

New Pd(II) Hemichelates Devoid of Incipient Bridging CO...Pd interactions

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Electronic Supporting Information

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Experimental Section

Complex 1c

$C_6D_6 - ^1H - 500\text{ MHz} - 293\text{ K.}$

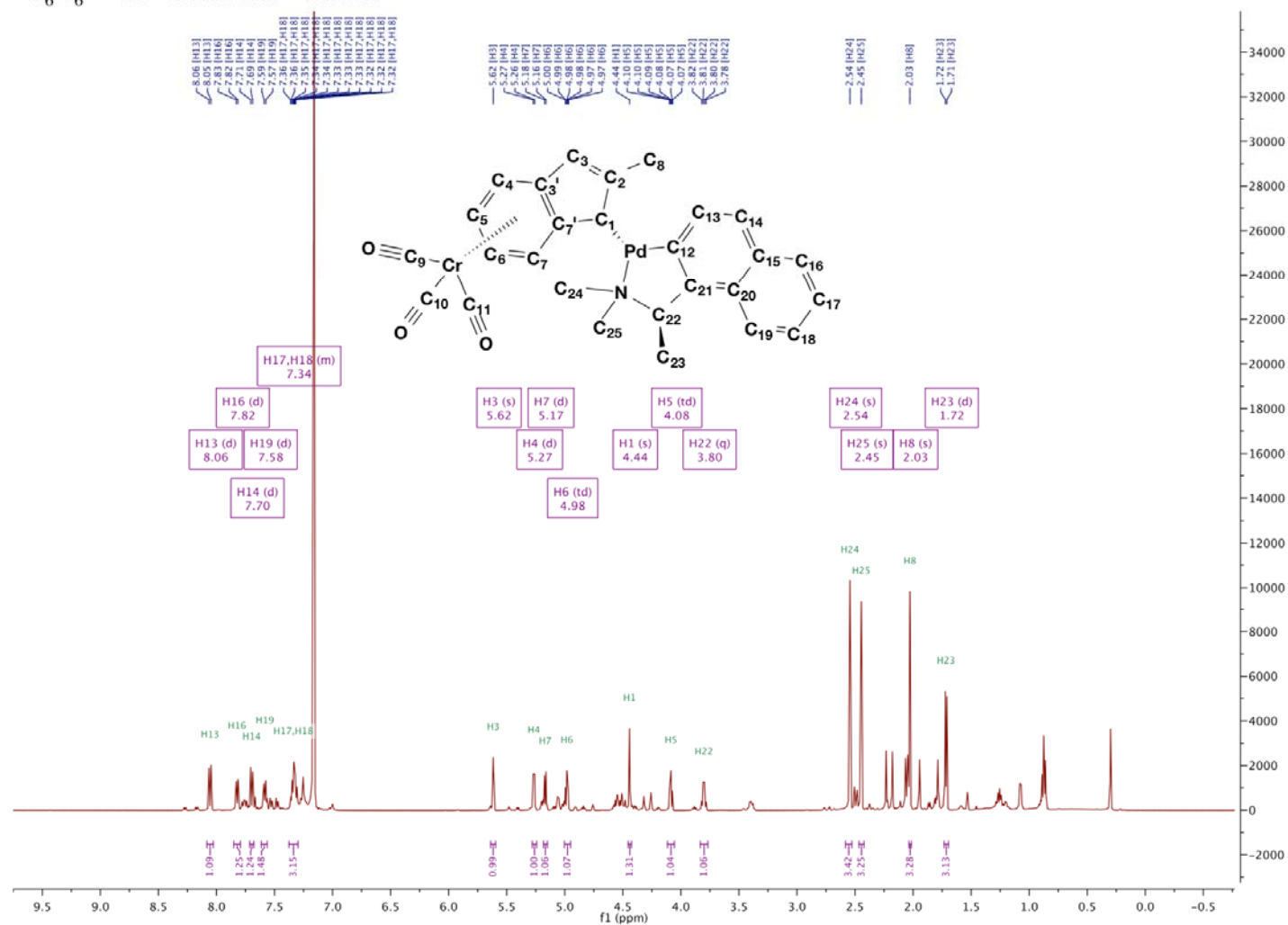


Figure 1. 1H NMR spectrum of **1c** in d_6 .benzene at 293 K

$C_6D_6 - ^{13}C - 126\text{ MHz} - 293\text{ K.}$

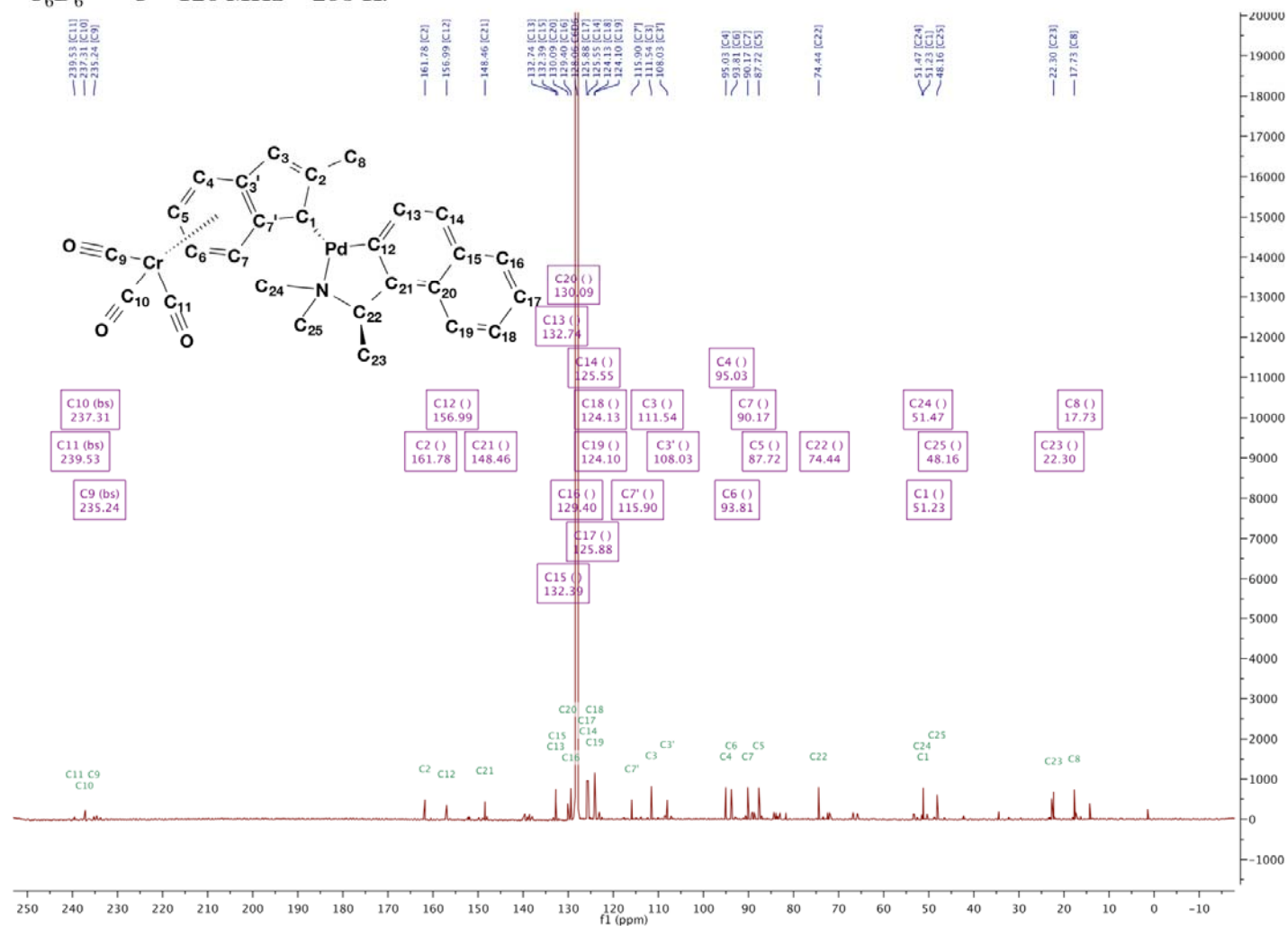


Figure 2. ^{13}C NMR spectrum of 1c in d_6 .benzene at 293 K

Tol – ^1H – 600 MHz – Variable Temperature.

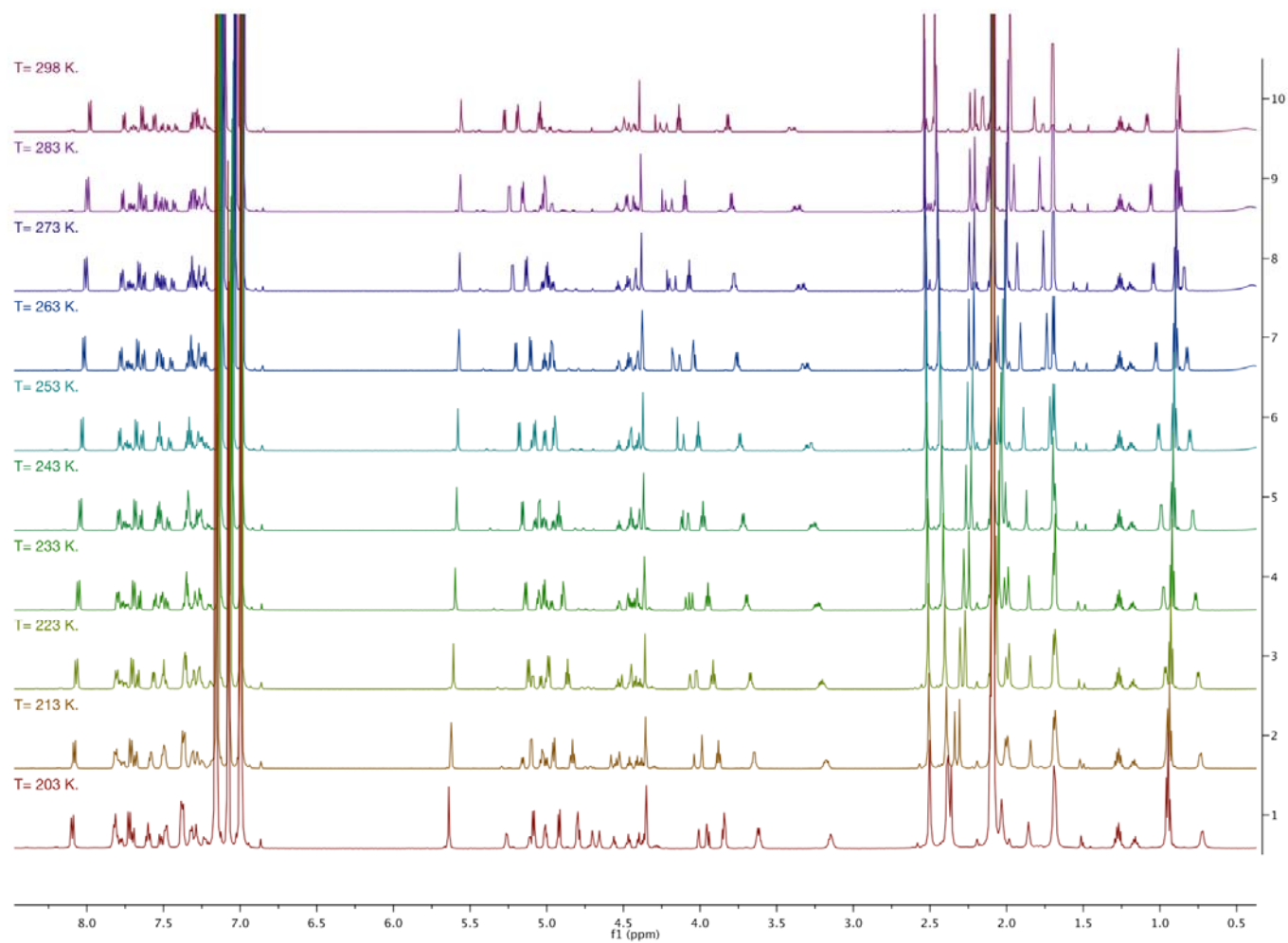


Figure 3. Variable temperature ^1H NMR spectrum of **1c** in d_8 -toluene

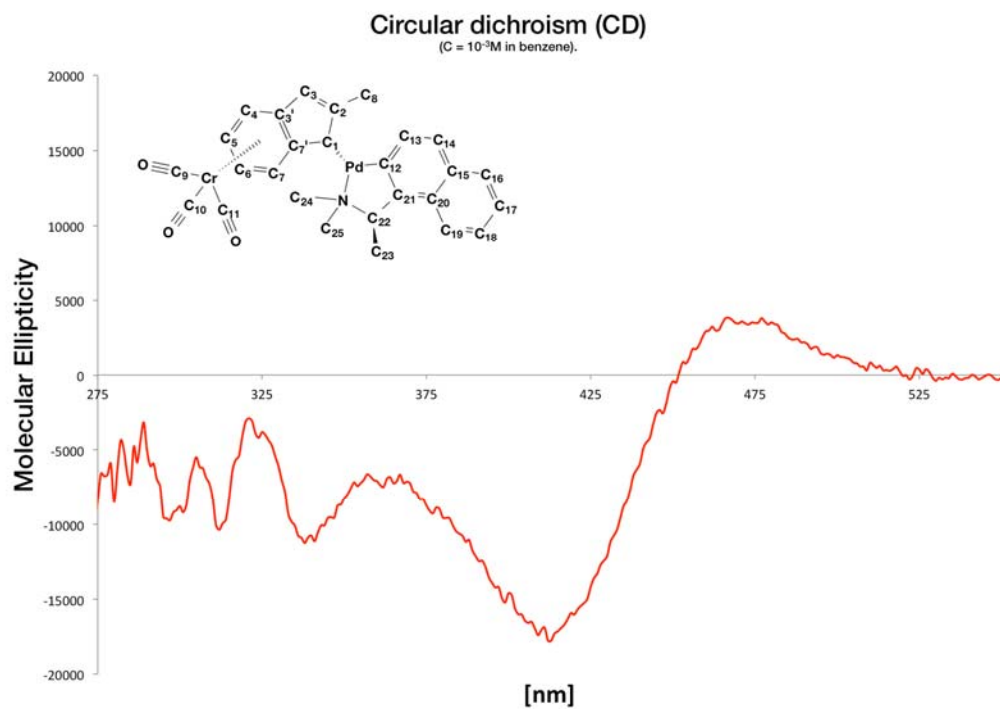


Figure 4. Circular dichrogram of **1c** in benzene at 20.0°C.

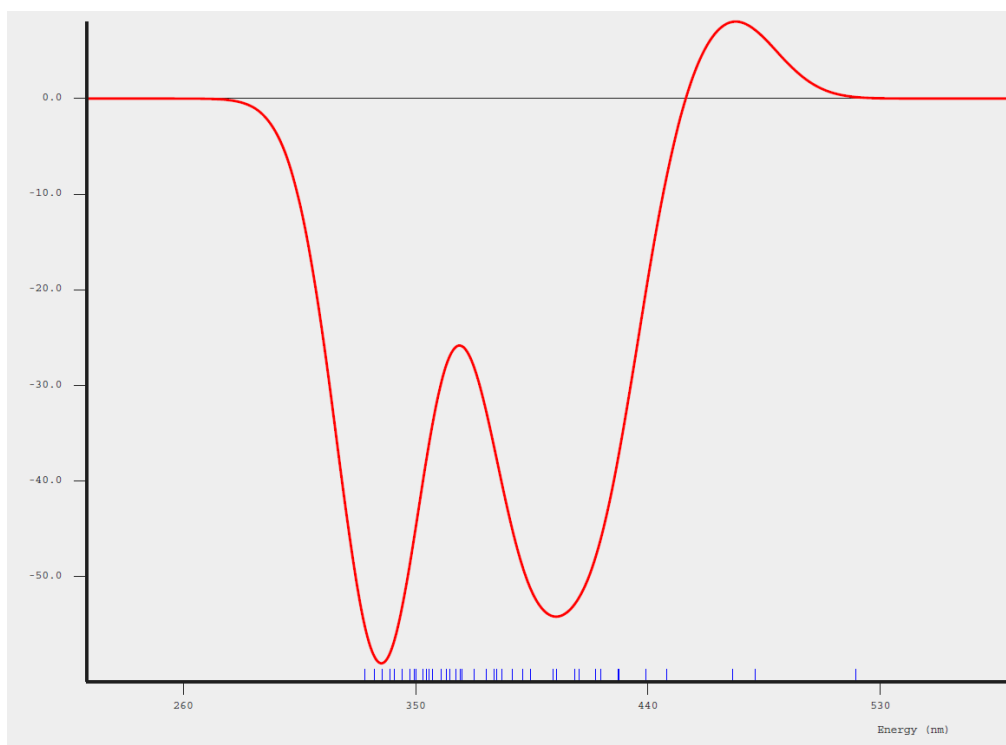


Figure 5. Computed CD response of a gas-phase model of (pS,1R)-**1c** (optimized from resolved X-ray diffraction structure coordinates) optimized at the ZORA-TPSS-D3(BJ)/all electron level using TD-DFT at the ZORA-SAOP/ all electron TZ2P level. No wavelength scaling was applied to the graph.

