

*Supplementary Data*

# New Bi-Nuclear Nickel(II) Complex-Based Salen Schiff Base: Synthesis, Crystal Structure, Spectroscopic, Thermal, and Electrical Investigations

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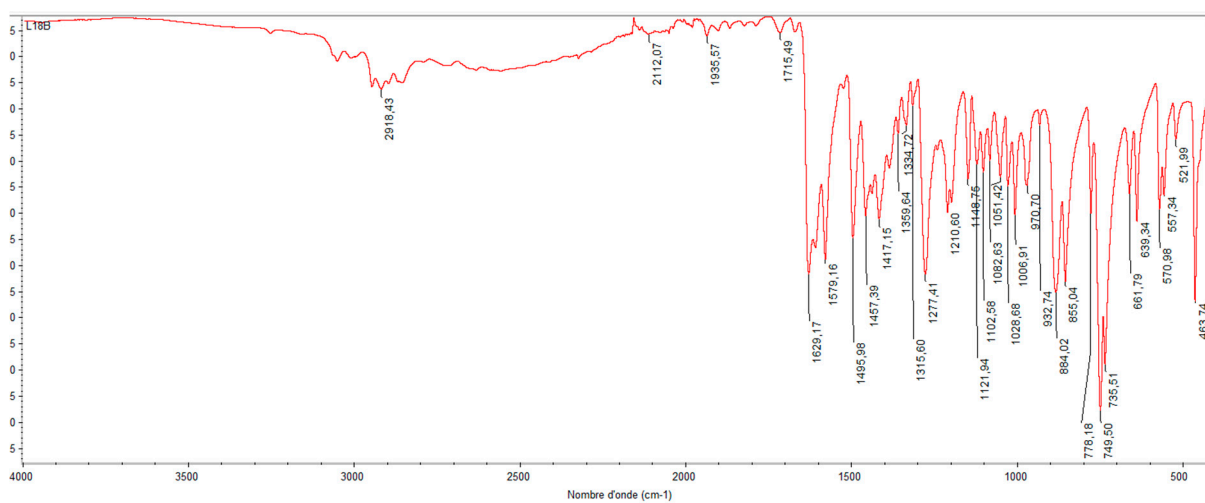


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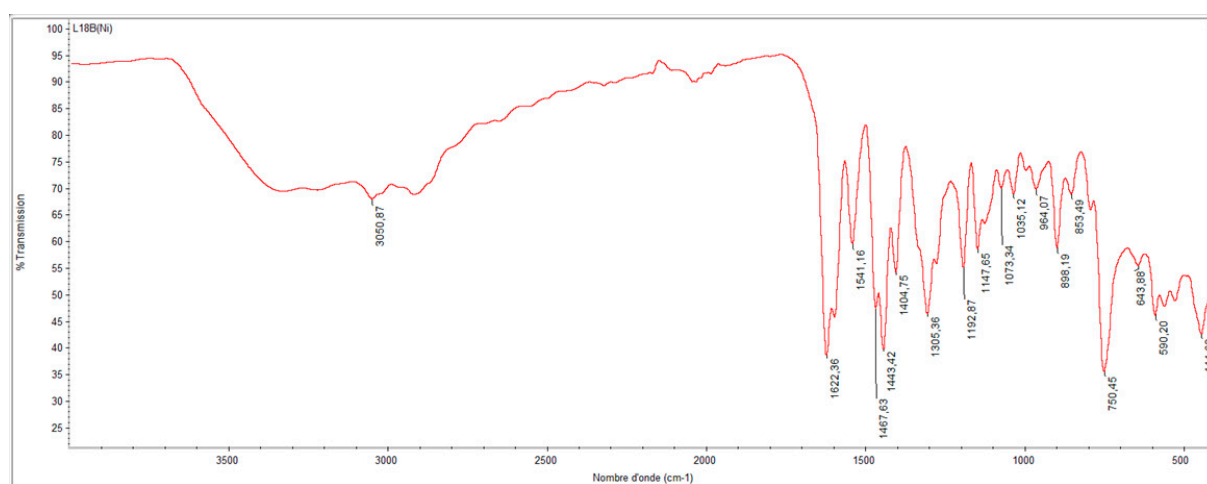
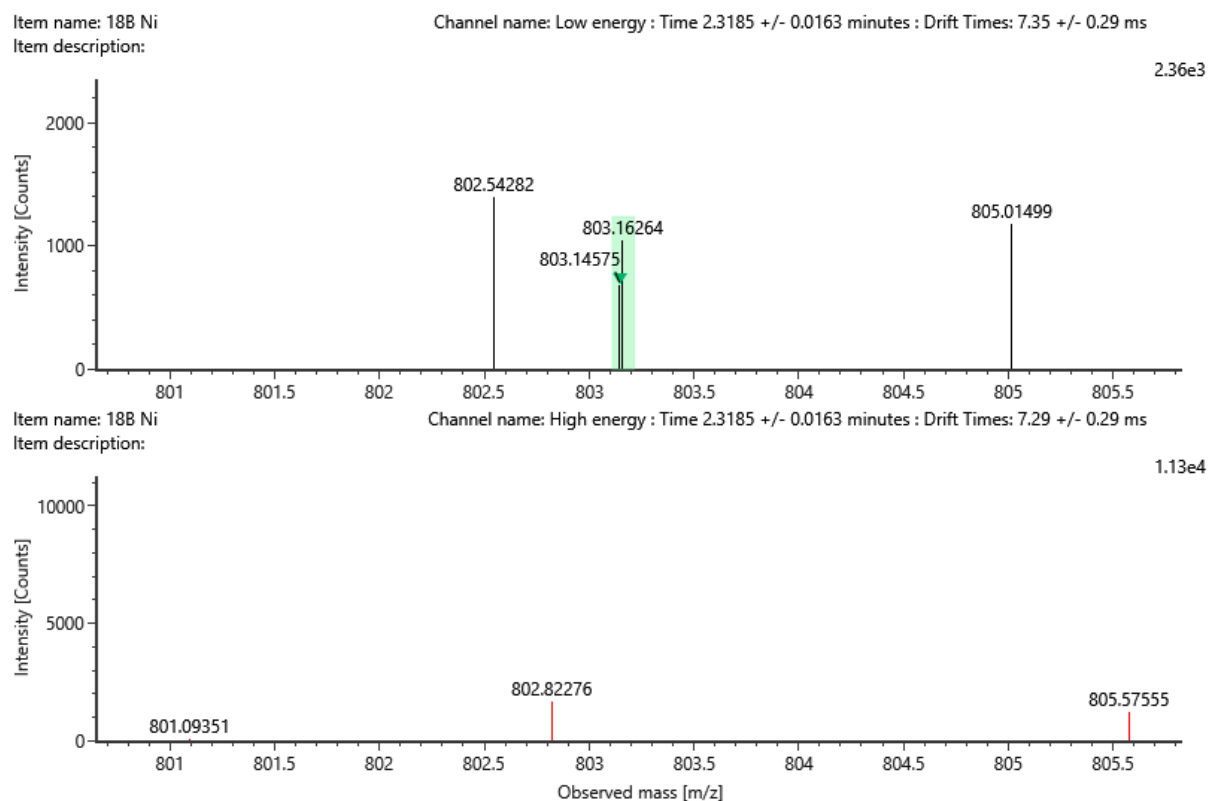
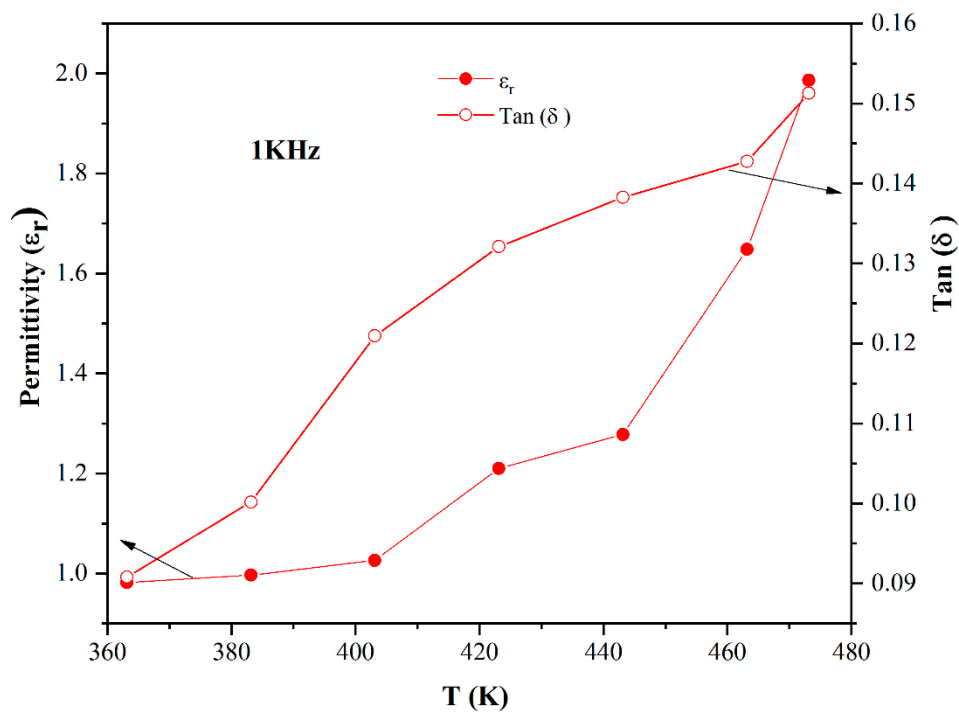


