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Supporting information for article:

Chiral one-dimensional hydrogen-bonded architectures constructed from single-enantiomer phosphoric triamides

Mahsa Eghbali Toularoud, Mehrdad Pourayoubi, Michal Dušek, Václav Eigner and Krishnan Damodaran

Table S1 Contribution of close contacts in fingerprint plots for L-1 and D-1.

	L-1a (%)	**L-1b (%)**	**D-1a (%)**	**D-1b (%)**
H…H	51.8	53.9	51.6	53.7
C…H/H…C	21.8	20.5	21.9	20.7
F…H/H…F	11.3	11.5	11.3	11.5
O…H/H…O	9.2	9.2	9.2	9.3
Others[a]	5.9	4.9	5.4	4.9

[a](F…O/O…F) + (F…C/C…F) + (O…C/C…O) + (N…H/H…N) + (C…C).

Table S2

^{31}P (L-1)				**^{31}P (D-1)**				
Run 1	Run 2	Run 3	STDEV	Run 1	Run 2	Run 3	STDEV	Atom
3.7780	3.7782	3.7780	0.0001	3.7963	3.7963	3.7963	0.0000	P1
^{19}F (L-1)				**^{19}F (D-1)**				
–113.4781	–113.4782	–113.4781	0.0000	–113.4659	–113.4659	–113.4658	0.0000	F1/F2
–113.4903	–113.4904	–113.4903	0.0000	–113.4781	–113.4780	–113.4780	0.0000	F1/F2
–113.5027	–113.5026	–113.5026	0.0000	–113.4904	–113.4904	–113.4903	0.0000	F1/F2
^{1}H (L-1)				**^{1}H (D-1)**				
9.7598	9.7595	9.7594	0.0002	9.7779	9.7783	9.7784	0.0002	HN1
--	--	--	--	9.7678	9.7683	9.7680	0.0002	HN1
7.5144	7.5144	7.5144	0.0000	7.5140	7.5139	7.5140	0.0000	HC5
7.5114	7.5114	7.5114	0.0000	7.5109	7.5109	7.5109	0.0000	HC5
7.5004	7.5004	7.5004	0.0000	7.4999	7.4999	7.4999	0.0000	HC5
7.4894	7.4893	7.4893	0.0000	7.4890	7.4889	7.4889	0.0000	HC5
7.4864	7.4864	7.4864	0.0000	7.4859	7.4859	7.4860	0.0000	HC5
7.3725	7.3725	7.3725	0.0000	7.3760	7.3760	7.3761	0.0000	HC11/HC15/HC19/HC23
7.3602	7.3602	7.3602	0.0000	7.3638	7.3638	7.3638	0.0000	HC11/HC15/HC19/HC23
7.3373	7.3373	7.3373	0.0000	7.3412	7.3412	7.3412	0.0000	HC11/HC15/HC19/HC23
7.3251	7.3251	7.3252	0.0000	7.3291	7.3290	7.3291	0.0000	HC11/HC15/HC19/HC23
7.3028	7.3027	7.3027	0.0000	7.3048	7.3047	7.3048	0.0000	HC11/HC15/HC19/HC23
7.2995	7.2995	7.2995	0.0000	7.3016	7.3015	7.3016	0.0000	HC12/HC14/HC20/HC22
7.2903	7.2903	7.2903	0.0000	7.2923	7.2923	7.2923	0.0000	HC12/HC14/HC20/HC22
7.2798	7.2797	7.2797	0.0000	7.2819	7.2818	7.2819	0.0000	HC12/HC14/HC20/HC22
7.2771	7.2771	7.2771	0.0000	7.2792	7.2791	7.2792	0.0000	HC12/HC14/HC20/HC22
7.2721	7.2721	7.2721	0.0000	7.2743	7.2743	7.2743	0.0000	HC12/HC14/HC20/HC22
7.2689	7.2689	7.2690	0.0000	7.2712	7.2711	7.2712	0.0000	HC12/HC14/HC20/HC22
7.2597	7.2597	7.2597	0.0000	7.2620	7.2619	7.2620	0.0000	HC12/HC14/HC20/HC22
7.2493	7.2493	7.2493	0.0000	7.2516	7.2515	7.2516	0.0000	HC12/HC14/HC20/HC22

