Supporting Information

Lewis Acids Catalyzed Rearrangement of Multi-substituted Arylvinyldenecyclopropanes

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General Remarks. ^1H and ^{13}C NMR spectra were recorded on a Bruker AM-300 spectrometer for solution in CDCl_3 with tetramethylsilane (TMS) as an internal standard; J -values are in Hz. Mass spectra were recorded by EI method, and HRMS was measured on a Finnigan MA^+ mass spectrometer. CHN microanalyses were recorded on a Carlo-Erba 1106 analyzer. THF and toluene were distilled from Na under Ar atmosphere. CH_3CN and 1,2-dichloroethane (DCE) were distilled from CaH_2 under Ar atmosphere. Commercially obtained reagents were used without further purification. All reactions were monitored by TLC with Huanghai GF_{254} silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

Typical Reaction Procedure for the Preparation of Diarylvinyldenecyclopropanes: A mixture of Bu_4NHSO_4 (10 mmol) and powdered NaOH (80 g) was added to a tetrahydrofuran (THF) solution containing 1,1-dibromo-2,2-diphenylcyclopropane (10 mmol) and an excess of 1-(but-2-en-2-yl)benzene (12 mmol). The reaction mixture was vigorously stirred at room temperature for 24 h. Flash column chromatography of the resulting mixture on silica gel gave the product **1a** (35%) as a colorless liquid.

Typical Reaction Procedure for the Rearrangement of Diarylvinyldenecyclopropanes in the Presence of Lewis acid: To a solution of diarylvinyldenecyclopropane **1d** (67 mg, 0.2 mmol) in 1,2-dichloroethane (2.0 mL) was added $\text{Sn}(\text{OTf})_2$ (8.0 mg, 0.02 mmol), the reaction mixture was stirred for 5 hour at 80 °C (monitored by TLC). After the starting materials (diarylvinyldenecyclopropanes **1**) were consumed, the solvent was removed under reduced pressure and the residue was subjected to a flash column chromatography to give the desired product **2d** (56 mg, 84%) as a colorless liquid.

1-(1,2-Dimethyl-3-(2,2-diphenylvinylidene)cyclopropyl)benzene (1a). A colorless liquid. IR (CH₂Cl₂): ν 3056, 3025, 2957, 2922, 2864, 1989, 1598, 1492, 1472, 1443, 1381, 1265, 1067, 1029, 766, 696, 628 cm⁻¹; Data for (*E*)-**1a**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.47 (3H, d, *J* = 6.0 Hz, CH₃), 1.67 (3H, s, CH₃), 2.17-2.26 (1H, m, CH), 7.14-7.50 (15H, m, ArH); Data for (*Z*)-**1a**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.02 (3H, d, *J* = 6.3 Hz, CH₃), 1.73 (3H, s, CH₃), 2.17-2.26 (1H, m, CH), 7.14-7.50 (15H, m, ArH); MS (EI) *m/z* (%): 322 (40.3) [M⁺], 307 (68.2), 292 (35.2), 229 (100), 215 (38.2), 202 (12.5), 165 (8.4), 128 (5.0), 115 (6.1), 91 (8.2); HRMS (EI) Calcd. for C₂₅H₂₂ (M⁺) requires 322.1722, Found: 322.1717.

1-Chloro-4-(1,2-dimethyl-3-(2,2-diphenylvinylidene)cyclopropyl)benzene (1b). A colorless solid, m.p. 100.3-102.1 °C; IR (CH₂Cl₂): ν 3058, 3028, 2959, 2922, 2852, 1989, 1596, 1492, 1471, 1443, 1398, 1378, 1091, 1067, 1030, 1013, 832, 767, 695, 628 cm⁻¹; Data for (*E*)-**1b**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.47 (3H, d, *J* = 6.0 Hz, CH₃), 1.65 (3H, s, CH₃), 2.13-2.26 (1H, m, CH), 7.19-7.52 (14H, m, ArH); Data for (*Z*)-**1b**: ¹H NMR (300 MHz, CDCl₃,

TMS): δ 1.02 (3H, d, $J = 6.0$ Hz, CH₃), 1.71 (3H, s, CH₃), 2.13-2.26 (1H, m, CH), 7.19-7.52 (14H, m, ArH); MS (EI) m/z (%): 358 (5.4) [M⁺], 356 (13.5) [M⁺], 343 (7.6), 341 (21.0), 321 (15.7), 306 (18.9), 291 (35.9), 263 (31.9), 229 (20.6), 215 (21.2), 202 (14.1), 191 (100), 165 (40.8), 128 (7.3), 115 (12.8), 91 (6.8); HRMS (EI) Calcd. for C₂₅H₂₁Cl (M⁺) requires 356.1332, Found: 356.1303.

NOE effect (NOESY spectrum) of 1b:

1c

1-Bromo-4-(1,2-dimethyl-3-(2,2-diphenylvinylidene)cyclopropyl)benzene (1c). A colorless solid, m.p. 108.5-109.7 °C; IR (CH₂Cl₂): ν 3057, 2957, 2923, 2864, 1990, 1596, 1491, 1471, 1442, 1393, 1381, 1264, 1074, 1030, 1010, 829, 767, 695, 627 cm⁻¹; Data for (*E*)-**1c**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.47 (3H, d, *J* = 6.3 Hz, CH₃), 1.65 (3H, s, CH₃), 2.13-2.26 (1H, m, CH), 7.11-7.44 (14H, m, ArH); Data for (*Z*)-**1c**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.02 (3H, d, *J* = 6.3 Hz, CH₃), 1.71 (3H, s, CH₃), 2.13-2.26 (1H, m, CH), 7.11-7.44 (14H, m, ArH); MS (EI) *m/z* (%): 402 (14.2) [M⁺], 400 (14.4) [M⁺], 387 (14.0), 385 (13.9), 321 (28.1), 306 (83.5), 291 (100), 243 (26.0), 229 (37.1), 215 (28.7), 202 (16.3), 165 (12.2), 128 (9.7), 115 (8.2), 91 (7.2); HRMS (EI) Calcd. for C₂₅H₂₁Br (M⁺) requires 400.0827, Found: 400.0797.

1c

1d

1-Methyl-4-(1,2-dimethyl-3-(2,2-diphenylvinylidene)cyclopropyl)benzene (1d). A colorless liquid. IR (CH₂Cl₂): ν 3054, 3026, 2956, 2921, 2864, 1990, 1597, 1514, 1492, 1472, 1442, 1375, 1069, 1030, 766, 695, 635 cm⁻¹; Data for (*E*)-**1d**: ¹H NMR (300 MHz, CDCl₃,

TMS): δ 1.47 (3H, d, J = 6.3 Hz, CH₃), 1.65 (3H, s, CH₃), 2.18-2.23 (1H, m, CH), 2.33 (3H, s, CH₃), 7.05-7.46 (14H, m, ArH); Data for (Z)-**1d**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.03 (3H, d, J = 6.3 Hz, CH₃), 1.71 (3H, s, CH₃), 2.18-2.23 (1H, m, CH), 2.31 (3H, s, CH₃), 7.05-7.46 (14H, m, ArH); MS (EI) m/z (%): 336 (44.2) [M⁺], 321 (90.6), 306 (40.0), 291 (46.0), 243 (100), 229 (52.8), 215 (32.4), 202 (18.3), 165 (17.7), 128 (13.6), 115 (13.3), 91 (13.6); HRMS (EI) Calcd. for C₂₆H₂₄ (M⁺) requires 336.1878, Found: 336.1865.

