	0.089122	-2.206292
65	1	1.683487	-3.406394	-3.637230
66	1	-3.680169	-3.789958	0.847509
67	1	-3.598452	1.874874	3.528965
68	1	2.811548	2.196932	-4.645269
69	1	4.158851	2.496069	2.653803
70	1	3.324714	2.785287	-3.051001
71	1	0.800534	3.788295	5.877894
72	1	-1.872427	1.773690	3.896542

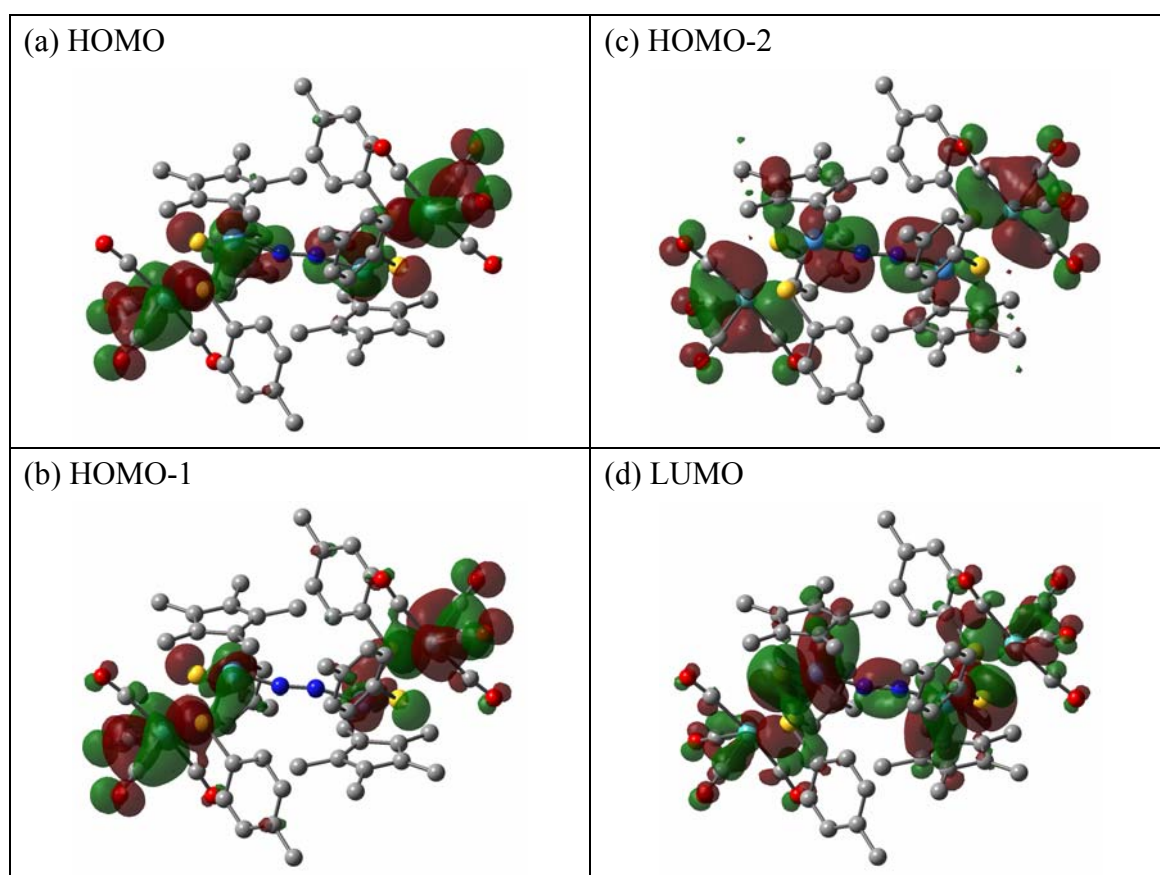
73	1	-5.440898	0.152980	-0.585601
74	1	5.410078	0.140341	0.670188
75	1	-7.880566	-0.265013	-0.704095
76	1	-3.050272	1.003829	4.973976
77	1	-0.062236	0.961262	-3.348781
78	1	5.326979	1.684302	-2.324140
79	1	0.022771	0.607977	3.447233
80	1	7.856605	-0.213670	0.842394
81	1	-0.644892	4.152888	4.913818
82	1	-5.442372	0.624795	2.625057
83	1	-9.739123	-2.048739	-0.765949
84	1	-9.595797	-2.086862	-2.528116
85	1	0.171786	-0.254631	-4.618257
86	1	0.491641	-2.764018	-2.495384
87	1	-4.689105	-3.809202	-2.130262
88	1	0.650886	-0.882256	2.750629
89	1	9.514378	-3.563824	1.110169
90	1	0.038515	-0.878429	4.411506
91	1	-0.431251	-0.729940	-3.021764
92	1	-9.434158	-3.585209	-1.599889
93	1	-0.041404	5.342198	-4.122218
94	1	-1.498666	5.001136	-5.068852
95	1	-2.274432	4.636111	0.423111
96	1	-1.445483	6.408748	-3.990158
97	1	9.539398	-2.387382	2.431451
98	1	-7.134664	-4.223986	-2.256799
99	1	-1.421563	6.035257	-1.440729
100	1	-5.937006	-0.992934	2.108458
101	1	4.750787	-4.057918	1.437529
102	1	4.922267	-2.954200	-3.273776
103	1	-1.300709	-3.790514	1.090611
104	1	5.644760	-2.094444	-1.902480
105	1	4.320371	-3.226422	-1.630020
106	1	0.053523	-2.901418	1.804028
107	1	-5.159232	-2.979682	1.365345
108	1	5.724317	0.784061	-3.795125
109	1	9.785566	-1.844071	0.766065

