

Appendix 1

NBS*AIDS83-Format Calculated Powder Pattern of Ni(C₁₂H₆O₄)(H₂O)₄

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10.08510	10.94290	6.26390	98.989	87.428	108.015									X R T	JAK445A1	2
0.00040	0.00050	0.00030	0.002	0.003	0.002											2
P-1	2	2	0.000	1.764				344.95		649.32						3
O																5
Nickel(II) 2,6-naphthalenedicarboxylate tetrahydrate														P 1		6
C12 H14 Ni O8																7
OPCOMC														C1		9
																2
																9
Prepared by mixing aqueous solutions of nickel acetate tetrahydrate														PRC1		B
and diammonium 2,6-naphthalenedicarboxylate at room temperature.														PR 2		B
Pale green.														CL 3		B
Structure solved by applying Monte Carlo simulated annealing														C4		B
techniques to laboratory powder data.																5
Pattern calculated using a symmetric Cauchy profile function.																6
CuKa1	1.54060E													D R17.66	C	F
C P	1.026													CC	0.045	G
10.2889960	0	1	0+	8.41864	13	-1	1	0	6.18693	22	0	0	1	1		I
6.13985	25	1	1	0	5.69225999*	0	-1	1	5.29630	17	1	-1	1	2		I
5.25299	26	-1	2	0	5.14446172	0	2	0+	4.96801321		-2	1	0M	3		I
4.96801321	0	1	1M	4.79531149		2	0	0+	4.57296	33	-1	-1	1	4		I
4.34079105	1	-2	1	4.28380189		0	-2	1	4.20932616		-2	2	0+	5		I
4.04642	11	1	2	0	4.01026	28	2	-1	1	3.91177	63	2	1	0	6	I
3.79691167	-2	0	1+	3.75023	36	-2	1	1+	3.69292105		0	2	1+	7		I
3.59762	10	-1	3	0+	3.39971	32	-2	-1	1+	3.34476	18	1	-3	1+	8	I
3.31037131	-2	3	0+	3.22026116		2	1	1+	3.10835757		2	-3	1+	9		I
3.02283	8	1	-1	2+	2.94726	13	-1	0	2+	2.91868	5	-1	3	1	10	I
2.84715	84	0	1	2+	2.82542	43	0	3	1+	2.76021	6	-2	3	1	11	I
2.73638	4	-3	2	1	2.71070	16	2	-1	2+	2.65470189		2	2	1+	12	I
2.62982	19	1	-4	1+	2.60385115		-2	0	2+	2.56075	55	2	-4	1+	13	I
2.54876131	-2	1	2+	2.50048	20	-2	-1	2+	2.48400	4	-4	2	0	14		I
2.44803	2	-3	3	1+	2.39398	10	-3	4	0+	2.35859	41	2	1	2+	15	I
2.35859	41	-2	2	2+	2.34309	43	3	-4	1+	2.32832	17	-4	3	0+	16	I
2.31344	6	1	4	0	2.30082	30	-4	1	1+	2.28648	14	-2	-2	2M	17	I
2.28648	14	-1	-3	2M	2.25238	23	-4	2	1+	2.25238	23	0	4	1+	18	I
2.22585	23	-3	1	2+	2.22585	23	-3	0	2+	2.21264	58	1	-4	2+	19	I
2.21264	58	3	-3	2+	2.20191161		2	3	1+	2.17039	22	2	-4	2	20	I
2.15173	6	-1	5	0	2.13837	18	1	-5	1+	2.13837	18	0	-4	2+	21	I
2.13075	35	-3	-1	2+	2.13075	35	2	-5	1+	2.11185	23	-4	3	1M	22	I
2.11185	23	-2	3	2M	2.10466	18	-4	4	0	2.08899	36	-4	-1	1+	23	I
2.08899	36	2	2	2+	2.07646	8	1	4	1	2.06928	12	4	-4	1	24	I
2.05778	20	0	5	0+	2.04312	65	4	1	1+	2.03254	36	3	-4	2M	25	I
2.03254	36	-2	-3	2M	2.02321	44	2	4	0+	2.02321	44	3	-5	1+	26	I
2.00513	24	4	-2	2+	1.98172	31	4	-1	2+	1.96611	5	0	1	3+	27	I
1.95589	25	4	2	0+	1.95589	25	2	-1	3+	1.94605	15	2	-2	3+	28	I
1.93320	16	-1	-2	3+	1.92373	32	-4	4	1+	1.91922	35	-4	1	2+	29	I
1.91163	15	1	-5	2	1.90530	32	2	-5	2+	1.89845104		-4	0	2+	30	I
1.89845104	-4	-2	1+	1.89172	49	4	0	2+	1.87511	35	-4	2	2+	31		I
1.87118	27	-2	-1	3+	1.87118	27	-2	4	2+	1.86012	82	4	-5	1+	32	I
1.84561	10	4	-4	2+	1.82869	46	3	-5	2+	1.82223	29	0	2	3+	33	I
1.80513	11	-1	-3	3+	1.79881	11	-2	6	0	1.79119	15	1	-6	1+	34	I
1.79119	15	-2	-2	3+	1.78547	9	-1	6	0+	1.77844	14	1	-4	3+	35	I
1.77844	14	-4	3	2+	1.77035	12	-2	2	3+	1.75572	14	3	-6	1+	36	I

