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(1η^5-Cyclopentadienyl)(μ-disulfur dinitrido)(triphenylphosphino-2κP)cobalt(II)gold(I) perchlorate

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Key indicators

Single-crystal X-ray study
T = 133 K
Mean σ(C–C) = 0.007 Å
R factor = 0.030
wR factor = 0.054
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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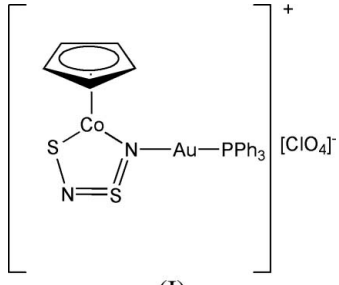
The title compound, [{Au($C_{18}H_{15}P$)}Co(C_5H_5)(N_2S_2)]ClO_4, has a planar CoS_2N_2 ring and a close-to-linear N—Au—P angle [176.54 (11)°].

Comment

The disulfur dinitride dianion is not known as a simple species but can be isolated in metal complexes (Kelly & Woollins, 1986; Jones *et al.*, 1985*a*,*b*; Bates *et al.*, 1986). These complexes may be protonated at the metal-coordinated N (Jones *et al.*, 1986) and we have previously commented on the structural consequences of this protonation (Jones *et al.*, 1987, 1988). Recently, we developed a new route to disulfur dinitrido complexes (Aucott *et al.*, 2002) and we examined the metallation of IrS_2N_2 rings using the AuPR_3 cation as a species which is isolobal with a proton (Aucott *et al.*, 2003). A comparison of metallacycle bond lengths for [(η^5-C_5Me_5)Ir(S_2N_2)] and [(C_5Me_5)$_2$Ir$_2$(S_2N_2)Cl(PPh_3)][PF_6] indicates that metallation appears to change the IrS_2N_2 bond lengths and angles in a similar fashion to protonation: both enlarge the M—S2, N1—S1 and N2—S2 distances. We have also recently carried out detailed studies of $CpCoS_2N_2$ (Van Droogenbroeck *et al.*, 2005). This led us to synthesize the title compound, (I), in order to allow us to investigate the effects of metallation on the CoS_2N_2 ring.



(I)

Compound (I) (Fig. 1) has a planar CoS_2N_2 ring and a close-to-linear N—Au—P angle [176.54 (11) Å]. Compared with the non-metallated parent, $CpCoS_2N_2$ (Van Droogenbroeck *et al.*, 2005), we note that (I) has statistically invariant Co—N, Co—S and S2—N2 distances, whilst the N1—S1 distance is longer in (I) than in the parent compound [1.599 (4) *versus* 1.556 (1) Å] and the S1—N2 distance is slightly shorter in (I) than in the parent molecule [1.580 (4) *versus* 1.597 (2) Å]. Within the CoS_2N_2 ring, it is noticeable that metallation results in an almost perfect trigonal Co—N—S internal angle [120.1 (2)° in (I) *versus* 118.32 (8)° in the parent compound]. In general, all internal angles in the CoS_2N_2 ring in (I) are closer to the idealized tetrahedral values at S and trigonal values at N

compared with the parent molecule. This work illustrates the difficulties in rationalizing bond lengths in S–N compounds and the continuing need for structural work in this area.

Experimental

Triphenylphosphinogold(disulfur dinitrido)(cyclopentadienyl)-cobalt(II) perchlorate was prepared as described in the literature (Aucott *et al.*, 2003) and was crystallized by vapour diffusion of diethyl ether into a dichloromethane solution, to give small dark-reddish–violet plates.

Crystal data

$[AuCo(C_5H_5)(N_2N_2)(C_{18}H_{15}P)]$-$ClO_4$	V = 2591.2 (11) Å^3
M_r = 774.85	Z = 4
Monoclinic, $P2_1/c$	D_x = 1.986 Mg m^{-3}
a = 14.646 (3) Å	Mo $K\alpha$ radiation
b = 14.186 (3) Å	μ = 6.65 mm^{-1}
c = 13.377 (3) Å	T = 133 (2) K
β = 111.20 (3)°	Block, red-violet
	0.26 × 0.25 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer	15021 measured reflections
ω scans	4718 independent reflections
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	3953 reflections with $I > 2\sigma(I)$
T_{min} = 0.203, T_{max} = 0.274	R_{int} = 0.048
	θ_{max} = 25.4°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0176P)^2 + 3.2524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$(\Delta/\sigma)_{max}$ = 0.007
$wR(F^2)$ = 0.054	$\Delta\rho_{max}$ = 0.70 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.77 e Å^{-3}
4718 reflections	
317 parameters	
H-atom parameters constrained	

All H atoms were included in calculated positions and refined as riding, with C—H = 0.95 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SCXmini Benchtop Crystallography System Software* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2004); software used to prepare material for publication: *CrystalStructure*.