110	1	-5.647849	-0.660658	3.824428
111	1	1.964403	-3.536207	-1.891701
112	1	-4.255552	-3.983150	2.512827
113	1	-0.960767	-3.933769	2.823198
114	1	7.202279	-4.408515	1.624069

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**Figure S10.** Molecular structure of **2** optimized by the DFT calculation.



**Figure S11.** (a) HOMO, (b) HOMO-1, (c) HOMO-2, and (d) LUMO of **2** calculated by DFT.

**Table S7.** Molecular coordinates of **2** optimized by the density functional calculation

	Atomic number	$x/\text{\AA}$	$y/\text{\AA}$	$z/\text{\AA}$
1	73	2.140257	0.002964	-1.210530
2	73	-2.141545	-0.004410	1.210965
3	42	5.148180	0.007054	0.444276
4	42	-5.146949	-0.006688	-0.444860
5	16	3.535107	-1.962722	-0.485096
6	16	3.526906	1.972363	-0.479837
7	16	-3.528327	-1.973362	0.479698
8	16	-3.533262	1.962699	0.484009
9	8	6.789896	0.019037	-2.322490
10	8	7.204476	-2.200731	1.389379
11	8	3.998521	-0.005447	3.450203
12	8	-3.997885	0.005935	-3.450801
13	8	-6.790677	-0.013045	2.320959
14	8	-7.199790	2.203420	-1.392197
15	8	7.187920	2.224285	1.403180
16	8	-7.189895	-2.221964	-1.401687
17	7	0.616342	0.000329	-0.215751
18	7	-0.617456	-0.002562	0.216277
19	6	3.064906	-4.268067	2.941566
20	6	1.950599	-5.081323	2.645948
21	6	2.843394	-3.093506	0.821425
22	6	-6.414356	-1.396942	-1.039669
23	6	-4.356201	0.000637	-2.321241
24	6	0.733640	-0.003103	3.136253
25	6	1.287999	-4.868719	1.416373
26	6	1.725741	-3.888524	0.507603
27	6	1.462519	6.159528	3.614380
28	6	3.516536	-3.286899	2.039265
29	6	1.496780	-6.169924	3.601118
30	6	6.126626	0.014876	-1.341491
31	6	-1.499645	6.174551	-3.599577
32	6	-6.126686	-0.011251	1.340489
33	6	-1.726852	3.892199	-0.505613
34	6	-4.127133	1.624170	3.895001
35	6	-2.829658	-3.098385	-0.828126

