

# Electronic Supplementary Data File

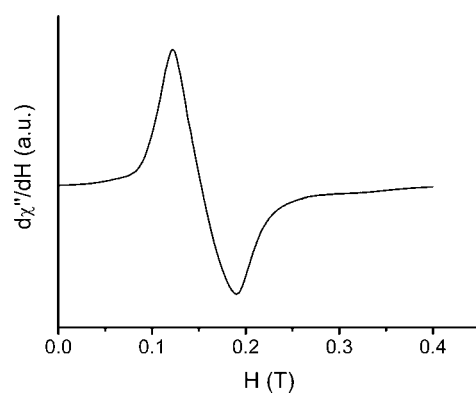
## The influence of ligand field effects on the magnetic exchange of high spin Co (II)- semiquinonate complexes

Alessandro Bencini,<sup>a</sup> Alessandra Beni,<sup>a</sup> Ferdinando Costantino,<sup>b</sup> Andrea Dei,<sup>a\*</sup> Dante Gatteschi,<sup>a</sup> Lorenzo Sorace<sup>a</sup>

<sup>a</sup> Udr INSTM and Dipartimento di Chimica, Università di Firenze, Via della Lastruccia 3 50019 Sesto Fiorentino (FI), Italy

*Fax:* +390554573372; *Tel:* +390554573328; *E-mail:* [andrea.dei@unifi.it](mailto:andrea.dei@unifi.it)

<sup>b</sup>UdR INSTM and Dipartimento di Chimica, Università di Perugia, Via Elce di Sotto 8, 06124 Perugia (Pg), Italy



**Figure S1** X-Band (9.23 GHz) EPR spectrum of a powder sample of **1** measured at 4 K.  $g=2.00$  is occurring at 0.3300 T.

**Table S1.** Atomic coordinates and equivalent isotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for **1**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

Atom name	$x/a$	$y/b$	$z/c$	$U_{eq}$
Co(1)	0.2875(1)	0.7424(1)	0.1641(1)	31(1)
Co(2)	0.3070(1)	0.2419(1)	0.0661(1)	30(1)
P(1)	0.1976(2)	0.5057(1)	0.3789(1)	46(1)
P(2)	0.1969(2)	0.4840(1)	-0.1552(1)	51(1)
F(2)	0.3020(5)	0.5334(4)	0.3540(2)	88(2)
F(3)	0.1634(7)	0.6040(3)	0.3798(3)	115(2)
F(4)	0.1232(6)	0.4942(4)	0.3283(2)	96(2)
F(5)	0.0952(4)	0.4764(3)	0.4045(2)	77(2)
F(6)	0.2293(6)	0.4049(4)	0.3763(3)	114(2)
F(7)	0.2755(6)	0.5131(6)	0.4283(2)	154(4)
F(8)	0.0989(5)	0.4845(3)	0.1242(2)	80(2)
F(9)	0.1114(6)	0.4758(4)	-0.2029(2)	100(2)
F(10)	0.1918(5)	0.5879(3)	-0.1597(2)	88(2)
F(11)	0.3001(6)	0.4856(4)	-0.1846(2)	106(2)
F(12)	0.2865(5)	0.4933(3)	-0.1081(2)	79(2)
O(4)	0.3264(4)	0.2030(3)	0.1367(1)	36(1)
O(1)	0.2629(4)	0.7982(3)	0.0961(1)	43(1)
O(3)	0.2039(4)	0.3283(3)	0.0948(2)	40(1)
O(2)	0.2140(5)	0.6420(3)	0.1199(2)	52(1)
N(1)	0.4593(7)	0.7126(5)	0.1512(2)	40(2)
N(2)	0.1182(6)	0.7712(5)	0.1796(3)	43(2)
N(3)	0.3344(7)	0.6494(5)	0.2264(3)	47(2)
N(4)	0.2428(6)	0.2852(4)	-0.0068(2)	48(2)
N(5)	0.4500(5)	0.1552(3)	0.0511(2)	41(1)
N(6)	0.1746(5)	0.1405(4)	0.0522(2)	44(1)
N(7)	0.4425(5)	0.3411(3)	0.0803(2)	40(1)
N(8)	0.3319(7)	0.8684(4)	0.1999(2)	38(2)
C(2)	0.2672(6)	0.2456(4)	0.1639(2)	34(1)
C(3)	0.1997(6)	0.3193(4)	0.1396(2)	37(2)
C(4)	0.1342(7)	0.3773(5)	0.1629(3)	53(2)
C(5)	0.1185(7)	0.3836(5)	0.2095(3)	57(2)
C(6)	0.1550(7)	0.3300(6)	0.2483(3)	59(2)
C(7)	0.2168(7)	0.2552(6)	0.2469(3)	59(2)
C(8)	0.2653(6)	0.2174(5)	0.2098(2)	46(2)
C(9)	0.1927(6)	0.6592(4)	0.0756(2)	40(2)
C(10)	0.2224(5)	0.7476(4)	0.0613(2)	30(1)
C(11)	0.1443(7)	0.5931(5)	0.0436(3)	55(2)
C(12)	0.1202(7)	0.5923(5)	-0.0054(3)	59(2)
C(13)	0.1335(6)	0.6545(5)	-0.0384(2)	50(2)
C(14)	0.1752(6)	0.7377(5)	-0.0287(2)	44(2)
C(15)	0.2108(6)	0.7776(4)	0.0141(2)	40(2)
C(18)	0.4283(10)	0.6014(7)	0.2092(5)	60(3)
C(19)	0.5165(8)	0.6704(8)	0.1940(4)	91(3)
C(20)	0.5281(10)	0.7932(8)	0.1392(4)	56(3)
C(21)	0.5249(9)	0.8706(7)	0.1737(4)	84(3)
C(22)	0.4051(8)	0.9180(5)	0.1703(3)	57(2)
C(23)	0.3819(10)	0.8774(7)	0.2524(3)	54(3)
C(24)	0.2146(10)	0.9133(6)	0.1894(5)	110(5)
C(25)	0.1319(8)	0.8455(6)	0.2136(3)	79(3)
C(26)	0.0635(10)	0.6948(8)	0.2023(4)	96(3)
C(27)	0.2422(9)	0.5924(6)	0.2281(3)	50(3)
C(28)	0.4669(7)	0.3653(5)	0.1313(2)	53(2)
C(29)	0.4101(8)	0.4257(5)	0.0547(3)	58(2)
C(30)	0.3552(8)	0.4206(5)	0.0027(3)	61(2)
C(31)	0.5430(6)	0.3000(5)	0.0663(3)	50(2)
C(32)	0.2351(8)	0.3788(5)	-0.0064(3)	64(2)
C(33)	0.5471(6)	0.2042(4)	0.0797(3)	46(2)

