Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Superconductivity in an organometallic compound

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1. The atomic positions of C and Bi in *o*-TTB

Table S1 The atomic positions of C and Bi in *o*-TTB.

Atom	Wyck.	x/a	y/b	z/c	U [Å²]
C1	1a	0.32481	0.22148	0.96460	0.0127
C2	1a	0.67519	0.77852	0.03540	0.0127
C3	1a	0.67519	0.22148	0.53540	0.0127
C4	1a	0.32481	0.77852	0.46460	0.0127
C5	1a	0.82481	0.72148	0.96460	0.0127
C6	1a	0.17519	0.27852	0.03540	0.0127
C7	1a	0.17519	0.72148	0.53540	0.0127
C8	1a	0.82481	0.27852	0.46460	0.0127
C9	1a	0.47611	0.88163	0.14048	0.0127
C10	1a	0.52389	0.11837	0.85952	0.0127
C11	1a	0.52389	0.88163	0.35951	0.0127
C12	1a	0.47611	0.11837	0.64048	0.0127
C13	1a	0.97611	0.38163	0.14048	0.0127
C14	1a	0.02389	0.61837	0.85952	0.0127
C15	1a	0.02389	0.38163	0.35951	0.0127
C16	1a	0.97611	0.61837	0.64048	0.0127
C17	1a	0.49575	0.95862	0.10200	0.0127
C18	1a	0.50425	0.04138	0.89800	0.0127
C19	1a	0.50425	0.95862	0.39800	0.0127
C20	1a	0.49575	0.04138	0.60200	0.0127
C21	1a	0.99575	0.45862	0.10200	0.0127
C22	1a	0.00425	0.54138	0.89800	0.0127
C23	1a	0.00425	0.45862	0.39800	0.0127
C24	1a	0.99575	0.54138	0.60200	0.0127
C25	1a	0.47959	0.15589	0.04809	0.0127
C26	1a	0.52041	0.84411	0.95191	0.0127
C27	1a	0.52041	0.15589	0.45191	0.0127
C28	1a	0.47959	0.84411	0.54809	0.0127
C29	1a	0.97959	0.65589	0.04809	0.0127
C30	1a	0.02041	0.34411	0.95191	0.0127
C31	1a	0.02041	0.65589	0.45191	0.0127
C32	1a	0.97959	0.34411	0.54809	0.0127
C33	1a	0.44453	0.28982	0.03326	0.0127
C34	1a	0.55547	0.71018	0.96674	0.0127
C35	1a	0.55547	0.28982	0.46674	0.0127
C36	1a	0.44453	0.71018	0.53326	0.0127
C37	1a	0.94453	0.78982	0.03326	0.0127
C38	1a	0.05547	0.21018	0.96674	0.0127
C39	1a	0.05547	0.78982	0.46674	0.0127