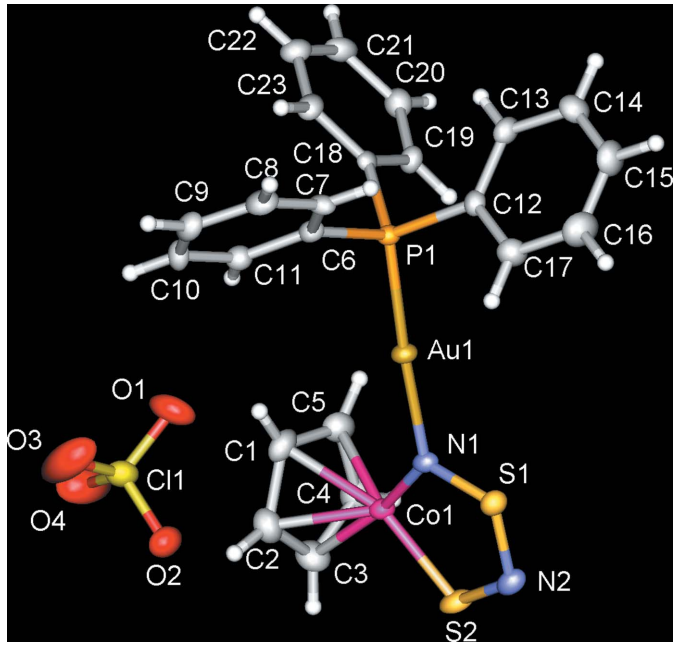


Figure 1
The structure and atom-labelling scheme for (I), with displacement ellipsoids drawn at the 50% probability level.

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Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
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15021 measured reflections
4718 independent reflections
3953 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 25.4°$, $\theta_{min} = 3.2°$
$h = -17\rightarrow17$
$k = -12\rightarrow17$
$l = -11\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.054$
$S = 1.04$
4718 reflections
317 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0176P)^2 + 3.2524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.007$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Au1	0.660192 (12)	0.597329 (13)	0.673981 (14)	0.01872 (6)
N1	0.5266 (3)	0.6296 (3)	0.5579 (3)	0.0204 (9)
S1	0.43958 (8)	0.57139 (8)	0.57449 (10)	0.0233 (3)
N2	0.3425 (3)	0.5926 (3)	0.4758 (3)	0.0259 (9)
S2	0.35506 (8)	0.66651 (10)	0.38578 (10)	0.0280 (3)
Co1	0.50197 (4)	0.70466 (4)	0.44071 (5)	0.01958 (15)
C1	0.6283 (4)	0.7851 (4)	0.4798 (4)	0.0347 (13)
H1A	0.6779	0.7932	0.5485	0.042*
C2	0.5432 (4)	0.8416 (4)	0.4351 (4)	0.0328 (13)
H2A	0.5249	0.8930	0.4695	0.039*
C3	0.4904 (4)	0.8081 (4)	0.3307 (4)	0.0351 (13)
H3A	0.4313	0.8340	0.2816	0.042*
C4	0.5411 (4)	0.7293 (4)	0.3121 (4)	0.0345 (13)
H4A	0.5216	0.6923	0.2486	0.041*
C5	0.6262 (4)	0.7151 (4)	0.4045 (4)	0.0341 (13)
H5A	0.6735	0.6668	0.4140	0.041*
P1	0.80157 (8)	0.55420 (8)	0.80220 (9)	0.0163 (3)
C6	0.8391 (3)	0.6366 (3)	0.9134 (3)	0.0175 (10)
C7	0.8577 (3)	0.6081 (3)	1.0179 (3)	0.0210 (11)
H7A	0.8507	0.5436	1.0329	0.025*
C8	0.8864 (3)	0.6732 (4)	1.1007 (4)	0.0281 (12)
H8A	0.8986	0.6537	1.1723	0.034*
C9	0.8974 (3)	0.7670 (3)	1.0782 (4)	0.0283 (12)
H9A	0.9192	0.8116	1.1349	0.034*
C10	0.8767 (3)	0.7961 (3)	0.9735 (4)	0.0262 (12)
H10A	0.8828	0.8608	0.9585	0.031*
C11	0.8471 (3)	0.7315 (3)	0.8908 (4)	0.0233 (11)
H11A	0.8322	0.7515	0.8188	0.028*
C12	0.7903 (3)	0.4395 (3)	0.8568 (4)	0.0184 (10)
C13	0.8595 (3)	0.3692 (3)	0.8686 (4)	0.0244 (11)
H13A	0.9159	0.3820	0.8516	0.029*
C14	0.8470 (4)	0.2808 (4)	0.9050 (4)	0.0325 (13)
H14A	0.8938	0.2325	0.9116	0.039*
C15	0.7661 (4)	0.2632 (4)	0.9315 (4)	0.0362 (14)
H15A	0.7579	0.2027	0.9575	0.043*

