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

Supporting Information

Superconductivity and phase stability of potassium-doped biphenyl

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Table S1 Optimized atomic coordinates for pristine biphenyl ($C_{12}H_{10}$).

atom	x	y	z	atom	x	y	z
C1	0.92402	-0.00111	0.95934	C13	0.63479	0.99152	0.80262
C2	0.07598	0.00111	0.04066	C14	0.36521	0.00848	0.19738
C3	0.07598	0.49889	0.54066	C15	0.36521	0.49152	0.69738
C4	0.92402	0.50111	0.45934	C16	0.63479	0.50848	0.30262
C5	0.8278	0.18384	0.82517	C17	0.72851	0.8081	0.93698
C6	0.1722	0.81616	0.17483	C18	0.27149	0.1919	0.06302
C7	0.1722	0.68384	0.67483	C19	0.27149	0.3081	0.56302
C8	0.8278	0.31616	0.32517	C20	0.72851	0.6919	0.43698
C9	0.68559	0.17954	0.74755	C21	0.87041	0.81124	0.0131
C10	0.31441	0.82046	0.25245	C22	0.12959	0.18876	0.9869
C11	0.31441	0.67954	0.75245	C23	0.12959	0.31124	0.4869
C12	0.68559	0.32046	0.24755	C24	0.87041	0.68876	0.5131
H1	0.86212	0.33272	0.77811	H11	0.47548	0.48777	0.75775
H2	0.13788	0.66728	0.22189	H12	0.52452	0.51223	0.24225
H3	0.13788	0.83272	0.72189	H13	0.6923	0.66188	0.98395
H4	0.86212	0.16728	0.27811	H14	0.3077	0.33812	0.01605
H5	0.61485	0.3236	0.64329	H15	0.3077	0.16188	0.51605
H6	0.38515	0.6764	0.35671	H16	0.6923	0.83812	0.48395
H7	0.38515	0.8236	0.85671	H17	0.93875	0.66464	0.11497
H8	0.61485	0.1764	0.14329	H18	0.06125	0.33536	0.88503
H9	0.52452	0.98777	0.74225	H19	0.06125	0.16464	0.38503
H10	0.47548	0.01223	0.25775	H20	0.93875	0.83536	0.61497

Figure S1 Bond lengths in pristine biphenyl.

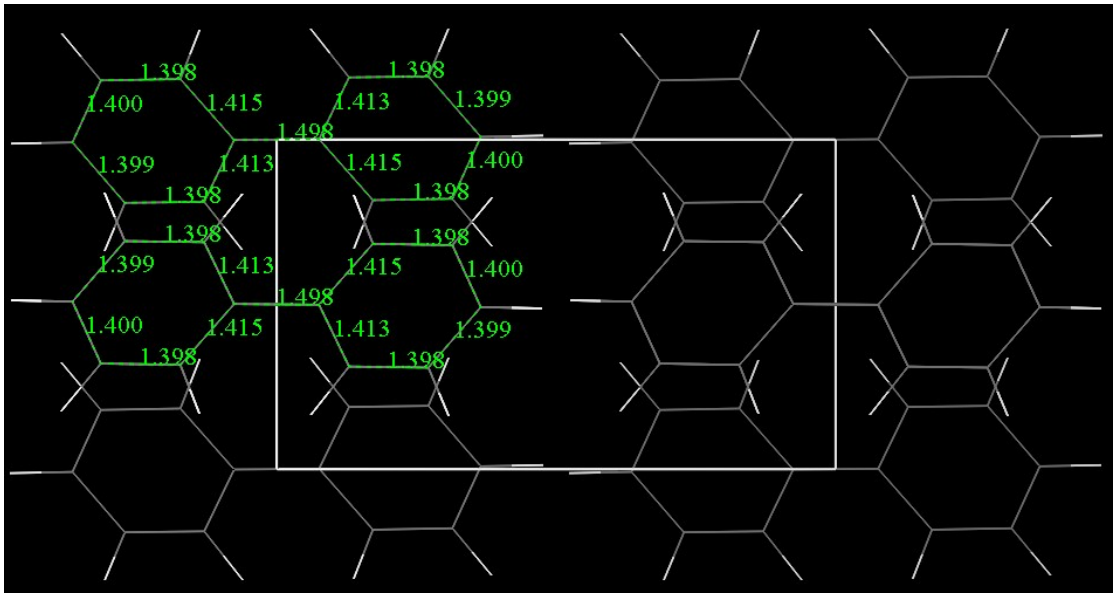

Table S2 Optimized atomic coordinates for $K_1C_{12}H_{10}$.

