crystals

Crystal Structure and Magnetism of Potassium-Intercalated 2,7-Dimethylnaphthalene

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Supplementary Materials

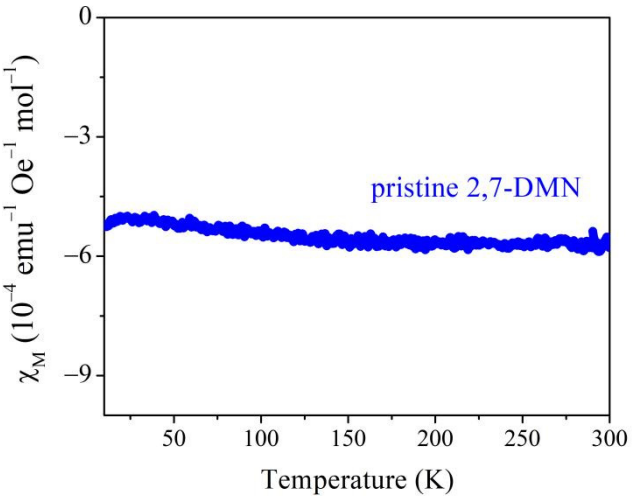


Figure S1. The relationship between molar magnetic susceptibility (χ_M) and temperature of pristine 2,7-DMN sample.

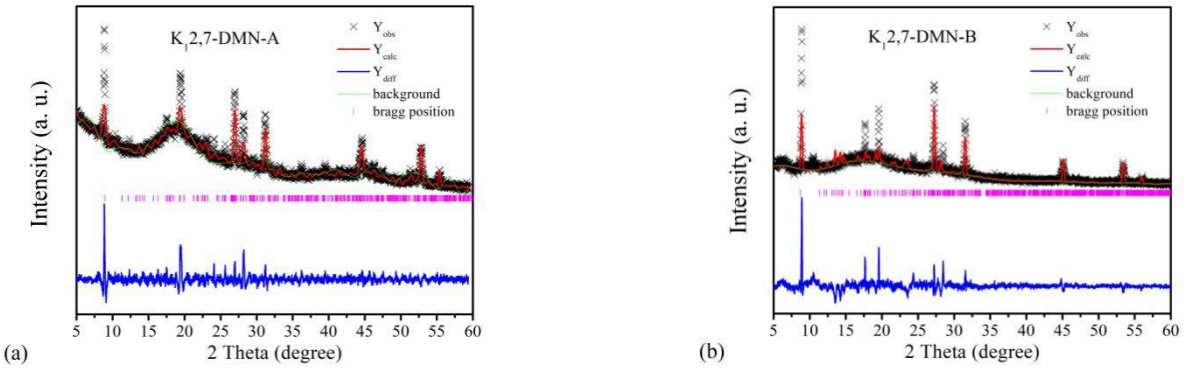


Figure S2. Comparison of the experimental XRD of the samples and the data of the refined theoretical structures. (**a**) K1 2,7-DMN-A sample. (**b**) K1 2,7-DMN-B sample.

Cif data of 2,7-DMN

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_symmetry_Int_Tables_number 1

_symmetry_cell_setting triclinic

loop_

_symmetry_equiv_pos_as_xyz

x,y,z

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_cell_length_b 7.8190

_cell_length_c 19.7870

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loop_

_atom_site_label

_atom_site_type_symbol

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_atom_site_adp_type

_atom_site_occupancy

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C3	C	0.16150	0.76098	0.08313	0.01267	Uiso	1.00
C4	C	0.91336	0.23902	0.82590	0.01267	Uiso	1.00
C5	C	0.01624	0.28586	0.40658	0.01267	Uiso	1.00
C6	C	1.05862	0.71414	0.50244	0.01267	Uiso	1.00
C7	C	1.05862	0.78586	0.04793	0.01267	Uiso	1.00
C8	C	0.01624	0.21414	0.86110	0.01267	Uiso	1.00
C9	C	0.16537	0.37412	0.37017	0.01267	Uiso	1.00