C16	0.6973 (4)	0.3317 (4)	0.9209 (4)	0.0376 (14)
H16A	0.6417	0.3183	0.9391	0.045*
C17	0.7084 (3)	0.4210 (3)	0.8835 (4)	0.0258 (12)
H17A	0.6608	0.4686	0.8763	0.031*
C18	0.9053 (3)	0.5441 (3)	0.7591 (3)	0.0155 (10)
C19	0.8910 (3)	0.4966 (3)	0.6622 (4)	0.0207 (11)
H19A	0.8281	0.4724	0.6208	0.025*
C20	0.9685 (3)	0.4852 (3)	0.6272 (4)	0.0248 (11)
H20A	0.9590	0.4514	0.5629	0.030*
C21	1.0592 (3)	0.5224 (4)	0.6850 (4)	0.0286 (12)
H21A	1.1117	0.5152	0.6597	0.034*
C22	1.0743 (3)	0.5710 (3)	0.7809 (4)	0.0274 (12)
H22A	1.1366	0.5970	0.8207	0.033*
C23	0.9968 (3)	0.5805 (3)	0.8172 (4)	0.0214 (11)
H23A	1.0069	0.6125	0.8827	0.026*
Cl1	0.66335 (9)	0.97334 (9)	0.70673 (10)	0.0320 (3)
O1	0.7129 (3)	0.8856 (3)	0.7190 (4)	0.0594 (13)
O2	0.5600 (2)	0.9577 (3)	0.6805 (3)	0.0436 (10)
O3	0.6772 (3)	1.0239 (4)	0.6216 (4)	0.0808 (17)
O4	0.7010 (3)	1.0237 (4)	0.8048 (4)	0.0850 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.01501 (9)	0.02417 (11)	0.01521 (10)	0.00228 (8)	0.00334 (7)	0.00008 (8)
N1	0.0154 (19)	0.024 (2)	0.020 (2)	0.0025 (16)	0.0044 (17)	−0.0047 (17)
S1	0.0199 (6)	0.0273 (7)	0.0241 (7)	−0.0013 (5)	0.0097 (5)	−0.0025 (5)
N2	0.017 (2)	0.033 (2)	0.027 (2)	−0.0014 (18)	0.0070 (17)	−0.0092 (19)
S2	0.0163 (6)	0.0442 (8)	0.0193 (7)	0.0009 (6)	0.0014 (5)	−0.0038 (6)
Co1	0.0159 (3)	0.0248 (4)	0.0174 (3)	0.0027 (3)	0.0053 (3)	−0.0007 (3)
C1	0.025 (3)	0.037 (3)	0.039 (3)	−0.014 (2)	0.007 (2)	0.006 (3)
C2	0.043 (3)	0.026 (3)	0.036 (3)	−0.004 (2)	0.022 (3)	0.000 (2)
C3	0.041 (3)	0.037 (3)	0.027 (3)	0.008 (3)	0.013 (3)	0.010 (2)
C4	0.045 (3)	0.037 (3)	0.032 (3)	−0.002 (3)	0.026 (3)	0.003 (3)
C5	0.028 (3)	0.035 (3)	0.046 (4)	0.002 (2)	0.021 (3)	0.008 (3)
P1	0.0146 (6)	0.0198 (7)	0.0143 (6)	0.0012 (5)	0.0049 (5)	0.0011 (5)
C6	0.014 (2)	0.025 (3)	0.013 (2)	−0.0006 (19)	0.0033 (19)	−0.0027 (19)
C7	0.017 (2)	0.023 (3)	0.019 (3)	0.004 (2)	0.0017 (19)	−0.001 (2)
C8	0.022 (3)	0.041 (3)	0.018 (3)	0.003 (2)	0.002 (2)	−0.001 (2)
C9	0.025 (3)	0.028 (3)	0.032 (3)	−0.006 (2)	0.011 (2)	−0.015 (2)
C10	0.027 (3)	0.018 (3)	0.035 (3)	−0.006 (2)	0.012 (2)	−0.006 (2)
C11	0.022 (2)	0.023 (3)	0.024 (3)	0.002 (2)	0.008 (2)	0.002 (2)
C12	0.022 (2)	0.019 (2)	0.014 (2)	−0.006 (2)	0.0058 (19)	−0.0009 (18)
C13	0.019 (2)	0.026 (3)	0.029 (3)	−0.005 (2)	0.008 (2)	0.004 (2)
C14	0.031 (3)	0.026 (3)	0.042 (3)	0.004 (2)	0.015 (3)	0.008 (2)
C15	0.039 (3)	0.027 (3)	0.047 (4)	−0.008 (3)	0.020 (3)	0.011 (3)
C16	0.036 (3)	0.045 (4)	0.040 (4)	−0.006 (3)	0.024 (3)	0.009 (3)
C17	0.027 (3)	0.028 (3)	0.028 (3)	0.002 (2)	0.017 (2)	0.001 (2)