C40	1a	0.94453	0.21018	0.53326	0.0127
C41	1a	0.42670	0.48608	0.96980	0.0127
C42	1a	0.57330	0.51392	0.03020	0.0127
C43	1a	0.57330	0.48608	0.53020	0.0127
C44	1a	0.42670	0.51392	0.46980	0.0127
C45	1a	0.92670	0.98608	0.96980	0.0127
C46	1a	0.07330	0.01392	0.03020	0.0127
C47	1a	0.07330	0.98608	0.53020	0.0127
C48	1a	0.92670	0.01392	0.46980	0.0127
C49	1a	0.37112	0.20502	0.15653	0.0127
C50	1a	0.62888	0.79498	0.84346	0.0127
C51	1a	0.62888	0.20502	0.34346	0.0127
C52	1a	0.37112	0.79498	0.65653	0.0127
C53	1a	0.87112	0.70502	0.15653	0.0127
C54	1a	0.12888	0.29498	0.84346	0.0127
C55	1a	0.12888	0.70502	0.34346	0.0127
C56	1a	0.87112	0.29498	0.65653	0.0127
C57	1a	0.39707	0.25083	0.23658	0.0127
C58	1a	0.60293	0.74917	0.76342	0.0127
C59	1a	0.60293	0.25083	0.26342	0.0127
C60	1a	0.39707	0.74917	0.73658	0.0127
C61	1a	0.89707	0.75083	0.23658	0.0127
C62	1a	0.10293	0.24917	0.76342	0.0127
C63	1a	0.10293	0.75083	0.26342	0.0127
C64	1a	0.89707	0.24917	0.73658	0.0127
C65	1a	0.39319	0.08887	0.28814	0.0127
C66	1a	0.60681	0.91113	0.71186	0.0127
C67	1a	0.60681	0.08887	0.21186	0.0127
C68	1a	0.39319	0.91113	0.78814	0.0127
C69	1a	0.89319	0.58887	0.28814	0.0127
C70	1a	0.10681	0.41113	0.71186	0.0127
C71	1a	0.10681	0.58887	0.21186	0.0127
C72	1a	0.89319	0.41113	0.78814	0.0127
C73	1a	0.36426	0.89379	0.26193	0.0127
C74	1a	0.63574	0.10621	0.73806	0.0127
C75	1a	0.63574	0.89379	0.23806	0.0127
C76	1a	0.36426	0.10621	0.76193	0.0127
C77	1a	0.86426	0.39379	0.26193	0.0127
C78	1a	0.13574	0.60621	0.73806	0.0127
C79	1a	0.13574	0.39379	0.23806	0.0127
C80	1a	0.86426	0.60621	0.76193	0.0127
C81	1a	0.34005	0.84373	0.18318	0.0127
C82	1a	0.65995	0.15627	0.81682	0.0127

C83	1a	0.65995	0.84373	0.31682	0.0127
C84	1a	0.34005	0.15627	0.68318	0.0127
C85	1a	0.84005	0.34373	0.18318	0.0127
C86	1a	0.15995	0.65627	0.81682	0.0127
C87	1a	0.15995	0.34373	0.31682	0.0127
C88	1a	0.84005	0.65627	0.68318	0.0127
C89	1a	0.28359	0.29754	0.92975	0.0127
C90	1a	0.71641	0.70246	0.07025	0.0127
C91	1a	0.71641	0.29754	0.57025	0.0127
C92	1a	0.28359	0.70246	0.42975	0.0127
C93	1a	0.78359	0.79754	0.92975	0.0127
C94	1a	0.21641	0.20246	0.07025	0.0127
C95	1a	0.21641	0.79754	0.57025	0.0127
C96	1a	0.78359	0.20246	0.42975	0.0127
C97	1a	0.34408	0.00052	0.13132	0.0127
C98	1a	0.65592	-0.00052	0.86868	0.0127
C99	1a	0.65592	0.00052	0.36868	0.0127
C100	1a	0.34408	-0.00052	0.63132	0.0127
C101	1a	0.84408	0.50052	0.13132	0.0127
C102	1a	0.15592	0.49948	0.86868	0.0127
C103	1a	0.15592	0.50052	0.36868	0.0127
C104	1a	0.84408	0.49948	0.63132	0.0127
C105	1a	0.43018	0.44808	0.26849	0.0127
C106	1a	0.56982	0.55192	0.73151	0.0127
C107	1a	0.56982	0.44808	0.23151	0.0127
C108	1a	0.43018	0.55192	0.76849	0.0127
C109	1a	0.93018	0.94808	0.26849	0.0127
C110	1a	0.06982	0.05192	0.73151	0.0127
C111	1a	0.06982	0.94808	0.23151	0.0127
C112	1a	0.93018	0.05192	0.76849	0.0127
C113	1a	0.25442	0.16023	0.86452	0.0127
C114	1a	0.74558	0.83977	0.13548	0.0127
C115	1a	0.74558	0.16023	0.63548	0.0127
C116	1a	0.25442	0.83977	0.36452	0.0127
C117	1a	0.75442	0.66023	0.86452	0.0127
C118	1a	0.24558	0.33977	0.13548	0.0127
C119	1a	0.24558	0.66023	0.63548	0.0127
C120	1a	0.75442	0.33977	0.36452	0.0127
C121	1a	0.26560	0.95797	0.83446	0.0127
C122	1a	0.73440	0.04203	0.16553	0.0127
C123	1a	0.73440	0.95797	0.66553	0.0127
C124	1a	0.26560	0.04203	0.33447	0.0127
C125	1a	0.76560	0.45797	0.83446	0.0127