atom	x	y	z	atom	x	y	z
C1	0.70531	0.74905	0.4265	C13	0.79652	0.75123	0.58164
C2	0.29469	0.24905	0.5735	C14	0.20348	0.25123	0.41836
C3	0.74851	0.88672	0.32695	C15	0.71578	0.65394	0.68727
C4	0.25149	0.38672	0.67305	C16	0.28422	0.15394	0.31273
C5	0.66464	0.88155	0.17723	C17	0.80512	0.6546	0.83625
C6	0.33536	0.38155	0.82277	C18	0.19488	0.1546	0.16375
C7	0.53174	0.74015	0.11573	C19	0.98025	0.75012	0.8903
C8	0.46826	0.24015	0.88427	C20	0.01975	0.25012	0.1097
C9	0.48648	0.60324	0.2103	C21	0.06331	0.84661	0.79005
C10	0.51352	0.10324	0.7897	C22	0.93669	0.34661	0.20995
C11	0.56717	0.60792	0.36109	C23	0.97447	0.84857	0.64075
C12	0.43283	0.10792	0.63891	C24	0.02553	0.34857	0.35925
H1	0.84223	0.0038	0.36914	H11	0.57671	0.58688	0.65195
H2	0.15777	0.5038	0.63086	H12	0.42329	0.08688	0.34805
H3	0.70148	0.9897	0.10789	H13	0.73607	0.58396	0.91189
H4	0.29852	0.4897	0.89211	H14	0.26393	0.08396	0.08811
H5	0.46852	0.73623	-0.00105	H15	0.05134	0.74788	0.0058
H6	0.53148	0.23623	0.00105	H16	0.94866	0.24788	0.9942
H7	0.38918	0.48954	0.16554	H17	0.19975	0.91776	0.82839
H8	0.61082	0.98954	0.83446	H18	0.80025	0.41776	0.17161
H9	0.53101	0.49638	0.42811	H19	0.04642	0.92263	0.56837
H10	0.46899	0.99638	0.57189	H20	0.95358	0.42263	0.43163
K1	0.13946	0.75018	0.31064	K2	0.86054	0.25018	0.68936

Figure S2 Bond lengths in $K_1C_{12}H_{10}$.

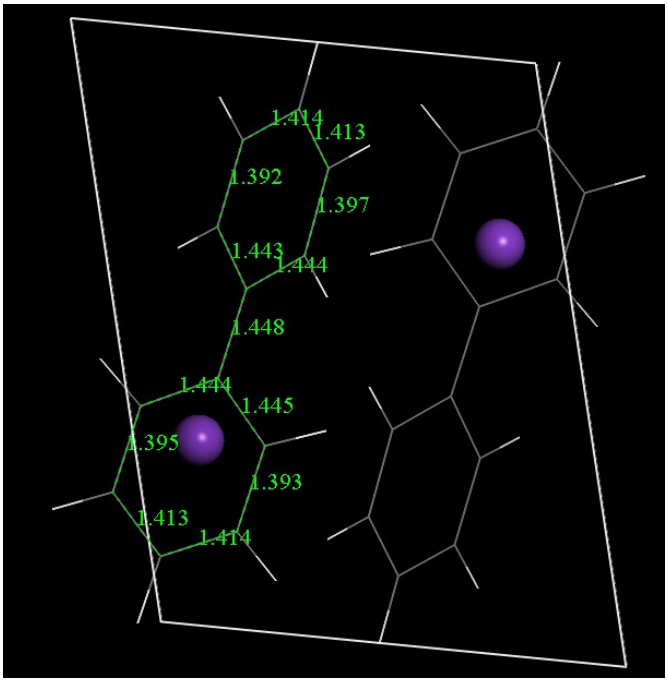

Table S3 Optimized atomic coordinates for $K_{1.5}C_{12}H_{10}$.

atom	x	y	z	atom	x	y	z
C1	0.13453	0.37108	0.23881	C13	0.93842	0.68469	0.81056
C2	0.2132	0.30876	0.39524	C14	0.79312	0.72031	0.61736
C3	0.17129	0.27508	0.17039	C15	0.91282	0.78749	0.88085
C4	0.34684	0.17094	0.49314	C16	0.61949	0.84347	0.49508
C5	0.29504	0.13496	0.26067	C17	0.74111	0.91166	0.76178
C6	0.41275	0.07829	0.44134	C18	0.58171	0.94815	0.55967
C7	0.85094	0.84175	0.24895	C19	0.11041	0.11933	0.71896
C8	0.74858	0.7921	0.08036	C20	0.2686	0.14856	0.9174
C9	0.81053	0.74206	0.31611	C21	0.09393	0.23806	0.62664
C10	0.60527	0.65392	0.97949	C22	0.40674	0.28795	0.01961
C11	0.67481	0.60156	0.22037	C23	0.23438	0.37731	0.72812
C12	0.55695	0.55106	0.04183	C24	0.40424	0.40944	0.93375
H1	0.01149	0.47228	0.15056	H11	0.09819	0.6002	0.91707
H2	0.1554	0.36493	0.43274	H12	0.82261	0.6518	0.56454
H3	0.09595	0.31313	0.04131	H13	0.03641	0.77015	0.03452
H4	0.39052	0.12747	0.60404	H14	0.51588	0.86345	0.35009
H5	0.31232	0.06777	0.19921	H15	0.74397	0.99109	0.82992
H6	0.96751	0.94807	0.33162	H16	0.00042	0.01181	0.63936
H7	0.79228	0.85705	0.03256	H17	0.28067	0.06028	0.98969
H8	0.89026	0.77605	0.44679	H18	0.96691	0.22047	0.47218
H9	0.53942	0.62009	0.85586	H19	0.52335	0.30402	0.16992
H10	0.64926	0.53029	0.27806	H20	0.20365	0.46635	0.64584
K1	0.77335	0.3541	0.62095	K3	0.32008	0.65434	0.49102
K2	0.69265	0.13954	0.00382				