C18	0.018 (2)	0.013 (2)	0.016 (2)	0.0004 (18)	0.0058 (19)	0.0067 (18)
C19	0.022 (2)	0.022 (3)	0.020 (3)	−0.004 (2)	0.009 (2)	−0.001 (2)
C20	0.030 (3)	0.027 (3)	0.020 (3)	0.000 (2)	0.011 (2)	−0.001 (2)
C21	0.027 (3)	0.034 (3)	0.031 (3)	0.006 (2)	0.017 (2)	0.011 (2)
C22	0.018 (2)	0.035 (3)	0.027 (3)	0.002 (2)	0.005 (2)	0.006 (2)
C23	0.023 (2)	0.026 (3)	0.013 (2)	−0.002 (2)	0.004 (2)	0.0029 (19)
Cl1	0.0258 (6)	0.0343 (8)	0.0390 (8)	0.0052 (6)	0.0155 (6)	0.0033 (6)
O1	0.053 (3)	0.050 (3)	0.070 (3)	0.030 (2)	0.015 (2)	0.003 (2)
O2	0.027 (2)	0.042 (2)	0.060 (3)	−0.0032 (18)	0.0146 (19)	0.008 (2)
O3	0.054 (3)	0.097 (4)	0.099 (4)	0.012 (3)	0.036 (3)	0.062 (3)
O4	0.038 (3)	0.134 (5)	0.085 (4)	−0.011 (3)	0.026 (3)	−0.077 (4)

Geometric parameters (Å, º)