C126	1a	0.23440	0.54203	0.16553	0.0127
C127	1a	0.23440	0.45797	0.66553	0.0127
C128	1a	0.76560	0.54203	0.33446	0.0127
C129	1a	0.30627	0.88213	0.87022	0.0127
C130	1a	0.69373	0.11787	0.12978	0.0127
C131	1a	0.69373	0.88213	0.62978	0.0127
C132	1a	0.30627	0.11787	0.37022	0.0127
C133	1a	0.80627	0.38213	0.87022	0.0127
C134	1a	0.19373	0.61787	0.12978	0.0127
C135	1a	0.19373	0.38213	0.62978	0.0127
C136	1a	0.80627	0.61787	0.37022	0.0127
C137	1a	0.33565	0.01490	0.93554	0.0127
C138	1a	0.66435	-0.01491	0.06446	0.0127
C139	1a	0.66435	0.01490	0.56446	0.0127
C140	1a	0.33566	-0.01491	0.43554	0.0127
C141	1a	0.83565	0.51490	0.93554	0.0127
C142	1a	0.16434	0.48510	0.06446	0.0127
C143	1a	0.16434	0.51490	0.56446	0.0127
C144	1a	0.83565	0.48510	0.43554	0.0127
C145	1a	0.27009	0.49959	0.96460	0.0127
C146	1a	0.72991	0.50041	0.03540	0.0127
C147	1a	0.72991	0.49959	0.53540	0.0127
C148	1a	0.27009	0.50041	0.46460	0.0127
C149	1a	0.77009	0.99959	0.96460	0.0127
C150	1a	0.22991	0.00041	0.03540	0.0127
C151	1a	0.22991	0.99959	0.53540	0.0127
C152	1a	0.77009	0.00041	0.46460	0.0127
C153	1a	0.42583	0.21763	0.07528	0.0127
C154	1a	0.57417	0.78237	0.92472	0.0127
C155	1a	0.57417	0.21763	0.42472	0.0127
C156	1a	0.42583	0.78237	0.57528	0.0127
C157	1a	0.92583	0.71763	0.07528	0.0127
C158	1a	0.07417	0.28238	0.92472	0.0127
C159	1a	0.07417	0.71763	0.42472	0.0127
C160	1a	0.92583	0.28238	0.57528	0.0127
C161	1a	0.44119	0.01362	0.12673	0.0127
C162	1a	0.55881	-0.01362	0.87327	0.0127
C163	1a	0.55881	0.01362	0.37327	0.0127
C164	1a	0.44119	-0.01362	0.62673	0.0127
C165	1a	0.94120	0.51362	0.12673	0.0127
C166	1a	0.05880	0.48638	0.87327	0.0127
C167	1a	0.05880	0.51362	0.37327	0.0127
C168	1a	0.94120	0.48638	0.62673	0.0127

Bi1	1a	0.37348	0.45428	0.06605	0.0127
Bi2	1a	0.62652	0.54572	0.93395	0.0127
Bi3	1a	0.62652	0.45428	0.43395	0.0127
Bi4	1a	0.37348	0.54572	0.56605	0.0127
Bi5	1a	0.87348	0.95428	0.06605	0.0127
Bi6	1a	0.12652	0.04572	0.93395	0.0127
Bi7	1a	0.12652	0.95428	0.43395	0.0127
Bi8	1a	0.87348	0.04572	0.56605	0.0127

2. The atomic positions of C, H, Bi, and K in K_3*o*-TTB

Table S2 The optimized atomic coordinates of C, H, Bi, and K in K_3*o*-TTB.