Figure S3 Bond lengths in $K_{1.5}C_{12}H_{10}$.

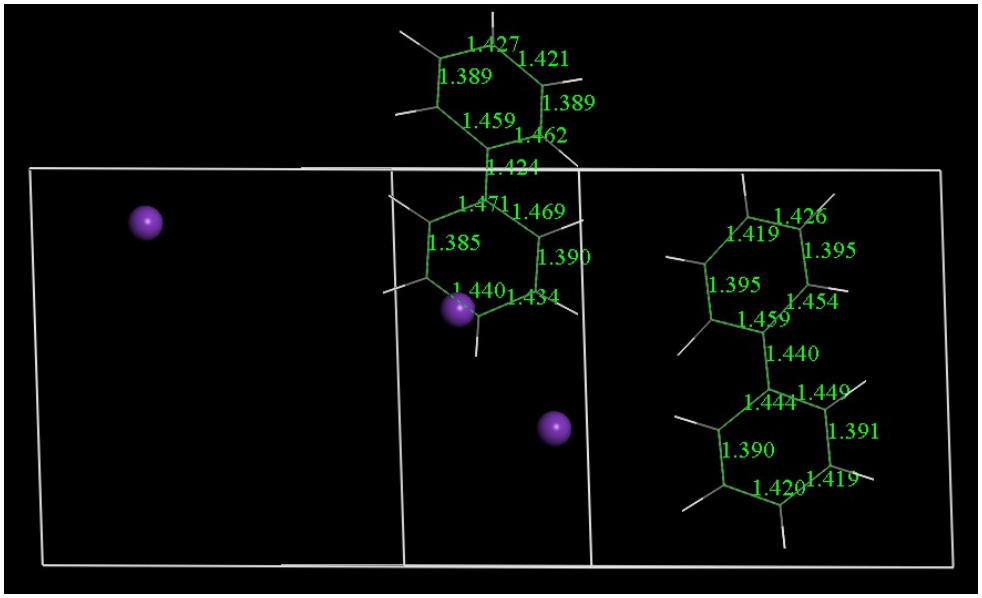

Table S4 Optimized atomic coordinates for $K_2C_{12}H_{10}$.

atom	x	y	z	atom	x	y	z
C1	0.92731	0.00249	0.95086	C13	0.62198	0.00106	0.74588
C2	0.07376	0.00288	0.05003	C14	0.37909	0.00172	0.25521
C3	0.07366	0.50023	0.54975	C15	0.37901	0.50082	0.75493
C4	0.92722	0.49978	0.45059	C16	0.62187	0.49956	0.24582
C5	0.85563	0.00042	0.78241	C17	0.68746	0.00021	0.90846
C6	0.14538	0.00097	0.21844	C18	0.31369	0.0014	0.09265
C7	0.14531	0.50059	0.71822	C19	0.31357	0.50058	0.59235
C8	0.85543	0.49954	0.28214	C20	0.68743	0.49969	0.40839
C9	0.7116	0.00018	0.68798	C21	0.83101	0.00049	0.00603
C10	0.28935	0.00086	0.31295	C22	0.17013	0.00157	0.99499
C11	0.2893	0.50084	0.81271	C23	0.17003	0.5004	0.49472
C12	0.71142	0.49943	0.18781	C24	0.83099	0.49979	0.50588
H1	0.91694	-0.00033	0.73008	H11	0.49097	0.50054	0.83067
H2	0.08402	0.0005	0.27071	H12	0.5099	0.49909	0.17014
H3	0.08397	0.50083	0.77051	H13	0.62228	-0.00101	0.95662
H4	0.9167	0.49908	0.22976	H14	0.37889	0.00082	0.04453
H5	0.66482	-0.00087	0.56514	H15	0.37878	0.50032	0.54423
H6	0.33604	-0.00002	0.43577	H16	0.62232	0.49957	0.45664
H7	0.336	0.50109	0.93554	H17	0.87415	-0.00028	0.12793
H8	0.66457	0.49899	0.06496	H18	0.12707	0.00139	0.87311
H9	0.51001	0.00024	0.67014	H19	0.12693	0.50014	0.37281
H10	0.49105	0.00128	0.33098	H20	0.8742	0.49988	0.6278
K1	0.23609	0.50131	0.1609	K3	0.76587	-0.00023	0.34085
K2	0.76591	0.50015	0.84088	K4	0.23609	0.00094	0.66086