Au1—N1	2.062 (4)	C9—C10	1.385 (7)
Au1—P1	2.2439 (14)	C9—H9A	0.9500
N1—S1	1.599 (4)	C10—C11	1.381 (6)
N1—Co1	1.821 (4)	C10—H10A	0.9500
S1—N2	1.580 (4)	C11—H11A	0.9500
N2—S2	1.657 (4)	C12—C13	1.390 (6)
S2—Co1	2.0782 (14)	C12—C17	1.395 (6)
Co1—C4	2.031 (5)	C13—C14	1.381 (7)
Co1—C2	2.044 (5)	C13—H13A	0.9500
Co1—C3	2.042 (5)	C14—C15	1.376 (7)
Co1—C5	2.050 (5)	C14—H14A	0.9500
Co1—C1	2.073 (5)	C15—C16	1.371 (7)
C1—C5	1.408 (7)	C15—H15A	0.9500
C1—C2	1.419 (7)	C16—C17	1.393 (7)
C1—H1A	0.9500	C16—H16A	0.9500
C2—C3	1.412 (7)	C17—H17A	0.9500
C2—H2A	0.9500	C18—C23	1.383 (6)
C3—C4	1.413 (7)	C18—C19	1.408 (6)
C3—H3A	0.9500	C19—C20	1.385 (6)
C4—C5	1.416 (7)	C19—H19A	0.9500
C4—H4A	0.9500	C20—C21	1.378 (6)
C5—H5A	0.9500	C20—H20A	0.9500
P1—C18	1.814 (4)	C21—C22	1.401 (7)
P1—C6	1.814 (4)	C21—H21A	0.9500
P1—C12	1.816 (5)	C22—C23	1.394 (7)
C6—C7	1.384 (6)	C22—H22A	0.9500
C6—C11	1.394 (6)	C23—H23A	0.9500
C7—C8	1.386 (6)	Cl1—O4	1.419 (4)
C7—H7A	0.9500	Cl1—O1	1.420 (4)
C8—C9	1.386 (7)	Cl1—O3	1.422 (4)
C8—H8A	0.9500	Cl1—O2	1.442 (4)
N1—Au1—P1	176.54 (11)	C6—P1—Au1	111.93 (15)
S1—N1—Co1	120.1 (2)	C12—P1—Au1	111.02 (15)

S1—N1—Au1	111.6 (2)	C7—C6—C11	120.0 (4)
Co1—N1—Au1	128.1 (2)	C7—C6—P1	122.0 (4)
N2—S1—N1	107.9 (2)	C11—C6—P1	117.9 (3)
S1—N2—S2	115.1 (2)	C6—C7—C8	120.2 (5)
N2—S2—Co1	106.31 (14)	C6—C7—H7A	119.9
N1—Co1—C4	143.30 (19)	C8—C7—H7A	119.9
N1—Co1—C2	128.21 (19)	C7—C8—C9	119.5 (5)
C4—Co1—C2	68.1 (2)	C7—C8—H8A	120.2
N1—Co1—C3	168.65 (19)	C9—C8—H8A	120.2
C4—Co1—C3	40.6 (2)	C10—C9—C8	120.4 (4)
C2—Co1—C3	40.4 (2)	C10—C9—H9A	119.8
N1—Co1—C5	109.25 (19)	C8—C9—H9A	119.8
C4—Co1—C5	40.6 (2)	C11—C10—C9	120.2 (5)
C2—Co1—C5	67.9 (2)	C11—C10—H10A	119.9
C3—Co1—C5	68.1 (2)	C9—C10—H10A	119.9
N1—Co1—C1	102.95 (19)	C10—C11—C6	119.6 (5)
C4—Co1—C1	67.6 (2)	C10—C11—H11A	120.2
C2—Co1—C1	40.3 (2)	C6—C11—H11A	120.2
C3—Co1—C1	67.7 (2)	C13—C12—C17	119.7 (4)
C5—Co1—C1	39.9 (2)	C13—C12—P1	121.4 (4)
N1—Co1—S2	90.54 (12)	C17—C12—P1	118.9 (4)
C4—Co1—S2	108.58 (16)	C14—C13—C12	120.5 (4)
C2—Co1—S2	121.08 (16)	C14—C13—H13A	119.8
C3—Co1—S2	97.29 (16)	C12—C13—H13A	119.8
C5—Co1—S2	145.98 (16)	C15—C14—C13	119.4 (5)
C1—Co1—S2	161.40 (15)	C15—C14—H14A	120.3
C5—C1—C2	108.0 (5)	C13—C14—H14A	120.3
C5—C1—Co1	69.2 (3)	C16—C15—C14	120.9 (5)
C2—C1—Co1	68.7 (3)	C16—C15—H15A	119.5
C5—C1—H1A	126.0	C14—C15—H15A	119.5
C2—C1—H1A	126.0	C15—C16—C17	120.3 (5)
Co1—C1—H1A	127.7	C15—C16—H16A	119.8
C3—C2—C1	108.0 (5)	C17—C16—H16A	119.8
C3—C2—Co1	69.7 (3)	C12—C17—C16	119.1 (5)
C1—C2—Co1	71.0 (3)	C12—C17—H17A	120.5
C3—C2—H2A	126.0	C16—C17—H17A	120.5
C1—C2—H2A	126.0	C23—C18—C19	119.1 (4)
Co1—C2—H2A	124.9	C23—C18—P1	123.0 (4)
C2—C3—C4	107.8 (5)	C19—C18—P1	117.9 (3)
C2—C3—Co1	69.8 (3)	C20—C19—C18	120.0 (4)
C4—C3—Co1	69.3 (3)	C20—C19—H19A	120.0
C2—C3—H3A	126.1	C18—C19—H19A	120.0
C4—C3—H3A	126.1	C21—C20—C19	120.5 (4)
Co1—C3—H3A	126.3	C21—C20—H20A	119.7
C3—C4—C5	108.1 (5)	C19—C20—H20A	119.7
C3—C4—Co1	70.1 (3)	C20—C21—C22	120.1 (4)
C5—C4—Co1	70.4 (3)	C20—C21—H21A	119.9
C3—C4—H4A	125.9	C22—C21—H21A	119.9