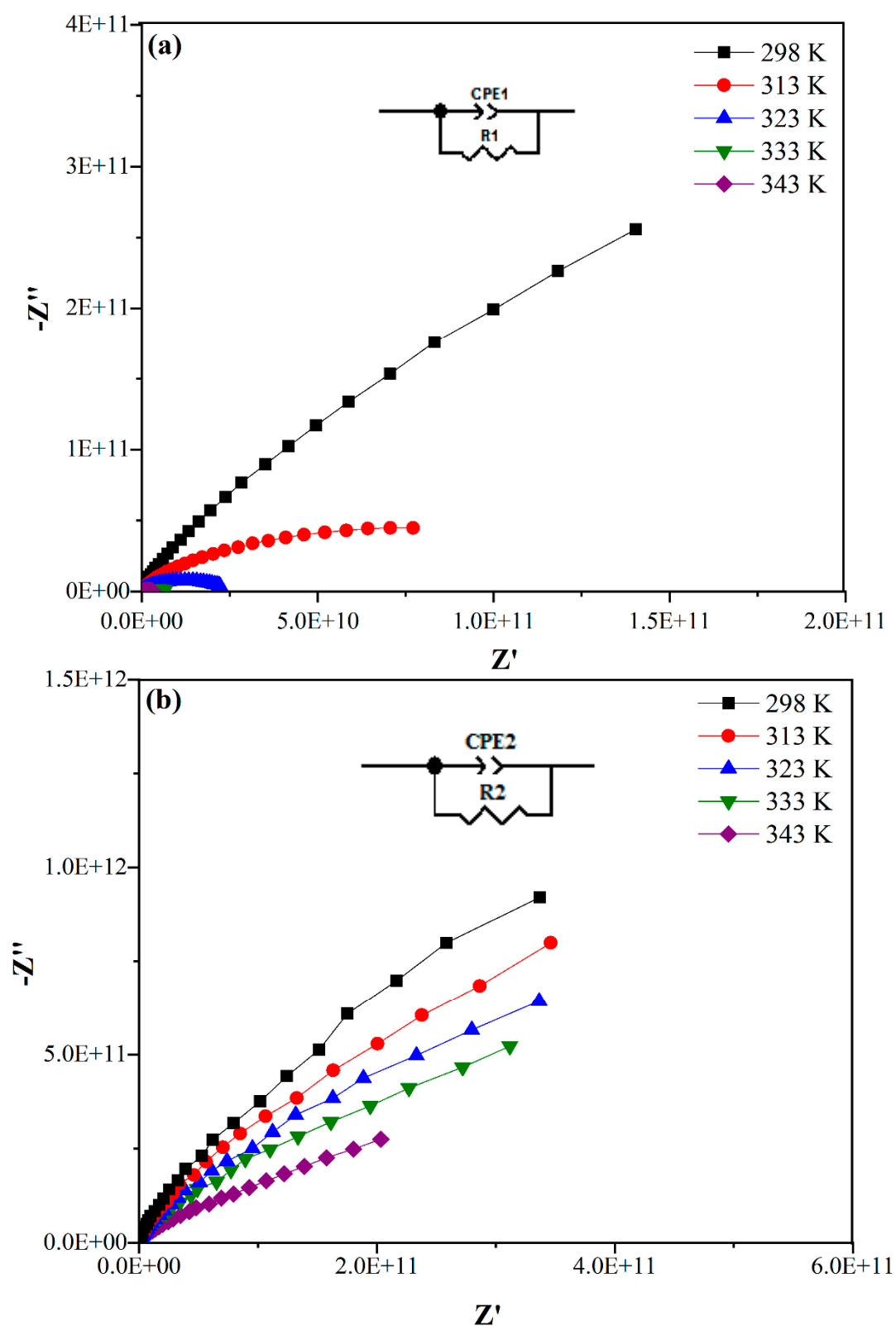
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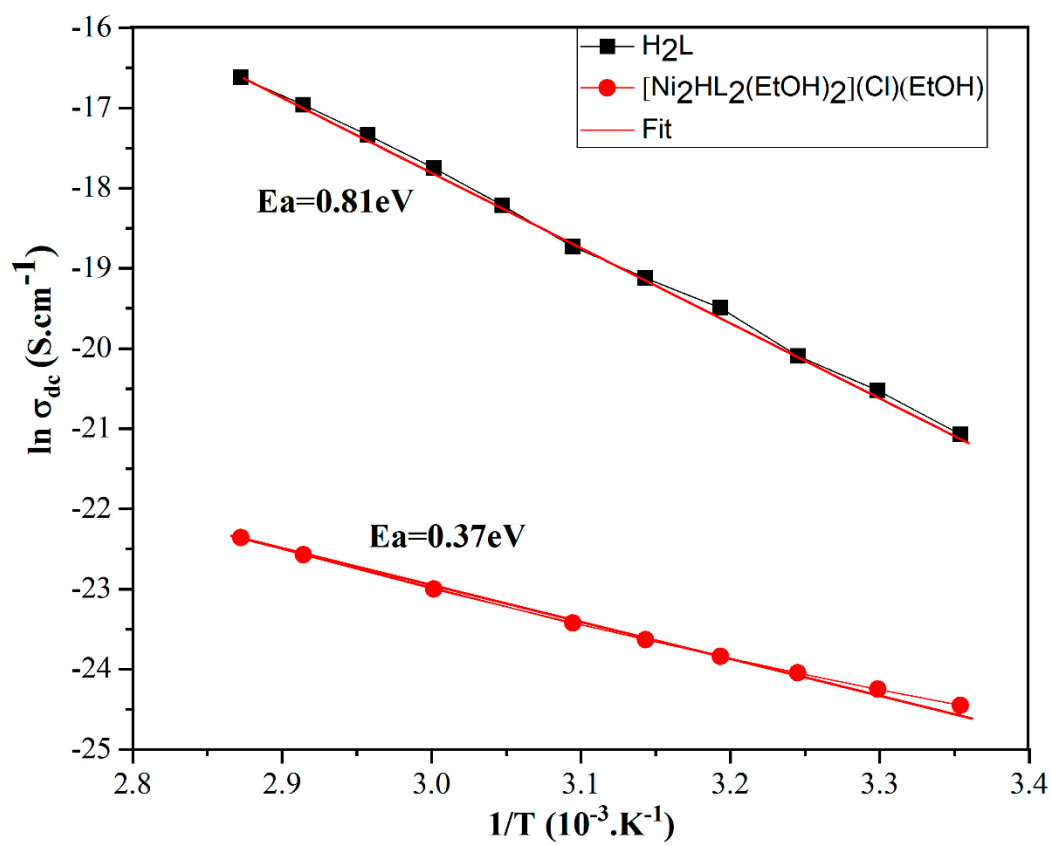