1-(2-(2-(4-Methoxyphenyl)-2,3-dimethylcyclopropylidene)-1-phenylvinyl)benzene(1e). A colorless liquid. IR (CH₂Cl₂): ν 3057, 3030, 2956, 2922, 2861, 2834, 1989, 1605, 1597, 1512, 1492, 1442, 1377, 1296, 1246, 1178, 1071, 1032, 833, 767, 696, 625 cm⁻¹; Data for (E)-**1e**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.47 (3H, d, J = 6.3 Hz, CH₃), 1.64 (3H, s, CH₃), 2.17-2.21 (1H, m, CH), 3.78 (3H, s, OCH₃), 6.77-6.80 (1H, m, ArH), 7.17-7.46 (13H, m, ArH); Data for (Z)-**1e**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.03 (3H, d, J = 6.6 Hz, CH₃), 1.70 (3H, s, CH₃), 2.17-2.21 (1H, m, CH), 3.76 (3H, s, OCH₃), 6.77-6.80 (1H, m, ArH), 7.17-7.46 (13H, m, ArH); MS (EI) m/z (%): 352 (31.8) [M⁺], 337 (100), 322 (28.8), 321 (29.0), 307 (10.8), 291 (17.5), 259 (43.6), 245 (11.7), 243 (9.5), 229 (18.3), 215 (17.3), 202 (11.8), 165 (10.7), 115 (5.8), 91 (7.1); HRMS (EI) Calcd. for C₂₆H₂₄O (M⁺) requires 352.1827, Found: 352.1819.

1-Fluoro-4-(1-(4-fluorophenyl)-2-(2,3-dimethyl-2-phenylcyclopropylidene)vinyl)benzene (1f). A colorless liquid. IR (CH₂Cl₂): ν 3059, 3030, 2956, 2924, 2844, 1601, 1506, 1466, 1224, 1157, 1095, 1015, 838, 761, 748 cm⁻¹; Data for (*E*)-**1f**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.48 (3H, d, J = 6.6 Hz, CH₃), 1.67 (3H, s, CH₃), 2.20-2.24 (1H, m, CH), 6.97-7.08 (4H, m, ArH), 7.18-7.37 (9H, m, ArH); Data for (*Z*)-**1f**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.03 (3H, d, J = 6.0 Hz, CH₃), 1.73 (3H, s, CH₃), 2.20-2.24 (1H, m, CH), 6.97-7.08 (4H, m, ArH), 7.18-7.37 (9H, m, ArH); MS (EI) m/z (%): 358 (66.6) [M⁺], 343 (96.6), 328 (43.8), 323 (14.2), 265 (17.7), 247 (100), 233 (28.1), 128 (7.7); HRMS (EI) Calcd. for C₂₅H₂₀F₂ (M⁺) requires 358.1533, Found: 358.1532.

1-Methyl-4-(2-(2,3-dimethyl-2-phenylcyclopropylidene)-1-*p*-tolylvinyl)benzene (1g). A colorless liquid. IR (CH₂Cl₂): ν 3056, 3023, 2955, 2922, 2864, 1989, 1603, 1509, 1494, 1445, 1387, 1277, 1067, 1030, 822, 700 cm⁻¹; Data for (*E*)-**1g**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.46 (3H, d, J = 6.3 Hz, CH₃), 1.67 (3H, s, CH₃), 2.14-2.21 (1H, m, CH), 2.37 (6H, s, CH₃), 7.10-7.36 (13H, m, ArH); Data for (*Z*)-**1g**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.01 (3H, d, J = 6.6 Hz, CH₃), 1.72 (3H, s, CH₃), 2.14-2.21 (1H, m, CH), 2.35 (6H, s, CH₃), 7.10-7.36 (13H, m, ArH); MS (EI) m/z (%): 350 (100) [M⁺], 335 (93.9), 320 (40.6), 305 (48.7), 290 (9.6), 257 (22.4), 243 (98.2), 229 (29.5), 215 (19.5), 202 (11.8), 165 (5.8), 128 (8.4), 115(7.3), 91 (6.0); HRMS (EI) Calcd. for C₂₇H₂₆ (M⁺) requires 350.2035, Found: 350.2043.

1-(1-Ethyl-2-methyl-3-(2,2-diphenylvinylidene)cyclopropyl)benzene (1h). A colorless liquid. IR (CH₂Cl₂): ν 3058, 3024, 2961, 2924, 2853, 1987, 1589, 1492, 1470, 1444, 1375, 1080, 1029, 767, 696, 629 cm⁻¹; Data for (*E*)-**1h**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 0.90-0.97 (3H, m, CH₃), 1.48 (3H, d, J = 6.6 Hz, CH₃), 1.84-2.10 (2H, m, CH₂), 2.20-2.30 (1H, m, CH), 7.14-7.51 (15H, m, ArH); Data for (*Z*)-**1h**: ¹H NMR (300 MHz, CDCl₃, TMS): δ 0.90-0.97 (3H, m, CH₃), 1.03 (3H, d, J = 6.0 Hz, CH₃), 1.59-1.71 (2H, m, CH₂), 2.20-2.30 (1H, m, CH), 7.14-7.51 (15H, m, ArH); MS (EI) m/z (%): 336 (38.0) [M⁺], 321 (18.9), 307 (61.6), 292 (44.0), 243 (12.9), 229 (100), 215 (43.8), 202 (17.5), 165 (13.4), 128 (9.0), 115 (11.0), 91 (15.8); HRMS (EI) Calcd. for C₂₆H₂₄ (M⁺) requires 336.1878, Found: 336.1884.

1-(2-Methyl-1-phenyl-3-(2,2-diphenylvinylidene)cyclopropyl)benzene (1i). A colorless solid, m.p. 124.2-125.0 °C; IR (CH₂Cl₂): ν 3056, 3026, 2986, 2923, 2864, 1989, 1597, 1493, 1471, 1445, 1377, 1265, 1090, 1075, 1029, 768, 696, 631 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.23 (3H, d, J = 6.3 Hz, CH₃), 2.79 (1H, q, J = 6.3 Hz, CH), 7.18-7.37 (18H, m, ArH), 7.44-7.47 (2H, m, ArH); ¹³C NMR (75 MHz, CDCl₃, TMS): δ 14.8, 44.5, 93.1, 113.2, 126.4, 126.8, 126.9, 127.0, 127.7, 128.2, 128.3, 128.4, 128.5, 130.2, 137.5, 137.5, 138.9, 144.3, 189.7; MS (EI) m/z (%): 384 (24.2) [M⁺], 369 (16.9), 292 (21.8), 291 (100), 229 (6.8), 215 (6.9), 202 (3.9), 165 (8.7); Anal. Calcd. for C₃₀H₂₄ requires C, 93.71; H, 6.29%. Found: C, 93.66; H, 6.24%.

7,11b-Dihydro-7,11b-dimethyl-5-phenyl-6aH-benzo[c]fluorene (2a). A colorless solid, m.p. 126.6-127.4 °C; IR (CH₂Cl₂): ν 3059, 3022, 2956, 2922, 2869, 1597, 1493, 1478, 1443, 1369, 1265, 1028, 778, 763, 754, 741, 704, 582 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.43 (3H, d, J = 6.6 Hz, CH₃), 1.58 (3H, s, CH₃), 2.46-2.52 (1H, m, CH), 2.91-2.97 (1H, m, CH), 6.19 (1H, d, J = 6.6 Hz, Ar₂C=CH), 7.00-7.44 (12H, m, ArH), 7.61 (1H, d, J = 7.5 Hz, ArH); ¹³C NMR (75 MHz, CDCl₃, TMS): δ 16.5, 27.4, 43.9, 48.3, 57.5, 122.5, 124.7, 125.8, 125.8, 126.3, 126.5, 126.9, 127.1, 127.3, 127.7, 128.2, 129.0, 132.6, 139.2, 140.2, 140.9, 147.6, 149.2; MS (EI) m/z (%): 322 (84.1) [M⁺], 307 (100), 292 (20.1), 229 (54.9), 215 (27.1), 202 (6.6), 115 (2.3); Anal. Calcd. for C₂₅H₂₂ requires C, 93.12; H, 6.88%. Found: C, 92.96; H, 6.72%.