C5—C4—H4A	125.9	C23—C22—C21	119.2 (4)
Co1—C4—H4A	125.2	C23—C22—H22A	120.4
C1—C5—C4	108.0 (5)	C21—C22—H22A	120.4
C1—C5—Co1	70.9 (3)	C18—C23—C22	121.0 (4)
C4—C5—Co1	69.0 (3)	C18—C23—H23A	119.5
C1—C5—H5A	126.0	C22—C23—H23A	119.5
C4—C5—H5A	126.0	O4—Cl1—O1	108.8 (3)
Co1—C5—H5A	125.7	O4—Cl1—O3	111.4 (4)
C18—P1—C6	105.7 (2)	O1—Cl1—O3	108.7 (3)
C18—P1—C12	105.4 (2)	O4—Cl1—O2	109.0 (3)
C6—P1—C12	107.0 (2)	O1—Cl1—O2	110.0 (2)
C18—P1—Au1	115.20 (14)	O3—Cl1—O2	108.9 (3)

Co1—N1—S1—N2	0.8 (3)	S2—Co1—C4—C3	79.2 (3)
Au1—N1—S1—N2	−174.22 (19)	N1—Co1—C4—C5	−44.2 (5)
N1—S1—N2—S2	−0.5 (3)	C2—Co1—C4—C5	81.1 (3)
S1—N2—S2—Co1	0.0 (3)	C3—Co1—C4—C5	118.7 (5)
S1—N1—Co1—C4	−123.7 (3)	C1—Co1—C4—C5	37.4 (3)
Au1—N1—Co1—C4	50.4 (4)	S2—Co1—C4—C5	−162.0 (3)
S1—N1—Co1—C2	131.0 (3)	C2—C1—C5—C4	1.4 (6)
Au1—N1—Co1—C2	−54.9 (3)	Co1—C1—C5—C4	59.3 (3)
S1—N1—Co1—C3	133.1 (9)	C2—C1—C5—Co1	−57.9 (3)
Au1—N1—Co1—C3	−52.8 (11)	C3—C4—C5—C1	−0.3 (6)
S1—N1—Co1—C5	−152.4 (3)	Co1—C4—C5—C1	−60.5 (3)
Au1—N1—Co1—C5	21.6 (3)	C3—C4—C5—Co1	60.2 (4)
S1—N1—Co1—C1	166.4 (3)	N1—Co1—C5—C1	−87.3 (3)
Au1—N1—Co1—C1	−19.5 (3)	C4—Co1—C5—C1	118.9 (4)
S1—N1—Co1—S2	−0.7 (2)	C2—Co1—C5—C1	37.1 (3)
Au1—N1—Co1—S2	173.4 (2)	C3—Co1—C5—C1	80.9 (3)
N2—S2—Co1—N1	0.32 (19)	S2—Co1—C5—C1	150.4 (3)
N2—S2—Co1—C4	148.4 (2)	N1—Co1—C5—C4	153.8 (3)
N2—S2—Co1—C2	−136.4 (2)	C2—Co1—C5—C4	−81.7 (3)
N2—S2—Co1—C3	−171.4 (2)	C3—Co1—C5—C4	−38.0 (3)
N2—S2—Co1—C5	127.4 (3)	C1—Co1—C5—C4	−118.9 (4)
N2—S2—Co1—C1	−136.6 (5)	S2—Co1—C5—C4	31.5 (5)
N1—Co1—C1—C5	104.6 (3)	C18—P1—C6—C7	−109.5 (4)
C4—Co1—C1—C5	−38.0 (3)	C12—P1—C6—C7	2.5 (4)
C2—Co1—C1—C5	−120.2 (4)	Au1—P1—C6—C7	124.3 (3)
C3—Co1—C1—C5	−82.1 (3)	C18—P1—C6—C11	71.8 (4)
S2—Co1—C1—C5	−119.9 (5)	C12—P1—C6—C11	−176.2 (3)
N1—Co1—C1—C2	−135.2 (3)	Au1—P1—C6—C11	−54.4 (4)
C4—Co1—C1—C2	82.1 (3)	C11—C6—C7—C8	−1.5 (6)
C3—Co1—C1—C2	38.1 (3)	P1—C6—C7—C8	179.8 (3)
C5—Co1—C1—C2	120.2 (4)	C6—C7—C8—C9	−0.6 (7)
S2—Co1—C1—C2	0.3 (7)	C7—C8—C9—C10	2.1 (7)
C5—C1—C2—C3	−2.0 (6)	C8—C9—C10—C11	−1.5 (7)
Co1—C1—C2—C3	−60.1 (4)	C9—C10—C11—C6	−0.6 (7)
C5—C1—C2—Co1	58.1 (3)	C7—C6—C11—C10	2.1 (7)