Complex 2a

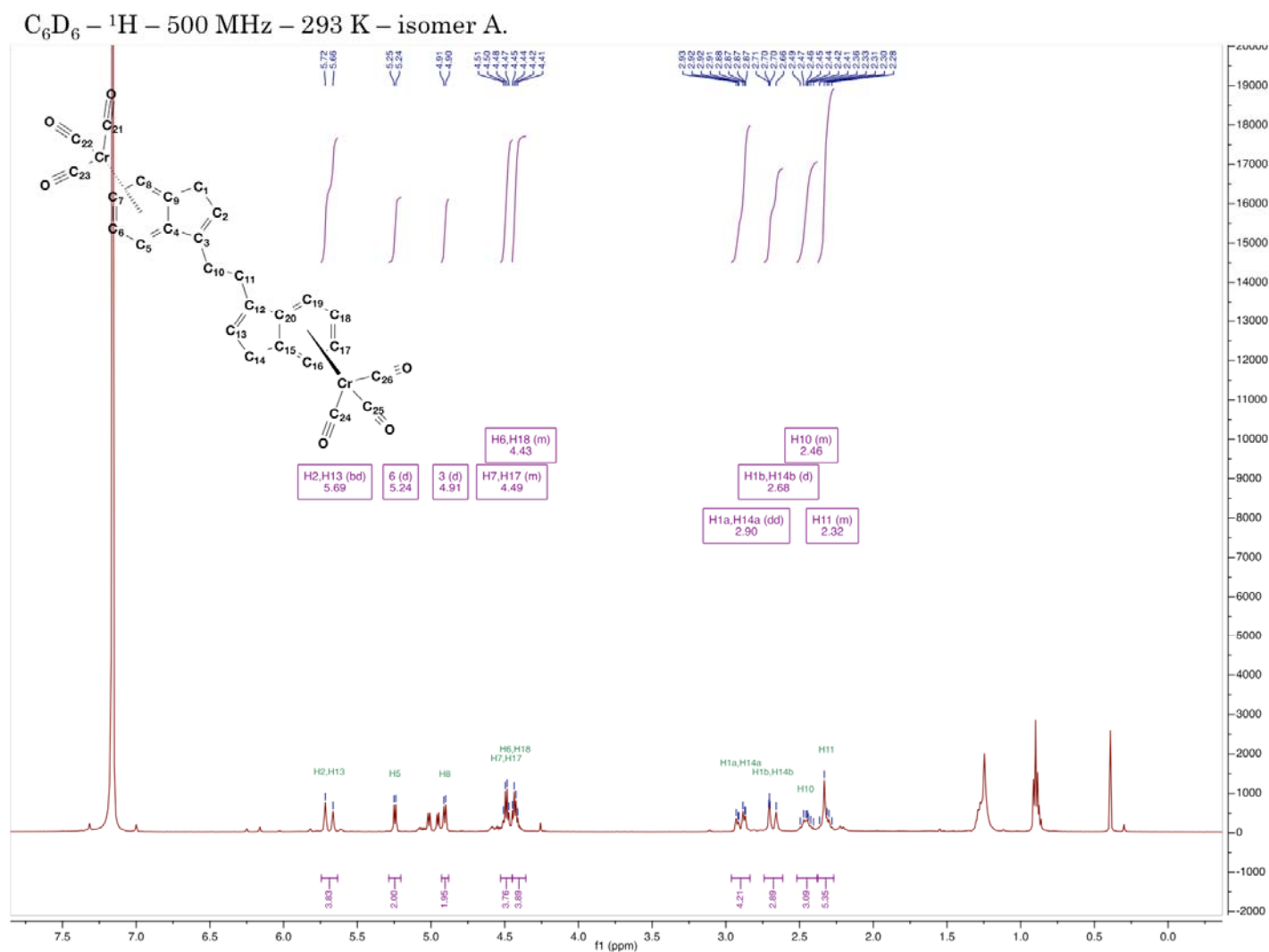


Figure 6. 1H NMR spectrum of isomer **A-2a** in d_6 -benzene at 293 K

$C_6D_6 - ^{13}C - 126 \text{ MHz} - 293 \text{ K} - \text{isomer A.}$

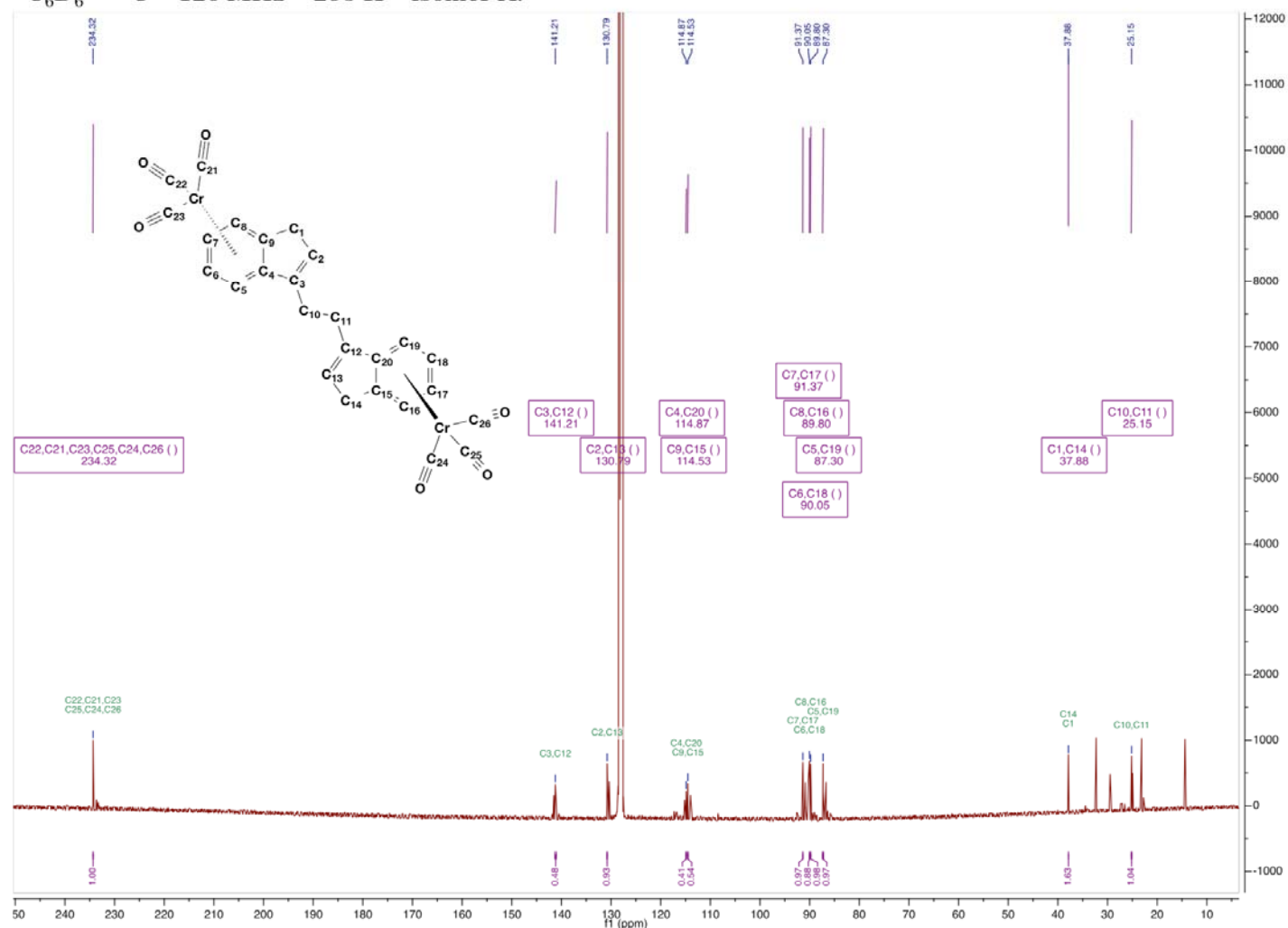


Figure 7. ^{13}C NMR spectrum of isomer A-2a in d_6 ,benzene at 293 K

$C_6D_6 - ^1H - 500\text{ MHz} - 293\text{ K} - \text{isomer B.}$

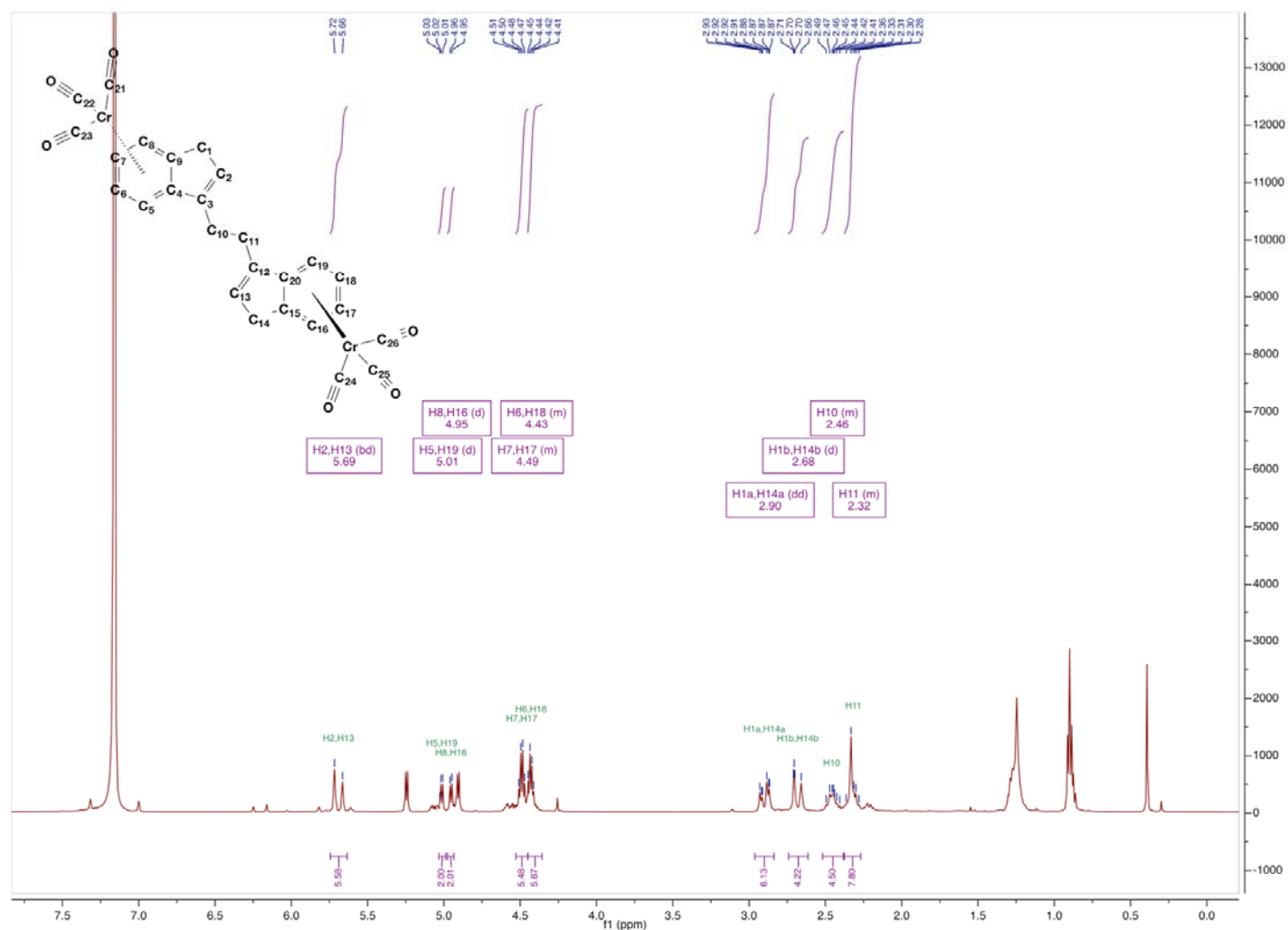


Figure 8. 1H NMR spectrum of isomer **B-2a** in d_6 -benzene at 293 K

$C_6D_6 - ^{13}C - 126 \text{ MHz} - 293 \text{ K} - \text{isomer B.}$

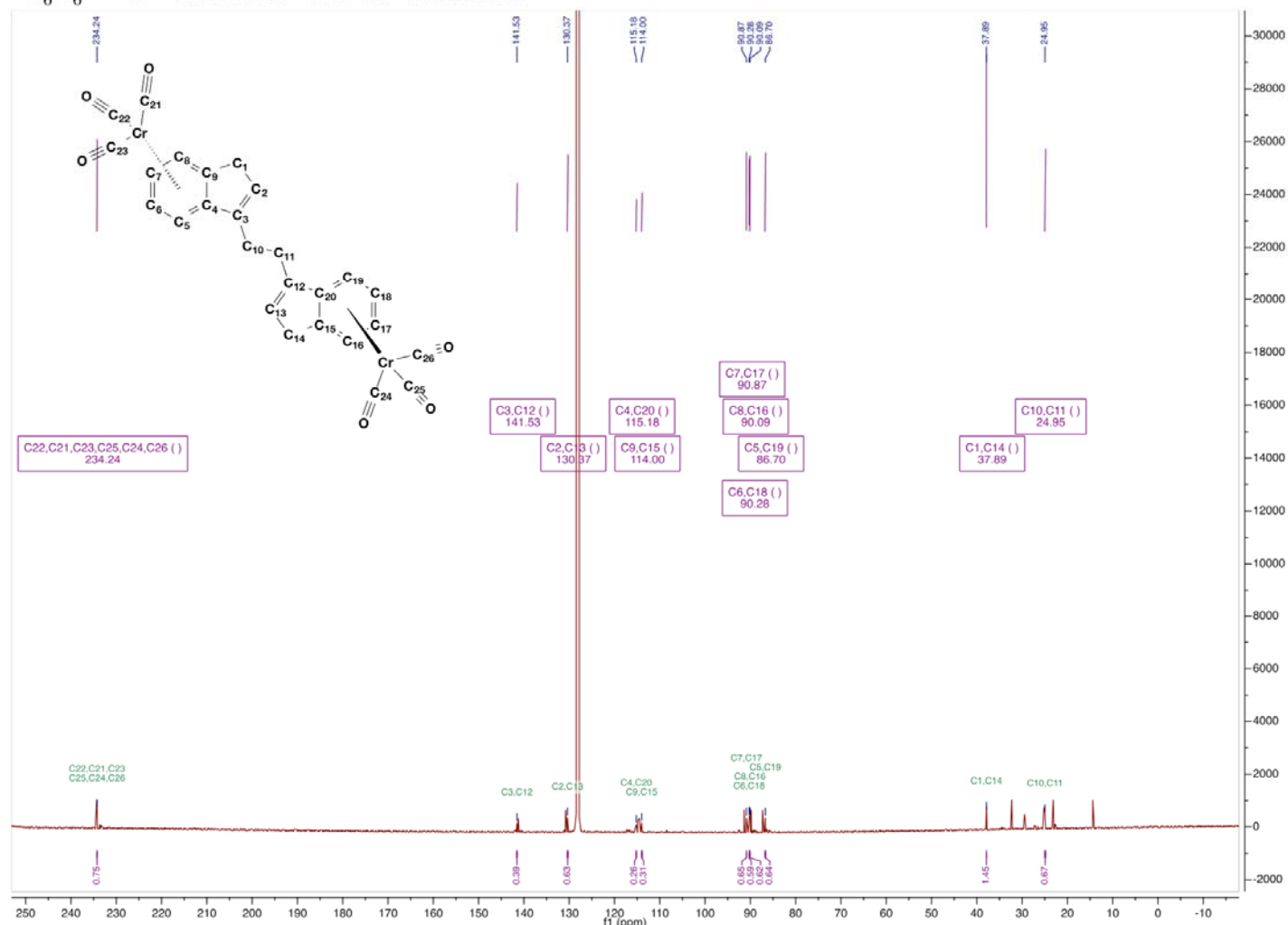


Figure 9. ^{13}C NMR spectrum of isomer **B-2a** in d_6 -benzene at 293 K

Complex 2c

$\text{CDCl}_3 - ^1\text{H} - 500 \text{ MHz} - 293 \text{ K.}$

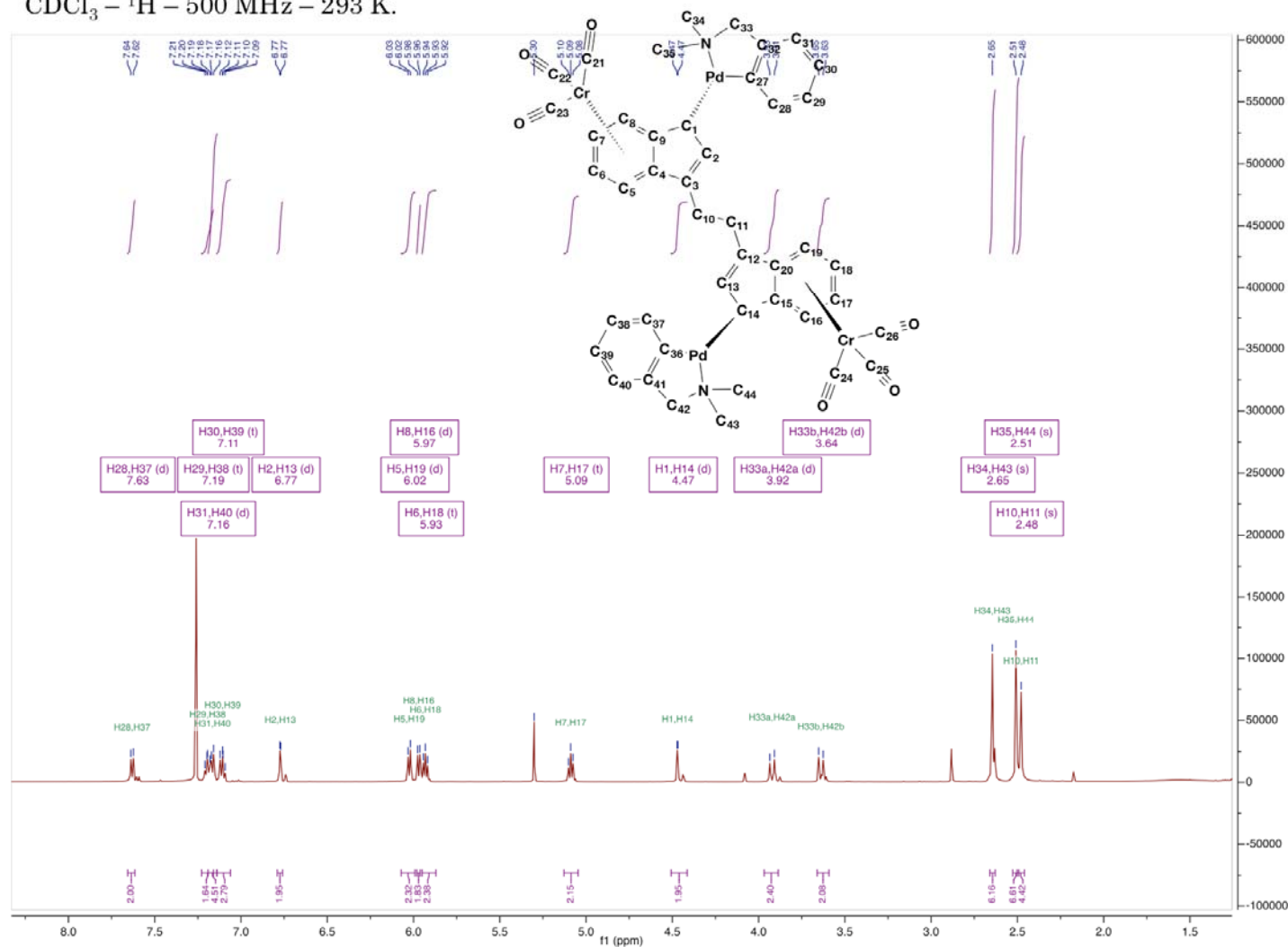


Figure 10. ^1H NMR spectrum of 2c in d_1 chloroform at 293 K.

$\text{CDCl}_3 - ^{13}\text{C} - 126 \text{ MHz} - 293 \text{ K}.$

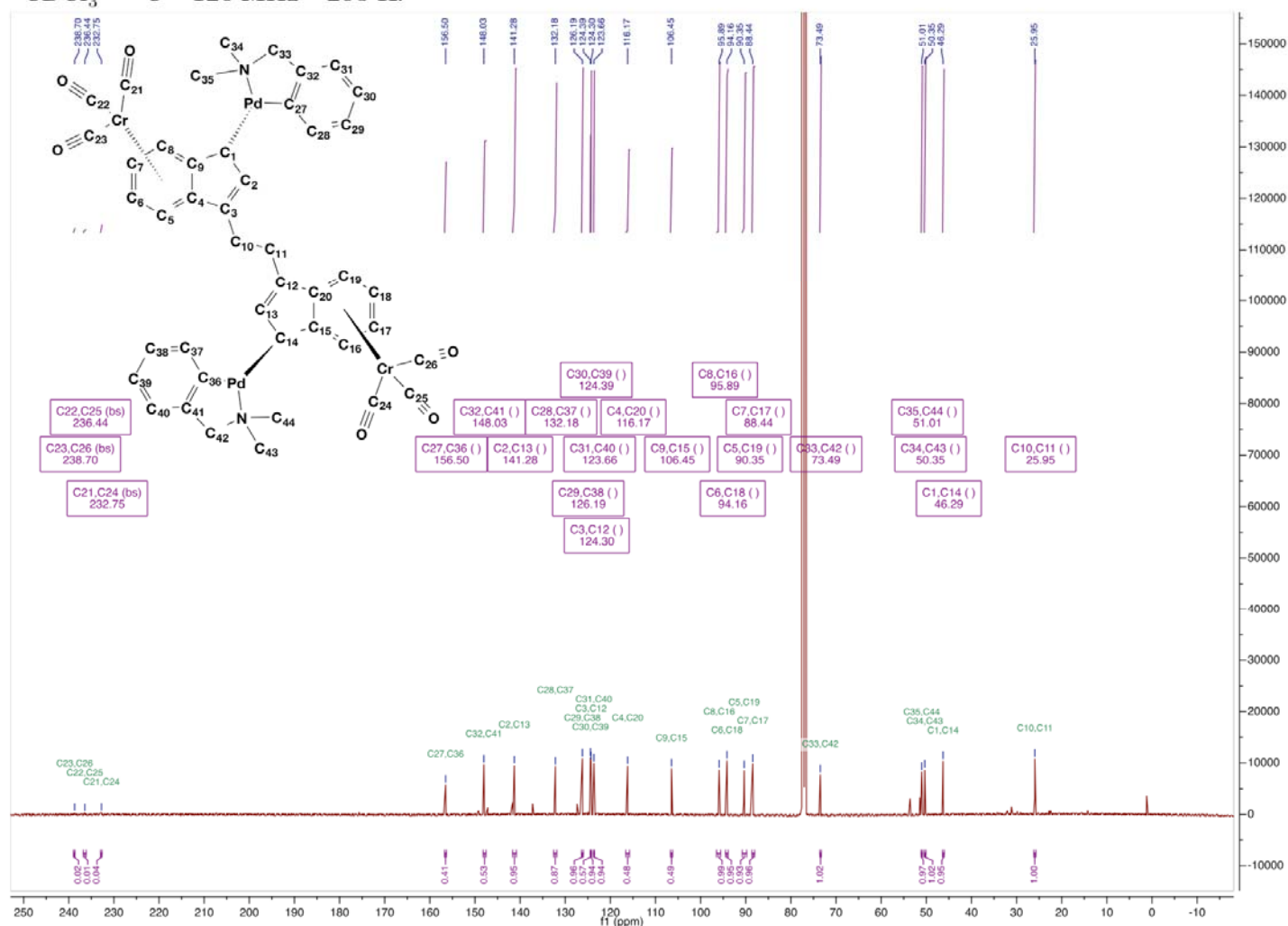


Figure 11. ^{13}C NMR spectrum of 2c in d_1 .chloroform at 293 K

$\text{CDCl}_3 - ^1\text{H} - 600 \text{ MHz} - \text{Variable Temperature.}$

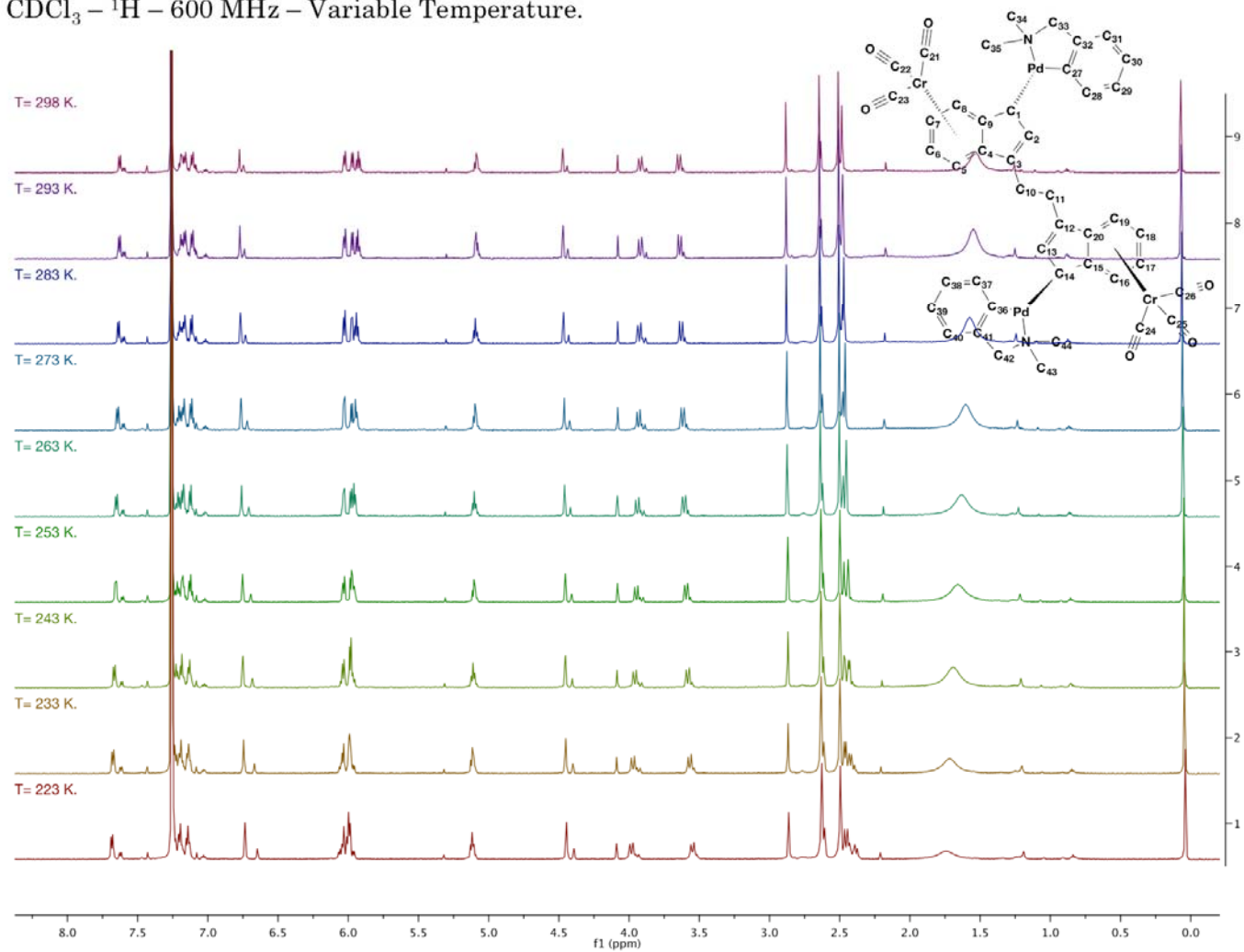


Figure 12. Variable temperature ^1H NMR spectra of **2c** in d_1 chloroform at 293 K