2a

2b

9-Chloro-7,11b-dihydro-7,11b-dimethyl-5-phenyl-6aH-benzo[c]fluorene (2b). A colorless liquid. IR (CH₂Cl₂): ν 3077, 3051, 3026, 2962, 2923, 2865, 1594, 1491, 1459, 1443, 1412, 1380, 1261, 1076, 1021, 817, 762, 746, 719, 695, 596 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, TMS): δ 0.97 (3H, d, J = 7.2 Hz, CH₃), 2.04 (3H, s, CH₃), 2.61-2.65 (1H, m, CH), 2.98-3.05 (1H, m, CH), 6.89 (1H, s, Ar₂C=CH), 7.03-7.25 (6H, m, ArH), 7.36-7.56 (6H, m, ArH); ¹³C NMR (75 MHz, CDCl₃, TMS): δ 11.1, 17.1, 34.4, 43.8, 119.5, 122.0, 122.8, 126.4, 127.3, 127.5, 127.6, 127.9, 128.1, 128.2, 128.4, 129.1, 130.9, 137.0, 140.8, 143.1, 143.4, 143.6, 145.2, 150.6; MS (EI) m/z (%): 358 (27.5) [M⁺], 356 (100) [M⁺], 343 (13.5), 341 (39.1), 326 (6.7), 321 (5.6), 306 (20.4), 291 (29.7), 263 (19.0), 229 (9.6), 215 (9.6), 191 (30.6), 165 (14.0); HRMS (EI) Calcd. for C₂₅H₂₁Cl (M⁺) requires 356.1332, Found: 356.1317.

9-Bromo-7,11b-dihydro-7,11b-dimethyl-5-phenyl-6aH-benzo[*c*]fluorene (2c). A colorless liquid. IR (CH₂Cl₂): ν 3077, 3045, 2955, 2924, 2852, 1587, 1486, 1457, 1441, 1407, 1383, 1268, 1067, 859, 834, 812, 760, 720, 698, 584 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, TMS): δ 0.97 (3H, d, J = 7.5 Hz, CH₃), 2.05 (3H, s, CH₃), 2.61-2.66 (1H, m, CH), 2.96-3.01 (1H, m, CH), 6.87 (1H, s, Ar₂C=CH), 7.05-7.12 (1H, m, ArH), 7.29-7.53 (11H, m, ArH); ¹³C NMR (75 MHz, CDCl₃, TMS): δ 11.1, 16.4, 17.1, 43.9, 119.2, 119.9, 122.0, 125.6, 127.5, 127.6, 127.9, 128.1, 129.3, 130.9, 137.0, 140.7, 143.2, 143.6, 143.8, 145.2, 150.9; MS (EI) m/z (%): 402 (92.5) [M⁺], 400 (100) [M⁺], 387 (20.6), 385 (20.3), 321 (7.5), 306 (47.5), 291 (55.2), 229 (13.3), 215 (8.9), 165 (8.6); HRMS (EI) Calcd. for C₂₅H₂₁Br (M⁺) requires 400.0827, Found: 400.0822.

7,11b-Dihydro-7,9,11b-trimethyl-5-phenyl-6aH-benzo[c]fluorene (2d). A colorless liquid. IR (CH₂Cl₂): ν 3056, 3024, 2957, 2923, 2869, 1599, 1492, 1479, 1443, 1369, 1265, 1029, 816, 776, 763, 739, 704, 596 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.42 (3H, d, J = 6.9 Hz, CH₃), 1.56 (3H, s, CH₃), 2.38 (3H, s, CH₃), 2.45-2.51 (1H, m, CH), 2.88-2.94 (1H, m, CH), 6.18 (1H, d, J = 6.3 Hz, Ar₂C=CH), 6.99-7.17 (4H, m, ArH), 7.24-7.42 (7H, m, ArH), 7.50 (1H, d, J = 7.5 Hz, ArH); ¹³C NMR (75 MHz, CDCl₃, TMS): δ 16.5, 21.4, 27.6, 43.8, 48.0, 57.7, 123.3, 124.4, 125.7, 125.8, 127.0, 127.1, 127.2, 127.3, 127.7, 128.2, 129.0, 132.6, 136.1, 139.2, 140.5, 141.0, 142.2, 146.4, 147.7; MS (EI) m/z (%): 336 (79.1) [M⁺], 321 (100), 306 (24.5), 291 (19.5), 243 (33.8), 229 (17.2), 215 (10.3), 193 (31.1), 165 (13.9), 115 (20.6); HRMS (EI) Calcd. for C₂₆H₂₄ (M⁺) requires 336.1878, Found: 336.1878.

2d

2e

7,11b-Dihydro-9-methoxy-7,11b-dimethyl-5-phenyl-6aH-benzo[c]fluorene (2e). A colorless liquid. IR (CH₂Cl₂): ν 3057, 3023, 2955, 2923, 2871, 2832, 1608, 1482, 1443, 1368, 1278, 1232, 1128, 1035, 774, 762, 738, 704, 578 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, TMS): δ 1.41 (3H, d, J = 6.6 Hz, CH₃), 1.55 (3H, s, CH₃), 2.45-2.51 (1H, m, CH), 2.86-2.94 (1H, m, CH), 3.79 (3H, s, OCH₃), 6.17 (1H, d, J = 6.6 Hz, Ar₂C=CH), 6.72-6.73 (1H, m, ArH), 6.85-6.88 (1H, m, ArH), 6.96-7.11 (3H, m, ArH), 7.15-7.40 (6H, m, ArH), 7.49 (1H, d, J = 8.1 Hz, ArH); ¹³C NMR (75 MHz, CDCl₃, TMS): δ 16.4, 27.7, 43.9, 47.6, 55.3, 57.8, 108.7, 111.5, 125.1, 125.7, 125.8, 126.9, 127.1, 127.3, 127.7, 128.2, 129.0, 132.5, 139.3, 140.6, 140.9, 141.4, 142.2, 149.1, 158.9; MS (EI) m/z (%): 352 (68.2) [M⁺], 337 (100), 322 (20.0), 321 (9.3), 307 (5.8), 291 (9.3), 259 (15.9), 229 (3.7), 215 (5.8), 202 (6.2); HRMS (EI) Calcd. for C₂₆H₂₄O (M⁺) requires 352.1827, Found: 352.1832.