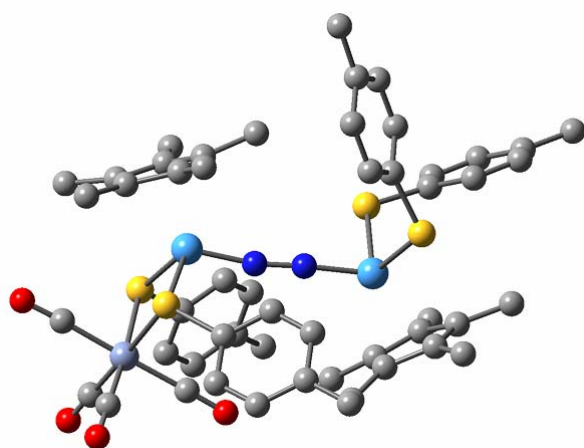
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37	6	-3.512638	3.286004	-2.041334
38	6	-2.841706	3.094665	-0.821596
39	6	-3.061637	4.267897	-2.942509
40	6	-1.950010	5.084558	-2.644377
41	6	-1.289463	4.873674	-1.413816
42	6	-6.420784	1.379934	-1.034028
43	6	-2.980525	-0.722527	3.550543
44	6	4.357158	-0.001291	2.320755
45	6	4.116885	1.646922	-3.892258
46	6	-2.982263	0.707569	3.551553
47	6	-1.622380	1.157665	3.297320
48	6	-1.619711	-1.168974	3.295728
49	6	1.624502	-1.160925	-3.297359
50	6	2.983111	-0.706928	-3.551332
51	6	-0.734791	-0.005918	-3.135899
52	6	6.423939	-1.378267	1.032147
53	6	6.413912	1.398162	1.040300
54	6	1.147575	2.596948	-3.369100
55	6	1.169586	-2.596111	-3.374498
56	6	3.033633	4.258400	2.957680
57	6	3.491032	3.281356	2.053297
58	6	2.828989	3.097838	0.828196
59	6	1.716856	3.898706	0.508593
60	6	4.130690	-1.620069	-3.895174
61	6	-0.769756	-0.004617	3.200427
62	6	2.977327	0.723204	-3.550048
63	6	1.615283	1.165670	-3.295022
64	6	1.273616	4.874460	1.419001
65	6	1.924834	5.076751	2.656673
66	6	0.768601	-0.001178	-3.199872
67	6	-3.031156	-4.257577	-2.958634
68	6	-1.458080	-6.157254	-3.614810
69	6	-1.922300	-5.075554	-2.656785
70	6	-1.272866	-4.874061	-1.418042
71	6	-4.123013	-1.642604	3.892570
72	6	-1.156563	-2.601696	3.370582