Selected structural parameters extracted from X-ray diffraction analyses

1c

Geometric parameters (Å, °)

Pd1—C3	2.017 (2)	C8—H8	0.97 (4)
Pd1—C15	2.117 (3)	C9—C10	1.371 (5)
Pd1—N1	2.170 (2)	C9—H9	0.89 (5)
Pd1—Cr1	2.9294 (5)	C10—C11	1.418 (4)
Cr1—C25	1.838 (3)	C10—H10	0.97 (4)
Cr1—C27	1.849 (5)	C12—H12A	0.98 (5)
Cr1—C26	1.861 (5)	C12—H12B	0.93 (5)
Cr1—C19	2.211 (3)	C12—H12C	0.97 (5)
Cr1—C17	2.226 (4)	C13—H13A	0.91 (6)
Cr1—C18	2.231 (5)	C13—H13B	1.05 (6)
Cr1—C16	2.244 (2)	C13—H13C	0.97 (4)
Cr1—C20	2.274 (4)	C14—H14A	0.96 (5)
Cr1—C21	2.326 (4)	C14—H14B	0.89 (5)
O1—C25	1.148 (4)	C14—H14C	0.95 (5)
O2—C26	1.149 (6)	C15—C16	1.460 (4)
O3—C27	1.156 (6)	C15—C23	1.479 (5)
N1—C14	1.489 (5)	C15—H15	0.93 (4)
N1—C13	1.492 (4)	C16—C17	1.407 (7)
N1—C1	1.505 (4)	C16—C21	1.436 (6)
C1—C2	1.512 (4)	C17—C18	1.421 (6)
C1—C12	1.515 (5)	C17—H17	0.89 (5)
C1—H1	1.00 (4)	C18—C19	1.394 (7)
C2—C3	1.386 (4)	C18—H18	0.89 (5)
C2—C11	1.422 (4)	C19—C20	1.405 (7)
C3—C4	1.417 (3)	C19—H19	1.01 (4)
C4—C5	1.374 (4)	C20—C21	1.414 (6)
C4—H4	0.96 (4)	C20—H20	1.02 (5)
C5—C6	1.411 (4)	C21—C22	1.428 (6)

C5—H5	0.99 (3)	C22—C23	1.368 (5)
C6—C7	1.420 (4)	C22—H22	0.88 (5)
C6—C11	1.424 (4)	C23—C24	1.484 (5)
C7—C8	1.363 (5)	C24—H24A	1.03 (6)
C7—H7	0.97 (4)	C24—H24B	1.00 (5)
C8—C9	1.410 (5)	C24—H24C	1.02 (5)
C3—Pd1—C15	90.63 (11)	C10—C9—C8	120.5 (3)
C3—Pd1—N1	79.85 (10)	C10—C9—H9	118 (3)
C15—Pd1—N1	170.46 (10)	C8—C9—H9	121 (3)
C3—Pd1—Cr1	169.05 (9)	C9—C10—C11	121.3 (3)
C15—Pd1—Cr1	78.77 (9)	C9—C10—H10	119 (3)
N1—Pd1—Cr1	110.70 (6)	C11—C10—H10	120 (3)
C25—Cr1—C27	85.2 (2)	C10—C11—C2	123.6 (3)
C25—Cr1—C26	86.1 (2)	C10—C11—C6	117.8 (3)
C27—Cr1—C26	99.68 (13)	C2—C11—C6	118.6 (3)
C25—Cr1—C19	89.38 (13)	C1—C12—H12A	110 (3)
C27—Cr1—C19	131.1 (2)	C1—C12—H12B	109 (3)
C26—Cr1—C19	128.4 (2)	H12A—C12—H12B	108 (4)
C25—Cr1—C17	137.9 (2)	C1—C12—H12C	113 (3)
C27—Cr1—C17	85.86 (19)	H12A—C12—H12C	113 (4)
C26—Cr1—C17	136.0 (2)	H12B—C12—H12C	103 (4)
C19—Cr1—C17	66.64 (15)	N1—C13—H13A	106 (4)
C25—Cr1—C18	104.27 (19)	N1—C13—H13B	115 (4)
C27—Cr1—C18	98.5 (2)	H13A—C13—H13B	105 (3)
C26—Cr1—C18	159.7 (2)	N1—C13—H13C	108 (2)
C19—Cr1—C18	36.58 (19)	H13A—C13—H13C	116 (5)
C17—Cr1—C18	37.18 (17)	H13B—C13—H13C	107 (5)
C25—Cr1—C16	167.10 (12)	N1—C14—H14A	112 (3)
C27—Cr1—C16	104.06 (19)	N1—C14—H14B	111 (3)
C26—Cr1—C16	100.82 (19)	H14A—C14—H14B	110 (4)

C19—Cr1—C16	77.78 (11)	N1—C14—H14C	108 (3)
C17—Cr1—C16	36.69 (17)	H14A—C14—H14C	106 (4)
C18—Cr1—C16	65.93 (16)	H14B—C14—H14C	110 (4)
C25—Cr1—C20	102.8 (2)	C16—C15—C23	104.8 (3)
C27—Cr1—C20	163.60 (19)	C16—C15—Pd1	95.61 (17)
C26—Cr1—C20	95.1 (2)	C23—C15—Pd1	105.4 (2)
C19—Cr1—C20	36.48 (18)	C16—C15—H15	115 (2)
C17—Cr1—C20	78.59 (16)	C23—C15—H15	122 (3)
C18—Cr1—C20	65.84 (18)	Pd1—C15—H15	110 (2)
C16—Cr1—C20	65.98 (15)	C17—C16—C21	120.7 (3)
C25—Cr1—C21	135.4 (2)	C17—C16—C15	131.5 (4)
C27—Cr1—C21	139.25 (18)	C21—C16—C15	107.6 (4)
C26—Cr1—C21	83.8 (2)	C17—C16—Cr1	71.0 (2)
C19—Cr1—C21	64.62 (16)	C21—C16—Cr1	74.9 (2)
C17—Cr1—C21	65.71 (13)	C15—C16—Cr1	122.10 (18)
C18—Cr1—C21	76.64 (17)	C16—C17—C18	118.9 (4)
C16—Cr1—C21	36.58 (16)	C16—C17—Cr1	72.3 (2)
C20—Cr1—C21	35.79 (15)	C18—C17—Cr1	71.6 (3)
C25—Cr1—Pd1	131.93 (9)	C16—C17—H17	120 (3)
C27—Cr1—Pd1	65.42 (13)	C18—C17—H17	121 (3)
C26—Cr1—Pd1	64.14 (15)	Cr1—C17—H17	123 (3)
C19—Cr1—Pd1	138.65 (9)	C19—C18—C17	119.9 (4)
C17—Cr1—Pd1	79.49 (11)	C19—C18—Cr1	70.9 (2)
C18—Cr1—Pd1	116.56 (13)	C17—C18—Cr1	71.2 (3)
C16—Cr1—Pd1	60.87 (7)	C19—C18—H18	125 (4)
C20—Cr1—Pd1	116.00 (12)	C17—C18—H18	115 (4)
C21—Cr1—Pd1	80.52 (11)	Cr1—C18—H18	128 (3)
C14—N1—C13	107.6 (3)	C18—C19—C20	122.0 (3)
C14—N1—C1	108.7 (3)	C18—C19—Cr1	72.5 (2)
C13—N1—C1	109.7 (3)	C20—C19—Cr1	74.2 (2)

C14—N1—Pd1	108.3 (2)	C18—C19—H19	119 (3)
C13—N1—Pd1	119.08 (18)	C20—C19—H19	119 (3)
C1—N1—Pd1	103.10 (16)	Cr1—C19—H19	127 (2)
N1—C1—C2	107.4 (2)	C19—C20—C21	118.8 (4)
N1—C1—C12	113.2 (3)	C19—C20—Cr1	69.3 (2)
C2—C1—C12	110.3 (3)	C21—C20—Cr1	74.1 (2)
N1—C1—H1	103 (2)	C19—C20—H20	120 (3)
C2—C1—H1	111.2 (19)	C21—C20—H20	121 (3)
C12—C1—H1	111 (3)	Cr1—C20—H20	127 (3)
C3—C2—C11	121.8 (2)	C20—C21—C22	132.4 (4)
C3—C2—C1	117.1 (2)	C20—C21—C16	119.3 (4)
C11—C2—C1	121.1 (3)	C22—C21—C16	108.2 (3)
C2—C3—C4	118.5 (2)	C20—C21—Cr1	70.1 (3)
C2—C3—Pd1	112.93 (18)	C22—C21—Cr1	128.8 (3)
C4—C3—Pd1	128.6 (2)	C16—C21—Cr1	68.6 (2)
C5—C4—C3	120.9 (3)	C23—C22—C21	109.2 (3)
C5—C4—H4	118 (2)	C23—C22—H22	125 (3)
C3—C4—H4	121 (2)	C21—C22—H22	126 (3)
C4—C5—C6	121.3 (2)	C22—C23—C15	109.7 (3)
C4—C5—H5	119 (2)	C22—C23—C24	125.6 (4)
C6—C5—H5	120 (2)	C15—C23—C24	124.8 (3)
C5—C6—C7	121.6 (3)	C23—C24—H24A	112 (3)
C5—C6—C11	118.7 (3)	C23—C24—H24B	111 (3)
C7—C6—C11	119.6 (3)	H24A—C24—H24B	112 (4)
C8—C7—C6	120.8 (3)	C23—C24—H24C	107 (3)
C8—C7—H7	121 (2)	H24A—C24—H24C	105 (5)
C6—C7—H7	118 (2)	H24B—C24—H24C	110 (4)
C7—C8—C9	120.0 (3)	O1—C25—Cr1	178.3 (3)
C7—C8—H8	123 (3)	O2—C26—Cr1	171.2 (4)
C9—C8—H8	117 (3)	O3—C27—Cr1	171.4 (4)

C3—Pd1—Cr1—C25	−154.9 (8)	Pd1—Cr1—C17—C18	175.6 (3)
C15—Pd1—Cr1—C25	−169.7 (3)	C16—C17—C18—C19	−3.2 (6)
N1—Pd1—Cr1—C25	9.1 (3)	Cr1—C17—C18—C19	53.5 (4)
C3—Pd1—Cr1—C27	147.3 (8)	C16—C17—C18—Cr1	−56.8 (3)
C15—Pd1—Cr1—C27	132.51 (18)	C25—Cr1—C18—C19	68.8 (3)
N1—Pd1—Cr1—C27	−48.68 (17)	C27—Cr1—C18—C19	156.0 (3)
C3—Pd1—Cr1—C26	−97.4 (8)	C26—Cr1—C18—C19	−50.4 (7)
C15—Pd1—Cr1—C26	−112.19 (19)	C17—Cr1—C18—C19	−132.5 (4)
N1—Pd1—Cr1—C26	66.62 (19)	C16—Cr1—C18—C19	−102.3 (3)
C3—Pd1—Cr1—C19	22.3 (8)	C20—Cr1—C18—C19	−29.0 (2)
C15—Pd1—Cr1—C19	7.5 (2)	C21—Cr1—C18—C19	−65.2 (3)
N1—Pd1—Cr1—C19	−173.7 (2)	Pd1—Cr1—C18—C19	−137.3 (2)
C3—Pd1—Cr1—C17	57.1 (8)	C25—Cr1—C18—C17	−158.7 (3)
C15—Pd1—Cr1—C17	42.28 (15)	C27—Cr1—C18—C17	−71.5 (3)
N1—Pd1—Cr1—C17	−138.91 (14)	C26—Cr1—C18—C17	82.1 (7)
C3—Pd1—Cr1—C18	60.0 (8)	C19—Cr1—C18—C17	132.5 (4)
C15—Pd1—Cr1—C18	45.22 (18)	C16—Cr1—C18—C17	30.2 (3)
N1—Pd1—Cr1—C18	−135.97 (17)	C20—Cr1—C18—C17	103.4 (3)
C3—Pd1—Cr1—C16	23.2 (7)	C21—Cr1—C18—C17	67.3 (3)
C15—Pd1—Cr1—C16	8.41 (18)	Pd1—Cr1—C18—C17	−4.8 (3)
N1—Pd1—Cr1—C16	−172.79 (17)	C17—C18—C19—C20	4.0 (5)
C3—Pd1—Cr1—C20	−14.6 (8)	Cr1—C18—C19—C20	57.7 (3)
C15—Pd1—Cr1—C20	−29.40 (16)	C17—C18—C19—Cr1	−53.7 (4)
N1—Pd1—Cr1—C20	149.41 (15)	C25—Cr1—C19—C18	−115.4 (3)
C3—Pd1—Cr1—C21	−9.7 (8)	C27—Cr1—C19—C18	−32.2 (3)
C15—Pd1—Cr1—C21	−24.57 (14)	C26—Cr1—C19—C18	160.1 (3)
N1—Pd1—Cr1—C21	154.24 (13)	C17—Cr1—C19—C18	29.0 (3)
C3—Pd1—N1—C14	−77.6 (3)	C16—Cr1—C19—C18	65.9 (3)
C15—Pd1—N1—C14	−81.6 (7)	C20—Cr1—C19—C18	131.8 (3)
Cr1—Pd1—N1—C14	105.5 (2)	C21—Cr1—C19—C18	102.1 (3)

C3—Pd1—N1—C13	159.2 (3)	Pd1—Cr1—C19—C18	66.7 (3)
C15—Pd1—N1—C13	155.2 (7)	C25—Cr1—C19—C20	112.8 (3)
Cr1—Pd1—N1—C13	−17.8 (3)	C27—Cr1—C19—C20	−164.1 (3)
C3—Pd1—N1—C1	37.4 (2)	C26—Cr1—C19—C20	28.3 (3)
C15—Pd1—N1—C1	33.4 (8)	C17—Cr1—C19—C20	−102.8 (3)
Cr1—Pd1—N1—C1	−139.51 (16)	C18—Cr1—C19—C20	−131.8 (3)
C14—N1—C1—C2	70.7 (3)	C16—Cr1—C19—C20	−66.0 (3)
C13—N1—C1—C2	−171.9 (3)	C21—Cr1—C19—C20	−29.7 (2)
Pd1—N1—C1—C2	−44.1 (3)	Pd1—Cr1—C19—C20	−65.1 (3)
C14—N1—C1—C12	−167.2 (3)	C18—C19—C20—C21	0.3 (5)
C13—N1—C1—C12	−49.8 (4)	Cr1—C19—C20—C21	57.3 (4)
Pd1—N1—C1—C12	78.0 (3)	C18—C19—C20—Cr1	−56.9 (3)
N1—C1—C2—C3	29.6 (4)	C25—Cr1—C20—C19	−71.0 (3)
C12—C1—C2—C3	−94.2 (4)	C27—Cr1—C20—C19	47.1 (7)
N1—C1—C2—C11	−150.6 (3)	C26—Cr1—C20—C19	−158.1 (3)
C12—C1—C2—C11	85.5 (4)	C17—Cr1—C20—C19	66.0 (2)
C11—C2—C3—C4	3.5 (7)	C18—Cr1—C20—C19	29.1 (2)
C1—C2—C3—C4	−176.7 (4)	C16—Cr1—C20—C19	102.3 (3)
C11—C2—C3—Pd1	−176.3 (3)	C21—Cr1—C20—C19	130.0 (4)
C1—C2—C3—Pd1	3.4 (5)	Pd1—Cr1—C20—C19	138.2 (2)
C15—Pd1—C3—C2	156.0 (3)	C25—Cr1—C20—C21	159.0 (3)
N1—Pd1—C3—C2	−23.3 (3)	C27—Cr1—C20—C21	−82.9 (7)
Cr1—Pd1—C3—C2	141.5 (5)	C26—Cr1—C20—C21	71.9 (3)
C15—Pd1—C3—C4	−23.8 (5)	C19—Cr1—C20—C21	−130.0 (4)
N1—Pd1—C3—C4	156.8 (5)	C17—Cr1—C20—C21	−64.0 (3)
Cr1—Pd1—C3—C4	−38.4 (12)	C18—Cr1—C20—C21	−100.9 (3)
C2—C3—C4—C5	−1.5 (8)	C16—Cr1—C20—C21	−27.7 (3)
Pd1—C3—C4—C5	178.3 (5)	Pd1—Cr1—C20—C21	8.2 (3)
C3—C4—C5—C6	0.3 (9)	C19—C20—C21—C22	−179.8 (4)
C4—C5—C6—C7	178.7 (5)	Cr1—C20—C21—C22	−124.9 (5)

C4—C5—C6—C11	−1.0 (8)	C19—C20—C21—C16	−5.4 (6)
C5—C6—C7—C8	178.8 (4)	Cr1—C20—C21—C16	49.5 (3)
C11—C6—C7—C8	−1.4 (5)	C19—C20—C21—Cr1	−54.9 (3)
C6—C7—C8—C9	−1.2 (6)	C17—C16—C21—C20	6.2 (4)
C7—C8—C9—C10	2.4 (6)	C15—C16—C21—C20	−169.7 (3)
C8—C9—C10—C11	−0.9 (6)	Cr1—C16—C21—C20	−50.2 (4)
C9—C10—C11—C2	178.0 (3)	C17—C16—C21—C22	−178.2 (4)
C9—C10—C11—C6	−1.7 (5)	C15—C16—C21—C22	6.0 (4)
C3—C2—C11—C10	176.1 (4)	Cr1—C16—C21—C22	125.5 (3)
C1—C2—C11—C10	−3.6 (5)	C17—C16—C21—Cr1	56.4 (2)
C3—C2—C11—C6	−4.2 (5)	C15—C16—C21—Cr1	−119.4 (2)
C1—C2—C11—C6	176.0 (3)	C25—Cr1—C21—C20	−29.8 (4)
C5—C6—C11—C10	−177.4 (4)	C27—Cr1—C21—C20	154.6 (3)
C7—C6—C11—C10	2.8 (5)	C26—Cr1—C21—C20	−107.8 (3)
C5—C6—C11—C2	2.9 (5)	C19—Cr1—C21—C20	30.3 (3)
C7—C6—C11—C2	−176.9 (3)	C17—Cr1—C21—C20	104.8 (3)
C3—Pd1—C15—C16	171.4 (3)	C18—Cr1—C21—C20	67.1 (3)
N1—Pd1—C15—C16	175.4 (6)	C16—Cr1—C21—C20	134.5 (4)
Cr1—Pd1—C15—C16	−11.4 (2)	Pd1—Cr1—C21—C20	−172.6 (3)
C3—Pd1—C15—C23	−81.6 (3)	C25—Cr1—C21—C22	99.1 (4)
N1—Pd1—C15—C23	−77.6 (7)	C27—Cr1—C21—C22	−76.5 (4)
Cr1—Pd1—C15—C23	95.6 (2)	C26—Cr1—C21—C22	21.1 (4)
C23—C15—C16—C17	177.4 (3)	C19—Cr1—C21—C22	159.2 (4)
Pd1—C15—C16—C17	−75.0 (4)	C17—Cr1—C21—C22	−126.3 (4)
C23—C15—C16—C21	−7.4 (3)	C18—Cr1—C21—C22	−164.0 (4)
Pd1—C15—C16—C21	100.2 (2)	C16—Cr1—C21—C22	−96.6 (4)
C23—C15—C16—Cr1	−90.2 (4)	C20—Cr1—C21—C22	128.9 (5)
Pd1—C15—C16—Cr1	17.3 (4)	Pd1—Cr1—C21—C22	−43.6 (3)
C25—Cr1—C16—C17	−72.8 (12)	C25—Cr1—C21—C16	−164.4 (3)
C27—Cr1—C16—C17	62.6 (3)	C27—Cr1—C21—C16	20.1 (4)