2-Fluoro-5-(4-fluorophenyl)-7,11b-dihydro-7,11b-dimethyl-6aH-benzo[*c*]fluorene (2f). A colorless liquid. IR (CH₂Cl₂): ν 3064, 3042, 2962, 2926, 2854, 1601, 1507, 1466, 1384, 1224, 1157, 1015, 838, 761, 748, 594 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, TMS): δ 0.99 (3H, d, J = 7.5 Hz, CH₃), 2.06 (3H, s, CH₃), 2.19-2.31 (1H, m, CH), 3.01-3.06 (1H, m, CH), 6.83 (1H, s, Ar₂C=CH), 6.90-7.06 (4H, m, ArH), 7.08-7.29 (7H, m, ArH); ¹³C NMR (75 MHz, CDCl₃, TMS): δ 11.2, 17.1, 28.5, 29.6, 43.8, 115.0 (d, J_{C-F} = 21.3 Hz), 115.2 (d, J_{C-F} = 21.2 Hz), 118.8, 122.5 (d, J_{C-F} = 15.2 Hz), 125.4, 126.4, 129.0 (d, J_{C-F} = 8.0 Hz), 129.4 (d, J_{C-F} = 7.2 Hz), 132.6 (d, J_{C-F} = 7.7 Hz), 136.7 (d, J_{C-F} = 3.5 Hz), 138.2, 139.8 (d, J_{C-F} = 3.3 Hz), 140.4, 144.2, 144.8, 148.7, 162.2 (d, J_{C-F} = 245.9 Hz), 162.4 (d, J_{C-F} = 246.5 Hz); MS (EI) m/z (%): 358 (75.0) [M⁺], 343 (18.8), 328 (6.0), 247 (13.8), 233 (7.4), 229 (8.6), 203 (100), 202 (6.2), 183 (17.3); HRMS (EI) Calcd. for C₂₅H₂₀F₂ (M⁺) requires 358.1533, Found: 358.1518.

S-20

The crystal data of **2a** has been deposited in CCDC with number 278658. Empirical Formula: $C_{25}H_{22}$; Formula Weight: 322.43; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.516 x 0.175 x 0.163 mm; Crystal System: Monoclinic; Lattice Type: Primitive; Lattice Parameters: $a = 10.3817(15)\text{\AA}$, $b = 20.576(3)\text{\AA}$, $c = 8.7912(13)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 101.985(3)^\circ$, $\gamma = 90^\circ$, $V = 1837.0(5)\text{\AA}^3$; Space group: $P2(1)/c$; $Z = 4$; $D_{calc} = 1.166\text{ g/cm}^3$; $F_{000} = 688$; Diffractometer: Rigaku AFC7R; Residuals: R; R_w : 0.0528, 0.0936.

Table 1. Crystal data and structure refinement for cd2535.

Identification code	cd2535
Empirical formula	C25 H22
Formula weight	322.43
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 10.3817(15) Å alpha = 90 deg. b = 20.576(3) Å beta = 101.985(3) deg. c = 8.7912(13) Å gamma = 90 deg.
Volume	1837.0(5) Å ³
Z, Calculated density	4, 1.166 Mg/m ³
Absorption coefficient	0.066 mm ⁻¹
F(000)	688
Crystal size	0.516 x 0.175 x 0.163 mm
Theta range for data collection	1.98 to 25.50 deg.
Limiting indices	-12<=h<=12, -24<=k<=22, -6<=l<=10
Reflections collected / unique	9656 / 3420 [R(int) = 0.1183]
Completeness to theta = 25.50	99.9 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.65564
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3420 / 3 / 315
Goodness-of-fit on F ²	0.738
Final R indices [I>2sigma(I)]	R1 = 0.0528, wR2 = 0.0936
R indices (all data)	R1 = 0.1395, wR2 = 0.1152
Extinction coefficient	0.0025(7)
Largest diff. peak and hole	0.144 and -0.162 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd2535. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	2833(3)	10568(1)	6004(3)	42(1)
C(2)	1363(3)	10688(2)	5290(4)	51(1)
C(3)	989(3)	11155(1)	6427(4)	50(1)
C(4)	1874(3)	11117(1)	7844(4)	47(1)
C(5)	2912(2)	10605(1)	7790(3)	41(1)
C(6)	2561(2)	9943(1)	8393(3)	40(1)
C(7)	2924(2)	9375(1)	7703(3)	40(1)
C(8)	3483(2)	9409(1)	6307(3)	41(1)
C(9)	3407(3)	9962(1)	5498(4)	46(1)
C(10)	2666(3)	8777(2)	8350(4)	51(1)
C(11)	2064(3)	8741(2)	9594(4)	57(1)
C(12)	1685(3)	9294(2)	10256(4)	57(1)
C(13)	1947(3)	9893(2)	9640(4)	52(1)
C(14)	1752(4)	11528(2)	9051(4)	63(1)
C(15)	731(4)	11981(2)	8839(6)	81(1)
C(16)	-156(4)	12004(2)	7434(6)	84(1)
C(17)	-40(3)	11599(2)	6226(5)	71(1)
C(18)	4093(3)	8823(1)	5769(3)	47(1)
C(19)	3646(3)	8560(2)	4305(4)	58(1)
C(20)	4217(4)	8017(2)	3800(4)	70(1)
C(21)	5272(4)	7730(2)	4758(5)	70(1)
C(22)	5758(4)	7986(2)	6201(4)	66(1)
C(23)	5185(3)	8528(2)	6699(4)	59(1)
C(24)	1089(5)	10896(2)	3586(5)	81(1)
C(25)	4296(3)	10793(2)	8679(5)	60(1)

Table 3. Bond lengths [Å] and angles [deg] for cd2535.

C(1)-C(9)	1.489(4)
C(1)-C(2)	1.544(3)
C(1)-C(5)	1.557(4)
C(1)-H(1)	1.012(19)
C(2)-C(3)	1.495(4)
C(2)-C(24)	1.526(5)
C(2)-H(2)	0.98(2)
C(3)-C(4)	1.387(4)
C(3)-C(17)	1.389(4)
C(4)-C(14)	1.383(4)
C(4)-C(5)	1.515(3)
C(5)-C(6)	1.533(3)
C(5)-C(25)	1.536(4)
C(6)-C(13)	1.382(4)
C(6)-C(7)	1.404(3)
C(7)-C(10)	1.405(4)
C(7)-C(8)	1.464(3)
C(8)-C(9)	1.336(3)
C(8)-C(18)	1.483(3)
C(9)-H(9)	1.00(2)
C(10)-C(11)	1.370(4)
C(10)-H(10)	1.01(3)
C(11)-C(12)	1.373(4)
C(11)-H(11)	1.00(3)
C(12)-C(13)	1.394(4)
C(12)-H(12)	1.01(2)
C(13)-H(13)	0.98(2)
C(14)-C(15)	1.395(5)
C(14)-H(14)	0.98(3)
C(15)-C(16)	1.379(5)
C(15)-H(15)	1.01(3)
C(16)-C(17)	1.374(5)
C(16)-H(16)	1.02(3)
C(17)-H(17)	0.98(3)
C(18)-C(19)	1.385(4)
C(18)-C(23)	1.393(4)
C(19)-C(20)	1.379(4)
C(19)-H(19)	0.95(2)
C(20)-C(21)	1.369(4)
C(20)-H(20)	1.03(3)
C(21)-C(22)	1.369(4)
C(21)-H(21)	0.987(16)
C(22)-C(23)	1.377(4)
C(22)-H(22)	0.98(3)
C(23)-H(23)	0.94(2)
C(24)-H(3)	1.017(18)
C(24)-H(4)	0.91(3)
C(24)-H(5)	1.024(19)
C(25)-H(6)	1.01(3)
C(25)-H(7)	1.02(3)
C(25)-H(8)	0.97(3)
C(9)-C(1)-C(2)	115.8(2)
C(9)-C(1)-C(5)	113.7(2)
C(2)-C(1)-C(5)	104.0(2)
C(9)-C(1)-H(1)	105.7(12)
C(2)-C(1)-H(1)	109.2(11)
C(5)-C(1)-H(1)	108.2(12)
C(3)-C(2)-C(24)	117.0(3)
C(3)-C(2)-C(1)	101.7(2)
C(24)-C(2)-C(1)	114.3(3)
C(3)-C(2)-H(2)	107.7(16)
C(24)-C(2)-H(2)	107.8(16)
C(1)-C(2)-H(2)	107.8(14)
C(4)-C(3)-C(17)	119.9(3)
C(4)-C(3)-C(2)	110.4(3)
C(17)-C(3)-C(2)	129.6(3)
C(14)-C(4)-C(3)	120.4(3)