Atom	Wyck.	x/a	y/b	z/c	U [Å²]
Bi1	1a	0.49625	0.49307	0.99311	0.0127
Bi2	1a	0.49625	0.99161	0.50268	0.0127
Bi3	1a	0.00000	0.49437	0.49250	0.0127
K4	1a	0.00001	0.19529	0.20402	0.0127
K5	1a	0.00001	0.79655	0.80298	0.0127
K7	1a	0.19700	0.19573	0.99165	0.0127
K8	1a	0.19700	0.99241	0.20165	0.0127
K9	1a	0.80052	0.99080	0.80878	0.0127
K10	1a	0.74814	0.24646	0.50177	0.0127
K12	1a	0.55590	0.74378	0.26953	0.0127
K13	1a	0.22780	0.74461	0.50491	0.0127
K14	1a	0.74814	0.49489	0.25095	0.0127
C16	1a	0.20306	0.37803	0.89211	0.0127
C17	1a	0.34030	0.34292	0.94219	0.0127
C18	1a	0.38378	0.20916	0.96676	0.0127
C19	1a	0.29495	0.10370	0.94208	0.0127
C20	1a	0.15267	0.12066	0.88642	0.0127
C21	1a	0.11245	0.26251	0.86412	0.0127
C22	1a	0.18385	0.79060	0.86277	0.0127
C23	1a	0.18252	0.64137	0.86672	0.0127
C24	1a	0.12802	0.56150	0.76202	0.0127
C25	1a	0.07347	0.62448	0.64812	0.0127
C26	1a	0.07060	0.77558	0.62496	0.0127
C27	1a	0.12755	0.85372	0.73821	0.0127
C28	1a	0.48936	0.15424	0.76370	0.0127
C29	1a	0.55108	0.24230	0.86736	0.0127
C30	1a	0.68148	0.29885	0.85523	0.0127
C31	1a	0.75677	0.27258	0.74020	0.0127
C32	1a	0.70783	0.18870	0.62219	0.0127
C33	1a	0.57165	0.13119	0.64123	0.0127
C34	1a	0.64006	0.65887	0.95866	0.0127

C35	1a	0.75908	0.60382	0.88733	0.0127
C36	1a	0.87000	0.68337	0.84636	0.0127
C37	1a	0.86973	0.82039	0.87465	0.0127
C38	1a	0.75884	0.89268	0.95071	0.0127
C39	1a	0.64511	0.80476	0.98966	0.0127
C40	1a	0.09497	0.31777	0.37560	0.0127
C41	1a	0.17219	0.18964	0.37569	0.0127
C42	1a	0.26335	0.15358	0.27260	0.0127
C43	1a	0.28384	0.24219	0.16535	0.0127
C44	1a	0.21718	0.37933	0.15127	0.0127
C45	1a	0.12206	0.41081	0.26110	0.0127
C46	1a	0.65077	0.04323	0.32801	0.0127
C47	1a	0.79981	0.04230	0.34464	0.0127
C48	1a	0.89025	0.07037	0.23818	0.0127
C49	1a	0.83851	0.10191	0.11086	0.0127
C50	1a	0.68911	0.11210	0.07678	0.0127
C51	1a	0.59966	0.08034	0.19148	0.0127
C52	1a	0.67009	0.55440	0.55355	0.0127
C53	1a	0.58751	0.50331	0.66715	0.0127
C54	1a	0.48879	0.58169	0.73327	0.0127
C55	1a	0.46573	0.71335	0.69010	0.0127
C56	1a	0.53737	0.78045	0.57267	0.0127
C57	1a	0.64022	0.69425	0.50852	0.0127
C58	1a	0.83433	0.71856	0.32440	0.0127
C59	1a	0.96444	0.64415	0.32549	0.0127
C60	1a	0.07170	0.66184	0.22680	0.0127
C61	1a	0.04882	0.75256	0.12142	0.0127
C62	1a	0.91633	0.83871	0.10508	0.0127
C63	1a	0.81521	0.81655	0.21205	0.0127
C64	1a	0.35910	0.79776	0.32917	0.0127
C65	1a	0.33175	0.70813	0.44608	0.0127
C66	1a	0.34372	0.56634	0.44112	0.0127
C67	1a	0.38430	0.50613	0.32161	0.0127
C68	1a	0.42087	0.58231	0.19376	0.0127
C69	1a	0.40509	0.72984	0.20454	0.0127
H70	1a	0.17202	0.49213	0.87691	0.0127
C71	1a	0.49435	0.18816	0.01470	0.0127
H72	1a	0.32875	0.98450	0.96470	0.0127
H73	1a	0.08534	0.02494	0.86504	0.0127
H74	1a	0.00206	0.28175	0.82184	0.0127
C75	1a	1.01798	0.81858	0.52157	0.0127
C76	1a	0.38613	0.06689	0.76494	0.0127
C77	1a	0.76454	0.48783	0.86196	0.0127