C26—Cr1—C16—C17	165.5 (3)	C26—Cr1—C21—C16	117.7 (3)
C19—Cr1—C16—C17	−67.1 (3)	C19—Cr1—C21—C16	−104.3 (3)
C18—Cr1—C16—C17	−30.6 (3)	C17—Cr1—C21—C16	−29.76 (19)
C20—Cr1—C16—C17	−103.6 (3)	C18—Cr1—C21—C16	−67.5 (2)
C21—Cr1—C16—C17	−130.8 (3)	C20—Cr1—C21—C16	−134.5 (4)
Pd1—Cr1—C16—C17	113.5 (3)	Pd1—Cr1—C21—C16	52.9 (2)
C25—Cr1—C16—C21	58.0 (12)	C20—C21—C22—C23	172.8 (4)
C27—Cr1—C16—C21	−166.7 (3)	C16—C21—C22—C23	−2.1 (4)
C26—Cr1—C16—C21	−63.7 (3)	Cr1—C21—C22—C23	74.7 (4)
C19—Cr1—C16—C21	63.6 (3)	C21—C22—C23—C15	−2.7 (4)
C17—Cr1—C16—C21	130.8 (3)	C21—C22—C23—C24	177.5 (3)
C18—Cr1—C16—C21	100.2 (3)	C16—C15—C23—C22	6.3 (3)
C20—Cr1—C16—C21	27.2 (2)	Pd1—C15—C23—C22	−93.9 (3)
Pd1—Cr1—C16—C21	−115.7 (3)	C16—C15—C23—C24	−174.0 (3)
C25—Cr1—C16—C15	159.5 (11)	Pd1—C15—C23—C24	85.8 (3)
C27—Cr1—C16—C15	−65.1 (4)	C27—Cr1—C25—O1	37 (25)
C26—Cr1—C16—C15	37.9 (4)	C26—Cr1—C25—O1	−63 (25)
C19—Cr1—C16—C15	165.2 (4)	C19—Cr1—C25—O1	168 (25)
C17—Cr1—C16—C15	−127.7 (5)	C17—Cr1—C25—O1	115 (25)
C18—Cr1—C16—C15	−158.3 (4)	C18—Cr1—C25—O1	134 (25)
C20—Cr1—C16—C15	128.7 (4)	C16—Cr1—C25—O1	174 (100)
C21—Cr1—C16—C15	101.5 (5)	C20—Cr1—C25—O1	−158 (25)
Pd1—Cr1—C16—C15	−14.2 (3)	C21—Cr1—C25—O1	−140 (25)
C21—C16—C17—C18	−1.8 (4)	Pd1—Cr1—C25—O1	−14 (25)
C15—C16—C17—C18	172.8 (3)	C25—Cr1—C26—O2	−53 (3)
Cr1—C16—C17—C18	56.4 (4)	C27—Cr1—C26—O2	−138 (3)
C21—C16—C17—Cr1	−58.2 (2)	C19—Cr1—C26—O2	33 (3)
C15—C16—C17—Cr1	116.4 (3)	C17—Cr1—C26—O2	128 (3)
C25—Cr1—C17—C16	161.5 (3)	C18—Cr1—C26—O2	69 (3)
C27—Cr1—C17—C16	−120.3 (3)	C16—Cr1—C26—O2	116 (3)

C26—Cr1—C17—C16	−20.7 (4)	C20—Cr1—C26—O2	49 (3)
C19—Cr1—C17—C16	101.2 (3)	C21—Cr1—C26—O2	83 (3)
C18—Cr1—C17—C16	129.8 (4)	Pd1—Cr1—C26—O2	166 (3)
C20—Cr1—C17—C16	64.9 (2)	C25—Cr1—C27—O3	59 (3)
C21—Cr1—C17—C16	29.68 (19)	C26—Cr1—C27—O3	144 (3)
Pd1—Cr1—C17—C16	−54.6 (2)	C19—Cr1—C27—O3	−26 (3)
C25—Cr1—C17—C18	31.7 (4)	C17—Cr1—C27—O3	−80 (3)
C27—Cr1—C17—C18	109.9 (3)	C18—Cr1—C27—O3	−45 (3)
C26—Cr1—C17—C18	−150.4 (3)	C16—Cr1—C27—O3	−112 (3)
C19—Cr1—C17—C18	−28.6 (3)	C20—Cr1—C27—O3	−61 (3)
C16—Cr1—C17—C18	−129.8 (4)	C21—Cr1—C27—O3	−124 (3)
C20—Cr1—C17—C18	−64.9 (3)	Pd1—Cr1—C27—O3	−160 (3)
C21—Cr1—C17—C18	−100.1 (3)		

Geometric parameters (Å, °)

C1—C2	1.394 (4)	C12—C13	1.397 (4)
C1—C6	1.400 (3)	C12—Cr1	2.238 (2)
C1—Pd1	2.020 (2)	C12—H12	0.9500
C2—C3	1.368 (4)	C13—C14	1.412 (4)
C2—H2	0.9500	C13—Cr1	2.236 (2)
C3—C4	1.382 (5)	C13—H13	0.9500
C3—H3	0.9500	C14—C15	1.407 (3)
C4—C5	1.378 (4)	C14—Cr1	2.220 (2)
C4—H4	0.9500	C14—H14	0.9500
C5—C6	1.394 (3)	C15—C16	1.408 (3)
C5—H5	0.9500	C15—Cr1	2.271 (2)
C6—C7	1.502 (3)	C15—H15	0.9500
C7—N1	1.485 (3)	C16—C17	1.456 (3)
C7—H7A	0.9900	C16—Cr1	2.2973 (19)
C7—H7B	0.9900	C17—C18	1.358 (3)
C8—N1	1.487 (3)	C17—C19	1.494 (3)
C8—H8A	0.9800	C18—H18	0.9500
C8—H8B	0.9800	C19—C19 ⁱ	1.521 (4)
C8—H8C	0.9800	C19—H19A	0.9900
C9—N1	1.476 (3)	C19—H19B	0.9900
C9—H9A	0.9800	C20—O1	1.151 (3)
C9—H9B	0.9800	C20—Cr1	1.853 (2)
C9—H9C	0.9800	C20—Pd1	2.647 (3)
C10—C11	1.443 (3)	C21—O2	1.156 (3)
C10—C18	1.471 (3)	C21—Cr1	1.837 (3)
C10—Pd1	2.111 (2)	C21—Pd1	2.649 (2)
C10—H10	1.0000	C22—O3	1.155 (3)
C11—C12	1.418 (3)	C22—Cr1	1.832 (3)

C11—C16	1.429 (3)	N1—Pd1	2.1915 (18)
C11—Cr1	2.231 (2)	Cr1—Pd1	2.8925 (4)
C2—C1—C6	116.6 (2)	C17—C18—H18	124.0
C2—C1—Pd1	131.03 (19)	C10—C18—H18	124.0
C6—C1—Pd1	112.31 (17)	C17—C19—C19 ⁱ	113.8 (2)
C3—C2—C1	122.2 (3)	C17—C19—H19A	108.8
C3—C2—H2	118.9	C19 ⁱ —C19—H19A	108.8
C1—C2—H2	118.9	C17—C19—H19B	108.8
C2—C3—C4	120.5 (3)	C19 ⁱ —C19—H19B	108.8
C2—C3—H3	119.7	H19A—C19—H19B	107.7
C4—C3—H3	119.7	O1—C20—Cr1	173.1 (2)
C5—C4—C3	119.2 (3)	O1—C20—Pd1	107.99 (17)
C5—C4—H4	120.4	Cr1—C20—Pd1	77.80 (9)
C3—C4—H4	120.4	O2—C21—Cr1	171.2 (2)
C4—C5—C6	120.1 (3)	O2—C21—Pd1	110.73 (19)
C4—C5—H5	120.0	Cr1—C21—Pd1	77.99 (8)
C6—C5—H5	120.0	O3—C22—Cr1	178.4 (3)
C5—C6—C1	121.3 (2)	C9—N1—C7	107.70 (18)
C5—C6—C7	121.6 (2)	C9—N1—C8	108.7 (2)
C1—C6—C7	117.0 (2)	C7—N1—C8	108.08 (19)
N1—C7—C6	110.32 (19)	C9—N1—Pd1	119.61 (15)
N1—C7—H7A	109.6	C7—N1—Pd1	102.35 (13)
C6—C7—H7A	109.6	C8—N1—Pd1	109.78 (15)
N1—C7—H7B	109.6	C22—Cr1—C21	83.50 (13)
C6—C7—H7B	109.6	C22—Cr1—C20	87.37 (11)
H7A—C7—H7B	108.1	C21—Cr1—C20	98.05 (10)
N1—C8—H8A	109.5	C22—Cr1—C14	89.26 (11)
N1—C8—H8B	109.5	C21—Cr1—C14	133.00 (10)
H8A—C8—H8B	109.5	C20—Cr1—C14	128.03 (11)
N1—C8—H8C	109.5	C22—Cr1—C11	167.28 (10)

H8A—C8—H8C	109.5	C21—Cr1—C11	103.87 (11)
H8B—C8—H8C	109.5	C20—Cr1—C11	101.61 (9)
N1—C9—H9A	109.5	C14—Cr1—C11	78.13 (9)
N1—C9—H9B	109.5	C22—Cr1—C13	103.06 (11)
H9A—C9—H9B	109.5	C21—Cr1—C13	100.10 (10)
N1—C9—H9C	109.5	C20—Cr1—C13	159.95 (9)
H9A—C9—H9C	109.5	C14—Cr1—C13	36.95 (10)
H9B—C9—H9C	109.5	C11—Cr1—C13	65.74 (9)
C11—C10—C18	103.86 (19)	C22—Cr1—C12	135.32 (11)
C11—C10—Pd1	98.01 (14)	C21—Cr1—C12	86.99 (10)
C18—C10—Pd1	103.09 (14)	C20—Cr1—C12	137.26 (9)
C11—C10—H10	116.4	C14—Cr1—C12	66.43 (10)
C18—C10—H10	116.4	C11—Cr1—C12	36.99 (8)
Pd1—C10—H10	116.4	C13—Cr1—C12	36.40 (10)
C12—C11—C16	120.0 (2)	C22—Cr1—C15	104.29 (11)
C12—C11—C10	131.1 (2)	C21—Cr1—C15	165.09 (10)
C16—C11—C10	108.45 (18)	C20—Cr1—C15	95.03 (9)
C12—C11—Cr1	71.76 (13)	C14—Cr1—C15	36.49 (8)
C16—C11—Cr1	74.13 (13)	C11—Cr1—C15	66.29 (9)
C10—C11—Cr1	119.59 (14)	C13—Cr1—C15	65.99 (9)
C13—C12—C11	118.9 (2)	C12—Cr1—C15	78.52 (9)
C13—C12—Cr1	71.72 (15)	C22—Cr1—C16	137.59 (12)
C11—C12—Cr1	71.25 (13)	C21—Cr1—C16	138.82 (11)
C13—C12—H12	120.5	C20—Cr1—C16	84.15 (8)
C11—C12—H12	120.5	C14—Cr1—C16	64.78 (8)
Cr1—C12—H12	128.7	C11—Cr1—C16	36.76 (8)
C12—C13—C14	120.8 (2)	C13—Cr1—C16	76.59 (8)
C12—C13—Cr1	71.88 (13)	C12—Cr1—C16	65.87 (8)
C14—C13—Cr1	70.91 (13)	C15—Cr1—C16	35.91 (8)
C12—C13—H13	119.6	C22—Cr1—Pd1	130.14 (9)

C14—C13—H13	119.6	C21—Cr1—Pd1	63.61 (8)
Cr1—C13—H13	130.2	C20—Cr1—Pd1	63.43 (8)
C15—C14—C13	121.1 (2)	C14—Cr1—Pd1	140.60 (7)
C15—C14—Cr1	73.75 (13)	C11—Cr1—Pd1	62.51 (6)
C13—C14—Cr1	72.14 (14)	C13—Cr1—Pd1	118.13 (8)
C15—C14—H14	119.5	C12—Cr1—Pd1	81.86 (7)
C13—C14—H14	119.5	C15—Cr1—Pd1	117.01 (6)
Cr1—C14—H14	126.6	C16—Cr1—Pd1	81.58 (5)
C14—C15—C16	118.6 (2)	C1—Pd1—C10	90.51 (9)
C14—C15—Cr1	69.76 (13)	C1—Pd1—N1	81.50 (8)
C16—C15—Cr1	73.05 (12)	C10—Pd1—N1	171.90 (8)
C14—C15—H15	120.7	C1—Pd1—C20	135.74 (8)
C16—C15—H15	120.7	C10—Pd1—C20	94.52 (8)
Cr1—C15—H15	128.6	N1—Pd1—C20	92.14 (7)
C15—C16—C11	120.34 (19)	C1—Pd1—C21	155.81 (9)
C15—C16—C17	131.3 (2)	C10—Pd1—C21	103.70 (8)
C11—C16—C17	108.17 (19)	N1—Pd1—C21	83.41 (7)
C15—C16—Cr1	71.04 (12)	C20—Pd1—C21	63.48 (8)
C11—C16—Cr1	69.10 (11)	C1—Pd1—Cr1	165.39 (6)
C17—C16—Cr1	127.22 (14)	C10—Pd1—Cr1	77.80 (6)
C18—C17—C16	106.72 (19)	N1—Pd1—Cr1	110.30 (5)
C18—C17—C19	129.34 (19)	C20—Pd1—Cr1	38.77 (5)
C16—C17—C19	123.69 (19)	C21—Pd1—Cr1	38.40 (6)
C17—C18—C10	112.05 (19)		
C6—C1—C2—C3	−1.2 (4)	C10—C11—C16—C15	−167.72 (18)
Pd1—C1—C2—C3	177.0 (2)	Cr1—C11—C16—C15	−51.22 (17)
C1—C2—C3—C4	0.8 (5)	C12—C11—C16—C17	−178.92 (18)
C2—C3—C4—C5	0.3 (5)	C10—C11—C16—C17	7.3 (2)
C3—C4—C5—C6	−1.1 (5)	Cr1—C11—C16—C17	123.80 (15)
C4—C5—C6—C1	0.7 (4)	C12—C11—C16—Cr1	57.29 (17)

C4—C5—C6—C7	−176.1 (3)	C10—C11—C16—Cr1	−116.51 (16)
C2—C1—C6—C5	0.4 (4)	C15—C16—C17—C18	171.6 (2)
Pd1—C1—C6—C5	−178.08 (19)	C11—C16—C17—C18	−2.7 (2)
C2—C1—C6—C7	177.4 (2)	Cr1—C16—C17—C18	74.5 (2)
Pd1—C1—C6—C7	−1.1 (3)	C15—C16—C17—C19	−3.2 (3)
C5—C6—C7—N1	−151.5 (2)	C11—C16—C17—C19	−177.45 (18)
C1—C6—C7—N1	31.5 (3)	Cr1—C16—C17—C19	−100.3 (2)
C18—C10—C11—C12	178.5 (2)	C16—C17—C18—C10	−3.0 (2)
Pd1—C10—C11—C12	−75.8 (2)	C19—C17—C18—C10	171.4 (2)
C18—C10—C11—C16	−8.6 (2)	C11—C10—C18—C17	7.3 (2)
Pd1—C10—C11—C16	97.06 (16)	Pd1—C10—C18—C17	−94.53 (18)
C18—C10—C11—Cr1	−90.46 (18)	C18—C17—C19—C19 ⁱ	26.0 (3)
Pd1—C10—C11—Cr1	15.22 (18)	C16—C17—C19—C19 ⁱ	−160.5 (2)
C16—C11—C12—C13	−2.9 (3)	C6—C7—N1—C9	−168.54 (19)
C10—C11—C12—C13	169.3 (2)	C6—C7—N1—C8	74.2 (2)
Cr1—C11—C12—C13	55.54 (19)	C6—C7—N1—Pd1	−41.6 (2)
C16—C11—C12—Cr1	−58.45 (17)	Pd1—C21—Cr1—C22	−141.33 (10)
C10—C11—C12—Cr1	113.7 (2)	Pd1—C21—Cr1—C20	−54.93 (9)
C11—C12—C13—C14	−1.8 (3)	Pd1—C21—Cr1—C14	135.79 (12)
Cr1—C12—C13—C14	53.5 (2)	Pd1—C21—Cr1—C11	49.21 (8)
C11—C12—C13—Cr1	−55.31 (18)	Pd1—C21—Cr1—C13	116.50 (8)
C12—C13—C14—C15	3.6 (3)	Pd1—C21—Cr1—C12	82.40 (8)
Cr1—C13—C14—C15	57.5 (2)	Pd1—C21—Cr1—C15	96.1 (4)
C12—C13—C14—Cr1	−53.9 (2)	Pd1—C21—Cr1—C16	35.37 (14)
C13—C14—C15—C16	−0.4 (3)	Pd1—C20—Cr1—C22	138.12 (10)
Cr1—C14—C15—C16	56.32 (18)	Pd1—C20—Cr1—C21	55.06 (10)
C13—C14—C15—Cr1	−56.7 (2)	Pd1—C20—Cr1—C14	−134.89 (10)
C14—C15—C16—C11	−4.4 (3)	Pd1—C20—Cr1—C11	−50.97 (7)
Cr1—C15—C16—C11	50.35 (17)	Pd1—C20—Cr1—C13	−99.6 (3)
C14—C15—C16—C17	−178.0 (2)	Pd1—C20—Cr1—C12	−39.24 (14)

Cr1—C15—C16—C17	−123.3 (2)	Pd1—C20—Cr1—C15	−117.76 (7)
C14—C15—C16—Cr1	−54.71 (18)	Pd1—C20—Cr1—C16	−83.49 (7)
C12—C11—C16—C15	6.1 (3)		

Geometric parameters (Å, °)

C1—N1	1.316 (12)	C16—Cr1	2.237 (9)
C1—C2	1.378 (14)	C16—H16	0.9500
C1—H1	0.9500	C17—C18	1.481 (12)
C2—C3	1.378 (15)	C17—Cr1	2.279 (9)
C2—H2	0.9500	C18—C19	1.527 (12)
C3—C4	1.413 (15)	C18—H18A	0.9900
C3—H3	0.9500	C18—H18B	0.9900
C4—C9	1.395 (14)	C19—C20	1.396 (12)
C4—C5	1.414 (13)	C19—C24	1.415 (12)
C5—N1	1.370 (11)	C19—Cr2	2.258 (9)
C5—C6	1.408 (13)	C20—C21	1.417 (12)
C6—C7	1.390 (13)	C20—Cr2	2.233 (10)
C6—C10	1.469 (14)	C20—H20	0.9500
C7—C8	1.386 (15)	C21—C22	1.377 (13)
C7—H7	0.9500	C21—Cr2	2.220 (10)
C8—C9	1.337 (15)	C21—H21	0.9500
C8—H8	0.9500	C22—C23	1.379 (12)
C9—H9	0.9500	C22—Cr2	2.213 (9)
C10—Pd1	2.034 (9)	C22—H22	0.9500
C10—H10A	0.9900	C23—C24	1.395 (12)
C10—H10B	0.9900	C23—Cr2	2.209 (9)
C11—C12	1.447 (13)	C23—H23	0.9500
C11—C24	1.505 (12)	C24—Cr2	2.278 (9)
C11—Pd1	2.057 (9)	C25—O1	1.149 (12)
C11—H11	1.0000	C25—Cr1	1.860 (13)
C12—C17	1.418 (12)	C26—O2	1.160 (11)
C12—C13	1.471 (13)	C26—Cr1	1.839 (10)
C12—Cr1	2.243 (9)	C26—Pd1	2.646 (10)

C12—Pd1	2.602 (10)	C27—O3	1.127 (11)
C13—C14	1.393 (13)	C27—Cr1	1.877 (12)
C13—Cr1	2.199 (9)	C28—O4	1.145 (11)
C13—H13	0.9500	C28—Cr2	1.860 (12)
C14—C15	1.378 (13)	C29—O5	1.148 (11)
C14—Cr1	2.206 (10)	C29—Cr2	1.843 (10)
C14—H14	0.9500	C30—O6	1.143 (11)
C15—C16	1.410 (12)	C30—Cr2	1.860 (12)
C15—Cr1	2.207 (9)	N1—Pd1	2.111 (8)
C15—H15	0.9500	Cr1—Pd1	2.8874 (16)
C16—C17	1.411 (12)		
N1—C1—C2	125.0 (10)	Cr2—C23—H23	126.2
N1—C1—H1	117.5	C23—C24—C19	117.8 (8)
C2—C1—H1	117.5	C23—C24—C11	123.1 (9)
C1—C2—C3	118.5 (10)	C19—C24—C11	118.9 (8)
C1—C2—H2	120.8	C23—C24—Cr2	69.2 (5)
C3—C2—H2	120.8	C19—C24—Cr2	71.1 (5)
C2—C3—C4	119.7 (11)	C11—C24—Cr2	126.4 (6)
C2—C3—H3	120.2	O1—C25—Cr1	172.6 (9)
C4—C3—H3	120.2	O2—C26—Cr1	171.9 (9)
C9—C4—C3	123.5 (10)	O2—C26—Pd1	108.5 (7)
C9—C4—C5	119.7 (10)	Cr1—C26—Pd1	77.9 (3)
C3—C4—C5	116.8 (9)	O3—C27—Cr1	178.5 (10)
N1—C5—C6	117.3 (9)	O4—C28—Cr2	176.7 (9)
N1—C5—C4	122.8 (9)	O5—C29—Cr2	179.3 (10)
C6—C5—C4	119.8 (9)	O6—C30—Cr2	176.0 (9)
C7—C6—C5	117.7 (10)	C1—N1—C5	117.1 (8)
C7—C6—C10	124.3 (10)	C1—N1—Pd1	130.9 (7)
C5—C6—C10	117.9 (8)	C5—N1—Pd1	111.9 (6)
C8—C7—C6	121.2 (10)	C26—Cr1—C25	97.7 (5)