C(14)-C(4)-C(5)	128.9(3)
C(3)-C(4)-C(5)	110.7(3)
C(4)-C(5)-C(6)	112.7(2)
C(4)-C(5)-C(25)	113.9(2)
C(6)-C(5)-C(25)	108.2(2)
C(4)-C(5)-C(1)	100.2(2)
C(6)-C(5)-C(1)	109.8(2)
C(25)-C(5)-C(1)	111.9(3)
C(13)-C(6)-C(7)	119.3(3)
C(13)-C(6)-C(5)	121.6(3)
C(7)-C(6)-C(5)	119.1(3)
C(6)-C(7)-C(10)	117.6(3)
C(6)-C(7)-C(8)	120.8(3)
C(10)-C(7)-C(8)	121.5(3)
C(9)-C(8)-C(7)	119.8(3)
C(9)-C(8)-C(18)	120.3(3)
C(7)-C(8)-C(18)	119.9(2)
C(8)-C(9)-C(1)	122.5(3)
C(8)-C(9)-H(9)	122.0(13)
C(1)-C(9)-H(9)	115.5(13)
C(11)-C(10)-C(7)	121.8(3)
C(11)-C(10)-H(10)	121.0(15)
C(7)-C(10)-H(10)	117.2(15)
C(10)-C(11)-C(12)	120.8(3)
C(10)-C(11)-H(11)	124.4(15)
C(12)-C(11)-H(11)	114.8(15)
C(11)-C(12)-C(13)	118.2(3)
C(11)-C(12)-H(12)	122.4(14)
C(13)-C(12)-H(12)	119.2(14)
C(6)-C(13)-C(12)	122.3(3)
C(6)-C(13)-H(13)	124.4(15)
C(12)-C(13)-H(13)	113.3(15)
C(4)-C(14)-C(15)	119.6(4)
C(4)-C(14)-H(14)	124.0(17)
C(15)-C(14)-H(14)	116.3(17)
C(16)-C(15)-C(14)	119.3(4)
C(16)-C(15)-H(15)	123.1(18)
C(14)-C(15)-H(15)	117.5(19)
C(17)-C(16)-C(15)	121.5(4)
C(17)-C(16)-H(16)	123.8(17)
C(15)-C(16)-H(16)	114.7(17)
C(16)-C(17)-C(3)	119.3(4)
C(16)-C(17)-H(17)	122.0(19)
C(3)-C(17)-H(17)	118.3(19)
C(19)-C(18)-C(23)	116.7(3)
C(19)-C(18)-C(8)	122.2(3)
C(23)-C(18)-C(8)	121.1(3)
C(20)-C(19)-C(18)	122.2(3)
C(20)-C(19)-H(19)	122.0(17)
C(18)-C(19)-H(19)	115.7(17)
C(21)-C(20)-C(19)	119.5(3)
C(21)-C(20)-H(20)	118.3(17)
C(19)-C(20)-H(20)	122.1(17)
C(20)-C(21)-C(22)	119.9(3)
C(20)-C(21)-H(21)	117.9(16)
C(22)-C(21)-H(21)	121.6(16)
C(21)-C(22)-C(23)	120.3(3)
C(21)-C(22)-H(22)	121.0(16)
C(23)-C(22)-H(22)	118.6(17)
C(22)-C(23)-C(18)	121.3(3)
C(22)-C(23)-H(23)	118.9(16)
C(18)-C(23)-H(23)	119.6(16)
C(2)-C(24)-H(3)	108(2)
C(2)-C(24)-H(4)	112(2)
H(3)-C(24)-H(4)	109(3)
C(2)-C(24)-H(5)	107(2)
H(3)-C(24)-H(5)	109(3)
H(4)-C(24)-H(5)	113(3)
C(5)-C(25)-H(6)	110.4(16)
C(5)-C(25)-H(7)	106.1(16)
H(6)-C(25)-H(7)	113(2)
C(5)-C(25)-H(8)	111.1(16)

H(6)-C(25)-H(8)	104(2)
H(7)-C(25)-H(8)	111(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd2535.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	43(2)	43(2)	42(2)	7(2)	11(1)	-4(1)
C(2)	48(2)	50(2)	51(2)	8(2)	1(2)	-3(2)
C(3)	45(2)	44(2)	64(2)	12(2)	16(2)	1(2)
C(4)	47(2)	39(2)	56(2)	2(2)	14(2)	-5(2)
C(5)	37(2)	39(2)	44(2)	-3(2)	6(1)	-1(1)
C(6)	37(2)	45(2)	35(2)	4(2)	3(1)	2(1)
C(7)	37(2)	44(2)	38(2)	2(2)	4(1)	-1(1)
C(8)	42(2)	43(2)	38(2)	-1(2)	5(1)	-2(1)
C(9)	51(2)	49(2)	39(2)	2(2)	11(2)	2(2)
C(10)	53(2)	48(2)	50(2)	1(2)	11(2)	2(2)
C(11)	66(2)	57(2)	49(2)	14(2)	16(2)	-1(2)
C(12)	68(2)	65(2)	43(2)	11(2)	18(2)	5(2)
C(13)	58(2)	56(2)	40(2)	-2(2)	10(2)	2(2)
C(14)	74(3)	47(2)	70(3)	-6(2)	21(2)	-4(2)
C(15)	94(3)	56(3)	105(4)	-7(3)	52(3)	6(2)
C(16)	80(3)	62(3)	121(4)	28(3)	48(3)	28(2)
C(17)	61(2)	69(3)	86(3)	30(2)	23(2)	15(2)
C(18)	59(2)	39(2)	44(2)	1(2)	14(2)	-2(2)
C(19)	65(2)	51(2)	55(2)	-5(2)	3(2)	5(2)
C(20)	94(3)	56(2)	59(3)	-20(2)	12(2)	1(2)
C(21)	100(3)	51(2)	66(3)	-3(2)	36(2)	16(2)
C(22)	87(3)	58(2)	54(2)	9(2)	21(2)	26(2)
C(23)	81(2)	55(2)	39(2)	0(2)	9(2)	16(2)
C(24)	75(3)	99(4)	59(3)	17(3)	-7(2)	16(3)
C(25)	53(2)	61(3)	60(3)	-7(2)	0(2)	-12(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd2535.

	x	y	z	U(eq)
H(1)	3374(19)	10937(9)	5700(20)	38(6)
H(2)	890(20)	10280(12)	5360(30)	67(9)
H(3)	1580(30)	11319(12)	3510(40)	133(17)
H(4)	210(30)	10963(14)	3210(40)	83(12)
H(5)	1470(30)	10541(14)	2990(40)	137(18)
H(6)	4980(30)	10493(13)	8390(30)	80(11)
H(7)	4270(30)	10775(13)	9830(30)	77(11)
H(8)	4540(20)	11223(14)	8380(30)	75(11)
H(9)	3770(20)	10002(10)	4540(30)	45(8)
H(10)	2930(20)	8371(13)	7840(30)	67(9)
H(11)	1840(20)	8326(12)	10070(30)	62(9)
H(12)	1170(20)	9282(11)	11110(30)	57(8)
H(13)	1640(20)	10264(12)	10160(30)	52(8)
H(14)	2320(30)	11510(13)	10090(30)	73(11)
H(15)	650(30)	12260(15)	9760(40)	103(13)
H(16)	-880(30)	12344(13)	7370(30)	82(10)
H(17)	-600(30)	11647(15)	5190(40)	93(12)
H(19)	2940(20)	8781(12)	3660(30)	65(9)
H(20)	3910(30)	7836(14)	2700(40)	102(12)
H(21)	5740(20)	7380(10)	4320(30)	73(10)
H(22)	6520(20)	7793(13)	6890(30)	73(10)
H(23)	5490(20)	8676(12)	7720(30)	59(9)

Table 6. Torsion angles [deg] for cd2535.