H78	1a	0.96134	0.63331	0.78887	0.0127
H79	1a	0.96032	0.88881	0.83868	0.0127
H80	1a	0.76873	0.01594	0.97349	0.0127
H81	1a	0.55521	0.85605	0.05528	0.0127
H82	1a	0.35755	0.21239	0.07697	0.0127
C83	1a	0.48206	0.08561	0.17037	0.0127
C84	1a	0.38559	0.78107	0.74606	0.0127
C85	1a	0.17452	0.60125	0.23300	0.0127
C86	1a	0.39213	0.38762	0.31497	0.0127
H87	1a	0.84865	0.01718	0.45112	0.0127
H88	1a	0.01563	0.06687	0.25626	0.0127
H89	1a	0.91270	0.12294	0.02017	0.0127
H90	1a	0.65416	0.14314	0.95954	0.0127
H91	1a	0.56891	0.18053	0.98122	0.0127
H92	1a	0.72518	0.36744	0.94217	0.0127
H93	1a	0.86699	0.31681	0.72973	0.0127
H94	1a	0.77729	0.17461	0.52669	0.0127
H95	1a	0.22792	0.85142	0.95521	0.0127
H96	1a	0.22862	0.58317	0.96084	0.0127
H97	1a	0.12921	0.44287	0.77197	0.0127
H98	1a	0.12683	0.97217	0.72609	0.0127
C99	1a	0.15908	0.11151	0.46513	0.0127
H100	1a	0.32097	0.04930	0.27825	0.0127
H101	1a	0.24337	0.44973	0.05845	0.0127
H102	1a	0.06630	0.51605	0.25468	0.0127
H103	1a	0.34389	0.91532	0.33906	0.0127
H104	1a	0.29804	0.75453	0.55017	0.0127
H105	1a	0.31936	0.50056	0.53777	0.0127
H106	1a	0.43115	0.79426	0.10745	0.0127
H107	1a	0.75335	0.48472	0.50493	0.0127
H108	1a	0.60257	0.39176	0.70683	0.0127
H109	1a	0.40856	0.54972	0.78719	0.0127
H110	1a	0.72001	0.77418	0.50520	0.0127
H111	1a	0.75381	0.69797	0.40962	0.0127
H112	1a	0.13101	0.76694	0.03655	0.0127
H113	1a	0.89451	0.91747	0.01760	0.0127
H114	1a	0.71517	0.88156	0.20507	0.0127
H115	1a	0.57300	0.20880	-0.07224	0.0000
H116	1a	0.50322	0.07475	0.05062	0.0000
H117	1a	0.51740	0.25992	0.10669	0.0000
H118	1a	0.98215	0.72790	0.45359	0.0000
H119	1a	1.10249	0.88009	0.46449	0.0000
H120	1a	0.92504	0.88994	0.54355	0.0000