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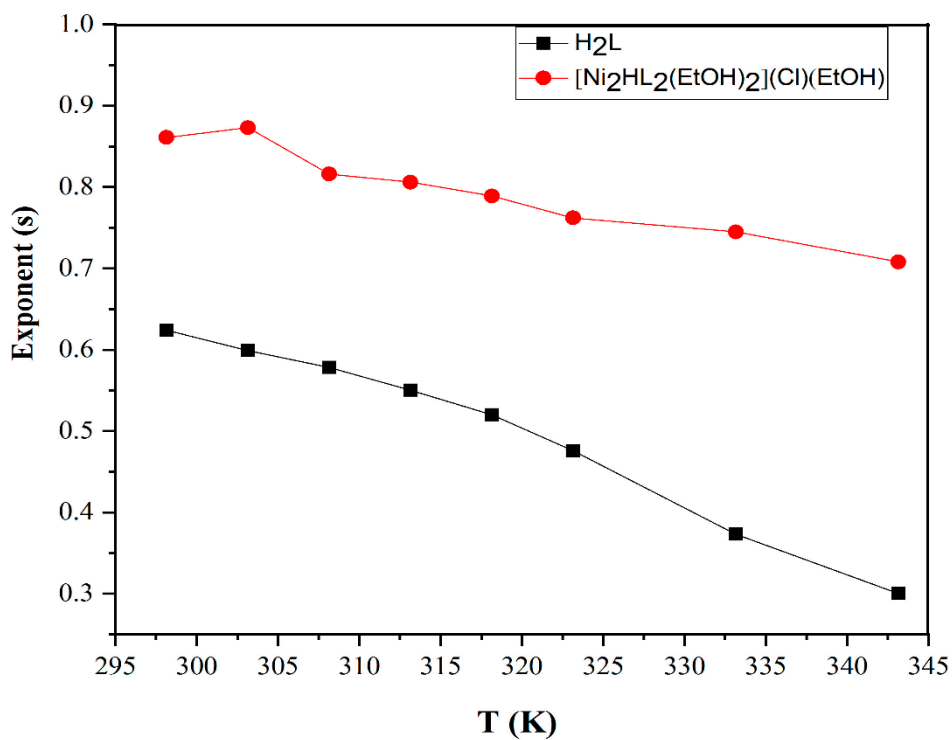


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**Table S1.** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) of  $[\text{Ni}_2\text{HL}_2(\text{EtOH})_2](\text{Cl})(\text{EtOH})$  complex.