N1—Co1—C2—C3	179.4 (3)	P1—C6—C11—C10	−179.2 (3)
C4—Co1—C2—C3	37.8 (3)	C18—P1—C12—C13	6.3 (4)
C5—Co1—C2—C3	81.7 (3)	C6—P1—C12—C13	−106.0 (4)
C1—Co1—C2—C3	118.5 (5)	Au1—P1—C12—C13	131.6 (3)
S2—Co1—C2—C3	−61.4 (3)	C18—P1—C12—C17	−171.4 (4)
N1—Co1—C2—C1	60.9 (4)	C6—P1—C12—C17	76.4 (4)
C4—Co1—C2—C1	−80.7 (3)	Au1—P1—C12—C17	−46.0 (4)
C3—Co1—C2—C1	−118.5 (5)	C17—C12—C13—C14	1.1 (7)
C5—Co1—C2—C1	−36.8 (3)	P1—C12—C13—C14	−176.6 (4)
S2—Co1—C2—C1	−179.9 (3)	C12—C13—C14—C15	−1.3 (8)
C1—C2—C3—C4	1.8 (6)	C13—C14—C15—C16	0.9 (8)
Co1—C2—C3—C4	−59.1 (4)	C14—C15—C16—C17	−0.4 (9)
C1—C2—C3—Co1	60.9 (3)	C13—C12—C17—C16	−0.5 (7)
N1—Co1—C3—C2	−2.6 (11)	P1—C12—C17—C16	177.2 (4)
C4—Co1—C3—C2	−119.1 (5)	C15—C16—C17—C12	0.2 (8)
C5—Co1—C3—C2	−81.2 (3)	C6—P1—C18—C23	10.6 (4)
C1—Co1—C3—C2	−37.9 (3)	C12—P1—C18—C23	−102.5 (4)
S2—Co1—C3—C2	130.7 (3)	Au1—P1—C18—C23	134.7 (3)
N1—Co1—C3—C4	116.6 (9)	C6—P1—C18—C19	−169.6 (3)
C2—Co1—C3—C4	119.1 (5)	C12—P1—C18—C19	77.3 (4)
C5—Co1—C3—C4	38.0 (3)	Au1—P1—C18—C19	−45.4 (4)
C1—Co1—C3—C4	81.2 (4)	C23—C18—C19—C20	1.3 (7)
S2—Co1—C3—C4	−110.2 (3)	P1—C18—C19—C20	−178.5 (3)
C2—C3—C4—C5	−1.0 (6)	C18—C19—C20—C21	−1.9 (7)
Co1—C3—C4—C5	−60.4 (4)	C19—C20—C21—C22	1.1 (7)
C2—C3—C4—Co1	59.4 (4)	C20—C21—C22—C23	0.3 (7)
N1—Co1—C4—C3	−162.9 (3)	C19—C18—C23—C22	0.1 (7)
C2—Co1—C4—C3	−37.6 (3)	P1—C18—C23—C22	179.9 (4)
C5—Co1—C4—C3	−118.7 (5)	C21—C22—C23—C18	−1.0 (7)
C1—Co1—C4—C3	−81.3 (3)		