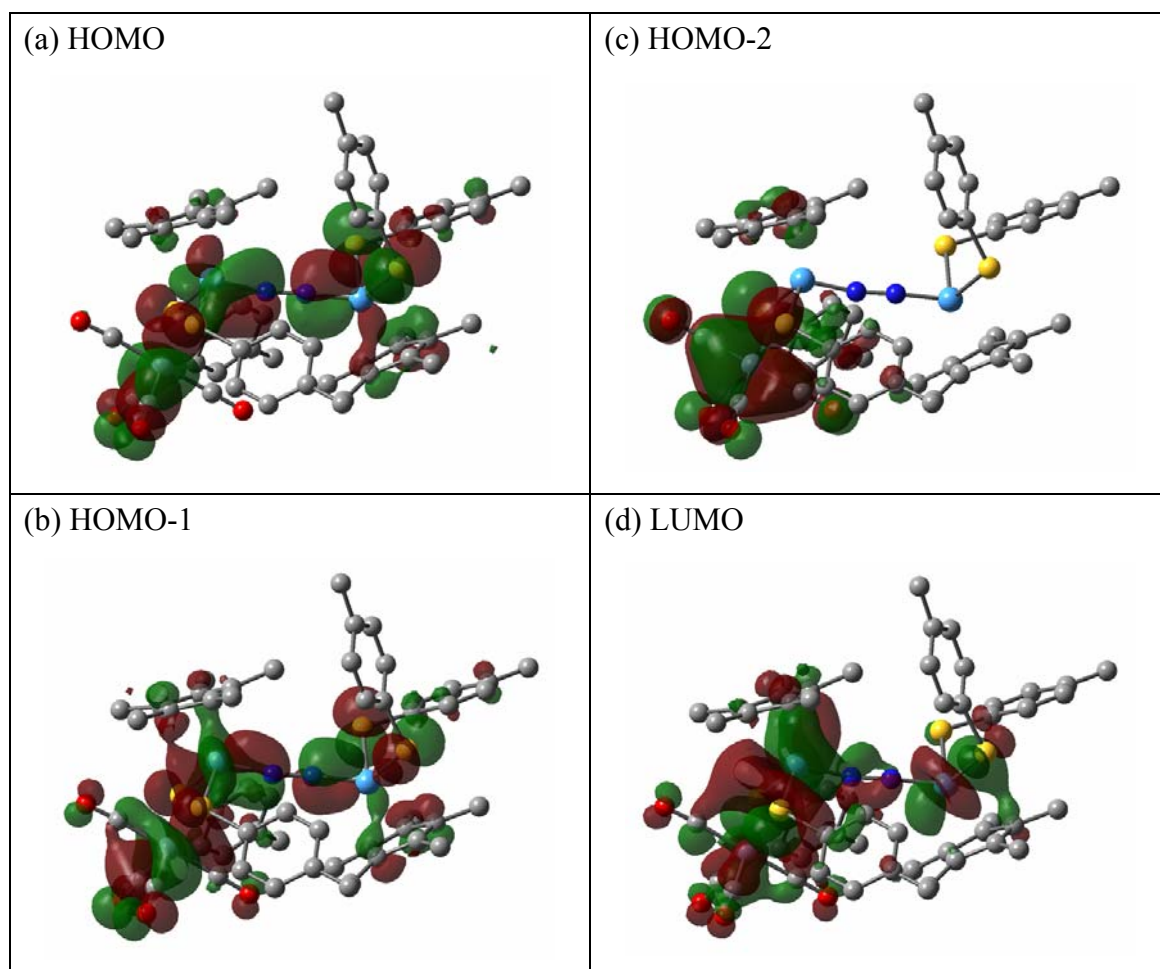
73	6	-3.490113	-3.281367	-2.054181
74	6	-1.717834	-3.899279	-0.507454
75	1	1.790118	-5.946139	4.633284
76	1	0.407817	-6.299515	3.577484
77	1	1.946209	-7.137535	3.335623
78	1	0.369047	6.248631	3.625115
79	1	1.796983	5.958821	4.638572
80	1	1.866083	7.139936	3.323582
81	1	0.261972	-2.775829	-2.789995
82	1	0.942741	-2.862685	-4.417665
83	1	1.946763	-3.282024	-3.020671
84	1	4.296001	-2.382422	-3.123679
85	1	3.916358	-2.147487	-4.835467
86	1	5.066576	-1.071605	-4.026625
87	1	5.056836	1.106735	-4.028726
88	1	3.896028	2.177171	-4.829417
89	1	4.278039	2.406774	-3.117376
90	1	1.919132	3.289352	-3.015630
91	1	0.916604	2.863249	-4.411423
92	1	0.239339	2.767535	-2.782842
93	1	-1.125389	0.866430	-2.603326
94	1	-1.158727	0.009962	-4.149212
95	1	-1.121178	-0.897247	-2.632592
96	1	4.362962	2.688997	2.301997
97	1	4.392386	-2.698335	2.283256
98	1	1.208677	-3.751035	-0.436333
99	1	0.426974	-5.485083	1.163687
100	1	3.597892	-4.403761	3.880188
101	1	3.558183	4.386613	3.902029
102	1	0.417309	5.495638	1.161996
103	1	1.209287	3.768558	-0.441493
104	1	-3.592885	4.402110	-3.882419
105	1	-0.430528	5.492059	-1.159281
106	1	-3.554367	-4.385405	-3.903777
107	1	1.122766	-0.882614	2.614567
108	1	-1.937948	3.279910	3.021008
109	1	-1.861899	-7.138077	-3.325760