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.60513 (18)	0.4545 (3)	0.36161 (15)	0.0417 (7)	
C2	0.6743 (2)	0.4428 (3)	0.32764 (17)	0.0535 (8)	
H2	0.714795	0.490120	0.338096	0.064*	
C3	0.6832 (2)	0.3629 (3)	0.27935 (19)	0.0615 (10)	
H3	0.729416	0.357180	0.257206	0.074*	
C4	0.6247 (3)	0.2909 (3)	0.2631 (2)	0.0680 (11)	
H4	0.631156	0.236610	0.230348	0.082*	
C5	0.5572 (3)	0.3003 (3)	0.29581 (19)	0.0610 (9)	
H5	0.517556	0.251797	0.284719	0.073*	
C6	0.5455 (2)	0.3812 (3)	0.34589 (16)	0.0456 (7)	
C7	0.46993 (19)	0.3876 (3)	0.37431 (16)	0.0483 (8)	
H7	0.433707	0.340075	0.355649	0.058*	
C8	0.36433 (19)	0.4454 (3)	0.43552 (19)	0.0546 (9)	
H8A	0.341576	0.386830	0.408478	0.065*	
H8B	0.341540	0.516678	0.422792	0.065*	
C9	0.34597 (19)	0.4226 (3)	0.5068 (2)	0.0564 (8)	
H9A	0.374293	0.356746	0.521150	0.068*	
H9B	0.292259	0.404918	0.510468	0.068*	
C10	0.3641 (2)	0.5203 (3)	0.55298 (19)	0.0556 (9)	
H10A	0.343833	0.589540	0.534508	0.067*	
H10B	0.339754	0.507610	0.595404	0.067*	
C11	0.60919 (18)	0.5815 (2)	0.60327 (15)	0.0383 (6)	
C12	0.68214 (18)	0.5899 (3)	0.63198 (15)	0.0444 (7)	
H12	0.722167	0.617260	0.606534	0.053*	
C13	0.6957 (2)	0.5590 (3)	0.69591 (17)	0.0560 (9)	
H13	0.744722	0.564775	0.712887	0.067*	
C14	0.6380 (2)	0.5195 (4)	0.73571 (17)	0.0627 (10)	
H14	0.647719	0.497746	0.779110	0.075*	
C15	0.5663 (2)	0.5130 (3)	0.71023 (16)	0.0575 (9)	
H15	0.526929	0.488377	0.737303	0.069*	
C16	0.55007 (19)	0.5425 (3)	0.64413 (15)	0.0442 (7)	
C17	0.47155 (19)	0.5319 (3)	0.62220 (17)	0.0472 (7)	
H17	0.435110	0.523753	0.655220	0.057*	
C18	0.6430 (2)	0.3466 (3)	0.5192 (2)	0.0621 (10)	
H18A	0.673035	0.414697	0.514087	0.074*	
H18B	0.655498	0.296347	0.482895	0.074*	

C19	0.6631 (3)	0.2912 (4)	0.5830 (2)	0.0752 (12)	
H19A	0.649621	0.340002	0.619064	0.113*	
H19B	0.716759	0.276543	0.584123	0.113*	
H19C	0.635766	0.221422	0.586928	0.113*	
C20	0.4336 (2)	0.7526 (3)	0.45966 (19)	0.0515 (9)	
C21	0.3843 (2)	0.7408 (4)	0.4054 (3)	0.0696 (11)	
H21	0.400197	0.700931	0.368258	0.083*	
C22	0.3121 (3)	0.7883 (4)	0.4068 (3)	0.0861 (16)	
H22	0.280194	0.779778	0.370351	0.103*	
C23	0.2871 (3)	0.8468 (4)	0.4604 (3)	0.0880 (17)	
H23	0.238416	0.877389	0.460715	0.106*	
C24	0.3335 (2)	0.8605 (3)	0.5132 (3)	0.0752 (12)	
H24	0.315796	0.900040	0.549835	0.090*	
C25	0.4078 (2)	0.8165 (3)	0.5142 (2)	0.0579 (9)	
C26	0.4535 (2)	0.8427 (3)	0.5718 (2)	0.0580 (9)	
H26	0.427665	0.872828	0.607865	0.070*	
C27	0.5579 (2)	0.8651 (3)	0.64167 (18)	0.0615 (10)	
H27A	0.573018	0.799140	0.666841	0.074*	
H27B	0.519935	0.905523	0.667152	0.074*	
C28	0.6264 (3)	0.9403 (3)	0.63134 (19)	0.0656 (11)	
H28A	0.613616	0.997463	0.598833	0.079*	
H28B	0.637698	0.978680	0.672605	0.079*	
C29	0.6968 (2)	0.8792 (3)	0.60859 (16)	0.0560 (9)	
H29A	0.740299	0.928902	0.613522	0.067*	
H29B	0.705015	0.814285	0.636912	0.067*	
C30	0.71351 (18)	0.7638 (2)	0.39692 (15)	0.0404 (7)	
C31	0.7288 (2)	0.7473 (3)	0.33015 (16)	0.0496 (8)	
H31	0.697016	0.701516	0.305013	0.059*	
C32	0.7909 (2)	0.7981 (3)	0.30084 (19)	0.0621 (10)	
H32	0.800561	0.786141	0.256139	0.074*	
C33	0.8380 (2)	0.8656 (3)	0.3365 (2)	0.0638 (10)	
H33	0.879199	0.900546	0.316199	0.077*	
C34	0.8246 (2)	0.8817 (3)	0.40251 (19)	0.0543 (9)	
H34	0.858127	0.926054	0.426851	0.065*	
C35	0.76220 (18)	0.8338 (3)	0.43431 (16)	0.0425 (7)	
C36	0.75131 (18)	0.8591 (2)	0.50387 (17)	0.0451 (7)	
H36	0.792305	0.892646	0.525262	0.054*	
C37	0.5526 (3)	0.9365 (4)	0.3838 (2)	0.0815 (13)	
H37A	0.499582	0.958399	0.380638	0.098*	
H37B	0.558339	0.863328	0.362893	0.098*	