1.75572	14	2	-4	3+	1.74645	3	1	5	1	1.74140	4	0	-4	3+	37	I
1.74140	4	-3	-4	1+	1.73170	14	4	3	0+	1.73170	14	-4	5	1+	38	I
1.71482	39	0	6	0+	1.70257	10	-4	-3	1+	1.70257	10	-3	-1	3+	39	I
1.68373	11	-5	5	0	1.67914	8	-6	2	0+	1.67914	8	-1	3	3+	40	I
1.67187	13	-2	-3	3+	1.66088	30	0	3	3+	1.65499	24	-1	-4	3+	41	I
1.64844	15	-2	3	3+	1.64844	15	-1	6	1+	1.64350	13	2	2	3+	42	I
1.64350	13	4	-2	3+	1.63471	12	4	3	1+	1.63471	12	3	-6	2+	43	I
1.62512	12	-3	-2	3+	1.62512	12	4	-3	3+	1.62039	10	1	-5	3+	44	I
1.62039	10	4	-1	3+	1.60968	18	-1	-6	1+	1.60968	18	2	4	2+	45	I
1.60590	13	-5	-2	1+	1.60590	13	-3	-4	2+	1.59844	9	6	0	0+	46	I
1.59844	9	2	5	1+	1.59409	9	-6	4	0+	1.58381	5	-2	-5	2	47	I
1.57985	5	0	-5	3+	1.57298	14	-6	3	1+	1.56968	11	4	-4	3+	48	I
1.56968	11	-4	0	3+	1.55909	4	5	-5	2+	1.55417	15	4	-6	2+	49	I
1.54507	15	-4	6	1+	1.54507	15	-2	7	0+	1.53652	13	1	-7	1+	50	I
1.53652	13	5	-6	1+	1.52449	11	-1	7	0+	1.52449	11	-4	-1	3+	51	I
1.51474	16	-2	4	3+	1.51144	17	-6	4	1+	1.51144	17	6	1	0+	52	I
1.50884	15	1	-3	4+	1.50445	30	6	-2	2+	1.50445	30	0	4	3+	53	I
1.49692	9	0	1	4+	1.48998	2	-1	1	4+	1.48051	13	5	-2	3+	54	I
1.48051	13	0	-7	1+	1.47641	15	-6	-1	1+	1.47641	15	5	-3	3+	55	I
1.47230	7	-5	-3	1+	1.47048	8	2	0	4+	1.47048	8	0	7	0+	56	I
1.46737	7	1	-6	3+	1.46300	4	4	3	2+	1.45934	7	-2	6	2+	57	I
1.45393	5	5	-1	3+	1.45017	5	-1	-3	4+	1.45017	5	-6	2	2+	58	I
1.44287	9	1	-4	4+	1.44287	9	3	-2	4+	1.43769	5	-3	-5	2+	59	I
1.42826	14	-6	5	1+	1.42826	14	-3	7	1+	1.42358	10	0	2	4+	60	I
1.42358	10	2	5	2+	1.41794	2	6	0	2+	1.41257	4	7	-2	1+	61	I
1.41257	4	7	-3	1+	1.40904	5	6	2	0+	1.40904	5	2	1	4+	62	I
1.40641	4	-2	-6	2+	1.39995	7	-1	-7	1+	1.39995	7	-7	4	0+	63	I
1.39434	4	-3	0	4	1.39050	5	1	7	0+	1.38723	9	-6	-2	1+	64	I
1.38335	5	-2	5	3+	1.38335	5	0	7	1+	1.37848	6	4	2	3+	65	I
1.37489	5	-1	-4	4+	1.37143	2	-6	-1	2+	1.37143	2	7	0	0+	66	I

K

Appendix 2

NBS*AIDS83-Format Powder Pattern of $\text{Co}(\text{C}_{12}\text{H}_6\text{O}_4)(\text{H}_2\text{O})_4$