C(34)	0.1237(7)	0.2450(6)	-0.0108(3)	64(2)
C(35)	0.4852(7)	0.1359(5)	0.0047(3)	55(2)
C(36)	0.1279(7)	0.1500(5)	0.0009(3)	57(2)
C(37)	0.4305(6)	0.0708(4)	0.0735(3)	47(2)
C(38)	0.3254(7)	0.0230(4)	0.0491(3)	50(2)
C(39)	0.2143(7)	0.494(5)	0.0643(3)	52(2)
C(40)	0.0805(7)	0.1540(5)	0.0794(3)	57(2)
C(42)	0.0402(7)	0.07941(6)	0.1365(3)	71(3)
C(43)	0.1373(10)	0.6474(9)	0.2435(4)	68(3)
C(46)	0.3805(11)	0.6770(8)	0.2783(3)	66(3)
Disordered group				
N(8B)	0.421(2)	0.844(2)	0.1922(9)	51(6)
C(46B)	0.314(3)	0.729(2)	0.285(1)	46(7)
N(2B)	0.150(2)	0.833(2)	0.1772(9)	52(6)
N(3B)	0.258(3)	0.690(2)	0.234(1)	67(7)
C(23B)	0.473(3)	0.860(2)	0.246(1)	51(7)
N(1B)	0.428(2)	0.663(2)	0.1580(9)	54(7)
C(18B)	0.416(2)	0.572(2)	0.174(1)	38(6)
C(26B)	0.280(4)	0.966(3)	0.190(2)	81(11)
C(43B)	0.142(3)	0.722(2)	0.238(1)	57(8)
C(27B)	0.404(4)	0.567(3)	0.226(2)	84(14)
C(20B)	0.525(3)	0.802(2)	0.164(1)	40(7)
C(46c)	0.360	0.630	0.250	25
C25b	0.08	0.780	0.20	25
C22b	0.360	0.920	0.170	25
C24b	0.180	0.920	0.210	25
C19b	0.530	0.710	0.170	25
C42b	0.110	0.830	0.130	25
C17b	0.390	0.640	0.110	25