

SUPPLEMENTAL TABLE 1. Bond distances in abelsonite

Bond	Distance (Å)	Bond	Distance (Å)
Ni1-N2	1.923(2)	C9-C10	1.367(4)
Ni1-N2	1.923(2)	C10-C1	1.371(4)
Ni1-N1	1.970(2)	C10-H10	0.95
Ni1-N1	1.970(2)	C14-H14A	0.98
N1-C4	1.328(12)	C14-H14B	0.98
N1-C1	1.397(3)	C14-H14C	0.98
N1-C4'	1.477(12)	C14-H14D	0.98
N2-C6	1.372(4)	C14-H14E	0.98
N2-C9	1.376(3)	C14-H14F	0.98
C1-C2"	1.32(4)	C2'-C3'	1.25(3)
C1-C10	1.371(4)	C2'-C11'	1.534(7)
C1-C2	1.376(11)	C3'-C4'	1.403(15)
C1-C2'	1.565(11)	C3'-C13'	1.510(15)
C2-C3	1.383(11)	C4'-C5'	1.390(10)
C2-C11	1.520(8)	C5'-H5'	0.95
C3-C4	1.434(9)	C11'-H11D	0.98
C3-C13	1.506(9)	C11'-H11E	0.98
C4-C5	1.387(10)	C11'-H11F	0.98
C5-C6	1.340(14)	C13'-C14'	1.21(3)
C5-H5	0.95	C13'-H13D	0.99
C11-C12	1.523(12)	C13'-H13E	0.99
C11-H11A	0.99	C14'-H14G	0.98
C11-H11B	0.99	C14'-H14H	0.98
C12-H12A	0.98	C14'-H14I	0.98
C12-H12B	0.98	C15'-H15D	0.98
C12-H12C	0.98	C15'-H15E	0.98
C13-H13A	0.98	C15'-H15F	0.98
C13-H13B	0.98	C2"-C11"	1.532(10)
C13-H13C	0.98	C2"-C3"	1.63(6)
C15-C8	1.436(12)	C11"-C12"	1.519(19)
C15-C16	1.578(13)	C11"-H11G	0.99
C15-H15A	0.99	C11"-H11H	0.99
C15-H15B	0.99	C12"-H12D	0.98
C16-C10	1.534(6)	C12"-H12E	0.98
C16-H16A	0.99	C12"-H12F	0.98
C16-H16B	0.99	C3"-C13"	1.522(15)
C6-C5'	1.440(14)	C13"-C14"	1.58(2)
C6-C7	1.453(4)	C13"-H13F	0.99
C7-C8	1.350(4)	C13"-H13G	0.99
C7-C14	1.491(4)	C14"-H14J	0.98
C8-C9	1.424(4)	C14"-H14 K	0.98
C8-C15'	1.571(11)	C14"-H14L	0.98

Notes: Numbers in parentheses indicate 1 σ errors in the final digits of the values.
Values without errors were fixed during refinement.

SUPPLEMENTAL TABLE 2. Bond angles in abelsonite

Bond pair	Angle (°)	Bond pair	Angle (°)
N2-Ni1-N2	180	C7-C14-H14B	109.5
N2-Ni1-N1	89.68(10)	H14A-C14-H14B	109.5
N2-Ni1-N1	90.32(10)	C7-C14-H14C	109.5
N2-Ni1-N1	90.32(10)	H14A-C14-H14C	109.5
N2-Ni1-N1	89.68(10)	H14B-C14-H14C	109.5
N1-Ni1-N1	180	C7-C14-H14D	109.5
C4-N1-C1	103.4(5)	H14A-C14-H14D	141.1
C1-N1-C4'	104.6(4)	H14B-C14-H14D	56.3
C4-N1-Ni1	127.1(5)	H14C-C14-H14D	56.3
C1-N1-Ni1	128.9(2)	C7-C14-H14E	109.5
C4'-N1-Ni1	125.7(4)	H14A-C14-H14E	56.3
C6-N2-C9	103.5(2)	H14B-C14-H14E	141.1
C6-N2-Ni1	130.27(18)	H14C-C14-H14E	56.3
C9-N2-Ni1	126.2(2)	H14D-C14-H14E	109.5
C2"-C1-C10	122.7(17)	C7-C14-H14F	109.5
C10-C1-C2	123.3(5)	H14A-C14-H14F	56.3
C2"-C1-N1	112.6(19)	H14B-C14-H14F	56.3
C10-C1-N1	122.8(3)	H14C-C14-H14F	141.1
C2-C1-N1	112.7(5)	H14D-C14-H14F	109.5
C10-C1-C2'	128.8(5)	H14E-C14-H14F	109.5
N1-C1-C2'	107.5(5)	C3'-C2'-C11'	135.7(13)
C1-C2-C3	105.1(7)	C3'-C2'-C1	105.0(10)
C1-C2-C11	129.9(9)	C11'-C2'-C1	118.5(9)
C3-C2-C11	123.7(10)	C2'-C3'-C4'	115.5(16)
C2-C3-C4	105.1(8)	C2'-C3'-C13'	121.1(17)
C2-C3-C13	129.4(9)	C4'-C3'-C13'	123.(2)
C4-C3-C13	125.5(9)	C5'-C4'-C3'	125.1(15)
N1-C4-C5	122.5(11)	C5'-C4'-N1	126.6(10)
N1-C4-C3	112.1(8)	C3'-C4'-N1	106.8(12)
C5-C4-C3	124.9(11)	C4'-C5'-C6	117.9(11)
C6-C5-C4	129.1(13)	C4'-C5'-H5'	121
C6-C5-H5	115.5	C6-C5'-H5'	121
C4-C5-H5	115.5	C2'-C11'-H11D	109.5
C2-C11-C12	110.8(8)	C2'-C11'-H11E	109.5
C2-C11-H11A	109.5	H11D-C11'-H11E	109.5
C12-C11-H11A	109.5	C2'-C11'-H11F	109.5
C2-C11-H11B	109.5	H11D-C11'-H11F	109.5
C12-C11-H11B	109.5	H11E-C11'-H11F	109.5
H11A-C11-H11B	108.1	C14'-C13'-C3'	119.2(17)
C11-C12-H12A	109.5	C14'-C13'-H13D	107.5
C11-C12-H12B	109.5	C3'-C13'-H13D	107.5
H12A-C12-H12B	109.5	C14'-C13'-H13E	107.5