C(9)-C(1)-C(2)-C(3)	159.4(3)
C(5)-C(1)-C(2)-C(3)	33.9(3)
C(9)-C(1)-C(2)-C(24)	-73.6(4)
C(5)-C(1)-C(2)-C(24)	160.9(3)
C(24)-C(2)-C(3)-C(4)	-145.9(3)
C(1)-C(2)-C(3)-C(4)	-20.7(3)
C(24)-C(2)-C(3)-C(17)	32.2(5)
C(1)-C(2)-C(3)-C(17)	157.4(3)
C(17)-C(3)-C(4)-C(14)	-1.2(4)
C(2)-C(3)-C(4)-C(14)	177.1(3)
C(17)-C(3)-C(4)-C(5)	-179.6(2)
C(2)-C(3)-C(4)-C(5)	-1.3(3)
C(14)-C(4)-C(5)-C(6)	87.6(3)
C(3)-C(4)-C(5)-C(6)	-94.2(3)
C(14)-C(4)-C(5)-C(25)	-36.2(4)
C(3)-C(4)-C(5)-C(25)	142.1(3)
C(14)-C(4)-C(5)-C(1)	-155.8(3)
C(3)-C(4)-C(5)-C(1)	22.4(3)
C(9)-C(1)-C(5)-C(4)	-161.0(2)
C(2)-C(1)-C(5)-C(4)	-34.1(3)
C(9)-C(1)-C(5)-C(6)	-42.2(3)
C(2)-C(1)-C(5)-C(6)	84.6(3)
C(9)-C(1)-C(5)-C(25)	77.9(3)
C(2)-C(1)-C(5)-C(25)	-155.3(3)
C(4)-C(5)-C(6)-C(13)	-37.7(3)
C(25)-C(5)-C(6)-C(13)	89.2(3)
C(1)-C(5)-C(6)-C(13)	-148.4(2)
C(4)-C(5)-C(6)-C(7)	145.1(2)
C(25)-C(5)-C(6)-C(7)	-88.0(3)
C(1)-C(5)-C(6)-C(7)	34.4(3)
C(13)-C(6)-C(7)-C(10)	-1.4(4)
C(5)-C(6)-C(7)-C(10)	175.8(2)
C(13)-C(6)-C(7)-C(8)	175.3(2)
C(5)-C(6)-C(7)-C(8)	-7.4(3)
C(6)-C(7)-C(8)-C(9)	-13.6(4)
C(10)-C(7)-C(8)-C(9)	163.0(3)
C(6)-C(7)-C(8)-C(18)	168.4(2)
C(10)-C(7)-C(8)-C(18)	-15.0(4)
C(7)-C(8)-C(9)-C(1)	3.4(4)
C(18)-C(8)-C(9)-C(1)	-178.6(2)
C(2)-C(1)-C(9)-C(8)	-94.7(3)
C(5)-C(1)-C(9)-C(8)	25.7(4)
C(6)-C(7)-C(10)-C(11)	1.1(4)
C(8)-C(7)-C(10)-C(11)	-175.6(3)
C(7)-C(10)-C(11)-C(12)	0.1(5)
C(10)-C(11)-C(12)-C(13)	-0.8(5)
C(7)-C(6)-C(13)-C(12)	0.8(4)
C(5)-C(6)-C(13)-C(12)	-176.5(2)
C(11)-C(12)-C(13)-C(6)	0.4(4)
C(3)-C(4)-C(14)-C(15)	0.1(5)
C(5)-C(4)-C(14)-C(15)	178.3(3)
C(4)-C(14)-C(15)-C(16)	1.1(5)
C(14)-C(15)-C(16)-C(17)	-1.4(6)
C(15)-C(16)-C(17)-C(3)	0.3(6)
C(4)-C(3)-C(17)-C(16)	1.0(5)
C(2)-C(3)-C(17)-C(16)	-177.0(3)
C(9)-C(8)-C(18)-C(19)	-56.8(4)
C(7)-C(8)-C(18)-C(19)	121.2(3)
C(9)-C(8)-C(18)-C(23)	120.5(3)
C(7)-C(8)-C(18)-C(23)	-61.5(4)
C(23)-C(18)-C(19)-C(20)	2.2(5)
C(8)-C(18)-C(19)-C(20)	179.6(3)
C(18)-C(19)-C(20)-C(21)	-0.9(5)
C(19)-C(20)-C(21)-C(22)	-0.5(5)
C(20)-C(21)-C(22)-C(23)	0.5(5)
C(21)-C(22)-C(23)-C(18)	0.9(5)
C(19)-C(18)-C(23)-C(22)	-2.2(5)
C(8)-C(18)-C(23)-C(22)	-179.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd2535 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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Table 1. Crystal data and structure refinement for cd25291.

Identification code	cd25291
Empirical formula	C30 H24
Formula weight	384.49
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 13.4641(13) Å alpha = 90 deg. b = 11.2411(11) Å beta = 99.602(2) deg. c = 14.4956(14) Å gamma = 90 deg.
Volume	2163.2(4) Å ³
Z, Calculated density	4, 1.181 Mg/m ³
Absorption coefficient	0.067 mm ⁻¹
F(000)	816
Crystal size	0.508 x 0.479 x 0.318 mm
Theta range for data collection	1.91 to 27.00 deg.
Limiting indices	-14<=h<=17, -13<=k<=14, -18<=l<=15
Reflections collected / unique	12406 / 4713 [R(int) = 0.1314]
Completeness to theta = 27.00	99.7 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.78765
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4713 / 0 / 280
Goodness-of-fit on F ²	0.998
Final R indices [I>2sigma(I)]	R1 = 0.0635, wR2 = 0.1540
R indices (all data)	R1 = 0.0886, wR2 = 0.1677
Largest diff. peak and hole	0.223 and -0.257 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd25291. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(4)	7903(1)	2010(2)	917(1)	41(1)
C(13)	8950(1)	1566(2)	1012(1)	40(1)
C(6)	6370(1)	2750(2)	170(1)	44(1)
C(1)	7203(1)	1666(2)	3278(1)	43(1)
C(25)	6209(1)	1054(2)	3088(1)	44(1)
C(3)	7338(1)	2138(2)	1595(1)	44(1)
C(5)	7315(1)	2375(2)	13(1)	43(1)
C(2)	7701(1)	2019(2)	2602(1)	47(1)
C(19)	7642(1)	1873(2)	4278(1)	44(1)
C(18)	9186(1)	405(2)	1268(1)	52(1)
C(14)	9724(1)	2296(2)	817(1)	52(1)
C(7)	6297(1)	2621(2)	1182(1)	45(1)
C(11)	5930(2)	3221(2)	-1450(1)	59(1)
C(9)	7562(1)	2396(2)	-872(1)	51(1)
C(20)	8064(1)	2967(2)	4561(1)	54(1)
C(12)	5673(1)	3182(2)	-571(1)	52(1)
C(30)	6030(2)	182(2)	2408(1)	57(1)
C(10)	6858(2)	2832(2)	-1604(1)	58(1)
C(26)	5450(1)	1296(2)	3596(1)	55(1)
C(17)	10153(1)	-26(2)	1331(1)	60(1)
C(16)	10905(1)	703(2)	1132(1)	58(1)
C(15)	10695(1)	1857(2)	883(1)	60(1)
C(24)	7639(1)	999(2)	4953(1)	56(1)
C(29)	5114(2)	-398(2)	2222(2)	69(1)
C(8)	6041(1)	3764(2)	1646(2)	62(1)
C(21)	8468(1)	3189(2)	5488(2)	69(1)
C(27)	4537(2)	707(2)	3416(2)	70(1)
C(22)	8463(2)	2315(3)	6141(2)	73(1)
C(28)	4371(2)	-133(2)	2724(2)	71(1)
C(23)	8060(2)	1225(2)	5883(1)	70(1)

Table 3. Bond lengths [Å] and angles [deg] for cd25291.