C10	C	0.90949	0.62588	0.53886	0.01267	Uiso	1.00
C11	C	0.90949	0.87412	0.08434	0.01267	Uiso	1.00
C12	C	0.16537	0.12588	0.82468	0.01267	Uiso	1.00
C13	C	0.12939	0.42727	0.30440	0.01267	Uiso	1.00
C14	C	0.94548	0.57273	0.60463	0.01267	Uiso	1.00
C15	C	0.94548	0.92727	0.15011	0.01267	Uiso	1.00
C16	C	0.12939	0.07273	0.75892	0.01267	Uiso	1.00
C17	C	0.97748	0.44384	0.20129	0.01267	Uiso	1.00
C18	C	0.09738	0.55616	0.70774	0.01267	Uiso	1.00
C19	C	0.09738	0.94384	0.25323	0.01267	Uiso	1.00
C20	C	0.97748	0.05616	0.65581	0.01267	Uiso	1.00
C21	C	0.79608	0.40643	0.16912	0.01267	Uiso	1.00
C22	C	0.27878	0.59357	0.73991	0.01267	Uiso	1.00
C23	C	0.27878	0.90643	0.28540	0.01267	Uiso	1.00
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C25	C	0.64191	0.32028	0.20282	0.01267	Uiso	1.00
C26	C	0.43295	0.67972	0.70621	0.01267	Uiso	1.00
C27	C	0.43295	0.82028	0.25170	0.01267	Uiso	1.00
C28	C	0.64191	0.17972	0.65734	0.01267	Uiso	1.00
C29	C	0.67579	0.27422	0.26988	0.01267	Uiso	1.00
C30	C	0.39907	0.72578	0.63915	0.01267	Uiso	1.00
C31	C	0.39907	0.77422	0.18464	0.01267	Uiso	1.00
C32	C	0.67579	0.22578	0.72439	0.01267	Uiso	1.00
C33	C	0.86221	0.30842	0.30462	0.01267	Uiso	1.00
C34	C	0.21265	0.69158	0.60442	0.01267	Uiso	1.00
C35	C	0.21265	0.80842	0.14991	0.01267	Uiso	1.00
C36	C	0.86221	0.19158	0.75913	0.01267	Uiso	1.00
C37	C	1.01781	0.39556	0.26960	0.01267	Uiso	1.00
C38	C	0.05705	0.60444	0.63944	0.01267	Uiso	1.00

C39	C	0.05705	0.89556	0.18492	0.01267	Uiso	1.00
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H48	H	0.76467	0.59973	0.51283	0.01267	Uiso	1.00
H49	H	0.76467	0.90027	0.05832	0.01267	Uiso	1.00
H50	H	0.31019	0.09973	0.85072	0.01267	Uiso	1.00
H51	H	0.24554	0.49545	0.27815	0.01267	Uiso	1.00
H52	H	0.82932	0.50456	0.63088	0.01267	Uiso	1.00
H53	H	0.82932	0.99545	0.17636	0.01267	Uiso	1.00
H54	H	0.24554	0.00456	0.73266	0.01267	Uiso	1.00
H55	H	0.01832	0.51101	0.17441	0.01267	Uiso	1.00
H56	H	1.05654	0.48899	0.73462	0.01267	Uiso	1.00
H57	H	1.05654	0.01101	0.28010	0.01267	Uiso	1.00
H58	H	0.01832	-0.01101	0.62892	0.01267	Uiso	1.00
H59	H	0.76976	0.44360	0.11629	0.01267	Uiso	1.00
H60	H	0.30510	0.55640	0.79274	0.01267	Uiso	1.00
H61	H	0.30510	0.94360	0.33823	0.01267	Uiso	1.00
H62	H	0.76976	0.05640	0.57080	0.01267	Uiso	1.00
H63	H	0.55831	0.20907	0.29674	0.01267	Uiso	1.00
H64	H	0.51655	0.79093	0.61229	0.01267	Uiso	1.00
H65	H	0.51655	0.70907	0.15777	0.01267	Uiso	1.00
H66	H	0.55831	0.29093	0.75126	0.01267	Uiso	1.00
H67	H	0.14549	0.10501	0.47813	0.01267	Uiso	1.00

H68	H	0.92938	0.89500	0.43091	0.01267	Uiso	1.00
H69	H	1.00049	0.20725	0.50539	0.01267	Uiso	1.00
H70	H	0.07438	0.79275	0.40363	0.01267	Uiso	1.00
H71	H	0.15576	0.32162	0.50521	0.01267	Uiso	1.00
H72	H	0.91910	0.67839	0.40382	0.01267	Uiso	1.00
H73	H	0.47437	0.19091	0.12277	0.01267	Uiso	1.00
H74	H	0.60050	0.80909	0.78627	0.01267	Uiso	1.00
H75	H	0.60050	0.69091	0.33175	0.01267	Uiso	1.00
H76	H	0.47437	0.30909	0.57728	0.01267	Uiso	1.00
H77	H	0.38244	0.39660	0.14167	0.01267	Uiso	1.00
H78	H	0.69242	0.60340	0.76737	0.01267	Uiso	1.00
H79	H	0.69242	0.89660	0.31286	0.01267	Uiso	1.00
H80	H	0.38244	0.10340	0.59618	0.01267	Uiso	1.00
H81	H	0.33864	0.22198	0.19706	0.01267	Uiso	1.00
H82	H	0.73622	0.77802	0.71197	0.01267	Uiso	1.00
H83	H	0.73622	0.72198	0.25745	0.01267	Uiso	1.00
H84	H	0.33864	0.27802	0.65158	0.01267	Uiso	1.00
C85	C	-0.00922	0.77035	-0.02579	0.00000	Uiso	1.00
C86	C	1.07548	0.24675	0.91680	0.00000	Uiso	1.00
H87	H	0.80641	0.32109	0.85545	0.00000	Uiso	1.00
H88	H	0.80641	0.17891	0.40094	0.00000	Uiso	1.00
H89	H	0.26845	0.67891	0.05357	0.00000	Uiso	1.00
H90	H	0.03983	0.63840	-0.04317	0.00000	Uiso	1.00
H91	H	0.07925	0.87271	-0.05268	0.00000	Uiso	1.00
H92	H	-0.17602	0.78795	-0.03851	0.00000	Uiso	1.00
H93	H	1.17871	0.36265	0.92140	0.00000	Uiso	1.00
H94	H	1.14957	0.13306	0.94389	0.00000	Uiso	1.00
H95	H	0.92746	0.27713	0.94081	0.00000	Uiso	1.00
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K97 K 0.42254 0.45740 0.84620 0.00000 Uiso 1.00