C8—C7—H7	119.4	C26—Cr1—C27	87.4 (4)
C6—C7—H7	119.4	C25—Cr1—C27	84.4 (4)
C9—C8—C7	121.4 (11)	C26—Cr1—C13	83.3 (4)
C9—C8—H8	119.3	C25—Cr1—C13	142.7 (4)
C7—C8—H8	119.3	C27—Cr1—C13	132.7 (4)
C8—C9—C4	120.0 (11)	C26—Cr1—C14	98.0 (4)
C8—C9—H9	120.0	C25—Cr1—C14	163.9 (4)
C4—C9—H9	120.0	C27—Cr1—C14	100.0 (4)
C6—C10—Pd1	110.2 (7)	C13—Cr1—C14	36.9 (3)
C6—C10—H10A	109.6	C26—Cr1—C15	131.4 (4)
Pd1—C10—H10A	109.6	C25—Cr1—C15	129.5 (4)
C6—C10—H10B	109.6	C27—Cr1—C15	86.8 (4)
Pd1—C10—H10B	109.6	C13—Cr1—C15	66.5 (4)
H10A—C10—H10B	108.1	C14—Cr1—C15	36.4 (3)
C12—C11—C24	114.5 (8)	C26—Cr1—C16	161.2 (4)
C12—C11—Pd1	94.3 (6)	C25—Cr1—C16	98.3 (4)
C24—C11—Pd1	113.2 (6)	C27—Cr1—C16	103.9 (4)
C12—C11—H11	111.3	C13—Cr1—C16	78.0 (4)
C24—C11—H11	111.3	C14—Cr1—C16	65.6 (4)
Pd1—C11—H11	111.3	C15—Cr1—C16	37.0 (3)
C17—C12—C11	121.4 (9)	C26—Cr1—C12	100.0 (4)
C17—C12—C13	117.5 (8)	C25—Cr1—C12	105.6 (4)
C11—C12—C13	120.9 (8)	C27—Cr1—C12	166.4 (4)
C17—C12—Cr1	73.1 (5)	C13—Cr1—C12	38.7 (3)
C11—C12—Cr1	124.7 (6)	C14—Cr1—C12	67.9 (4)
C13—C12—Cr1	69.0 (5)	C15—Cr1—C12	79.8 (4)
C17—C12—Pd1	106.5 (6)	C16—Cr1—C12	66.1 (3)
C11—C12—Pd1	52.0 (5)	C26—Cr1—C17	134.9 (4)
C13—C12—Pd1	107.1 (6)	C25—Cr1—C17	88.0 (4)
Cr1—C12—Pd1	72.7 (3)	C27—Cr1—C17	137.7 (4)

C14—C13—C12	120.4 (9)	C13—Cr1—C17	67.0 (3)
C14—C13—Cr1	71.8 (6)	C14—Cr1—C17	78.3 (4)
C12—C13—Cr1	72.3 (5)	C15—Cr1—C17	66.7 (3)
C14—C13—H13	119.8	C16—Cr1—C17	36.4 (3)
C12—C13—H13	119.8	C12—Cr1—C17	36.5 (3)
Cr1—C13—H13	128.3	C26—Cr1—Pd1	63.6 (3)
C15—C14—C13	121.3 (9)	C25—Cr1—Pd1	66.7 (3)
C15—C14—Cr1	71.8 (6)	C27—Cr1—Pd1	134.1 (3)
C13—C14—Cr1	71.3 (6)	C13—Cr1—Pd1	81.0 (3)
C15—C14—H14	119.4	C14—Cr1—Pd1	117.8 (3)
C13—C14—H14	119.4	C15—Cr1—Pd1	139.1 (3)
Cr1—C14—H14	130.2	C16—Cr1—Pd1	114.5 (2)
C14—C15—C16	119.3 (9)	C12—Cr1—Pd1	59.4 (3)
C14—C15—Cr1	71.8 (6)	C17—Cr1—Pd1	78.4 (2)
C16—C15—Cr1	72.7 (5)	C29—Cr2—C30	87.2 (4)
C14—C15—H15	120.3	C29—Cr2—C28	87.5 (4)
C16—C15—H15	120.3	C30—Cr2—C28	92.0 (4)
Cr1—C15—H15	127.2	C29—Cr2—C23	111.8 (4)
C15—C16—C17	122.0 (9)	C30—Cr2—C23	161.0 (4)
C15—C16—Cr1	70.3 (5)	C28—Cr2—C23	89.1 (4)
C17—C16—Cr1	73.4 (5)	C29—Cr2—C22	147.8 (4)
C15—C16—H16	119.0	C30—Cr2—C22	124.8 (4)
C17—C16—H16	119.0	C28—Cr2—C22	87.5 (4)
Cr1—C16—H16	129.9	C23—Cr2—C22	36.3 (3)
C16—C17—C12	119.4 (9)	C29—Cr2—C21	159.0 (4)
C16—C17—C18	121.2 (8)	C30—Cr2—C21	96.8 (4)
C12—C17—C18	119.4 (8)	C28—Cr2—C21	112.8 (4)
C16—C17—Cr1	70.2 (5)	C23—Cr2—C21	65.5 (4)
C12—C17—Cr1	70.4 (5)	C22—Cr2—C21	36.2 (3)
C18—C17—Cr1	130.9 (6)	C29—Cr2—C20	122.3 (4)

C17—C18—C19	112.6 (8)	C30—Cr2—C20	92.7 (4)
C17—C18—H18A	109.1	C28—Cr2—C20	149.9 (4)
C19—C18—H18A	109.1	C23—Cr2—C20	77.3 (4)
C17—C18—H18B	109.1	C22—Cr2—C20	65.6 (4)
C19—C18—H18B	109.1	C21—Cr2—C20	37.1 (3)
H18A—C18—H18B	107.8	C29—Cr2—C19	93.8 (4)
C20—C19—C24	120.5 (8)	C30—Cr2—C19	115.3 (4)
C20—C19—C18	119.8 (8)	C28—Cr2—C19	152.7 (4)
C24—C19—C18	119.5 (8)	C23—Cr2—C19	65.2 (3)
C20—C19—Cr2	70.9 (5)	C22—Cr2—C19	77.0 (3)
C24—C19—Cr2	72.6 (5)	C21—Cr2—C19	65.8 (3)
C18—C19—Cr2	134.3 (6)	C20—Cr2—C19	36.2 (3)
C19—C20—C21	119.8 (9)	C29—Cr2—C24	88.9 (4)
C19—C20—Cr2	72.9 (5)	C30—Cr2—C24	150.9 (4)
C21—C20—Cr2	71.0 (6)	C28—Cr2—C24	116.6 (4)
C19—C20—H20	120.1	C23—Cr2—C24	36.2 (3)
C21—C20—H20	120.1	C22—Cr2—C24	65.3 (3)
Cr2—C20—H20	128.3	C21—Cr2—C24	77.6 (3)
C22—C21—C20	119.2 (9)	C20—Cr2—C24	65.5 (3)
C22—C21—Cr2	71.6 (6)	C19—Cr2—C24	36.4 (3)
C20—C21—Cr2	71.9 (5)	C10—Pd1—C11	88.7 (4)
C22—C21—H21	120.4	C10—Pd1—N1	82.3 (4)
C20—C21—H21	120.4	C11—Pd1—N1	170.1 (3)
Cr2—C21—H21	128.2	C10—Pd1—C12	122.2 (4)
C21—C22—C23	120.9 (9)	C11—Pd1—C12	33.7 (3)
C21—C22—Cr2	72.2 (6)	N1—Pd1—C12	155.5 (3)
C23—C22—Cr2	71.7 (5)	C10—Pd1—C26	149.2 (4)
C21—C22—H22	119.6	C11—Pd1—C26	100.9 (3)
C23—C22—H22	119.6	N1—Pd1—C26	85.0 (3)
Cr2—C22—H22	128.9	C12—Pd1—C26	73.5 (3)

C22—C23—C24	121.7 (9)	C10—Pd1—Cr1	169.5 (3)
C22—C23—Cr2	72.0 (5)	C11—Pd1—Cr1	81.5 (3)
C24—C23—Cr2	74.6 (5)	N1—Pd1—Cr1	107.7 (2)
C22—C23—H23	119.1	C12—Pd1—Cr1	47.9 (2)
C24—C23—H23	119.1	C26—Pd1—Cr1	38.5 (2)
N1—C1—C2—C3	−3.3 (17)	C16—C17—Cr1—C25	106.9 (6)
C1—C2—C3—C4	3.7 (16)	C12—C17—Cr1—C25	−120.0 (6)
C2—C3—C4—C9	175.7 (10)	C18—C17—Cr1—C25	−7.7 (9)
C2—C3—C4—C5	−3.1 (16)	C16—C17—Cr1—C27	27.5 (9)
C9—C4—C5—N1	−176.9 (9)	C12—C17—Cr1—C27	160.6 (7)
C3—C4—C5—N1	2.0 (14)	C18—C17—Cr1—C27	−87.1 (10)
C9—C4—C5—C6	−1.1 (14)	C16—C17—Cr1—C13	−101.4 (6)
C3—C4—C5—C6	177.8 (9)	C12—C17—Cr1—C13	31.7 (6)
N1—C5—C6—C7	177.9 (8)	C18—C17—Cr1—C13	144.0 (9)
C4—C5—C6—C7	1.8 (14)	C16—C17—Cr1—C14	−64.5 (6)
N1—C5—C6—C10	−4.9 (13)	C12—C17—Cr1—C14	68.6 (6)
C4—C5—C6—C10	179.0 (9)	C18—C17—Cr1—C14	−179.1 (9)
C5—C6—C7—C8	0.2 (15)	C16—C17—Cr1—C15	−28.2 (6)
C10—C6—C7—C8	−176.8 (10)	C12—C17—Cr1—C15	104.9 (7)
C6—C7—C8—C9	−3.2 (18)	C18—C17—Cr1—C15	−142.8 (9)
C7—C8—C9—C4	4.0 (19)	C12—C17—Cr1—C16	133.1 (9)
C3—C4—C9—C8	179.3 (12)	C18—C17—Cr1—C16	−114.6 (11)
C5—C4—C9—C8	−1.8 (17)	C16—C17—Cr1—C12	−133.1 (9)
C7—C6—C10—Pd1	−175.7 (8)	C18—C17—Cr1—C12	112.3 (11)
C5—C6—C10—Pd1	7.3 (11)	C16—C17—Cr1—Pd1	173.5 (6)
C24—C11—C12—C17	30.9 (12)	C12—C17—Cr1—Pd1	−53.4 (5)
Pd1—C11—C12—C17	−86.9 (8)	C18—C17—Cr1—Pd1	58.9 (8)
C24—C11—C12—C13	−153.9 (8)	C22—C23—Cr2—C29	−174.1 (6)
Pd1—C11—C12—C13	88.2 (8)	C24—C23—Cr2—C29	54.4 (7)
C24—C11—C12—Cr1	121.4 (8)	C22—C23—Cr2—C30	6.3 (15)

Pd1—C11—C12—Cr1	3.5 (8)	C24—C23—Cr2—C30	−125.3 (12)
C24—C11—C12—Pd1	117.9 (9)	C22—C23—Cr2—C28	−87.1 (6)
C17—C12—C13—C14	1.0 (13)	C24—C23—Cr2—C28	141.3 (6)
C11—C12—C13—C14	−174.3 (9)	C24—C23—Cr2—C22	−131.6 (9)
Cr1—C12—C13—C14	−55.5 (8)	C22—C23—Cr2—C21	28.6 (6)
Pd1—C12—C13—C14	−118.7 (8)	C24—C23—Cr2—C21	−102.9 (6)
C17—C12—C13—Cr1	56.5 (7)	C22—C23—Cr2—C20	65.9 (6)
C11—C12—C13—Cr1	−118.8 (8)	C24—C23—Cr2—C20	−65.7 (6)
Pd1—C12—C13—Cr1	−63.2 (4)	C22—C23—Cr2—C19	102.1 (7)
C12—C13—C14—C15	1.9 (15)	C24—C23—Cr2—C19	−29.5 (5)
Cr1—C13—C14—C15	−53.8 (9)	C22—C23—Cr2—C24	131.6 (9)
C12—C13—C14—Cr1	55.7 (8)	C21—C22—Cr2—C29	142.8 (8)
C13—C14—C15—C16	−3.4 (15)	C23—C22—Cr2—C29	10.4 (11)
Cr1—C14—C15—C16	−57.0 (8)	C21—C22—Cr2—C30	−45.2 (8)
C13—C14—C15—Cr1	53.5 (9)	C23—C22—Cr2—C30	−177.5 (6)
C14—C15—C16—C17	2.0 (14)	C21—C22—Cr2—C28	−135.8 (6)
Cr1—C15—C16—C17	−54.5 (8)	C23—C22—Cr2—C28	91.8 (6)
C14—C15—C16—Cr1	56.5 (8)	C21—C22—Cr2—C23	132.4 (9)
C15—C16—C17—C12	1.0 (14)	C23—C22—Cr2—C21	−132.4 (9)
Cr1—C16—C17—C12	−52.2 (8)	C21—C22—Cr2—C20	30.3 (6)
C15—C16—C17—C18	179.6 (8)	C23—C22—Cr2—C20	−102.1 (6)
Cr1—C16—C17—C18	126.5 (8)	C21—C22—Cr2—C19	66.7 (6)
C15—C16—C17—Cr1	53.2 (8)	C23—C22—Cr2—C19	−65.6 (6)
C11—C12—C17—C16	172.9 (8)	C21—C22—Cr2—C24	103.3 (6)
C13—C12—C17—C16	−2.4 (13)	C23—C22—Cr2—C24	−29.1 (6)
Cr1—C12—C17—C16	52.1 (8)	C22—C21—Cr2—C29	−116.0 (11)
Pd1—C12—C17—C16	117.7 (8)	C20—C21—Cr2—C29	14.4 (14)
C11—C12—C17—C18	−5.8 (13)	C22—C21—Cr2—C30	144.1 (6)
C13—C12—C17—C18	178.9 (8)	C20—C21—Cr2—C30	−85.5 (6)
Cr1—C12—C17—C18	−126.6 (8)	C22—C21—Cr2—C28	49.0 (7)

Pd1—C12—C17—C18	−61.0 (9)	C20—C21—Cr2—C28	179.5 (6)
C11—C12—C17—Cr1	120.8 (9)	C22—C21—Cr2—C23	−28.8 (6)
C13—C12—C17—Cr1	−54.5 (7)	C20—C21—Cr2—C23	101.7 (6)
Pd1—C12—C17—Cr1	65.6 (3)	C20—C21—Cr2—C22	130.4 (9)
C16—C17—C18—C19	155.2 (8)	C22—C21—Cr2—C20	−130.4 (9)
C12—C17—C18—C19	−26.1 (12)	C22—C21—Cr2—C19	−101.2 (6)
Cr1—C17—C18—C19	−114.8 (8)	C20—C21—Cr2—C19	29.2 (5)
C17—C18—C19—C20	−152.0 (8)	C22—C21—Cr2—C24	−64.8 (6)
C17—C18—C19—C24	33.9 (12)	C20—C21—Cr2—C24	65.6 (6)
C17—C18—C19—Cr2	−60.2 (11)	C19—C20—Cr2—C29	−42.9 (7)
C24—C19—C20—C21	0.1 (13)	C21—C20—Cr2—C29	−173.9 (6)
C18—C19—C20—C21	−174.0 (8)	C19—C20—Cr2—C30	−131.2 (6)
Cr2—C19—C20—C21	55.2 (8)	C21—C20—Cr2—C30	97.7 (6)
C24—C19—C20—Cr2	−55.2 (8)	C19—C20—Cr2—C28	130.1 (8)
C18—C19—C20—Cr2	130.8 (8)	C21—C20—Cr2—C28	−1.0 (11)
C19—C20—C21—C22	−0.3 (14)	C19—C20—Cr2—C23	65.1 (5)
Cr2—C20—C21—C22	55.8 (8)	C21—C20—Cr2—C23	−66.0 (6)
C19—C20—C21—Cr2	−56.1 (8)	C19—C20—Cr2—C22	101.5 (6)
C20—C21—C22—C23	−1.1 (14)	C21—C20—Cr2—C22	−29.6 (5)
Cr2—C21—C22—C23	54.8 (8)	C19—C20—Cr2—C21	131.1 (8)
C20—C21—C22—Cr2	−56.0 (8)	C21—C20—Cr2—C19	−131.1 (8)
C21—C22—C23—C24	2.9 (14)	C19—C20—Cr2—C24	28.9 (5)
Cr2—C22—C23—C24	58.0 (8)	C21—C20—Cr2—C24	−102.2 (6)
C21—C22—C23—Cr2	−55.0 (8)	C20—C19—Cr2—C29	144.8 (6)
C22—C23—C24—C19	−3.1 (14)	C24—C19—Cr2—C29	−83.0 (6)
Cr2—C23—C24—C19	53.7 (8)	C18—C19—Cr2—C29	31.5 (9)
C22—C23—C24—C11	−177.5 (9)	C20—C19—Cr2—C30	56.2 (6)
Cr2—C23—C24—C11	−120.7 (9)	C24—C19—Cr2—C30	−171.6 (5)
C22—C23—C24—Cr2	−56.8 (8)	C18—C19—Cr2—C30	−57.1 (10)
C20—C19—C24—C23	1.6 (13)	C20—C19—Cr2—C28	−123.3 (9)

C18—C19—C24—C23	175.6 (8)	C24—C19—Cr2—C28	8.9 (11)
Cr2—C19—C24—C23	−52.8 (8)	C18—C19—Cr2—C28	123.4 (10)
C20—C19—C24—C11	176.2 (8)	C20—C19—Cr2—C23	−102.9 (6)
C18—C19—C24—C11	−9.8 (13)	C24—C19—Cr2—C23	29.3 (5)
Cr2—C19—C24—C11	121.8 (8)	C18—C19—Cr2—C23	143.8 (10)
C20—C19—C24—Cr2	54.4 (8)	C20—C19—Cr2—C22	−66.4 (6)
C18—C19—C24—Cr2	−131.6 (8)	C24—C19—Cr2—C22	65.8 (6)
C12—C11—C24—C23	151.9 (9)	C18—C19—Cr2—C22	−179.7 (9)
Pd1—C11—C24—C23	−101.6 (9)	C20—C19—Cr2—C21	−29.9 (5)
C12—C11—C24—C19	−22.4 (12)	C24—C19—Cr2—C21	102.3 (6)
Pd1—C11—C24—C19	84.1 (9)	C18—C19—Cr2—C21	−143.2 (10)
C12—C11—C24—Cr2	64.5 (11)	C24—C19—Cr2—C20	132.2 (8)
Pd1—C11—C24—Cr2	171.0 (5)	C18—C19—Cr2—C20	−113.3 (11)
C2—C1—N1—C5	2.1 (15)	C20—C19—Cr2—C24	−132.2 (8)
C2—C1—N1—Pd1	−174.6 (8)	C18—C19—Cr2—C24	114.5 (11)
C6—C5—N1—C1	−177.4 (9)	C23—C24—Cr2—C29	−131.0 (6)
C4—C5—N1—C1	−1.4 (13)	C19—C24—Cr2—C29	97.9 (6)
C6—C5—N1—Pd1	0.0 (10)	C11—C24—Cr2—C29	−14.5 (8)
C4—C5—N1—Pd1	175.9 (7)	C23—C24—Cr2—C30	146.9 (8)
Pd1—C26—Cr1—C25	59.1 (4)	C19—C24—Cr2—C30	15.8 (10)
Pd1—C26—Cr1—C27	143.1 (4)	C11—C24—Cr2—C30	−96.6 (10)
Pd1—C26—Cr1—C13	−83.3 (3)	C23—C24—Cr2—C28	−44.3 (7)
Pd1—C26—Cr1—C14	−117.2 (3)	C19—C24—Cr2—C28	−175.4 (5)
Pd1—C26—Cr1—C15	−133.5 (4)	C11—C24—Cr2—C28	72.2 (9)
Pd1—C26—Cr1—C16	−88.9 (12)	C19—C24—Cr2—C23	−131.1 (8)
Pd1—C26—Cr1—C12	−48.3 (3)	C11—C24—Cr2—C23	116.5 (11)
Pd1—C26—Cr1—C17	−35.7 (6)	C23—C24—Cr2—C22	29.2 (6)
C14—C13—Cr1—C26	−113.1 (6)	C19—C24—Cr2—C22	−101.9 (6)
C12—C13—Cr1—C26	115.3 (6)	C11—C24—Cr2—C22	145.7 (9)
C14—C13—Cr1—C25	153.1 (7)	C23—C24—Cr2—C21	65.2 (6)

C12—C13—Cr1—C25	21.5 (9)	C19—C24—Cr2—C21	−65.9 (6)
C14—C13—Cr1—C27	−33.0 (8)	C11—C24—Cr2—C21	−178.3 (9)
C12—C13—Cr1—C27	−164.5 (6)	C23—C24—Cr2—C20	102.4 (6)
C12—C13—Cr1—C14	−131.6 (8)	C19—C24—Cr2—C20	−28.8 (5)
C14—C13—Cr1—C15	28.0 (6)	C11—C24—Cr2—C20	−141.1 (9)
C12—C13—Cr1—C15	−103.6 (6)	C23—C24—Cr2—C19	131.1 (8)
C14—C13—Cr1—C16	65.1 (6)	C11—C24—Cr2—C19	−112.4 (10)
C12—C13—Cr1—C16	−66.5 (5)	C6—C10—Pd1—C11	170.5 (7)
C14—C13—Cr1—C12	131.6 (8)	C6—C10—Pd1—N1	−5.4 (7)
C14—C13—Cr1—C17	101.6 (6)	C6—C10—Pd1—C12	174.7 (6)
C12—C13—Cr1—C17	−30.0 (5)	C6—C10—Pd1—C26	61.1 (11)
C14—C13—Cr1—Pd1	−177.3 (6)	C6—C10—Pd1—Cr1	−167.1 (12)
C12—C13—Cr1—Pd1	51.1 (5)	C12—C11—Pd1—C10	173.7 (6)
C15—C14—Cr1—C26	−159.2 (6)	C24—C11—Pd1—C10	54.7 (7)
C13—C14—Cr1—C26	67.3 (6)	C24—C11—Pd1—C12	−119.0 (9)
C15—C14—Cr1—C25	34.1 (17)	C12—C11—Pd1—C26	−35.7 (6)
C13—C14—Cr1—C25	−99.4 (15)	C24—C11—Pd1—C26	−154.7 (6)
C15—C14—Cr1—C27	−70.5 (6)	C12—C11—Pd1—Cr1	−2.3 (5)
C13—C14—Cr1—C27	156.1 (6)	C24—C11—Pd1—Cr1	−121.2 (7)
C15—C14—Cr1—C13	133.5 (9)	C1—N1—Pd1—C10	−179.9 (9)
C13—C14—Cr1—C15	−133.5 (9)	C5—N1—Pd1—C10	3.2 (6)
C15—C14—Cr1—C16	30.4 (6)	C1—N1—Pd1—C12	−0.1 (13)
C13—C14—Cr1—C16	−103.0 (6)	C5—N1—Pd1—C12	−176.9 (6)
C15—C14—Cr1—C12	103.2 (6)	C1—N1—Pd1—C26	28.2 (9)
C13—C14—Cr1—C12	−30.3 (5)	C5—N1—Pd1—C26	−148.7 (6)
C15—C14—Cr1—C17	66.4 (6)	C1—N1—Pd1—Cr1	−3.4 (9)
C13—C14—Cr1—C17	−67.0 (6)	C5—N1—Pd1—Cr1	179.8 (5)
C15—C14—Cr1—Pd1	136.4 (5)	C17—C12—Pd1—C10	109.8 (7)
C13—C14—Cr1—Pd1	3.0 (7)	C11—C12—Pd1—C10	−7.4 (7)
C14—C15—Cr1—C26	28.0 (8)	C13—C12—Pd1—C10	−123.6 (7)