C(4)-C(3)	1.347(2)
C(4)-C(5)	1.472(2)
C(4)-C(13)	1.479(2)
C(13)-C(18)	1.379(3)
C(13)-C(14)	1.392(2)
C(6)-C(12)	1.390(2)
C(6)-C(5)	1.393(2)
C(6)-C(7)	1.494(3)
C(1)-C(2)	1.337(3)
C(1)-C(25)	1.488(2)
C(1)-C(19)	1.489(2)
C(25)-C(30)	1.383(2)
C(25)-C(26)	1.383(3)
C(3)-C(2)	1.465(2)
C(3)-C(7)	1.530(2)
C(5)-C(9)	1.379(3)
C(2)-H(2)	0.977(18)
C(19)-C(20)	1.387(3)
C(19)-C(24)	1.388(3)
C(18)-C(17)	1.377(2)
C(18)-H(18)	0.9300
C(14)-C(15)	1.386(3)
C(14)-H(14)	0.9300
C(7)-C(8)	1.516(3)
C(7)-H(7)	1.012(18)
C(11)-C(12)	1.376(3)
C(11)-C(10)	1.376(3)
C(11)-H(11)	0.9300
C(9)-C(10)	1.389(3)
C(9)-H(9)	0.9300
C(20)-C(21)	1.386(3)
C(20)-H(20)	0.9300
C(12)-H(12)	0.9300
C(30)-C(29)	1.381(3)
C(30)-H(30)	0.9300
C(10)-H(10)	0.9300
C(26)-C(27)	1.382(3)
C(26)-H(26)	0.9300
C(17)-C(16)	1.371(3)
C(17)-H(17)	0.9300
C(16)-C(15)	1.363(3)
C(16)-H(16)	0.9300
C(15)-H(15)	0.9300
C(24)-C(23)	1.395(3)
C(24)-H(24)	0.9300
C(29)-C(28)	1.364(3)
C(29)-H(29)	0.9300
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(21)-C(22)	1.365(3)
C(21)-H(21)	0.9300
C(27)-C(28)	1.369(3)
C(27)-H(27)	0.9300
C(22)-C(23)	1.367(3)
C(22)-H(22)	0.9300
C(28)-H(28)	0.9300
C(23)-H(23)	0.9300
C(3)-C(4)-C(5)	109.51(15)
C(3)-C(4)-C(13)	127.79(15)
C(5)-C(4)-C(13)	122.70(14)
C(18)-C(13)-C(14)	117.75(16)
C(18)-C(13)-C(4)	121.19(15)
C(14)-C(13)-C(4)	121.03(16)
C(12)-C(6)-C(5)	119.79(17)
C(12)-C(6)-C(7)	130.18(17)
C(5)-C(6)-C(7)	110.03(14)

C(2)-C(1)-C(25)	123.14(16)
C(2)-C(1)-C(19)	120.07(15)
C(25)-C(1)-C(19)	116.79(14)
C(30)-C(25)-C(26)	117.52(17)
C(30)-C(25)-C(1)	120.31(16)
C(26)-C(25)-C(1)	122.13(16)
C(4)-C(3)-C(2)	125.58(15)
C(4)-C(3)-C(7)	110.13(15)
C(2)-C(3)-C(7)	123.65(15)
C(9)-C(5)-C(6)	120.99(15)
C(9)-C(5)-C(4)	130.95(16)
C(6)-C(5)-C(4)	108.05(15)
C(1)-C(2)-C(3)	129.25(16)
C(1)-C(2)-H(2)	117.7(10)
C(3)-C(2)-H(2)	113.1(10)
C(20)-C(19)-C(24)	117.90(17)
C(20)-C(19)-C(1)	120.17(16)
C(24)-C(19)-C(1)	121.92(17)
C(17)-C(18)-C(13)	121.59(17)
C(17)-C(18)-H(18)	119.2
C(13)-C(18)-H(18)	119.2
C(15)-C(14)-C(13)	120.34(18)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(6)-C(7)-C(8)	114.23(16)
C(6)-C(7)-C(3)	102.26(14)
C(8)-C(7)-C(3)	112.79(14)
C(6)-C(7)-H(7)	108.4(10)
C(8)-C(7)-H(7)	109.9(10)
C(3)-C(7)-H(7)	109.0(10)
C(12)-C(11)-C(10)	121.00(17)
C(12)-C(11)-H(11)	119.5
C(10)-C(11)-H(11)	119.5
C(5)-C(9)-C(10)	118.48(19)
C(5)-C(9)-H(9)	120.8
C(10)-C(9)-H(9)	120.8
C(21)-C(20)-C(19)	121.4(2)
C(21)-C(20)-H(20)	119.3
C(19)-C(20)-H(20)	119.3
C(11)-C(12)-C(6)	119.01(18)
C(11)-C(12)-H(12)	120.5
C(6)-C(12)-H(12)	120.5
C(29)-C(30)-C(25)	121.18(19)
C(29)-C(30)-H(30)	119.4
C(25)-C(30)-H(30)	119.4
C(11)-C(10)-C(9)	120.70(19)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(27)-C(26)-C(25)	121.23(19)
C(27)-C(26)-H(26)	119.4
C(25)-C(26)-H(26)	119.4
C(16)-C(17)-C(18)	119.9(2)
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-H(17)	120.0
C(15)-C(16)-C(17)	119.73(18)
C(15)-C(16)-H(16)	120.1
C(17)-C(16)-H(16)	120.1
C(16)-C(15)-C(14)	120.64(18)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(19)-C(24)-C(23)	120.3(2)
C(19)-C(24)-H(24)	119.9
C(23)-C(24)-H(24)	119.9
C(28)-C(29)-C(30)	120.3(2)
C(28)-C(29)-H(29)	119.9
C(30)-C(29)-H(29)	119.9
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5