C38	0.6001 (5)	1.0197 (6)	0.3492 (3)	0.132 (3)	
H38A	0.600315	1.089094	0.373716	0.197*	
H38B	0.579811	1.032850	0.305806	0.197*	
H38C	0.651097	0.991524	0.345615	0.197*	
C39	0.3975 (7)	0.1939 (8)	0.6742 (6)	0.239 (7)	
H39A	0.363314	0.182911	0.711345	0.287*	
H39B	0.376356	0.252505	0.646221	0.287*	
C40A	0.4719 (10)	0.229 (2)	0.6986 (13)	0.30 (2)	0.6011
H40A	0.465361	0.279439	0.735549	0.444*	0.6011
H40B	0.498840	0.267927	0.663960	0.444*	0.6011
H40C	0.500422	0.164512	0.712284	0.444*	0.6011
C40B	0.4684 (12)	0.191 (4)	0.7118 (17)	0.27 (3)	0.3989
H40D	0.502331	0.248120	0.695113	0.409*	0.3989
H40E	0.491675	0.118497	0.707297	0.409*	0.3989
H40F	0.457901	0.205779	0.757625	0.409*	0.3989
N1	0.44666 (15)	0.4499 (2)	0.42155 (13)	0.0436 (6)	
N2	0.44717 (15)	0.5326 (2)	0.56289 (14)	0.0438 (6)	
N3	0.52479 (17)	0.8293 (2)	0.57883 (14)	0.0496 (7)	
N4	0.69263 (17)	0.8411 (2)	0.53942 (12)	0.0446 (6)	
O1	0.59666 (13)	0.5334 (2)	0.40779 (12)	0.0493 (6)	
O2	0.59963 (11)	0.60982 (18)	0.54106 (10)	0.0380 (4)	
O3	0.56373 (13)	0.3748 (2)	0.51604 (13)	0.0502 (6)	
O4	0.50098 (12)	0.70281 (19)	0.45858 (11)	0.0454 (5)	
O5	0.65403 (13)	0.7147 (2)	0.42592 (11)	0.0503 (6)	
H50	0.646939	0.652424	0.409362	0.076*	
O6	0.57418 (17)	0.9286 (2)	0.45239 (13)	0.0609 (7)	
O7	0.4035 (4)	0.0906 (6)	0.6371 (4)	0.201 (3)	
H7A	0.432482	0.099890	0.605801	0.301*	
Ni1	0.51975 (2)	0.53345 (3)	0.48375 (2)	0.03755 (10)	
Ni2	0.59223 (2)	0.77388 (3)	0.50365 (2)	0.03901 (10)	
Cl1	0.49158 (7)	0.13811 (9)	0.50978 (8)	0.0903 (4)	
H3O	0.534 (2)	0.315 (4)	0.513 (2)	0.072 (13)*	
H6O	0.553 (3)	0.985 (4)	0.475 (3)	0.091 (16)*	

**Table S2.** Atomic displacement parameters ( $\text{\AA}^2$ ) for  $[\text{Ni}_2\text{HL}_2(\text{EtOH})_2](\text{Cl})(\text{EtOH})$  complex.

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0535 (17)	0.0358 (16)	0.0354 (14)	-0.0009 (13)	-0.0012 (13)	0.0027 (12)
C2	0.060 (2)	0.052 (2)	0.0475 (18)	-0.0102 (16)	0.0071 (15)	-0.0028 (15)
C3	0.070 (2)	0.054 (2)	0.059 (2)	0.0048 (18)	0.0194 (18)	-0.0044 (17)
C4	0.095 (3)	0.048 (2)	0.061 (2)	0.001 (2)	0.008 (2)	-0.0175 (17)