110	1	-0.255104	2.768094	2.788583
111	1	-4.361994	-2.689146	-2.303390
112	1	-1.211408	3.756021	0.439398
113	1	-4.386281	2.695042	-2.287334
114	1	1.157815	-0.006924	4.149595
115	1	-1.211838	-3.769502	0.443529
116	1	-0.416738	-5.495204	-1.160378
117	1	1.121165	0.881365	2.621864
118	1	-0.933954	2.857244	4.416964
119	1	-3.905572	-2.170828	4.831714
120	1	-0.928626	-2.868780	4.413354
121	1	-0.247693	-2.774956	2.786107
122	1	-3.911667	2.150672	4.835564
123	1	-5.064896	1.078738	4.025697
124	1	-5.061984	-1.099847	4.025363
125	1	-4.289403	2.387186	3.123494
126	1	-1.710844	5.907459	-4.641775
127	1	-0.424580	6.371215	-3.509966
128	1	-1.790811	-5.955561	-4.639373
129	1	-0.364573	-6.246066	-3.623726
130	1	-4.283972	-2.404258	3.119420
131	1	-1.929623	-3.291583	3.015404
132	1	-2.023324	7.118801	-3.392335

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**Figure S12.** Molecular structure of **5** optimized by the DFT calculation.



**Figure S13.** (a) HOMO, (b) HOMO-1, (c) HOMO-2, and (d) LUMO of **5** calculated by DFT.

**Table S8.** Molecular coordinates of **5** optimized by the density functional calculation

	Atomic number	$x/\text{\AA}$	$y/\text{\AA}$	$z/\text{\AA}$
1	73	-2.321869	0.096031	0.839953
2	73	2.186266	-0.364797	-1.088203
3	24	4.423345	1.102872	0.678709
4	16	-3.120037	0.870193	-1.360406
5	16	-3.257197	-2.180195	1.137202
6	16	3.067290	1.946184	-1.356805
7	16	3.604542	-1.363784	0.694309
8	8	6.202240	0.301364	2.989453
9	8	5.636719	3.871423	0.767535
10	8	6.638488	0.253134	-1.266149
11	8	2.221473	1.994282	2.610277
12	7	-0.636219	-0.091484	0.180462
13	7	0.588097	-0.137947	-0.256594
14	6	-5.463554	2.170350	-2.201399
15	6	-4.955097	1.074006	-1.472854
16	6	0.767467	-3.570785	5.758731
17	6	-7.238491	0.277457	-1.145135
18	6	-7.763283	1.374353	-1.862247
19	6	-6.849049	2.315084	-2.390155
20	6	1.359370	-2.391802	2.136933
21	6	3.363950	-1.928456	3.442255
22	6	2.670335	-1.892912	2.215929
23	6	-0.878249	6.711357	-0.915211
24	6	0.748694	-2.932116	3.285508
25	6	1.423135	-2.980323	4.523329
26	6	2.737269	-2.461774	4.581086
27	6	5.761762	0.564495	-0.534572
28	6	-2.107411	-6.356175	-3.306680
29	6	-1.940118	-4.409970	0.012698
30	6	5.155421	2.786648	0.722888
31	6	5.500812	0.605382	2.080624
32	6	3.062515	1.636662	1.860491
33	6	-1.704164	-5.375401	-0.985053
34	6	-2.799321	-3.324053	-0.244636
35	6	-9.259368	1.549678	-2.050739