loop_

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C1 C5 0.977 1_655 D

C2 C34 1.401 . D

C2 C6 0.977 1_455 D

C3 C35 1.401 . S

C3 H89 1.140 . S

C3 C7 0.977 1_455 D

C4 C36 1.401 . S

C4 H87 1.140 . S

C4 C8 0.977 1_655 D

C5 C9 1.431 . S

C5 C41 1.501 . S

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C6 C2 0.977 1_655 D

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C7 C85 1.514 1_655 S

C8 C12 1.431 . S

C8 C4 0.977 1_455 D

C8	C86	1.183	1_455	S
C9	C13	1.378	.	D
C9	H47	1.095	.	S
C10	C14	1.377	.	D
C10	H48	1.096	.	S
C11	C15	1.378	.	D
C11	H49	1.095	.	S
C12	C16	1.377	.	D
C12	H50	1.096	.	S
C13	H51	1.091	.	S
C13	C37	1.023	1_455	S
C14	H52	1.091	.	S
C14	C38	1.023	1_655	S
C15	H53	1.091	.	S
C15	C39	1.023	1_655	S
C16	H54	1.091	.	S
C16	C40	1.024	1_455	S
C17	C21	1.376	.	S
C17	C37	1.418	.	D
C17	H55	0.803	1_655	S
C18	C22	1.376	.	S
C18	C38	1.418	.	D
C18	H56	0.803	1_455	S
C19	C23	1.376	.	S
C19	C39	1.418	.	D
C19	H57	0.803	1_465	S
C20	C24	1.376	.	S
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C20	H58	0.803	1_655	S

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C21	H59	1.092	.	S
C22	C26	1.420	.	D
C22	H60	1.092	.	S
C23	C27	1.420	.	D
C23	H61	1.092	.	S
C24	C28	1.420	.	D
C24	H62	1.092	.	S
C25	C29	1.384	.	S
C25	C43	1.502	.	S
C26	C30	1.384	.	S
C26	C44	1.502	.	S
C27	C31	1.384	.	S
C27	C45	1.502	.	S
C28	C32	1.384	.	S
C28	C46	1.502	.	S
C29	C33	1.422	.	D
C29	H63	1.092	.	S
C30	C34	1.422	.	S
C30	H64	1.092	.	S
C31	C35	1.422	.	D
C31	H65	1.092	.	S
C32	C36	1.422	.	D
C32	H66	1.092	.	S
C33	C37	1.444	.	S
C34	C38	1.444	.	S
C35	C39	1.444	.	S
C36	C40	1.444	.	S
C37	C13	1.023	1_655	S

C38	C14	1.023	1_455	S
C39	C15	1.023	1_455	S
C40	C16	1.024	1_655	S
C41	H67	1.103	.	S
C41	H71	1.099	.	S
C41	H69	0.716	1_455	S
C42	H68	1.103	.	S
C42	H72	1.099	.	S
C42	H70	0.716	1_655	S
C43	H73	1.101	.	S
C43	H77	1.100	.	S
C43	H81	1.096	.	S
C44	H74	1.101	.	S
C44	H78	1.100	.	S
C44	H82	1.096	.	S
C45	H75	1.101	.	S
C45	H79	1.100	.	S
C45	H83	1.096	.	S
C46	H76	1.101	.	S
C46	H80	1.100	.	S
C46	H84	1.096	.	S
H55	C17	0.803	1_455	S
H56	C18	0.803	1_655	S
H57	C19	0.803	1_645	S
H58	C20	0.803	1_455	S
H69	C41	0.716	1_655	S
H70	C42	0.716	1_455	S
C85	H90	1.140	.	S
C85	H91	1.140	.	S

C85	H92	1.140	.	S
C85	C7	1.514	1_455	S
C86	H93	1.140	.	S
C86	H94	1.140	.	S
C86	H95	1.140	.	S
C86	C8	1.183	1_655	S

Supplementary Materials: The following are available online at www.mdpi.com/xxx/s1, Figure S1: The relationship between molar magnetic susceptibility (χ_M) and temperature of pristine 2,7-DMN sample, Figure S2: Comparison of the experimental XRD of the samples and the data of the refined theoretical structures, Cif data of 2,7-DMN.

Author Contributions: Conceptualization, X.-L.W. and Z.-B.H.; data curation, Z.-B.H.; formal analysis, Y.G.; investigation, X.-J.C.; methodology, R.-S.W. and M.-A.F.; resources, H.L.; software, H.Y.; validation, H.-Q.Y.; writing—original draft, X.-L.W.; review and editing all authors. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: Data are contained within the article.

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Conflicts of Interest: The authors declare no conflict of interest.



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