C5	0.076 (2)	0.045 (2)	0.060 (2)	-0.0056 (17)	-0.0066 (19)	-0.0099 (16)
C6	0.0565 (18)	0.0386 (16)	0.0394 (15)	-0.0010 (14)	-0.0029 (14)	-0.0024 (13)
C7	0.0542 (18)	0.0448 (18)	0.0464 (17)	-0.0124 (15)	-0.0096 (15)	-0.0027 (14)
C8	0.0420 (17)	0.058 (2)	0.063 (2)	-0.0117 (16)	-0.0046 (15)	-0.0012 (17)
C9	0.0441 (16)	0.0564 (19)	0.069 (2)	-0.0139 (15)	0.0054 (17)	-0.0025 (19)
C10	0.0420 (17)	0.059 (2)	0.066 (2)	-0.0080 (16)	0.0081 (16)	-0.0069 (18)
C11	0.0507 (17)	0.0274 (14)	0.0361 (15)	0.0039 (12)	0.0006 (12)	-0.0015 (11)
C12	0.0473 (16)	0.0441 (17)	0.0411 (16)	0.0028 (14)	-0.0017 (13)	-0.0022 (13)
C13	0.060 (2)	0.062 (2)	0.0461 (18)	0.0069 (17)	-0.0118 (16)	-0.0017 (17)
C14	0.083 (3)	0.072 (3)	0.0334 (15)	0.005 (2)	-0.0044 (16)	0.0027 (16)
C15	0.071 (2)	0.064 (2)	0.0357 (16)	0.0010 (18)	0.0088 (16)	-0.0018 (15)
C16	0.0537 (17)	0.0425 (17)	0.0348 (15)	-0.0005 (14)	0.0057 (13)	-0.0017 (13)
C17	0.0501 (17)	0.0453 (18)	0.0456 (17)	-0.0024 (14)	0.0162 (14)	-0.0037 (14)
C18	0.0531 (19)	0.060 (2)	0.073 (2)	0.0117 (16)	0.0054 (17)	0.0002 (18)
C19	0.071 (3)	0.068 (3)	0.086 (3)	0.012 (2)	-0.017 (2)	0.004 (2)
C20	0.0475 (18)	0.0370 (17)	0.068 (2)	-0.0050 (14)	-0.0059 (16)	0.0170 (15)
C21	0.062 (2)	0.060 (2)	0.087 (3)	-0.0082 (19)	-0.025 (2)	0.015 (2)
C22	0.062 (3)	0.063 (3)	0.131 (5)	-0.011 (2)	-0.038 (3)	0.027 (3)
C23	0.056 (2)	0.055 (3)	0.155 (5)	0.001 (2)	-0.013 (3)	0.022 (3)
C24	0.056 (2)	0.047 (2)	0.122 (4)	0.0061 (17)	0.007 (2)	0.013 (2)
C25	0.0541 (18)	0.0355 (15)	0.084 (3)	0.0030 (15)	0.0102 (19)	0.0112 (18)
C26	0.072 (2)	0.0368 (18)	0.066 (2)	0.0071 (17)	0.0148 (19)	0.0045 (16)
C27	0.084 (3)	0.056 (2)	0.0452 (19)	0.010 (2)	0.0100 (18)	-0.0055 (16)
C28	0.107 (3)	0.046 (2)	0.0455 (19)	-0.005 (2)	-0.002 (2)	-0.0120 (16)
C29	0.074 (2)	0.052 (2)	0.0407 (17)	-0.0123 (18)	-0.0070 (16)	-0.0054 (15)
C30	0.0476 (16)	0.0327 (15)	0.0402 (15)	-0.0023 (13)	0.0002 (13)	0.0050 (12)
C31	0.059 (2)	0.0493 (19)	0.0387 (16)	-0.0039 (15)	0.0009 (14)	0.0007 (13)
C32	0.082 (3)	0.059 (2)	0.0459 (18)	-0.007 (2)	0.0193 (18)	0.0046 (16)
C33	0.062 (2)	0.057 (2)	0.071 (2)	-0.0123 (19)	0.0225 (19)	0.0051 (19)
C34	0.0496 (18)	0.045 (2)	0.067 (2)	-0.0087 (15)	0.0057 (16)	-0.0039 (16)
C35	0.0492 (17)	0.0332 (15)	0.0445 (16)	-0.0007 (13)	-0.0029 (13)	0.0020 (13)
C36	0.0537 (16)	0.0351 (14)	0.0454 (15)	-0.0084 (12)	-0.0066 (16)	0.0017 (14)
C37	0.108 (3)	0.072 (3)	0.064 (3)	0.005 (3)	-0.016 (3)	0.020 (2)
C38	0.198 (7)	0.096 (4)	0.098 (4)	-0.009 (4)	0.003 (4)	0.045 (4)
C39A	0.178 (9)	0.185 (9)	0.211 (9)	-0.035 (8)	0.076 (8)	-0.074 (8)
C40A	0.215 (13)	0.198 (11)	0.232 (13)	-0.109 (10)	0.048 (11)	-0.044 (10)
C39B	0.197 (11)	0.173 (11)	0.217 (11)	-0.044 (10)	0.068 (11)	-0.062 (10)
C40B	0.198 (18)	0.131 (16)	0.224 (17)	-0.076 (16)	0.061 (17)	-0.045 (16)
N1	0.0437 (14)	0.0432 (15)	0.0432 (14)	-0.0063 (12)	-0.0027 (11)	0.0023 (11)
N2	0.0396 (14)	0.0415 (15)	0.0500 (15)	-0.0030 (11)	0.0055 (11)	-0.0045 (12)

N3	0.0623 (18)	0.0397 (15)	0.0466 (15)	0.0041 (13)	0.0098 (13)	0.0030 (12)
N4	0.0626 (17)	0.0342 (14)	0.0368 (13)	-0.0054 (12)	-0.0059 (12)	0.0000 (10)
O1	0.0595 (13)	0.0457 (14)	0.0426 (12)	-0.0139 (10)	0.0115 (10)	-0.0136 (10)
O2	0.0447 (11)	0.0360 (11)	0.0326 (10)	-0.0028 (9)	-0.0018 (8)	0.0034 (8)
O3	0.0484 (12)	0.0365 (11)	0.0645 (15)	0.0028 (10)	0.0000 (11)	0.0017 (10)
O4	0.0478 (12)	0.0382 (12)	0.0490 (12)	-0.0002 (9)	-0.0073 (9)	0.0040 (9)
O5	0.0597 (13)	0.0473 (13)	0.0426 (11)	-0.0200 (11)	0.0118 (10)	-0.0093 (10)
O6	0.0835 (18)	0.0464 (15)	0.0536 (15)	0.0020 (14)	-0.0060 (13)	0.0128 (12)
O7	0.193 (6)	0.169 (6)	0.230 (7)	-0.020 (4)	0.064 (5)	-0.056 (5)
Ni1	0.03971 (17)	0.03510 (18)	0.03730 (17)	-0.00415 (15)	0.00034 (15)	-0.00075 (15)
Ni2	0.04793 (19)	0.03328 (17)	0.03531 (16)	-0.00276 (15)	-0.00071 (16)	0.00100 (16)
Cl1	0.1048 (8)	0.0455 (5)	0.1200 (10)	-0.0024 (5)	-0.0245 (8)	-0.0082 (6)

**Table S3.** Selected bond distances (Å) and angles (°) for the  $[\text{Ni}_2\text{HL}_2(\text{EtOH})_2](\text{Cl})(\text{EtOH})$  complex.