36	6	-5.852744	0.122950	-0.949742
37	6	-2.322959	-5.286409	-2.251375
38	6	-3.172214	-4.183691	-2.495835
39	6	-3.410185	-3.210806	-1.508955
40	6	4.823341	-2.612932	-2.342314
41	6	4.365120	0.130274	-4.029974
42	6	1.235664	0.558704	-4.358181
43	6	-4.131159	0.890580	2.533259
44	6	-3.505318	2.035326	1.933520
45	6	-2.095724	2.017048	2.289845
46	6	-0.278099	-1.924497	-2.985819
47	6	1.877748	-0.517383	-3.517233
48	6	1.197006	-1.633523	-2.903015
49	6	2.205244	-2.483631	-2.310675
50	6	1.974825	-3.825727	-1.660166
51	6	3.511567	-1.932663	-2.638114
52	6	3.310454	-0.726362	-3.379095
53	6	-0.380603	4.256307	-1.412601
54	6	0.491234	3.153029	-1.467008
55	6	1.827598	3.300458	-1.057559
56	6	2.283697	4.543484	-0.577376
57	6	1.396484	5.632231	-0.515703
58	6	0.054801	5.514046	-0.944163
59	6	-0.601757	0.555251	3.891369
60	6	-1.116843	3.139467	2.053011
61	6	-1.866676	0.861396	3.130506
62	6	-3.120520	0.164113	3.269505
63	6	-3.383452	-0.992591	4.197987
64	6	-5.603660	0.566608	2.549440
65	6	-4.201843	3.169669	1.227417
66	1	-6.050110	0.887794	3.502554
67	1	-6.142236	1.072715	1.743778
68	1	-5.114568	2.844443	0.720685
69	1	-5.784954	-0.510076	2.450690
70	1	-2.465464	-1.543529	4.424523
71	1	-3.791228	-0.617739	5.148801
72	1	-4.105323	-1.703380	3.782750

73	1	-0.081641	2.790367	2.061866
74	1	4.869176	-2.977273	-1.309210
75	1	4.952150	-3.481536	-3.004465
76	1	-1.217033	3.893274	2.848879
77	1	-4.479672	3.946081	1.955885
78	1	-3.554100	3.635544	0.477628
79	1	-1.287478	3.642631	1.097704
80	1	-0.409105	-0.519214	3.965841
81	1	-9.795544	0.605344	-1.901749
82	1	-9.667316	2.276763	-1.333564
83	1	0.740887	-2.844702	6.582559
84	1	-9.496279	1.918034	-3.056722
85	1	-2.098054	-5.929084	-4.317060
86	1	-1.160628	-6.887567	-3.153657
87	1	-2.912011	-7.105185	-3.277369
88	1	-0.659629	7.402297	-1.741936
89	1	0.274067	1.015874	3.431669
90	1	-0.682222	0.949650	4.915877
91	1	-0.773621	7.279094	0.018107
92	1	-0.262143	-3.885861	5.554561
93	1	1.319469	-4.449304	6.119941
94	1	-1.926728	6.405863	-1.010674
95	1	-7.222113	3.165961	-2.957833
96	1	-4.776973	2.898591	-2.625050
97	1	0.809243	-2.357823	1.202712
98	1	-7.915980	-0.470749	-0.737427
99	1	-3.655849	-4.082604	-3.465761
100	1	-4.062933	-2.370263	-1.723484
101	1	-5.478257	-0.734671	-0.397316
102	1	1.759533	6.587136	-0.139936
103	1	-1.409691	4.124800	-1.740816
104	1	0.123115	2.195469	-1.820488
105	1	3.315762	4.672047	-0.267526
106	1	-0.267467	-3.314535	3.208950
107	1	3.282948	-2.481118	5.522768
108	1	4.381386	-1.557282	3.511815
109	1	-1.041560	-6.211535	-0.768305

110	1	1.756285	1.517520	-4.260093
111	1	1.263078	0.275528	-5.421171
112	1	0.185270	0.714190	-4.089174
113	1	4.191751	1.197787	-3.849310
114	1	5.676808	-1.946929	-2.496579
115	1	5.369323	-0.108247	-3.668484
116	1	4.355028	-0.026102	-5.118509
117	1	2.071663	-4.629526	-2.405574
118	1	2.705534	-4.020865	-0.867462
119	1	-1.473204	-4.512029	0.988850
120	1	0.973331	-3.903552	-1.225357
121	1	-0.891371	-1.020586	-2.914074
122	1	-0.508783	-2.407281	-3.946854
123	1	-0.605758	-2.602202	-2.194487

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