C(22)-C(21)-C(20)	119.8(2)
C(22)-C(21)-H(21)	120.1
C(20)-C(21)-H(21)	120.1
C(28)-C(27)-C(26)	120.0(2)
C(28)-C(27)-H(27)	120.0
C(26)-C(27)-H(27)	120.0
C(21)-C(22)-C(23)	120.2(2)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(29)-C(28)-C(27)	119.8(2)
C(29)-C(28)-H(28)	120.1
C(27)-C(28)-H(28)	120.1
C(22)-C(23)-C(24)	120.4(2)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd25291.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(4)	37(1)	46(1)	39(1)	0(1)	0(1)	-6(1)
C(13)	36(1)	52(1)	31(1)	0(1)	1(1)	-4(1)
C(6)	37(1)	44(1)	46(1)	-1(1)	-3(1)	-8(1)
C(1)	38(1)	48(1)	42(1)	-2(1)	4(1)	4(1)
C(25)	45(1)	43(1)	44(1)	2(1)	4(1)	2(1)
C(3)	35(1)	52(1)	42(1)	-2(1)	0(1)	-3(1)
C(5)	40(1)	43(1)	41(1)	-1(1)	-2(1)	-6(1)
C(2)	34(1)	62(1)	43(1)	-3(1)	1(1)	-1(1)
C(19)	34(1)	56(1)	42(1)	-1(1)	4(1)	8(1)
C(18)	42(1)	56(1)	58(1)	4(1)	6(1)	-6(1)
C(14)	44(1)	61(1)	51(1)	9(1)	1(1)	-8(1)
C(7)	32(1)	56(1)	47(1)	-3(1)	2(1)	-5(1)
C(11)	57(1)	62(1)	49(1)	9(1)	-15(1)	-11(1)
C(9)	50(1)	57(1)	44(1)	0(1)	1(1)	-4(1)
C(20)	47(1)	64(1)	50(1)	-1(1)	2(1)	0(1)
C(12)	39(1)	55(1)	57(1)	3(1)	-8(1)	-4(1)
C(30)	67(1)	47(1)	59(1)	-6(1)	13(1)	-4(1)
C(10)	63(1)	67(1)	39(1)	4(1)	-4(1)	-9(1)
C(26)	47(1)	60(1)	58(1)	-7(1)	7(1)	1(1)
C(17)	52(1)	60(1)	65(1)	3(1)	2(1)	6(1)
C(16)	38(1)	84(2)	51(1)	-3(1)	2(1)	7(1)
C(15)	36(1)	88(2)	55(1)	8(1)	4(1)	-15(1)
C(24)	59(1)	59(1)	49(1)	5(1)	8(1)	15(1)
C(29)	81(2)	51(1)	71(1)	-8(1)	-1(1)	-15(1)
C(8)	55(1)	67(1)	64(1)	-9(1)	5(1)	6(1)
C(21)	47(1)	93(2)	62(1)	-22(1)	-4(1)	-4(1)
C(27)	46(1)	74(2)	92(2)	1(1)	18(1)	0(1)
C(22)	51(1)	117(2)	47(1)	-9(1)	-8(1)	21(1)
C(28)	52(1)	62(1)	95(2)	3(1)	-3(1)	-13(1)
C(23)	69(1)	94(2)	46(1)	16(1)	5(1)	34(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd25291.

	x	y	z	U(eq)
H(18)	8681	-99	1401	63
H(14)	9588	3083	640	63
H(11)	5470	3515	-1948	70
H(9)	8186	2123	-977	61
H(20)	8075	3564	4119	65
H(12)	5043	3441	-473	62
H(30)	6535	-18	2069	69
H(10)	7014	2861	-2205	69
H(26)	5556	1865	4068	66
H(17)	10295	-811	1509	72
H(16)	11557	412	1166	70
H(15)	11208	2354	757	72
H(24)	7356	259	4786	67
H(29)	5003	-970	1753	83
H(8A)	6572	4332	1636	94
H(8B)	5969	3603	2281	94
H(8C)	5422	4080	1313	94
H(21)	8742	3930	5664	83
H(27)	4035	882	3765	84
H(22)	8734	2462	6763	88
H(28)	3754	-523	2596	85
H(23)	8066	630	6329	84
H(7)	5773(14)	1993(17)	1243(13)	54(5)
H(2)	8413(14)	2222(15)	2781(12)	48(5)

Table 6. Torsion angles [deg] for cd25291.

C(3)-C(4)-C(13)-C(18)	65.6(3)
C(5)-C(4)-C(13)-C(18)	-113.69(19)
C(3)-C(4)-C(13)-C(14)	-116.5(2)
C(5)-C(4)-C(13)-C(14)	64.2(2)
C(2)-C(1)-C(25)-C(30)	41.7(3)
C(19)-C(1)-C(25)-C(30)	-137.83(17)
C(2)-C(1)-C(25)-C(26)	-140.6(2)
C(19)-C(1)-C(25)-C(26)	39.9(2)
C(5)-C(4)-C(3)-C(2)	-171.35(16)
C(13)-C(4)-C(3)-C(2)	9.3(3)
C(5)-C(4)-C(3)-C(7)	-0.3(2)
C(13)-C(4)-C(3)-C(7)	-179.66(16)
C(12)-C(6)-C(5)-C(9)	-1.8(3)
C(7)-C(6)-C(5)-C(9)	179.22(16)
C(12)-C(6)-C(5)-C(4)	177.85(15)
C(7)-C(6)-C(5)-C(4)	-1.15(19)
C(3)-C(4)-C(5)-C(9)	-179.52(19)
C(13)-C(4)-C(5)-C(9)	-0.1(3)
C(3)-C(4)-C(5)-C(6)	0.9(2)
C(13)-C(4)-C(5)-C(6)	-179.69(15)
C(25)-C(1)-C(2)-C(3)	14.6(3)
C(19)-C(1)-C(2)-C(3)	-165.81(17)
C(4)-C(3)-C(2)-C(1)	-150.6(2)
C(7)-C(3)-C(2)-C(1)	39.5(3)
C(2)-C(1)-C(19)-C(20)	45.1(2)
C(25)-C(1)-C(19)-C(20)	-135.36(17)
C(2)-C(1)-C(19)-C(24)	-135.36(19)
C(25)-C(1)-C(19)-C(24)	44.2(2)
C(14)-C(13)-C(18)-C(17)	0.1(3)
C(4)-C(13)-C(18)-C(17)	178.00(16)
C(18)-C(13)-C(14)-C(15)	-0.2(2)
C(4)-C(13)-C(14)-C(15)	-178.12(16)
C(12)-C(6)-C(7)-C(8)	-55.7(2)
C(5)-C(6)-C(7)-C(8)	123.11(16)
C(12)-C(6)-C(7)-C(3)	-177.91(18)
C(5)-C(6)-C(7)-C(3)	0.94(18)
C(4)-C(3)-C(7)-C(6)	-0.38(19)
C(2)-C(3)-C(7)-C(6)	170.90(16)
C(4)-C(3)-C(7)-C(8)	-123.53(18)
C(2)-C(3)-C(7)-C(8)	47.7(2)
C(6)-C(5)-C(9)-C(10)	1.9(3)
C(4)-C(5)-C(9)-C(10)	-177.68(17)
C(24)-C(19)-C(20)-C(21)	-0.3(3)
C(1)-C(19)-C(20)-C(21)	179.33(16)
C(10)-C(11)-C(12)-C(6)	0.5(3)
C(5)-C(6)-C(12)-C(11)	0.6(3)
C(7)-C(6)-C(12)-C(11)	179.34(18)
C(26)-C(25)-C(30)-C(29)	2.1(3)
C(1)-C(25)-C(30)-C(29)	179.91(18)
C(12)-C(11)-C(10)-C(9)	-0.4(3)
C(5)-C(9)-C(10)-C(11)	-0.8(3)
C(30)-C(25)-C(26)-C(27)	-1.5(3)
C(1)-C(25)-C(26)-C(27)	-179.27(17)
C(13)-C(18)-C(17)-C(16)	-0.4(3)
C(18)-C(17)-C(16)-C(15)	0.8(3)
C(17)-C(16)-C(15)-C(14)	-1.0(3)
C(13)-C(14)-C(15)-C(16)	0.6(3)
C(20)-C(19)-C(24)-C(23)	-0.6(3)
C(1)-C(19)-C(24)-C(23)	179.83(16)
C(25)-C(30)-C(29)-C(28)	-1.3(3)
C(19)-C(20)-C(21)-C(22)	0.6(3)
C(25)-C(26)-C(27)-C(28)	0.1(3)
C(20)-C(21)-C(22)-C(23)	0.0(3)
C(30)-C(29)-C(28)-C(27)	-0.2(3)
C(26)-C(27)-C(28)-C(29)	0.8(3)
C(21)-C(22)-C(23)-C(24)	-0.8(3)
C(19)-C(24)-C(23)-C(22)	1.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd25291 [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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