C1—O1	1.330 (4)	C27—N3	1.460 (5)
C1—C6	1.399 (5)	C27—C28	1.513 (6)
C1—C2	1.404 (5)	C27—H27A	0.9700
C2—C3	1.369 (5)	C27—H27B	0.9700
C2—H2	0.9300	C28—C29	1.506 (6)
C3—C4	1.376 (6)	C28—H28A	0.9700
C3—H3	0.9300	C28—H28B	0.9700
C4—C5	1.363 (6)	C29—N4	1.471 (4)
C4—H4	0.9300	C29—H29A	0.9700
C5—C6	1.409 (5)	C29—H29B	0.9700
C5—H5	0.9300	C30—O5	1.333 (4)
C6—C7	1.449 (5)	C30—C31	1.390 (4)
C7—N1	1.275 (4)	C30—C35	1.411 (4)
C7—H7	0.9300	C31—C32	1.380 (5)
C8—N1	1.475 (4)	C31—H31	0.9300
C8—C9	1.501 (6)	C32—C33	1.359 (6)
C8—H8A	0.9700	C32—H32	0.9300
C8—H8B	0.9700	C33—C34	1.367 (5)
C9—C10	1.522 (5)	C33—H33	0.9300
C9—H9A	0.9700	C34—C35	1.393 (5)
C9—H9B	0.9700	C34—H34	0.9300
C10—N2	1.481 (4)	C35—C36	1.450 (5)
C10—H10A	0.9700	C36—N4	1.275 (4)
C10—H10B	0.9700	C36—H36	0.9300

C11—O2	1.312 (3)	C37—O6	1.440 (5)
C11—C16	1.406 (4)	C37—C38	1.469 (8)
C11—C12	1.411 (4)	C37—H37A	0.9700
C12—C13	1.364 (5)	C37—H37B	0.9700
C12—H12	0.9300	C38—H38A	0.9600
C13—C14	1.377 (5)	C38—H38B	0.9600
C13—H13	0.9300	C38—H38C	0.9600
C14—C15	1.363 (5)	C39—O7	1.4399 (15)
C14—H14	0.9300	C39—C40A	1.4596 (15)
C15—C16	1.410 (5)	C39—C40B	1.4597 (15)
C15—H15	0.9300	C39—H39A	0.9700
C16—C17	1.455 (5)	C39—H39B	0.9700
C17—N2	1.273 (4)	C40A—H40A	0.9600
C17—H17	0.9300	C40A—H40B	0.9600
C18—O3	1.435 (4)	C40A—H40C	0.9600
C18—C19	1.489 (6)	C40B—H40D	0.9600
C18—H18A	0.9700	C40B—H40E	0.9600
C18—H18B	0.9700	C40B—H40F	0.9600
C19—H19A	0.9600	N1—Ni1	2.052 (3)
C19—H19B	0.9600	N2—Ni1	2.046 (3)
C19—H19C	0.9600	N3—Ni2	2.036 (3)
C20—O4	1.323 (4)	N4—Ni2	2.067 (3)
C20—C21	1.404 (6)	O1—Ni1	2.045 (2)
C20—C25	1.412 (6)	O2—Ni1	2.033 (2)
C21—C22	1.390 (6)	O2—Ni2	2.091 (2)
C21—H21	0.9300	O3—Ni1	2.135 (2)
C22—C23	1.359 (8)	O3—H3O	0.88 (5)
C22—H22	0.9300	O4—Ni2	2.028 (2)
C23—C24	1.353 (7)	O4—Ni1	2.097 (2)
C23—H23	0.9300	O5—Ni2	2.035 (2)
C24—C25	1.406 (5)	O5—H5O	0.8200
C24—H24	0.9300	O6—Ni2	2.130 (3)
C25—C26	1.448 (6)	O6—H6O	0.89 (5)
C26—N3	1.272 (5)	O7—H7A	0.8200
C26—H26	0.9300		
O1—C1—C6	120.9 (3)	O5—C30—C31	121.2 (3)
O1—C1—C2	120.6 (3)	O5—C30—C35	119.8 (3)
C6—C1—C2	118.5 (3)	C31—C30—C35	119.0 (3)
C3—C2—C1	121.0 (3)	C32—C31—C30	120.5 (3)

C3—C2—H2	119.5	C32—C31—H31	119.7
C1—C2—H2	119.5	C30—C31—H31	119.7
C2—C3—C4	121.0 (4)	C33—C32—C31	120.8 (3)
C2—C3—H3	119.5	C33—C32—H32	119.6
C4—C3—H3	119.5	C31—C32—H32	119.6
C5—C4—C3	119.0 (4)	C32—C33—C34	119.7 (3)
C5—C4—H4	120.5	C32—C33—H33	120.2
C3—C4—H4	120.5	C34—C33—H33	120.2
C4—C5—C6	122.0 (4)	C33—C34—C35	121.9 (3)
C4—C5—H5	119.0	C33—C34—H34	119.1
C6—C5—H5	119.0	C35—C34—H34	119.1
C1—C6—C5	118.5 (3)	C34—C35—C30	118.1 (3)
C1—C6—C7	124.3 (3)	C34—C35—C36	117.8 (3)
C5—C6—C7	117.0 (3)	C30—C35—C36	124.1 (3)
N1—C7—C6	128.4 (3)	N4—C36—C35	128.2 (3)
N1—C7—H7	115.8	N4—C36—H36	115.9
C6—C7—H7	115.8	C35—C36—H36	115.9
N1—C8—C9	113.6 (3)	O6—C37—C38	110.6 (5)
N1—C8—H8A	108.8	O6—C37—H37A	109.5
C9—C8—H8A	108.8	C38—C37—H37A	109.5
N1—C8—H8B	108.8	O6—C37—H37B	109.5
C9—C8—H8B	108.8	C38—C37—H37B	109.5
H8A—C8—H8B	107.7	H37A—C37—H37B	108.1
C8—C9—C10	114.0 (3)	C37—C38—H38A	109.5
C8—C9—H9A	108.8	C37—C38—H38B	109.5
C10—C9—H9A	108.8	H38A—C38—H38B	109.5
C8—C9—H9B	108.8	C37—C38—H38C	109.5
C10—C9—H9B	108.8	H38A—C38—H38C	109.5
H9A—C9—H9B	107.7	H38B—C38—H38C	109.5
N2—C10—C9	111.4 (3)	O7—C39—C40A	110.8 (13)
N2—C10—H10A	109.4	O7—C39—C40B	101 (2)
C9—C10—H10A	109.4	O7—C39—H39A	109.5
N2—C10—H10B	109.4	C40A—C39—H39A	109.5
C9—C10—H10B	109.4	O7—C39—H39B	109.5
H10A—C10—H10B	108.0	C40A—C39—H39B	109.5
O2—C11—C16	123.5 (3)	H39A—C39—H39B	108.1
O2—C11—C12	119.5 (3)	C39—C40A—H40A	109.5
C16—C11—C12	117.0 (3)	C39—C40A—H40B	109.5
C13—C12—C11	122.0 (3)	H40A—C40A—H40B	109.5
C13—C12—H12	119.0	C39—C40A—H40C	109.5