H121	1a	0.71295	0.46862	0.75587	0.0000
H122	1a	0.71119	0.45884	0.94438	0.0000
H123	1a	0.87880	0.45316	0.85855	0.0000
H124	1a	0.43350	-0.02098	0.19156	0.0000
H125	1a	0.46254	0.11668	0.05648	0.0000
H126	1a	0.43253	0.16638	0.24195	0.0000
H127	1a	0.31302	0.71178	0.81028	0.0000
H128	1a	0.32137	0.84240	0.66545	0.0000
H129	1a	0.44222	0.85676	0.81842	0.0000
H130	1a	0.39722	0.32325	0.22804	0.0000
H131	1a	0.33303	0.33835	0.40599	0.0000
H132	1a	0.50691	0.35473	0.32042	0.0000
H133	1a	0.21068	0.00834	0.43608	0.0000
H134	1a	0.04278	0.09389	0.48484	0.0000
H135	1a	0.21066	0.15415	0.56391	0.0000
H136	1a	0.25042	0.64478	0.14591	0.0000
H137	1a	0.13644	0.53301	0.18773	0.0000
H138	1a	0.24892	0.65506	0.30918	0.0000
H139	1a	0.42361	-0.03752	0.80943	0.0000
H140	1a	0.31765	0.03673	0.66812	0.0000
H141	1a	0.29142	0.02718	0.82772	0.0000

3. Magnetic susceptibility measurement for sample B

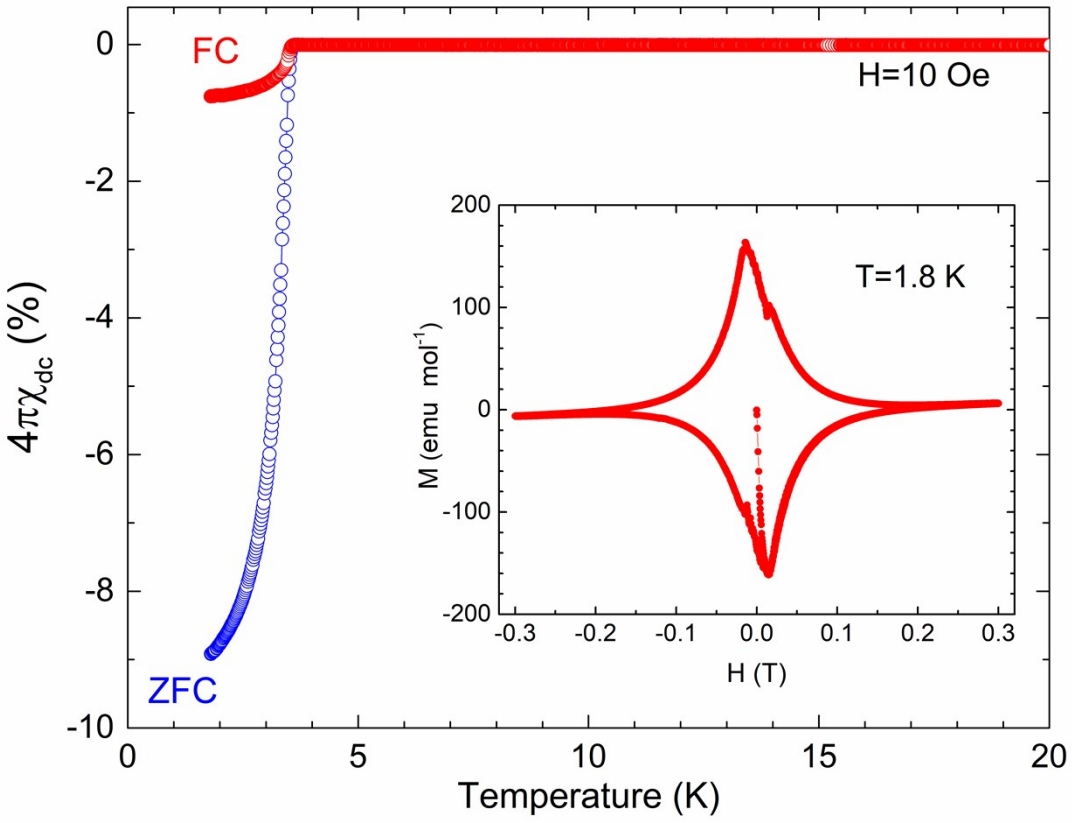

Fig. S1 The temperature dependence of the *dc* magnetic susceptibility for sample B with ZFC and FC runs in the applied magnetic field of 10 Oe. The inset shows the magnetization loop of sample B at 1.8 K.