Figure S4 Bond lengths in $K_2C_{12}H_{10}$.

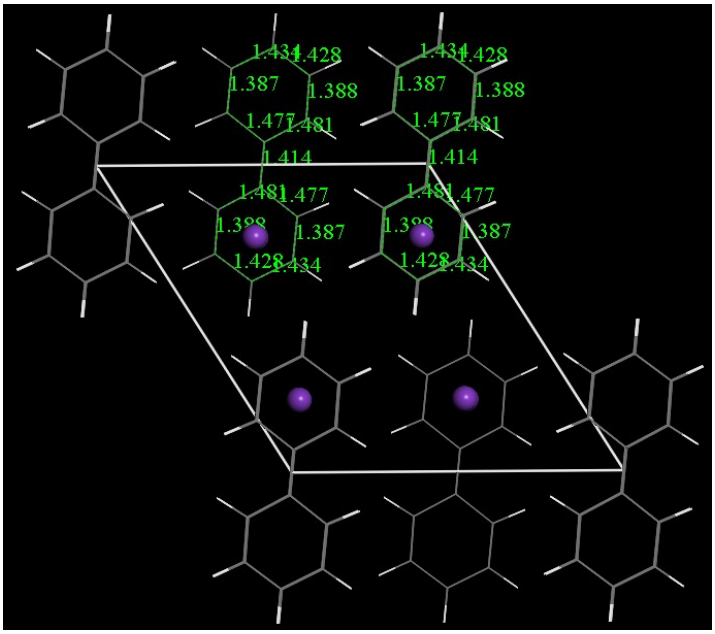

Table S5 Optimized atomic coordinates for $K_3C_{12}H_{10}$.

atom	x	y	z	atom	x	y	z
C1	0.94802	0.00103	0.95507	C13	0.73192	0.9815	0.75799
C2	0.05352	0.99774	0.04558	C14	0.2698	0.01721	0.2421
C3	0.05332	0.49938	0.54617	C15	0.26946	0.47777	0.74308
C4	0.94788	0.49802	0.4554	C16	0.73193	0.52159	0.25789
C5	0.91932	0.10791	0.80478	C17	0.75494	0.88878	0.90676
C6	0.08237	0.89118	0.19594	C18	0.24659	0.10988	0.09328
C7	0.08195	0.6063	0.69626	C19	0.24648	0.38477	0.59449
C8	0.91925	0.39165	0.3051	C20	0.75487	0.61396	0.40667
C9	0.81718	0.09426	0.71273	C21	0.85593	0.89775	0.00134
C10	0.1846	0.90476	0.28774	C22	0.14548	0.10106	0.999
C11	0.18414	0.59171	0.78828	C23	0.14545	0.39461	0.49996
C12	0.81718	0.40717	0.21285	C24	0.85578	0.60313	0.50148
H1	0.97937	0.20221	0.7636	H11	0.34918	0.46754	0.81606
H2	0.02237	0.79687	0.23724	H12	0.65228	0.53214	0.18474
H3	0.02188	0.70188	0.73718	H13	0.69032	0.8096	0.94877
H4	0.97935	0.29642	0.26399	H14	0.31113	0.18881	0.05092
H5	0.80228	0.17637	0.60264	H15	0.31119	0.30512	0.55234
H6	0.19965	0.82283	0.39789	H16	0.69023	0.6942	0.44862
H7	0.19906	0.67414	0.89815	H17	0.86574	0.82714	0.11396
H8	0.80233	0.32551	0.10269	H18	0.13554	0.17158	0.88635
H9	0.65224	0.97219	0.68494	H19	0.1357	0.32424	0.38731
H10	0.34961	0.02617	0.31483	H20	0.86549	0.67354	0.6141
K1	0.35639	0.96546	0.78573	K4	0.35552	0.52703	0.28494
K2	0.64607	0.03367	0.21475	K5	0.00058	-0.00131	0.50024
K3	0.6449	0.47013	0.71339	K6	0.00049	0.49908	0.00047

Figure S5 Bond lengths in $K_3C_{12}H_{10}$.