C16—C15—Cr1—C26	158.0 (6)	Cr1—C12—Pd1—C10	175.6 (4)
C14—C15—Cr1—C25	−168.3 (6)	C17—C12—Pd1—C11	117.2 (9)
C16—C15—Cr1—C25	−38.3 (8)	C13—C12—Pd1—C11	−116.2 (9)
C14—C15—Cr1—C27	111.6 (6)	Cr1—C12—Pd1—C11	−177.0 (7)
C16—C15—Cr1—C27	−118.4 (6)	C17—C12—Pd1—N1	−70.1 (10)
C14—C15—Cr1—C13	−28.4 (6)	C11—C12—Pd1—N1	172.7 (7)
C16—C15—Cr1—C13	101.7 (6)	C13—C12—Pd1—N1	56.5 (10)
C16—C15—Cr1—C14	130.0 (9)	Cr1—C12—Pd1—N1	−4.3 (8)
C14—C15—Cr1—C16	−130.0 (9)	C17—C12—Pd1—C26	−99.5 (6)
C14—C15—Cr1—C12	−66.5 (6)	C11—C12—Pd1—C26	143.3 (6)
C16—C15—Cr1—C12	63.5 (6)	C13—C12—Pd1—C26	27.1 (6)
C14—C15—Cr1—C17	−102.2 (6)	Cr1—C12—Pd1—C26	−33.7 (3)
C16—C15—Cr1—C17	27.8 (6)	C17—C12—Pd1—Cr1	−65.8 (5)
C14—C15—Cr1—Pd1	−68.6 (7)	C11—C12—Pd1—Cr1	177.0 (7)
C16—C15—Cr1—Pd1	61.4 (7)	C13—C12—Pd1—Cr1	60.8 (5)
C15—C16—Cr1—C26	−60.9 (14)	O2—C26—Pd1—C10	−7.4 (12)
C17—C16—Cr1—C26	73.0 (13)	Cr1—C26—Pd1—C10	167.4 (6)
C15—C16—Cr1—C25	151.1 (6)	O2—C26—Pd1—C11	−113.7 (8)
C17—C16—Cr1—C25	−75.1 (6)	Cr1—C26—Pd1—C11	61.1 (4)
C15—C16—Cr1—C27	64.8 (7)	O2—C26—Pd1—N1	58.4 (8)
C17—C16—Cr1—C27	−161.3 (6)	Cr1—C26—Pd1—N1	−126.8 (4)
C15—C16—Cr1—C13	−66.6 (6)	O2—C26—Pd1—C12	−133.4 (8)
C17—C16—Cr1—C13	67.2 (6)	Cr1—C26—Pd1—C12	41.4 (3)
C15—C16—Cr1—C14	−29.9 (6)	O2—C26—Pd1—Cr1	−174.8 (10)
C17—C16—Cr1—C14	103.9 (6)	C26—Cr1—Pd1—C10	−142.2 (18)
C17—C16—Cr1—C15	133.9 (9)	C25—Cr1—Pd1—C10	105.7 (18)
C15—C16—Cr1—C12	−105.5 (7)	C27—Cr1—Pd1—C10	161.2 (18)
C17—C16—Cr1—C12	28.4 (6)	C13—Cr1—Pd1—C10	−55.3 (18)
C15—C16—Cr1—C17	−133.9 (9)	C14—Cr1—Pd1—C10	−57.1 (18)
C15—C16—Cr1—Pd1	−140.8 (5)	C15—Cr1—Pd1—C10	−18.5 (18)

C17—C16—Cr1—Pd1	−7.0 (6)	C16—Cr1—Pd1—C10	17.1 (18)
C17—C12—Cr1—C26	164.9 (6)	C12—Cr1—Pd1—C10	−20.9 (18)
C11—C12—Cr1—C26	48.1 (9)	C17—Cr1—Pd1—C10	12.8 (18)
C13—C12—Cr1—C26	−65.7 (6)	C26—Cr1—Pd1—C11	−119.6 (4)
Pd1—C12—Cr1—C26	51.0 (4)	C25—Cr1—Pd1—C11	128.3 (4)
C17—C12—Cr1—C25	64.0 (6)	C27—Cr1—Pd1—C11	−176.2 (5)
C11—C12—Cr1—C25	−52.9 (8)	C13—Cr1—Pd1—C11	−32.7 (4)
C13—C12—Cr1—C25	−166.7 (6)	C14—Cr1—Pd1—C11	−34.5 (4)
Pd1—C12—Cr1—C25	−50.0 (4)	C15—Cr1—Pd1—C11	4.1 (5)
C17—C12—Cr1—C27	−72.6 (18)	C16—Cr1—Pd1—C11	39.7 (4)
C11—C12—Cr1—C27	170.5 (14)	C12—Cr1—Pd1—C11	1.7 (4)
C13—C12—Cr1—C27	56.7 (17)	C17—Cr1—Pd1—C11	35.4 (3)
Pd1—C12—Cr1—C27	173.4 (15)	C26—Cr1—Pd1—N1	56.8 (4)
C17—C12—Cr1—C13	−129.3 (8)	C25—Cr1—Pd1—N1	−55.3 (4)
C11—C12—Cr1—C13	113.8 (10)	C27—Cr1—Pd1—N1	0.3 (5)
Pd1—C12—Cr1—C13	116.7 (5)	C13—Cr1—Pd1—N1	143.7 (3)
C17—C12—Cr1—C14	−100.4 (6)	C14—Cr1—Pd1—N1	141.9 (4)
C11—C12—Cr1—C14	142.8 (9)	C15—Cr1—Pd1—N1	−179.4 (5)
C13—C12—Cr1—C14	29.0 (5)	C16—Cr1—Pd1—N1	−143.9 (4)
Pd1—C12—Cr1—C14	145.7 (4)	C12—Cr1—Pd1—N1	178.1 (4)
C17—C12—Cr1—C15	−64.4 (6)	C17—Cr1—Pd1—N1	−148.1 (3)
C11—C12—Cr1—C15	178.7 (8)	C26—Cr1—Pd1—C12	−121.3 (5)
C13—C12—Cr1—C15	64.9 (5)	C25—Cr1—Pd1—C12	126.6 (4)
Pd1—C12—Cr1—C15	−178.4 (3)	C27—Cr1—Pd1—C12	−177.9 (5)
C17—C12—Cr1—C16	−28.3 (5)	C13—Cr1—Pd1—C12	−34.4 (4)
C11—C12—Cr1—C16	−145.2 (9)	C14—Cr1—Pd1—C12	−36.2 (4)
C13—C12—Cr1—C16	101.0 (6)	C15—Cr1—Pd1—C12	2.4 (5)
Pd1—C12—Cr1—C16	−142.3 (4)	C16—Cr1—Pd1—C12	38.0 (4)
C11—C12—Cr1—C17	−116.9 (11)	C17—Cr1—Pd1—C12	33.7 (4)
C13—C12—Cr1—C17	129.3 (8)	C25—Cr1—Pd1—C26	−112.1 (5)

Pd1—C12—Cr1—C17	−113.9 (6)	C27—Cr1—Pd1—C26	−56.5 (5)
C17—C12—Cr1—Pd1	113.9 (6)	C13—Cr1—Pd1—C26	86.9 (4)
C11—C12—Cr1—Pd1	−2.9 (6)	C14—Cr1—Pd1—C26	85.1 (5)
C13—C12—Cr1—Pd1	−116.7 (5)	C15—Cr1—Pd1—C26	123.8 (6)
C16—C17—Cr1—C26	−154.2 (7)	C16—Cr1—Pd1—C26	159.3 (5)
C12—C17—Cr1—C26	−21.2 (8)	C12—Cr1—Pd1—C26	121.3 (5)
C18—C17—Cr1—C26	91.2 (10)	C17—Cr1—Pd1—C26	155.1 (4)

Theoretical Section

1a ZORA-PBE-D3(BJ)/AE-TZP

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H	2.771438	2.054336	4.219046
Cr	4.051294	2.079827	0.872466
O	4.038472	2.176920	-2.129407
O	1.799715	4.072510	0.909639
O	1.981169	-0.088766	0.714795
C	5.054659	3.349536	2.460810
C	4.522831	4.450448	3.259972
H	4.680451	5.503290	3.030227
C	3.811619	3.965177	4.304072
C	3.099815	4.745696	5.357203
H	3.244636	5.824691	5.224273
H	3.454040	4.468773	6.362909
C	2.787592	0.759801	0.770250
C	4.033745	2.143299	-0.958529
C	2.678777	3.300371	0.887426
C	3.797256	2.450129	4.275014
H	4.251627	2.030824	5.189385
C	4.614367	2.122847	3.052587
C	4.981634	0.888680	2.482485
H	4.614883	-0.048006	2.901298
C	5.840957	0.868807	1.346965
H	6.119317	-0.077830	0.890105
C	6.238065	2.089628	0.746589
H	6.829208	2.064937	-0.167354
C	5.857635	3.345377	1.296446
H	6.151239	4.273671	0.811424
H	2.018235	4.537594	5.333674

	hartree	eV	kcal/mol	kJ/mol

Pauli Repulsion				
Kinetic (Delta T^0):	71.944188738899129	1957.7010	45145.66	188889.44
Delta V^Pauli Coulomb:	-36.282606110387462	-987.2999	-22767.68	-95259.97
Delta V^Pauli LDA-XC:	-9.106911193876115	-247.8117	-5714.67	-23910.19
Delta V^Pauli GGA-Exchange:	0.439704984229587	11.9650	275.92	1154.45
Delta V^Pauli GGA-Correlation:	-0.099094231191074	-2.6965	-62.18	-260.17

Total Pauli Repulsion:	26.895282187674063	731.8579	16877.05	70613.55
(Total Pauli Repulsion =				
Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	26.895282187674063	731.8579	16877.05	70613.55
Electrostatic Interaction:	-5.798907994859269	-157.7963	-3638.87	-15225.03
(Electrostatic Interaction =				
Delta V_elstat in the BB paper)				

Total Steric Interaction:	21.096374192814793	574.0616	13238.18	55388.52
(Total Steric Interaction =				
Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-27.808670770501426	-756.7124	-17450.21	-73011.65

Total Orbital Interactions:	-27.812680044252449	-756.8215	-17452.72	-73022.18
Alternative Decomposition Orb.Int.				
Kinetic:	-65.785201203849596	-1790.1064	-41280.84	-172719.02
Coulomb:	35.069056379799250	954.2776	22006.17	92073.79
XC:	2.903464779797899	79.0073	1821.95	7623.05

Total Orbital Interactions:	-27.812680044252446	-756.8215	-17452.72	-73022.18
Residu (E=Steric+OrbInt+Res):	0.000003293450019	0.0001	0.00	0.01
Dispersion Energy:	-0.038399769872803	-1.0449	-24.10	-100.82
Total Bonding Energy:	-6.754702327860440	-183.8048	-4238.64	-17734.47

List of All Frequencies:

Intensities
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Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
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-10.278931	0.000000	0.000000

61.002326	127.033940	1.942425
86.009450	17.054351	0.367671
88.179802	34.172512	0.755308
101.293980	40.536424	1.029217
103.698958	11.141913	0.289609
127.756064	28.626065	0.916687
151.647947	15.983625	0.607561
195.725647	22.916283	1.124268
226.801375	109.037557	6.198689
242.011202	10.799709	0.655127
308.616826	153.594002	11.881518
323.992644	44.992957	3.653909
354.261792	32.102968	2.850674
406.202497	1.082836	0.110251
409.886142	43.684588	4.488173
417.510180	5.337398	0.558566
428.131342	8.996245	0.965420
468.430239	16.594050	1.948388
487.271706	15.761754	1.925102
490.049548	5.297931	0.650765
503.697761	71.960400	9.085350
519.208927	54.644712	7.111617
544.246712	91.001424	12.414295
555.143303	144.293824	20.078484
592.072089	16.339166	2.424837
632.854166	90.108468	14.293787
644.200013	354.582475	57.255349
649.694837	207.777421	33.836531
664.222209	23.667663	3.940459
687.474122	517.657488	89.202479
774.225089	33.847520	6.568590
785.058282	34.337382	6.756895
814.128043	51.077281	10.423140
825.225407	42.216270	8.732338
858.758606	11.235511	2.418477
871.979825	0.723847	0.158209
884.194929	12.550757	2.781609
901.200187	11.122641	2.512507
919.702499	1.964298	0.452827
979.619143	6.537315	1.605221
991.772335	20.893180	5.193912
1015.703001	1.626228	0.414025
1062.751199	3.385149	0.901753
1120.509647	2.578166	0.724110
1127.033328	2.959880	0.836159
1132.970533	5.318250	1.510308
1149.442492	12.399086	3.572358
1184.209081	10.120212	3.003973
1214.315812	25.097030	7.638922
1279.152366	9.064793	2.906419
1305.157000	9.399403	3.074972
1365.675992	6.196875	2.121282
1380.859958	56.106390	19.419589
1398.879716	2.210117	0.774950
1409.620020	17.010589	6.010346
1423.857284	55.248026	19.717929
1434.677851	23.831466	8.570047
1439.206449	23.035960	8.310123
1494.296476	1.656434	0.620425
1526.565789	23.152379	8.859092
1615.399619	82.559429	33.429103
1896.452542	1804.919085	857.981229
1901.176690	1812.607053	863.782133
1956.563008	2352.382982	1153.665585
2948.796385	4.168325	3.080949
2953.201597	50.961270	37.723450
2995.848651	0.649572	0.487782
3001.195120	7.532781	5.666666
3054.298410	13.461905	10.306141
3120.054229	2.286966	1.788545
3129.202545	1.221983	0.958466
3137.253485	6.670160	5.245223
3145.246739	0.951456	0.750104
3152.019712	3.418615	2.700954

3a ZORA-PBE-D3(BJ)/AE-TZP

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C	3.486458	4.644574	12.644728
H	2.693783	5.308614	12.986608
C	3.308982	3.915259	11.427421
C	1.849283	0.487923	8.195705
C	-0.059727	1.939973	9.058020
C	0.203535	1.556038	6.527337
C	6.391310	6.382934	11.888170
C	4.168668	6.540126	10.602340
C	6.076585	5.058754	9.715387
H	1.300979	3.284499	11.091037
O	2.239845	-0.588384	8.443031
O	-0.898548	1.794363	9.862384
O	-0.487912	1.155524	5.673913
O	7.184180	7.154545	12.267236
O	3.512841	7.406426	10.169417
O	6.661486	4.961051	8.707245
Cr	1.297204	2.200685	7.855059
Cr	5.154638	5.155802	11.301775
C	2.012142	4.014960	10.669629
H	1.570046	5.008165	10.828726
C	2.173410	3.776171	9.188116
C	1.263131	4.370046	8.260291
H	0.431757	4.963244	8.638255
C	1.410373	4.174655	6.874119
H	0.690735	4.608570	6.183207
C	2.470117	3.358298	6.387177
H	2.567066	3.163738	5.321205
C	3.359467	2.756401	7.297101
H	4.149100	2.102024	6.930663
C	3.226028	2.966094	8.704444
C	4.203602	2.330442	9.663034
H	5.180617	2.233027	9.169839
H	3.874491	1.306785	9.909574
C	4.362324	3.105741	10.943771
C	5.585085	3.029598	11.681705
H	6.413010	2.447081	11.279922
C	5.747385	3.737482	12.887643
H	6.698406	3.703620	13.415258
C	4.686723	4.553609	13.374706
H	4.822323	5.146768	14.276719

	hartree	eV	kcal/mol	kJ/mol

Pauli Repulsion				
Kinetic (Delta T^0):	116.724436138100387	3176.2335	73245.70	306459.96
Delta V^Pauli Coulomb:	-60.189376372140458	-1637.8363	-37769.41	-158027.19
Delta V^Pauli LDA-XC:	-14.661926693041389	-398.9713	-9200.50	-38494.88
Delta V^Pauli GGA-Exchange:	0.738459066074054	20.0945	463.39	1938.82
Delta V^Pauli GGA-Correlation:	-0.178157226539973	-4.8479	-111.80	-467.75

Total Pauli Repulsion:	42.433434912452626	1154.6725	26627.39	111408.97
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	42.433434912452626	1154.6725	26627.39	111408.97
Electrostatic Interaction:	-9.445299157752361	-257.0197	-5927.02	-24798.63
(Electrostatic Interaction = Delta V_elstat in the BB paper)				

Total Steric Interaction:	32.988135754700266	897.6528	20700.37	86610.34
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-43.380128556999260	-1180.4334	-27221.44	-113894.51

Total Orbital Interactions:	-43.386638102159516	-1180.6105	-27225.53	-113911.60
Alternative Decomposition Orb.Int.				
Kinetic:	-107.179242688006468	-2916.4956	-67256.00	-281399.06
Coulomb:	58.693113668661631	1597.1209	36830.49	154098.75

XC:	5.099490917185292	138.7642	3199.98	13388.71
Total Orbital Interactions:	-43.386638102159544	-1180.6105	-27225.53	-113911.60
Residu (E=Steric+OrbInt+Res):	-0.000009000389363	-0.0002	-0.01	-0.02
Dispersion Energy:	-0.068609427935584	-1.8670	-43.05	-180.13
Total Bonding Energy:	-10.467120775784197	-284.8248	-6568.22	-27481.42

Intensities
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Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-----	-----	-----
-3.628359	88.783799	-0.080746
25.723501	519.264326	3.348086
55.098556	16.770937	0.231620
77.546392	1.732953	0.033684
80.379526	33.262230	0.670154
80.814065	15.478024	0.313531
82.494065	38.454353	0.795145
94.474032	123.376075	2.921605
97.257569	8.555704	0.208573
106.434024	5.887556	0.157070
110.103891	0.314038	0.008667
138.427763	22.395823	0.777085
152.127805	5.341677	0.203687
180.729970	0.050370	0.002282
221.228338	310.850554	17.237349
273.941657	1.848017	0.126894
281.199970	32.401927	2.283832
297.483108	1.352754	0.100869
313.841332	223.361078	17.570969
323.850335	100.105419	8.126060
331.117218	70.495085	5.850846
362.193314	51.166106	4.645162
386.860741	0.039541	0.003834
411.022364	0.989975	0.101992
411.388255	1.470096	0.151592
412.470210	0.019661	0.002033
430.017617	7.110587	0.766425
444.794164	52.587555	5.863003
457.248600	2.025781	0.232179
479.918423	14.227829	1.711528
485.687850	10.998493	1.338963
488.626260	1.203388	0.147387
490.299133	7.503878	0.922200
492.892402	28.858225	3.565331
496.820530	135.141349	16.829292
497.018485	18.250538	2.273664
524.185402	6.989472	0.918348
537.008697	283.744746	38.193303
540.262083	76.234477	10.323667
541.543281	82.146862	11.150702
543.433271	27.291243	3.717471
604.708415	0.148166	0.022458
606.333223	105.528238	16.038292
607.487172	30.279184	4.610620
641.700041	3.720488	0.598425
644.395289	308.134081	49.770289
646.294695	212.479464	34.421170
648.093432	214.579693	34.858148
649.108484	539.272452	87.741204
663.599200	43.358232	7.211996
684.152065	576.036885	98.782726
686.463387	434.738883	74.803847
724.470629	9.666373	1.755345
766.935781	15.404271	2.961272
799.267826	94.178705	18.867880
802.196433	3.162691	0.635939
844.555352	3.298491	0.698267
848.011094	16.999130	3.613319
858.536542	3.390530	0.729633
860.474438	8.918274	1.923521
891.573847	18.791534	4.199500
895.406108	8.675227	1.947058
908.809630	41.622996	9.481659
917.425440	0.129029	0.029671
924.049010	0.074109	0.017165
928.765183	3.627672	0.844524
1004.846866	14.637052	3.686647
1005.980877	18.539886	4.674927
1060.690290	0.161915	0.043048
1097.773079	26.448206	7.277578
1134.875312	6.403418	1.821537
1139.217839	0.207108	0.059140
1156.471991	1.390958	0.403206