Table S2 continue

7.2467	7.2467	7.2467	0.0000	7.2490	7.2489	7.2490	0.0000	HC12/HC14/HC20/HC22
7.211	7.2110	7.2109	0.0000	7.2129	7.2128	7.2129	0.0000	HC13/HC21 or HC4/HC6
7.2089	7.2089	7.2089	0.0000	7.2108	7.2107	7.2108	0.0000	HC13/HC21 or HC4/HC6
7.2068	7.2068	7.2068	0.0000	7.2087	7.2086	7.2087	0.0000	HC13/HC21 or HC4/HC6
7.1995	7.1995	7.1994	0.0000	7.2014	7.2013	7.2014	0.0000	HC13/HC21 or HC4/HC6
7.1966	7.1966	7.1966	0.0000	7.1984	7.1984	7.1985	0.0000	HC13/HC21 or HC4/HC6
7.1935	7.1935	7.1935	0.0000	7.1954	7.1954	7.1954	0.0000	HC13/HC21 or HC4/HC6
7.1913	7.1913	7.1914	0.0000	7.1933	7.1932	7.1933	0.0000	HC13/HC21 or HC4/HC6
7.1866	7.1866	7.1865	0.0000	7.1885	7.1884	7.1885	0.0000	HC13/HC21 or HC4/HC6
7.1845	7.1845	7.1845	0.0000	7.1864	7.1863	7.1864	0.0000	HC13/HC21 or HC4/HC6
7.1814	7.1814	7.1814	0.0000	7.1833	7.1833	7.1833	0.0000	HC13/HC21 or HC4/HC6
7.1782	7.1782	7.1782	0.0000	7.1801	7.1800	7.1801	0.0000	HC13/HC21 or HC4/HC6
7.1712	7.1712	7.1712	0.0000	7.1732	7.1731	7.1732	0.0000	HC13/HC21 or HC4/HC6
7.1692	7.1692	7.1692	0.0000	7.1711	7.1710	7.1711	0.0000	HC13/HC21 or HC4/HC6
7.1671	7.1670	7.1671	0.0000	7.1689	7.1689	7.1690	0.0000	HC13/HC21 or HC4/HC6
7.1507	7.1507	7.1507	0.0000	7.1506	7.1506	7.1506	0.0000	HC13/HC21 or HC4/HC6
7.1372	7.1371	7.1372	0.0000	7.1370	7.1370	7.1371	0.0000	HC13/HC21 or HC4/HC6
7.1237	7.1237	7.1237	0.0000	7.1236	7.1235	7.1236	0.0000	HC13/HC21 or HC4/HC6
4.9277	4.9278	4.9278	0.0000	4.9328	4.9328	4.9330	0.0001	HN2/HN3
4.9105	4.9106	4.9107	0.0001	4.9156	4.9157	4.9158	0.0001	HN2/HN3
4.8934	4.8933	4.8934	0.0000	4.8984	4.8983	4.8985	0.0001	HN2/HN3
4.8408	4.8408	4.8409	0.0000	4.8468	4.8468	4.8470	0.0001	HN2/HN3
4.8245	4.8245	4.8246	0.0000	4.8305	4.8305	4.8307	0.0001	HN2/HN3
4.8077	4.8077	4.8078	0.0000	4.8136	4.8137	4.8138	0.0001	HN2/HN3
4.4063	4.4061	4.4062	0.0001	4.4113	4.4113	4.4114	0.0000	HC8/HC16
4.3947	4.3946	4.3945	0.0001	4.3997	4.3997	4.3997	0.0000	HC8/HC16
4.3552	4.3553	4.3551	0.0001	4.3608	4.3607	4.3607	0.0000	HC8/HC16
4.3437	4.3439	4.3437	0.0001	4.3494	4.3493	4.3494	0.0000	HC8/HC16
3.3070	3.3070	3.3071	0.0000	3.3169	3.3169	3.3171	0.0001	H_2O
2.5061	2.5061	2.5061	0.0000	2.5062	2.5061	2.5062	0.0000	solvent
2.5031	2.5031	2.5031	0.0000	2.5031	2.5030	2.5031	0.0000	solvent
2.5000	2.5000	2.5000	0.0000	2.5000	2.5000	2.5000	0.0000	solvent
2.4969	2.4969	2.4969	0.0000	2.4969	2.4969	2.4969	0.0000	solvent
2.4938	2.4938	2.4938	0.0000	2.4938	2.4938	2.4938	0.0000	solvent
1.4115	1.4115	1.4115	0.0000	1.4151	1.4151	1.4151	0.0000	HC9/HC17
1.4000	1.4000	1.4000	0.0000	1.4036	1.4036	1.4036	0.0000	HC9/HC17
1.3962	1.3962	1.3962	0.0000	1.4009	1.4008	1.4009	0.0000	HC9/HC17
1.3847	1.3847	1.3847	0.0000	1.3893	1.3893	1.3893	0.0000	HC9/HC17