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10.18550	10.89210	6.29080	98.519	87.563	108.304													X R T P	JAK440A1
0.00060	0.00060	0.00050	0.004	0.004	0.003														2
P-1	2	2	0.000	1.749														655.28	3
O																			5
Cobalt(II) 2,6-naphthalenedicarboxylate tetrahydrate																		P 1	6
C12 H14 Co O8																			7
OPCOMC																		C1	9
																			2
																			9
Prepared by mixing aqueous solutions of cobalt acetate tetrahydrate																		PRC1	B
and diammonium 2,6-naphthalenedicarboxylate at room temperature.																		PR 2	B
Pink.																		CL 3	B
Structure solved by applying Monte Carlo simulated annealing																		C4	B
techniques to laboratory powder data.																			5
Pattern calculated using a symmetric Cauchy profile function.																			6
CuKa1	1.54060E																	D R17.66	C
C P	1.125																		G
																		CC 0.119	
10.2361827	0	1	0+	8.46831	8	-1	1	0	6.22134	29	0	0	1	1					I
6.13929 20	1	1	0	5.68716999*	0	-1	1	1	5.31043	15	1	-1	1	2					I
5.22193 28	1	0	1+	5.22193 28	-1	0	1+	1	5.11803142	0	2	0	3						I
5.01676307	-2	1	0M	5.01676307	0	1	1M	1	4.83503143	2	0	0	4						I
4.76180 15	-1	1	1	4.57563 26	-1	-1	1	1	4.33001 87	1	-2	1	5						I
4.23415547	-2	2	0+	4.03598 34	2	-1	1+	1	3.92513 63	2	1	0	6						I
3.82558146	-2	0	1+	3.78644 31	-2	1	1+	1	3.70274 83	0	2	1M	7						I
3.70274 83	2	-2	1M	3.58724 4	-1	3	0+	1	3.41002 30	-2	-1	1+	8						I
3.31657112	-2	3	0+	3.23610 96	2	1	1+	1	3.18877 10	0	-3	1	9						I
3.10619740	2	-3	1+	3.03381 9	1	-1	2M	1	3.03381 9	3	-1	1M	10						I
2.96491 8	-1	0	2+	2.94282 4	1	3	0	1	2.92612 7	-1	3	1+	11						I
2.86516 68	0	1	2+	2.84358 24	0	-2	2	1	2.82706 31	0	3	1+	12						I
2.79751 8	-1	-3	1	2.77507 12	-2	3	1+	1	2.72447 6	2	-1	2	13						I
2.66150168	2	2	1+	2.62112106	-2	0	2+	1	2.56971109	-2	1	2+	14						I
2.55319 43	2	-4	1	2.54359 25	1	-3	2+	1	2.54359 25	-4	1	0+	15						I
2.50974 19	-2	-1	2+	2.50974 19	-4	2	0+	1	2.48095 2	0	-3	2	16						I
2.46706 3	-3	3	1	2.45120 2	2	3	0	1	2.43940 2	2	-3	2	17						I
2.41752 2	4	0	0	2.40126 7	-3	4	0+	1	2.37193 38	2	1	2+	18						I
2.37193 38	4	-1	1+	2.34506 39	3	-4	1+	1	2.32365 19	-4	1	1	19						I
2.30304 6	-2	4	1+	2.30304 6	1	4	0+	1	2.28782 7	-2	-2	2M	20						I
2.28782 7	-1	-3	2M	2.27550 14	-4	2	1	1	2.26749 10	4	-3	1	21						I
2.25651 13	0	4	1+	2.24546 15	-3	1	2+	1	2.24546 15	-3	0	2+	22						I
2.21991 24	3	-3	2	2.20358167	2	3	1+	1	2.16500 31	2	-4	2	23						I
2.14058 22	-3	-1	2+	2.13134 33	-4	3	1+	1	2.13134 33	-2	3	2+	24						I
2.11708 21	-4	4	0+	2.11708 21	2	-5	1+	1	2.10059 26	-4	-1	1	25						I
2.09478 21	2	2	2+	2.07763 10	4	-4	1+	1	2.05547 53	4	1	1+	26						I
2.04721 28	0	5	0+	2.03311 29	3	-4	2+	1	2.03311 29	-2	-3	2+	27						I
2.01690 49	2	4	0+	2.01690 49	4	-2	2+	1	1.99590 29	4	-1	2+	28						I
1.98602 7	-2	-4	1	1.97851 6	0	1	3+	1	1.97851 6	-1	-4	2+	29						I
1.96256 25	4	2	0+	1.96256 25	2	-1	3+	1	1.95224 12	2	-2	3	30						I
1.93669 54	-4	1	2+	1.93669 54	-4	4	1+	1	1.91279 54	-4	0	2+	31						I
1.90490 61	4	0	2+	1.90490 61	-4	-2	1+	1	1.89753 46	2	-5	2+	32						I
1.89753 46	-4	2	2+	1.88725 16	1	5	0	1	1.87913 22	-2	-1	3+	33						I
1.87913 22	-2	1	3+	1.86363 51	4	-5	1+	1	1.85092 11	4	-4	2+	34						I
1.84128 16	4	2	1+	1.84128 16	-5	4	0+	1	1.83346 25	0	2	3+	35						I
1.82569 22	3	-5	2+	1.80360 7	-1	-3	3+	1	1.79362 12	-2	6	0+	36						I