SUPPLEMENTAL TABLE 2.—CONTINUED

Bond pair	Angle (°)	Bond pair	Angle (°)
C11-C12-H12C	109.5	C3'-C13'-H13E	107.5
H12A-C12-H12C	109.5	H13D-C13'-H13E	107
H12B-C12-H12C	109.5	C13'-C14'-H14G	109.5
C3-C13-H13A	109.5	C13'-C14'-H14H	109.5
C3-C13-H13B	109.5	H14G-C14'-H14H	109.5
H13A-C13-H13B	109.5	C13'-C14'-H14I	109.5
C3-C13-H13C	109.5	H14G-C14'-H14I	109.5
H13A-C13-H13C	109.5	H14H-C14'-H14I	109.5
H13B-C13-H13C	109.5	C8-C15'-H15D	109.5
C8-C15-C16	101.5(6)	C8-C15'-H15E	109.5
C8-C15-H15A	111.5	H15D-C15'-H15E	109.5
C16-C15-H15A	111.5	C8-C15'-H15F	109.5
C8-C15-H15B	111.5	H15D-C15'-H15F	109.5
C16-C15-H15B	111.5	H15E-C15'-H15F	109.5
H15A-C15-H15B	109.3	C1-C2"-C11"	135.(3)
C10-C16-C15	110.6(6)	C1-C2"-C3"	114.(2)
C10-C16-H16A	109.5	C11"-C2"-C3"	108.(3)
C15-C16-H16A	109.5	C12"-C11"-C2"	108.(2)
C10-C16-H16B	109.5	C12"-C11"-H11G	110
C15-C16-H16B	109.5	C2"-C11"-H11G	110
H16A-C16-H16B	108.1	C12"-C11"-H11H	110
C5-C6-N2	119.9(6)	C2"-C11"-H11H	110
N2-C6-C5'	127.3(6)	H11G-C11"-H11H	108.4
C5-C6-C7	127.9(7)	C11"-C12"-H12D	109.5
N2-C6-C7	111.5(2)	C11"-C12"-H12E	109.5
C5'-C6-C7	120.3(6)	H12D-C12"-H12E	109.5
C8-C7-C6	105.9(3)	C11"-C12"-H12F	109.5
C8-C7-C14	128.6(3)	H12D-C12"-H12F	109.5
C6-C7-C14	125.5(3)	H12E-C12"-H12F	109.5
C7-C8-C9	106.7(2)	C13"-C3"-C2"	139.(2)
C7-C8-C15	144.3(5)	C3"-C13"-C14"	110.5(19)
C9-C8-C15	108.8(5)	C3"-C13"-H13F	109.6
C7-C8-C15'	128.9(5)	C14"-C13"-H13F	109.6
C9-C8-C15'	124.1(5)	C3"-C13"-H13G	109.6
C10-C9-N2	128.5(3)	C14"-C13"-H13G	109.6
C10-C9-C8	119.2(3)	H13F-C13"-H13G	108.1
N2-C9-C8	112.3(3)	C13"-C14"-H14J	109.5
C9-C10-C1	123.3(3)	C13"-C14"-H14 K	109.5
C9-C10-C16	99.7(3)	H14J-C14"-H14 K	109.5
C1-C10-C16	136.8(3)	C13"-C14"-H14L	109.5
C9-C10-H10	118.3	H14J-C14"-H14L	109.5
C1-C10-H10	118.3	H14 K-C14"-H14L	109.5
C7-C14-H14A	109.5		

Notes: Numbers in parentheses indicate 1 σ errors in the final digits of the values. Values without errors were fixed during refinement.