1171.325786	6.331092	1.858807
1173.538636	9.815581	2.887297
1183.647483	9.711495	2.881287
1188.339936	0.193496	0.057636
1195.167912	51.465805	15.417919
1215.664541	3.877581	1.181552
1240.715432	14.538681	4.521424
1306.546636	5.940029	1.945322
1325.709781	0.637541	0.211853
1392.055435	0.216543	0.075558
1397.972240	4.750285	1.664548
1398.802241	17.311316	6.069662
1417.043550	0.180620	0.064155
1422.047415	5.046458	1.798783
1422.874009	35.621017	12.704303
1442.187939	60.858589	21.999956
1446.934927	1.169931	0.424314
1486.853591	56.502702	21.057921
1511.290881	0.099429	0.037665
1513.296232	0.003978	0.001509
1517.624109	2.812898	1.070031
1895.801584	1251.277400	594.599518
1904.960054	822.675756	392.819142
1905.379137	1935.164257	924.224144
1907.037668	3122.555230	1492.613861
1958.986063	3683.952968	1808.937215
1963.020132	777.241095	382.435834
2953.149906	2.105019	1.558187
2955.120291	4.834423	3.580947
3010.534127	4.151027	3.132400
3011.777550	3.038876	2.294109
3122.620252	0.486319	0.380644
3124.042827	0.528859	0.414128
3124.199872	0.785479	0.615108
3125.939786	0.456386	0.357595
3137.112525	0.183739	0.144481
3139.147485	0.029820	0.023464
3147.822349	3.634136	2.867408
3149.960670	1.573840	1.242636

1c ZORA PBE-D3(BJ)/AE-TZP

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Pd	1.943218	2.101849	3.004103
Cr	3.980085	2.056819	0.928226
O	3.806133	2.140237	-2.063379
O	2.091828	4.396568	0.725780
O	2.249231	-0.367127	0.592030
N	-0.033541	1.752428	2.113788
C	-0.939736	2.636755	2.937764
H	-1.971304	2.288536	2.747745
C	-0.567073	2.440185	4.386564
C	0.775225	2.176196	4.665872
C	1.151980	1.955279	6.018641
H	2.185539	1.723708	6.274627
C	0.230327	2.025971	7.042566
H	0.539928	1.848042	8.075457
C	-1.129997	2.333426	6.783688
C	-2.087046	2.430288	7.8277610
H	-1.756217	2.261545	8.854783
C	-3.406009	2.732324	7.559720
H	-4.130865	2.805216	8.371500
C	-3.818599	2.951095	6.224496
H	-4.861046	3.195041	6.013588
C	-2.912951	2.861902	5.186444
H	-3.257432	3.045712	4.168421
C	-1.543909	2.546950	5.424075
C	-0.836687	4.113200	2.555763
H	0.209456	4.443918	2.617294
H	-1.425174	4.698342	3.274903
H	-1.223042	4.319634	1.548740
C	-0.208449	2.016971	0.665811
H	0.374190	1.284003	0.099236
H	0.137928	3.020945	0.411510
H	-1.274040	1.913388	0.389528
C	-0.409827	0.333018	2.362157
H	-1.435822	0.149432	1.993852
H	-0.364865	0.127514	3.435473
H	0.289570	-0.320506	1.832304
C	3.707877	2.462373	4.163212
H	3.650969	1.813687	5.038730
C	4.627133	2.140226	3.077840
C	5.016456	0.906296	2.505476
H	4.664543	-0.030654	2.934610
C	5.832540	0.898992	1.346413
H	6.114008	-0.044553	0.883870
C	6.180915	2.123738	0.721070
H	6.724888	2.103128	-0.222164
C	5.808794	3.370547	1.282556
H	6.069642	4.296756	0.773176
C	5.086969	3.389638	2.499658
C	4.575997	4.457885	3.311659
H	4.737100	5.516956	3.120971
C	3.796764	3.926265	4.315703
C	3.117638	4.704602	5.393811
H	3.338034	5.775705	5.308103
H	3.443938	4.361990	6.387705
H	2.028743	4.558252	5.353695
C	3.879630	2.116141	-0.894290
C	2.742900	3.432952	0.895333
C	2.860835	0.621773	0.780800

	hartree	eV	kcal/mol	kJ/mol

Pauli Repulsion				
Kinetic (Delta T^0):	147.344433883099413	4009.4460	92460.04	386852.76
Delta V^Pauli Coulomb:	-73.896794924458987	-2010.8341	-46370.94	-194016.01
Delta V^Pauli LDA-XC:	-19.036802385734436	-518.0177	-11945.78	-49981.12
Delta V^Pauli GGA-Exchange:	0.940188120517600	25.5838	589.98	2468.46
Delta V^Pauli GGA-Correlation:	-0.214979828473442	-5.8499	-134.90	-564.43

Total Pauli Repulsion:	55.136044864950151	1500.3281	34598.39	144759.67
(Total Pauli Repulsion =				
Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	55.136044864950151	1500.3281	34598.39	144759.67
Electrostatic Interaction:	-11.620803340942640	-316.2181	-7292.16	-30510.41
(Electrostatic Interaction =				
Delta V_elstat in the BB paper)				

Total Steric Interaction:	43.515241524007507	1184.1100	27306.23	114249.25

(Total Steric Interaction =
Delta E^0 in the BB paper)

Orbital Interactions				
A:	-57.247614086309476	-1557.7868	-35923.42	-150303.59

Total Orbital Interactions:	-57.257787884959669	-1558.0637	-35929.81	-150330.30
Alternative Decomposition Orb.Int.				
Kinetic:	-134.433581775858897	-3658.1239	-84358.36	-352955.32
Coulomb:	71.047187432333075	1933.2923	44582.79	186534.36
XC:	6.128606458566157	166.7679	3845.76	16090.65

Total Orbital Interactions:	-57.257787884959669	-1558.0637	-35929.81	-150330.30
Residu (E=Steric+OrbInt+Res):	0.000019875669135	0.0005	0.01	0.05
Dispersion Energy:	-0.105414770057775	-2.8685	-66.15	-276.77
Total Bonding Energy:	-13.847941255340801	-376.8217	-8689.72	-36357.76

Intensities
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Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole

30.686813	34.732500	0.267157
36.765152	75.854541	0.699030
48.584572	28.577657	0.348019
61.386051	25.088987	0.386039
78.351674	13.395467	0.263078
85.306227	32.101056	0.686401
92.076639	12.731270	0.293832
96.424477	46.443103	1.122501
102.115713	41.963594	1.074097
107.665203	13.187388	0.355887
109.219876	15.753966	0.431290
123.159914	25.360838	0.782909
127.352810	103.791069	3.313192
135.002500	4.796762	0.162319
140.697576	17.077389	0.602263
148.026757	14.108840	0.523491
175.321103	14.120788	0.620542
178.329798	42.527932	1.900974
186.511208	20.837431	0.974153
207.017308	4.725244	0.245193
215.930465	67.508757	3.653862
219.706880	42.396284	2.334799
232.070754	33.652580	1.957568
239.169268	6.452985	0.386851
254.909127	5.991084	0.382797
266.289474	3.725935	0.248695
273.358683	0.410575	0.028132
280.069500	17.147051	1.203742
311.712744	123.491346	9.648708
317.231234	35.297952	2.806749
322.769198	10.629610	0.859978
329.181501	29.645326	2.446075
364.023640	39.605024	3.613749
373.328424	5.104336	0.477648
390.088727	105.943814	10.358982
395.643487	31.256787	3.099748
403.362468	75.617375	7.645311
418.715208	23.290161	2.444383
437.233615	26.347568	2.887567
449.609973	35.162168	3.962686
452.196457	21.690980	2.458580
465.839741	52.477411	6.127552
473.615274	3.203639	0.380318
482.452421	49.372088	5.970546
492.090114	7.905276	0.975079
495.138485	5.707322	0.708332
499.512327	24.428039	3.058531
507.276082	60.246680	7.660473
521.004249	13.366035	1.745508
529.588678	115.054170	15.272816
540.809470	50.243786	6.810903
558.480323	81.495914	11.408322
558.978347	15.816890	2.216125
572.619998	22.384016	3.212792
597.060520	30.335674	4.539940
616.774911	660.700704	102.143219
631.029854	14.265447	2.256386
635.981737	365.143757	58.208525
638.064264	260.421203	41.650367
643.514949	8.286074	1.336551
658.690407	14.682272	2.424112
678.165324	146.655261	24.929370
687.640836	201.355353	34.705868

720.453408	77.690450	14.029804
728.911728	11.932048	2.180058
766.890730	75.751150	14.561321
772.940142	68.236383	13.220258
781.195618	78.785125	15.427022
786.730368	139.905859	27.589250
793.334628	121.736010	24.207701
806.870225	122.201698	24.714908
820.148491	23.060707	4.740708
824.039460	241.114145	49.802228
841.324285	12.122003	2.556324
846.400929	23.902106	5.070962
854.281034	29.330527	6.280565
878.913020	58.862410	12.967672
902.421635	9.985066	2.258596
917.195519	6.730435	1.547331
923.143114	4.744597	1.097859
925.801145	90.568605	21.017133
931.564651	5.301050	1.237807
936.046737	5.121982	1.201749
954.511614	0.791028	0.189257
974.609009	19.681191	4.807949
980.837671	27.988970	6.881167
995.248047	20.068318	5.006340
999.249665	22.674241	5.679170
1011.629590	0.782635	0.198454
1013.217860	19.559244	4.967444
1027.257711	65.059843	16.752148
1062.253684	22.034425	5.866891
1067.066580	59.538904	15.924669
1070.679507	11.833544	3.175794
1090.916657	4.600844	1.258077
1107.905912	52.073776	14.461056
1116.600333	10.810090	3.025556
1135.862441	30.403268	8.656136
1138.711679	3.439041	0.981588
1150.577180	13.131883	3.787223
1153.778059	15.851602	4.584305
1159.870710	11.050509	3.212698
1173.908385	6.467272	1.902976
1187.333752	43.438543	12.927845
1190.989088	18.620610	5.558783
1220.406669	6.522989	1.995397
1221.645679	5.910856	1.809980
1238.962857	87.987659	27.324871
1242.409572	93.812583	29.214870
1286.317365	8.702029	2.805736
1292.626374	33.113683	10.728983
1320.910966	2.006674	0.664398
1327.287872	39.943041	13.288756
1348.092339	10.591814	3.579053
1356.504278	20.826697	7.081408
1357.073193	19.862223	6.756304
1360.461520	48.773596	16.632178
1375.783368	80.187986	27.652693
1377.670537	28.069408	9.692966
1382.327347	16.096998	5.577427
1407.766523	25.299113	8.927174
1415.237411	20.848605	7.395787
1420.168611	14.613295	5.201950
1430.885638	13.118391	4.705043
1434.172213	11.064344	3.977453
1435.828376	25.290119	9.101888
1436.445415	105.757148	38.078246
1438.548030	19.436102	7.008283
1442.999336	22.268657	8.054493
1448.668150	10.456459	3.796922
1455.212211	26.999267	9.848189
1460.827022	46.086789	16.875370
1476.091632	12.025316	4.449261
1496.488220	57.266210	21.480768
1496.885084	6.287768	2.359191
1524.343250	168.504450	64.383149
1541.747931	36.241933	14.005635
1542.443972	19.965223	7.719011
1565.236594	104.795877	41.115186
1606.990218	49.510159	19.942777
1856.581252	1600.080357	744.618504
1876.388287	807.513443	379.796138
1936.424076	2475.947993	1201.766413
2913.458698	17.319747	12.648193
2919.403081	16.574947	12.128980
2924.775832	192.882296	141.404432
2962.046621	24.445281	18.149514
2968.881903	21.935984	16.324057
3019.738742	4.428928	3.352325
3048.346918	16.528703	12.629357
3052.915273	4.664618	3.569512
3053.776975	1.964676	1.503857

3055.953275	16.784712	12.856971
3059.673310	2.352564	1.804241
3076.569270	7.032790	5.423410
3087.413919	7.073958	5.474386
3093.671416	7.500656	5.816363
3095.703969	4.742319	3.679834
3101.115333	0.823995	0.640502
3106.495233	35.973292	28.011021
3110.381181	18.019899	14.048956
3112.554071	1.008108	0.786506
3122.592862	34.686296	27.148845
3123.687192	0.819802	0.641881
3127.272712	0.339024	0.265751
3136.713142	1.462820	1.150121
3142.977897	3.139882	2.473618
3148.171662	6.400806	5.050928

2c ZORA-PBE-D3/AE-TZP

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C	-0.584066	2.481577	-4.586655
C	-1.698154	3.208883	-4.140647
H	-2.614743	2.699779	-3.836462
C	-1.666517	4.608295	-4.067398
H	-2.547345	5.151853	-3.718330
C	-0.519154	5.309706	-4.445543
H	-0.495889	6.399315	-4.393944
C	0.598455	4.603728	-4.901144
H	1.497520	5.144199	-5.210409
C	0.569685	3.206347	-4.964289
C	1.755351	2.406079	-5.416663
H	2.429633	2.987912	-6.072260
H	2.336202	2.066048	-4.546403
C	0.694769	1.534655	-7.433117
H	-0.124594	2.242398	-7.269935
H	0.306693	0.629478	-7.911421
H	1.460272	1.997552	-8.083895
C	2.465514	0.292710	-6.363777
H	2.141959	-0.617046	-6.879260
H	2.930340	0.025891	-5.409939
H	3.205937	0.816472	-6.995356
C	-2.009120	0.139030	-3.521747
H	-2.843792	0.688183	-3.959862
C	-1.957078	-1.315336	-3.577195
C	-2.354594	-2.234735	-4.578416
H	-2.905525	-1.888998	-5.452062
C	-1.994523	-3.598740	-4.455113
H	-2.271183	-4.307692	-5.232450
C	-1.169530	-4.016847	-3.376750
H	-0.814778	-5.046262	-3.348124
C	-0.771093	-3.115478	-2.361195
H	-0.120066	-3.455626	-1.557410
C	-1.218266	-1.770817	-2.416227
C	-0.949575	-0.629209	-1.568204
C	-1.453454	0.479161	-2.210994
H	-1.385666	1.502974	-1.852003
C	-0.131602	-0.685052	-0.312835
H	0.835745	-1.166939	-0.539071
H	-0.625872	-1.332799	0.430246
C	1.224660	-1.283369	-3.776987
C	-0.153253	-1.807248	-6.182853
C	1.135951	-3.523302	-4.960036
N	1.297386	1.171854	-6.123163
O	2.156888	-0.783929	-3.260314
O	-0.184516	-1.646647	-7.352210
O	1.955679	-4.278899	-5.325400
Cr	-0.155424	-2.342678	-4.427722
Pd	-0.323653	0.472688	-4.798889
C	2.009120	-0.139030	3.521747
H	2.843792	-0.688183	3.959862
C	1.957078	1.315336	3.577195
C	2.354594	2.234735	4.578416
H	2.905525	1.888998	5.452062
C	1.994523	3.598740	4.455113
H	2.271183	4.307692	5.232450
C	1.169530	4.016847	3.376750
H	0.814778	5.046262	3.348124
C	0.771093	3.115478	2.361195
H	0.120066	3.455626	1.557410
C	1.218266	1.770817	2.416227
C	0.949575	0.629209	1.568204
C	1.453454	-0.479161	2.210994
H	1.385666	-1.502974	1.852003
C	0.131602	0.685052	0.312835
H	-0.835745	1.166939	0.539071
H	0.625872	1.332799	-0.430246
C	0.584066	-2.481577	4.586655
C	1.698154	-3.208883	4.140647
H	2.614743	-2.699779	3.836462
C	1.666517	-4.608295	4.067398
H	2.547345	-5.151853	3.718330
C	0.519154	-5.309706	4.445543
H	0.495889	-6.399315	4.393944
C	-0.598455	-4.603728	4.901144
H	-1.497520	-5.144199	5.210409
C	-0.569685	-3.206347	4.964289
C	-1.755351	-2.406079	5.416663
H	-2.429633	-2.987912	6.072260
H	-2.336202	-2.066048	4.546403
C	-0.694769	-1.534655	7.433117
H	-0.124594	-2.242398	7.269935
H	-0.306693	-0.629478	7.911421
H	-1.460272	-1.997552	8.083895

C	-2.465514	-0.292710	6.363777
H	-2.141959	0.617046	6.879260
H	-2.930340	-0.025891	5.409939
H	-3.205937	-0.816472	6.995356
C	-1.224660	1.283369	3.776987
C	0.153253	1.807248	6.182853
C	-1.135951	3.523302	4.960036
N	-1.297386	-1.171854	6.123163
O	-2.156888	0.783929	3.260314
O	0.184516	1.646647	7.352210
O	-1.955679	4.278899	5.325400
Cr	0.155424	2.342678	4.427722
Pd	0.323653	-0.472688	4.798889

	hartree	eV	kcal/mol	kJ/mol

Pauli Repulsion				
Kinetic (Delta T^0):	247.930980278188059	6746.5452	155579.06	650942.70
Delta V^APauli Coulomb:	-126.146070719951069	-3432.6092	-79157.86	-331196.46
Delta V^APauli LDA-XC:	-31.914222030124009	-868.4302	-20026.48	-83790.78
Delta V^APauli GGA-Exchange:	1.618113661228115	44.0311	1015.38	4248.36
Delta V^APauli GGA-Correlation:	-0.386792911554085	-10.5252	-242.72	-1015.52

Total Pauli Repulsion:	91.102008277787007	2479.0118	57167.38	239188.29
(Total Pauli Repulsion =				
Delta E^APauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^APauli):	91.102008277787007	2479.0118	57167.38	239188.29
Electrostatic Interaction:	-19.545943164329429	-531.8722	-12265.27	-51317.87
(Electrostatic Interaction =				
Delta V_elstat in the BB paper)				

Total Steric Interaction:	71.556065113457578	1947.1396	44902.11	187870.42
(Total Steric Interaction =				
Delta E^0 in the BB paper)				
Orbital Interactions				
A.g:	-47.156715681971207	-1283.1995	-29591.29	-123809.94
A.u:	-47.199069873705149	-1284.3520	-29617.87	-123921.14

Total Orbital Interactions:	-94.380048294751575	-2568.2118	-59224.38	-247794.78
Alternative Decomposition Orb.Int.				
Kinetic:	-226.667774947095296	-6167.9440	-142236.19	-595116.16
Coulomb:	121.690121560623396	3311.3567	76361.71	319497.37
XC:	10.597605091720375	288.3755	6650.10	27824.01

Total Orbital Interactions:	-94.380048294751532	-2568.2118	-59224.38	-247794.78
Residu (E=Steric+OrbInt+Res):				
Dispersion Energy:	0.000067742960734	0.0018	0.04	0.18
Dispersion Energy:	-0.180779563562241	-4.9193	-113.44	-474.64
Total Bonding Energy:				
	-23.004695001895502	-625.9896	-14435.67	-60398.82

Intensities

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Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole

-12.654564	0.000000	0.000000
-5.686016	0.000000	0.000000
15.943483	0.000000	0.000000
19.784735	0.000000	0.000000
20.601873	0.000000	0.000000
29.062618	110.362433	0.803959
30.604017	0.000000	0.000000
41.798375	70.982336	0.743683
46.354658	0.000000	0.000000
52.489614	47.432507	0.624062
69.092145	0.000000	0.000000
76.985476	0.000000	0.000000
77.571394	16.291491	0.316767
89.830307	0.000000	0.000000
90.913591	69.884216	1.592524
94.162153	16.913642	0.399201
94.275807	0.000000	0.000000
95.662208	59.157062	1.418486
100.229493	0.000000	0.000000
100.424176	138.954364	3.497748
104.652180	73.778529	1.935336
106.635789	0.000000	0.000000
111.846287	0.000000	0.000000

124.587124	71.802455	2.242284
125.583265	0.000000	0.000000
128.324809	30.727329	0.988356
129.641663	0.000000	0.000000
134.356244	253.794199	8.547077
136.355254	0.000000	0.000000
144.758409	157.880324	5.728618
154.967821	0.000000	0.000000
155.566175	46.579641	1.816308
157.881311	0.000000	0.000000
182.932525	123.083228	5.643751
186.242771	0.000000	0.000000
190.079435	0.000000	0.000000
203.572215	0.000000	0.000000
204.321407	16.771679	0.858951
215.877859	0.000000	0.000000
216.110784	48.260590	2.614250
233.144623	0.000000	0.000000
235.666503	27.474849	1.622973
249.781306	0.000000	0.000000
256.244735	28.529324	1.832418
265.951116	0.000000	0.000000
268.649781	39.157173	2.636792
271.245571	0.000000	0.000000
278.890162	17.461958	1.220687
279.122831	0.000000	0.000000
280.010680	18.506954	1.298936
289.322814	60.459730	4.384569
295.131236	0.000000	0.000000
298.243784	39.926216	2.984748
304.565242	0.000000	0.000000
304.609865	5.798803	0.442752
314.657272	131.375102	10.361650
317.231354	0.000000	0.000000
337.209832	0.000000	0.000000
338.256009	124.613382	10.565457
352.841816	61.013299	5.396133
352.853806	0.000000	0.000000
385.659912	0.000000	0.000000
385.791011	8.494681	0.821443
387.796069	40.243831	3.911837
387.881513	0.000000	0.000000
405.552144	0.000000	0.000000
408.718781	11.495147	1.177653
420.379744	0.000000	0.000000
420.406734	90.248264	9.510133
442.701560	0.000000	0.000000
443.950677	197.929336	22.025357
451.987500	0.000000	0.000000
459.716502	59.831368	6.894410
460.118670	0.000000	0.000000
463.084007	3.240231	0.376109
463.421964	0.000000	0.000000
468.702375	215.540212	25.322322
468.941976	0.000000	0.000000
481.419412	118.717991	14.325778
491.009636	0.000000	0.000000
494.292040	86.641229	10.734611
500.573242	0.000000	0.000000
502.942911	64.429797	8.122384
503.003528	0.000000	0.000000
504.196712	43.504185	5.498055
530.098463	125.138983	16.627511
530.456525	0.000000	0.000000
538.100419	270.318769	36.460079
540.065180	0.000000	0.000000
549.973401	0.000000	0.000000
550.137659	12.620989	1.740375
559.724164	6.167737	0.865322
563.983806	0.000000	0.000000
572.757898	131.309734	18.851507
602.499285	0.000000	0.000000
609.022744	0.000000	0.000000
609.576983	1086.095673	165.949028
612.780398	77.052961	11.835109
612.786020	0.000000	0.000000
620.902840	465.593780	72.461761
623.969030	0.000000	0.000000
631.276280	702.289545	111.125504
636.632198	0.000000	0.000000
648.199299	16.913140	2.747963
648.234268	0.000000	0.000000
678.045169	526.232316	89.436380
679.789493	0.000000	0.000000
690.323040	218.380493	37.787162
693.640673	0.000000	0.000000
695.849545	105.889765	18.469171
702.026163	0.000000	0.000000
702.055722	16.594764	2.920255