1.79362	12	-2	-2	3+	1.78392	11	-2	2	3+	1.77970	11	1	-6	1M	37	I
1.77970	11	-1	6	0M	1.77436	8	1	-4	3+	1.76450	2	1	2	3	38	I
1.75133	8	3	-6	1+	1.74741	5	-3	0	3+	1.74335	6	-5	-1	1+	39	I
1.74335	6	3	0	3+	1.73416	9	4	3	0+	1.72303	4	5	-3	2+	40	I
1.70601	41	0	6	0+	1.69366	10	-5	5	0+	1.69366	10	-6	2	0+	41	I
1.68347	3	5	-5	1+	1.66994	27	0	3	3+	1.66389	8	2	-6	2+	42	I
1.66033	10	-2	3	3+	1.66033	10	4	-6	1+	1.65042	20	-1	-4	3+	43	I
1.65042	20	4	-2	3+	1.63887	8	4	3	1+	1.63181	11	4	-3	3+	44	I
1.63181	11	-3	-2	3+	1.62492	7	-3	6	1M	1.62492	7	6	-1	1M	45	I
1.61805	6	4	2	2M	1.61805	6	-6	2	1M	1.61235	12	-5	-2	1+	46	I
1.61235	12	6	0	0+	1.60821	10	-6	4	0+	1.59931	9	-1	-6	1+	47	I
1.58916	12	-6	3	1+	1.58175	2	-4	1	3	1.57629	6	-2	-5	2+	48	I
1.57629	6	-4	0	3+	1.57370	7	4	-4	3+	1.57370	7	0	-5	3+	49	I
1.56689	3	3	-5	3+	1.56179	4	-6	0	1+	1.55310	21	4	-6	2+	50	I
1.55310	21	-4	6	1+	1.53878	8	-2	7	0+	1.53878	8	-4	-1	3+	51	I
1.52590	16	-6	4	1+	1.52590	16	-2	4	3+	1.52094	11	6	1	0+	52	I
1.52094	11	-3	-5	1+	1.51648	26	6	-2	2+	1.51648	26	-6	5	0+	53	I
1.50964	16	0	4	3+	1.50964	16	2	3	3+	1.50623	11	0	1	4+	54	I
1.49784	3	0	-3	4+	1.49784	3	-1	-5	3+	1.48993	6	5	-2	3+	55	I
1.48607	13	-6	-1	1+	1.47878	5	2	0	4+	1.47710	5	1	1	4	56	I
1.47540	5	-5	-3	1+	1.47081	8	0	-7	1+	1.46306	10	-2	6	2+	57	I
1.45136	6	-1	-3	4+	1.45136	6	3	-2	4+	1.44026	10	-6	5	1+	58	I
1.44026	10	1	-4	4+	1.43258	11	0	2	4+	1.43258	11	-3	7	1+	59	I
1.42443	6	2	5	2+	1.42443	6	7	-2	1+	1.42179	4	0	-4	4+	60	I
1.41808	3	2	1	4+	1.41351	4	-7	4	0+	1.41138	5	-6	6	0+	61	I
1.41138	5	-2	2	4+	1.40313	3	-3	0	4+	1.39876	3	-2	-6	2+	62	I
1.39876	3	1	2	4+	1.39381	10	-6	-2	1+	1.39095	8	-1	-7	1+	63	I
1.39095	8	-2	5	3+	1.38591	4	4	2	3+	1.38355	4	1	7	0+	64	I
1.38355	4	-5	-3	2+	1.37362	4	-1	-4	4+	1.37004	4	2	4	3+	65	I
1.36327	2	0	5	3+	1.36327	2	4	-2	4+	1.35766	4	1	-5	4+	66	I
1.35766	4	-1	-6	3+											67	I
				JAK												K