C11—C12—H12	119.0	H40A—C40A—H40C	109.5
C12—C13—C14	121.1 (3)	H40B—C40A—H40C	109.5
C12—C13—H13	119.5	C39—C40B—H40D	109.5
C14—C13—H13	119.5	C39—C40B—H40E	109.5
C15—C14—C13	118.6 (3)	H40D—C40B—H40E	109.5
C15—C14—H14	120.7	C39—C40B—H40F	109.5
C13—C14—H14	120.7	H40D—C40B—H40F	109.5
C14—C15—C16	122.1 (3)	H40E—C40B—H40F	109.5
C14—C15—H15	119.0	C7—N1—C8	115.9 (3)
C16—C15—H15	119.0	C7—N1—Ni1	122.5 (2)
C11—C16—C15	119.2 (3)	C8—N1—Ni1	121.0 (2)
C11—C16—C17	123.4 (3)	C17—N2—C10	117.3 (3)
C15—C16—C17	117.4 (3)	C17—N2—Ni1	121.7 (2)
N2—C17—C16	127.3 (3)	C10—N2—Ni1	120.6 (2)
N2—C17—H17	116.4	C26—N3—C27	117.0 (3)
C16—C17—H17	116.4	C26—N3—Ni2	122.1 (3)
O3—C18—C19	111.8 (3)	C27—N3—Ni2	120.7 (2)
O3—C18—H18A	109.3	C36—N4—C29	116.3 (3)
C19—C18—H18A	109.3	C36—N4—Ni2	123.9 (2)
O3—C18—H18B	109.3	C29—N4—Ni2	119.6 (2)
C19—C18—H18B	109.3	C1—O1—Ni1	126.9 (2)
H18A—C18—H18B	107.9	C11—O2—Ni1	121.35 (19)
C18—C19—H19A	109.5	C11—O2—Ni2	126.33 (19)
C18—C19—H19B	109.5	Ni1—O2—Ni2	99.52 (8)
H19A—C19—H19B	109.5	C18—O3—Ni1	124.8 (2)
C18—C19—H19C	109.5	C18—O3—H3O	113 (3)
H19A—C19—H19C	109.5	Ni1—O3—H3O	118 (3)
H19B—C19—H19C	109.5	C20—O4—Ni2	121.0 (2)
O4—C20—C21	119.7 (4)	C20—O4—Ni1	124.3 (2)
O4—C20—C25	122.7 (3)	Ni2—O4—Ni1	99.47 (9)
C21—C20—C25	117.7 (4)	C30—O5—Ni2	127.42 (19)
C22—C21—C20	120.6 (5)	C30—O5—H5O	109.5
C22—C21—H21	119.7	Ni2—O5—H5O	123.0
C20—C21—H21	119.7	C37—O6—Ni2	124.3 (3)
C23—C22—C21	121.1 (5)	C37—O6—H6O	109 (3)
C23—C22—H22	119.4	Ni2—O6—H6O	117 (4)
C21—C22—H22	119.4	C39—O7—H7A	109.5
C24—C23—C22	119.7 (4)	O2—Ni1—O1	88.33 (9)
C24—C23—H23	120.1	O2—Ni1—N2	89.30 (9)
C22—C23—H23	120.1	O1—Ni1—N2	177.19 (11)

C23—C24—C25	121.8 (5)	O2—Ni1—N1	175.08 (10)
C23—C24—H24	119.1	O1—Ni1—N1	87.39 (10)
C25—C24—H24	119.1	N2—Ni1—N1	94.92 (11)
C24—C25—C20	119.1 (4)	O2—Ni1—O4	79.65 (8)
C24—C25—C26	116.6 (4)	O1—Ni1—O4	85.53 (10)
C20—C25—C26	124.3 (3)	N2—Ni1—O4	95.52 (10)
N3—C26—C25	127.6 (4)	N1—Ni1—O4	102.42 (10)
N3—C26—H26	116.2	O2—Ni1—O3	88.17 (9)
C25—C26—H26	116.2	O1—Ni1—O3	89.42 (10)
N3—C27—C28	111.7 (3)	N2—Ni1—O3	89.00 (10)
N3—C27—H27A	109.3	N1—Ni1—O3	89.36 (10)
C28—C27—H27A	109.3	O4—Ni1—O3	166.93 (9)
N3—C27—H27B	109.3	O4—Ni2—O5	86.12 (9)
C28—C27—H27B	109.3	O4—Ni2—N3	90.49 (11)
H27A—C27—H27B	107.9	O5—Ni2—N3	176.61 (11)
C29—C28—C27	114.4 (3)	O4—Ni2—N4	173.03 (10)
C29—C28—H28A	108.7	O5—Ni2—N4	86.95 (10)
C27—C28—H28A	108.7	N3—Ni2—N4	96.43 (11)
C29—C28—H28B	108.7	O4—Ni2—O2	79.92 (8)
C27—C28—H28B	108.7	O5—Ni2—O2	85.69 (9)
H28A—C28—H28B	107.6	N3—Ni2—O2	93.83 (9)
N4—C29—C28	113.4 (3)	N4—Ni2—O2	100.31 (9)
N4—C29—H29A	108.9	O4—Ni2—O6	91.24 (10)
C28—C29—H29A	108.9	O5—Ni2—O6	90.07 (11)
N4—C29—H29B	108.9	N3—Ni2—O6	89.90 (12)
C28—C29—H29B	108.9	N4—Ni2—O6	88.01 (11)
H29A—C29—H29B	107.7	O2—Ni2—O6	170.43 (10)