718.665141	0.000000	0.000000
721.834049	456.553775	82.605197
721.839972	0.000000	0.000000
749.612421	51.613816	9.697969
758.561025	15.610395	2.968127
795.997802	0.000000	0.000000
803.961802	0.000000	0.000000
804.254889	229.032013	46.170861
811.082377	0.000000	0.000000
815.032442	114.052573	23.300114
823.230162	0.000000	0.000000
823.757300	63.760683	13.165286
830.760470	231.671160	48.242062
830.815081	0.000000	0.000000
842.884184	0.000000	0.000000
843.238445	253.258225	53.529357
845.272502	0.000000	0.000000
850.482003	104.603421	22.299190
853.391583	0.000000	0.000000
853.748183	50.227398	10.748517
864.700330	206.468363	44.750430
865.937238	0.000000	0.000000
905.795323	0.000000	0.000000
905.805336	16.704054	3.792581
907.434199	17.000076	3.866732
907.472268	0.000000	0.000000
937.402870	0.000000	0.000000
937.728966	12.950183	3.043906
952.041542	2.336042	0.557461
952.042736	0.000000	0.000000
957.904096	0.000000	0.000000
957.913046	27.527097	6.609439
977.036896	0.000000	0.000000
980.895185	115.230286	28.331353
980.909730	0.000000	0.000000
993.210048	11.775967	2.931675
994.721035	0.000000	0.000000
997.344357	95.312319	23.827158
1006.166634	0.000000	0.000000
1006.269341	113.428299	28.609728
1006.762564	0.000000	0.000000
1007.047380	295.064195	74.480826
1017.333902	0.000000	0.000000
1023.520643	0.000000	0.000000
1038.874919	23.426154	6.100176
1040.189274	0.000000	0.000000
1043.986562	128.851299	33.717998
1065.595134	0.000000	0.000000
1080.457327	50.242829	13.606918
1082.671816	0.000000	0.000000
1082.712498	14.181410	3.848670
1083.438161	0.000000	0.000000
1101.319448	26.710203	7.373413
1101.320638	0.000000	0.000000
1131.041910	5.736676	1.626362
1131.080939	0.000000	0.000000
1139.286447	21.504743	6.141087
1139.762909	0.000000	0.000000
1147.149087	1.681232	0.483421
1147.188069	0.000000	0.000000
1157.026356	16.984043	4.925637
1157.049812	0.000000	0.000000
1165.129337	16.458020	4.806509
1168.585280	11.001481	3.222476
1170.162814	0.000000	0.000000
1191.204827	198.763851	59.347430
1193.651975	0.000000	0.000000
1194.115720	41.914285	12.545459
1196.806967	0.000000	0.000000
1226.080244	25.097063	7.712938
1229.749409	0.000000	0.000000
1229.875852	5.176577	1.595813
1230.826700	6.186432	1.908601
1230.843816	0.000000	0.000000
1241.561821	37.038618	11.526599
1244.390617	0.000000	0.000000
1265.261511	9.528013	3.021765
1265.261529	0.000000	0.000000
1275.672198	0.000000	0.000000
1292.604062	0.000000	0.000000
1299.311257	42.999364	14.004039
1308.270633	0.000000	0.000000
1312.833452	12.962424	4.265539
1312.916330	0.000000	0.000000
1338.153634	30.331521	10.173684
1338.199890	0.000000	0.000000
1345.784291	139.516491	47.062942
1365.583622	0.000000	0.000000
1377.110436	48.284530	16.666901

1380.270701	0.000000	0.000000
1380.318631	44.376356	15.353559
1381.118609	0.000000	0.000000
1407.354106	59.126751	20.857655
1407.386806	0.000000	0.000000
1420.970245	0.000000	0.000000
1420.981054	30.134491	10.733224
1426.837655	0.000000	0.000000
1426.848195	75.763749	27.096756
1429.156219	149.028423	53.385938
1429.239710	0.000000	0.000000
1433.207565	0.000000	0.000000
1433.208427	1.405973	0.505085
1436.442426	0.000000	0.000000
1436.452824	50.876447	18.318344
1440.120739	0.000000	0.000000
1445.215433	23.887771	8.653390
1445.524439	0.000000	0.000000
1445.583627	46.613176	16.890013
1450.713955	3.272666	1.190040
1450.723300	0.000000	0.000000
1460.236270	0.000000	0.000000
1460.245033	137.258242	50.239145
1467.710501	0.000000	0.000000
1467.720788	58.781779	21.625405
1491.753497	39.431312	14.744035
1491.909896	0.000000	0.000000
1513.262833	101.442973	38.478170
1515.969592	0.000000	0.000000
1549.401326	22.750321	8.835467
1551.001954	0.000000	0.000000
1555.291035	40.733810	15.879791
1555.305118	0.000000	0.000000
1570.122665	0.000000	0.000000
1570.156756	195.370855	76.891947
1838.320536	3631.735665	1673.453079
1839.071805	0.000000	0.000000
1861.108768	0.000000	0.000000
1861.299659	1481.351693	691.118544
1923.240312	0.000000	0.000000
1923.247851	4608.859974	2221.809604
2913.880744	41.016724	29.957862
2913.882675	0.000000	0.000000
2915.943055	250.285562	182.933358
2915.999154	0.000000	0.000000
2929.876246	357.943428	262.870433
2929.958303	0.000000	0.000000
2930.936836	0.000000	0.000000
2937.775578	25.344684	18.663091
2956.906576	0.000000	0.000000
2977.327954	10.150071	7.574846
2994.850380	4.498336	3.376798
2994.851673	0.000000	0.000000
3044.952021	0.000000	0.000000
3044.953110	3.123427	2.383911
3049.406775	0.000000	0.000000
3049.407627	1.994478	1.524484
3068.832032	39.533226	30.409792
3068.832739	0.000000	0.000000
3076.282175	0.670053	0.516670
3076.284722	0.000000	0.000000
3091.463515	14.794954	11.464518
3091.526006	0.000000	0.000000
3091.640962	0.974495	0.755173
3091.641002	0.000000	0.000000
3092.708351	0.000000	0.000000
3092.731853	45.879271	35.566149
3099.281039	0.000000	0.000000
3099.282978	1.697889	1.319011
3113.992310	0.000000	0.000000
3114.007025	93.636084	73.087129
3120.817214	1.011775	0.791462
3120.830704	0.000000	0.000000
3125.111968	0.969642	0.759548
3125.113466	0.000000	0.000000
3132.666930	2.042744	1.604007
3132.670647	0.000000	0.000000
3147.315281	9.267017	7.310689
3147.324753	0.000000	0.000000
3153.114512	0.000000	0.000000
3153.432985	19.327142	15.276692

3c ZORA-PBE-D3(BJ)/AE-TZP

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Frame 30: Geometry 31, SCF Bond Energy: -15.14014 Hartree

C	-0.955590	-0.275441	10.427579
H	-0.626727	-0.268119	9.389015
C	-1.906372	-1.218463	10.867160
H	-2.300170	-1.944962	10.157122
C	-2.325551	-1.191476	12.180007
H	-3.071008	-1.899874	12.547510
C	-1.791205	-0.223242	13.063882
C	-0.815252	0.685273	12.547961
C	-0.230451	1.686029	13.363818
C	-0.674441	1.789282	14.675171
H	-0.248756	2.561043	15.319811
C	-1.647757	0.908061	15.198841
H	-1.963802	1.018440	16.236575
C	-2.191858	-0.090139	14.417458
H	-2.941279	-0.773931	14.818710
C	0.842558	2.546639	12.767341
H	1.840353	2.203041	13.095505
H	0.727101	3.600943	13.063457
C	2.106934	3.970787	10.501640
H	1.504990	4.830996	10.815700
C	2.228046	3.839540	9.048856
C	1.230655	4.366335	8.170053
H	0.429893	4.965844	8.600363
C	1.235330	4.098435	6.787245
H	0.441031	4.488172	6.154104
C	2.220177	3.232405	6.254096
H	2.189966	2.950828	5.203018
C	3.241499	2.732257	7.090395
H	4.003868	2.072205	6.678129
C	3.255794	3.025054	8.475779
C	4.349916	2.468478	9.352338
H	5.303897	2.531996	8.810517
H	4.160389	1.396284	9.530783
C	4.478655	3.144148	10.692026
C	5.678522	3.020521	11.424503
H	6.529401	2.516131	10.967254
C	5.801499	3.566919	12.732710
H	6.742691	3.489762	13.272122
C	4.717664	4.279984	13.279912
H	4.818271	4.759065	14.251784
C	3.507763	4.421523	12.545236
H	2.691689	5.009644	12.957382
C	3.359945	3.837812	11.263335
C	1.787756	0.669423	8.834387
C	-0.481060	2.342198	8.632140
C	0.471053	1.049285	6.703023
C	5.196284	6.808754	12.153395
C	4.631954	5.982118	9.788173
C	6.951798	5.509511	10.862475
N	-0.424392	0.646938	11.225927
O	2.242153	-0.318249	9.276936
O	-1.620367	2.533105	8.840568
O	-0.037960	0.326519	5.935307
O	5.189841	7.841153	12.705625
O	4.223538	6.490019	8.816527
O	8.077016	5.717117	10.608938
Cr	1.229479	2.176977	7.927702
Cr	5.215487	5.171249	11.332003
Pd	0.879561	2.250466	10.717387

	hartree	eV	kcal/mol	kJ/mol
	-----	-----	-----	-----
Pauli Repulsion				
Kinetic (Delta T^0):	172.025353114769416	4681.0480	107947.55	451652.50
Delta V^Pauli Coulomb:	-88.641719051008607	-2412.0639	-55623.52	-232728.80
Delta V^Pauli LDA-XC:	-21.688729790338254	-590.1804	-13609.88	-56943.75
Delta V^Pauli GGA-Exchange:	1.095988236355382	29.8234	687.74	2877.52
Delta V^Pauli GGA-Correlation:	-0.258987346038575	-7.0474	-162.52	-679.97
	-----	-----	-----	-----
Total Pauli Repulsion:	62.531905163739360	1701.5797	39239.37	164177.49
(Total Pauli Repulsion =				
Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	62.531905163739360	1701.5797	39239.37	164177.49
Electrostatic Interaction:	-13.690387523990646	-372.5344	-8590.85	-35944.11
(Electrostatic Interaction =				
Delta V_elstat in the BB paper)				
	-----	-----	-----	-----
Total Steric Interaction:	48.841517639748716	1329.0453	30648.52	128233.39
(Total Steric Interaction =				
Delta E^0 in the BB paper)				

Orbital Interactions				
A:	-63.867957908184756	-1737.9356	-40077.75	-167685.30
	-----	-----	-----	-----
Total Orbital Interactions:	-63.867865962767176	-1737.9331	-40077.70	-167685.06
Alternative Decomposition Orb.Int.				
Kinetic:	-157.971860284570937	-4298.6330	-99128.85	-414755.06
Coulomb:	86.396441346650846	2350.9668	54214.59	226833.82
XC:	7.707552975152923	209.7332	4836.56	20236.18
	-----	-----	-----	-----
Total Orbital Interactions:	-63.867865962767169	-1737.9331	-40077.70	-167685.06
Residu (E=Steric+OrbInt+Res):	0.000043313510734	0.0012	0.03	0.11
Dispersion Energy:	-0.113834140372027	-3.0976	-71.43	-298.87
Total Bonding Energy:	-15.140139149879754	-411.9841	-9500.58	-39750.43

Intensities
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Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-----	-----	-----
-26.711033	16.779935	-0.112346
-2.183436	0.000000	0.000000
24.704739	281.132251	1.740881
28.386759	151.215816	1.075948
34.590191	8.053403	0.069825
37.272071	91.426306	0.854147
53.146744	119.662371	1.594088
67.149394	56.006060	0.942660
74.991648	22.006191	0.413653
79.660748	2.828586	0.056480
81.730620	4.748629	0.097282
90.629041	67.180178	1.526113
93.272825	55.060200	1.287274
97.204187	51.650352	1.258451
100.293153	56.816839	1.428323
105.969679	48.626442	1.291612
118.696032	31.715501	0.943595
124.294005	138.707036	4.321423
125.334151	9.507688	0.298691
141.204214	90.219022	3.193183
146.356110	44.107224	1.618075
162.881454	14.349965	0.585869
174.461204	5.541247	0.242317
196.156300	49.371090	2.427465
204.331805	93.388711	4.783089
217.112335	136.324733	7.418861
240.087566	33.359384	2.007547
240.722253	48.745751	2.941244
254.380531	36.555585	2.330857
288.365358	2.840364	0.205303
296.973244	7.571107	0.563579
317.974390	177.460188	14.143964
329.544617	68.835506	5.685973
341.499992	139.353240	11.928500
346.413623	73.098409	6.347182
369.558538	45.043637	4.172485
391.618576	12.654651	1.242200
396.686703	3.858015	0.383610
408.477286	5.483764	0.561468
412.821931	2.542712	0.263110
421.458686	11.780905	1.244548
427.199379	15.068517	1.613538
441.268349	4.615114	0.510462
450.885512	56.204852	6.352112
454.067325	56.579933	6.439628
466.180536	6.201913	0.724699
484.606427	59.684803	7.249883
487.289183	14.875731	1.816951
490.618780	52.713028	6.482465
493.751207	46.027781	5.696476
497.509168	43.064272	5.370272
499.408954	15.837798	1.982573
503.891049	65.384623	8.258294
509.930988	20.589484	2.631691
523.877243	20.196791	2.652101
526.573816	27.015804	3.565786
534.909232	72.819771	9.763544
536.740661	59.175874	7.961360
541.374366	191.182715	25.943250
546.349776	76.896783	10.530694
565.025680	85.186653	12.064736
582.204991	57.980577	8.461289
601.548985	62.408597	9.410084
604.108593	204.109511	30.906963

606.695181	95.286691	14.490416
615.222327	586.946276	90.512489
621.001506	193.908366	30.183338
626.593892	327.528501	51.441465
633.467064	238.303222	37.838336
639.195300	76.786986	12.302667
643.861966	399.248342	64.433832
650.974118	91.196386	14.880565
658.960272	65.128474	10.757422
668.844433	247.020469	41.412946
681.065645	23.470393	4.006705
687.904473	777.028695	133.981014
721.840950	5.251944	0.950254
725.901761	0.398124	0.072439
742.853394	46.731442	8.701425
775.373552	136.328789	26.495775
781.475236	37.391861	7.324372
801.518733	56.053124	11.261379
806.528827	10.629031	2.148778
808.740140	79.961144	16.209367
810.733631	68.734138	13.967824
835.902948	8.547037	1.790810
847.150730	39.625690	8.414254
855.335717	2.584784	0.554165
878.068156	10.600161	2.333022
879.710712	4.777685	1.053502
879.996584	0.978375	0.215806
892.733666	0.367462	0.082227
906.189954	28.243476	6.415278
912.306729	10.705414	2.448062
917.504603	14.243067	3.275592
926.678219	4.420565	1.026797
934.741047	9.018525	2.113026
936.302529	5.074786	1.191001
953.395165	0.851221	0.203420
966.059405	1.707979	0.413585
1009.530298	15.519049	3.927015
1013.096904	25.711235	6.529080
1020.918248	177.228591	45.352666
1037.079729	14.120282	3.670571
1056.003958	3.917515	1.036941
1061.781971	8.943306	2.380189
1073.746070	36.749891	9.890898
1082.978300	9.692105	2.630970
1090.766873	10.985893	3.003623
1132.889424	10.851574	3.081473
1133.797294	1.412937	0.401547
1140.171983	1.156732	0.330584
1158.636449	4.520759	1.312915
1170.421813	56.270221	16.508176
1172.301961	15.490964	4.551934
1184.178174	5.001633	1.484591
1191.370190	51.112065	15.263292
1200.353839	53.633537	16.137037
1213.772188	3.327912	1.012482
1224.346653	17.655653	5.418340
1226.230808	7.664426	2.355754
1246.489844	8.651248	2.702997
1247.405855	10.484948	3.278326
1310.926474	19.910762	6.542508
1321.257785	10.082073	3.338993
1335.930923	14.116166	4.726926
1363.032593	93.822695	32.054737
1371.844675	19.791149	6.805406
1386.810105	19.556021	6.797912
1395.329047	29.155558	10.197086
1400.368853	5.184447	1.819797
1401.815739	17.722452	6.227200
1414.167038	30.405431	10.777795
1417.773414	2.599281	0.923715
1426.238120	4.389440	1.569203
1435.994532	254.565415	91.628433
1451.448175	26.733486	9.726021
1461.114900	56.700404	20.765796
1486.051996	25.482177	9.491801
1495.759265	3.220792	1.207543
1500.363200	164.634572	61.914948
1516.854382	79.732130	30.314843
1523.171547	12.513199	4.777440
1567.311430	54.696286	21.487763
1583.946412	0.175645	0.069735
1599.589857	17.375069	6.966478
1872.409622	1461.995238	686.159203
1884.357815	670.197156	316.551244
1893.476838	2173.522166	1031.578165
1898.252539	2191.919925	1042.933803
1938.334793	2394.508063	1163.384211
1952.679735	2488.074416	1217.790144
2938.450196	16.998037	12.519736

2947.755745	8.260383	6.103371
3000.149922	20.209935	15.197983
3006.871647	4.744809	3.576117
3034.176142	1.565951	1.190960
3092.732514	4.889059	3.790057
3097.275752	4.428932	3.438404
3102.258845	5.309815	4.128911
3114.801977	2.138428	1.669565
3115.166982	0.217920	0.170160
3120.299907	0.135649	0.106094
3121.732453	0.827170	0.647245
3122.007316	28.746701	22.495725
3127.990465	1.238878	0.971341
3132.592403	15.179657	11.919112
3133.362306	0.666304	0.523312
3140.774753	2.506855	1.973531
3146.403788	2.679507	2.113233
3148.048278	3.248014	2.562933

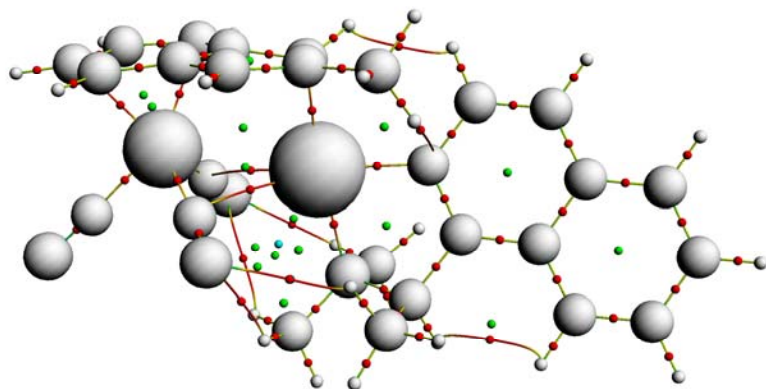


Figure 13. Plot of bond critical points (red dots) and ring critical points (green dots). Atom size is scaled by density. AIM was computed from a model geometry optimized at the ZORA-PBE0-dDsC/all electron TZP level using the PBE0-dDsC/TZP (all electron for all elements except for Pd for which a frozen core up to 3d was used) level.

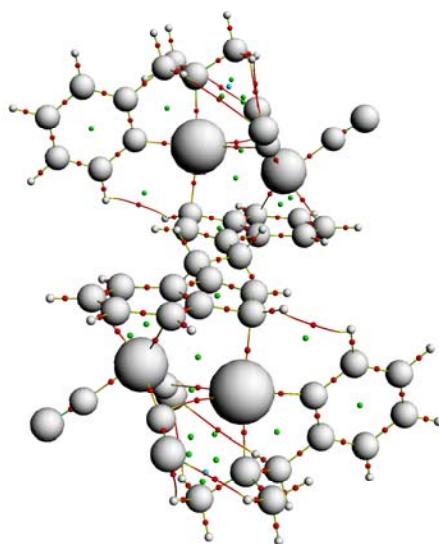


Figure 14 Plot of bond critical points (red dots) and ring critical points (green dots). Atom size is scaled by density. AIM was computed from a model geometry optimized at the ZORA-TPSS-D3(BJ)/all electron TZP level using the PBE0-dDsC/TZP (all electron for all elements except for Pd for which a frozen core up to 3d was used) level.

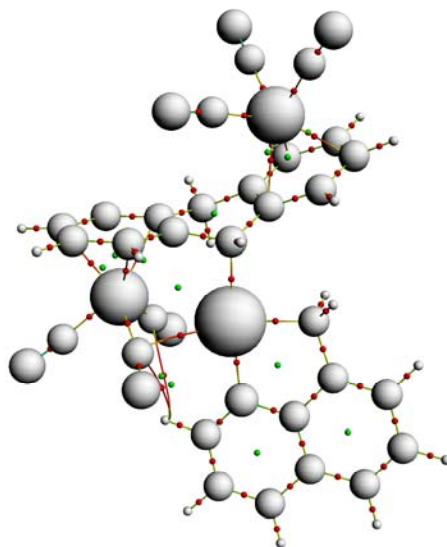


Figure 15 Plot of bond critical points (red dots) and ring critical points (green dots). Atom size is scaled by density. AIM was computed from a model geometry optimized at the ZORA-PBE0-dDsC/all electron TZP level using the PBE0-dDsC/TZP (all electron for all elements except for Pd for which a frozen core up to 3d was used) level.