Table S2 continue

^{13}C (L-1)				^{13}C (D-1)				
161.6624	161.6806	161.6758	0.0077	161.6884	161.6905	161.6902	0.0009	C1
159.6516	159.6501	159.6521	0.0008	159.6629	159.6632	159.6640	0.0005	C3/C7
159.5991	159.6000	159.5996	0.0004	159.6127	159.6119	159.6126	0.0004	C3/C7
158.0022	158.0025	158.0019	0.0002	158.0145	158.0136	158.0144	0.0004	C3/C7
157.9509	157.9513	157.9518	0.0004	157.9628	157.9619	157.9620	0.0004	C3/C7
146.2603	146.2604	146.2603	0.0000	146.2636	146.2633	146.2635	0.0001	C10/C18
146.2236	146.2233	146.2229	0.0003	146.2263	146.2263	146.2262	0.0000	C10/C18
145.9081	145.9087	145.9080	0.0003	145.9119	145.9116	145.9113	0.0002	C10/C18
145.8706	145.8707	145.8699	0.0004	145.8737	145.8739	145.8737	0.0001	C10/C18
131.8322	131.8291	131.8292	0.0015	131.8328	131.8330	131.8372	0.0001	C5[a]
127.9944	127.9945	127.9941	0.0002	128.0019	128.0019	128.0019	0.0000	C12/C14/C20/C22
127.9829	127.9830	127.9827	0.0001	127.9905	127.9905	127.9904	0.0000	C12/C14/C20/C22
126.3599	126.3601	126.3596	0.0002	126.3683	126.3683	126.3682	0.0000	C13/C21
126.3226	126.3228	126.3223	0.0002	126.3311	126.3310	126.3310	0.0000	C13/C21
126.0595	126.0596	126.0592	0.0002	126.0677	126.0678	126.0677	0.0000	C11/C15/C19/C23
125.9774	125.9775	125.9771	0.0002	125.9860	125.9860	125.9859	0.0000	C11/C15/C19/C23
111.9114	111.9125	111.9120	0.0004	111.9161	111.9155	111.9155	0.0003	C4/C6
111.7507	111.7506	111.7501	0.0003	111.7539	111.7541	111.7531	0.0001	C4/C6
50.0446	50.0438	50.0440	0.0003	50.0551	50.0555	50.0552	0.0002	C8/C16
49.7068	49.7080	49.7083	0.0006	49.7165	49.7168	49.7166	0.0001	C8/C16
25.4627	25.4626	25.4615	0.0005	25.4654	25.4660	25.4655	0.0000	C9/C17
25.4277	25.4276	25.4272	0.0002	25.4312	25.4315	25.4311	0.0002	C9/C17
24.9121	24.9115	24.9112	0.0004	24.9131	24.9134	24.9133	0.0001	C9/C17
24.8790	24.8792	24.8782	0.0004	24.8805	24.8808	24.8801	0.0003	C9/C17

[a] The signal around 131.8 are triplet (C5) and the S/N of the triplet wasn't good enough to report reproducibility. So I used just the center signal. Moreover, for the signal about 115.3 (double of triplets, C2), the peak had a very low S/N to report reliably.

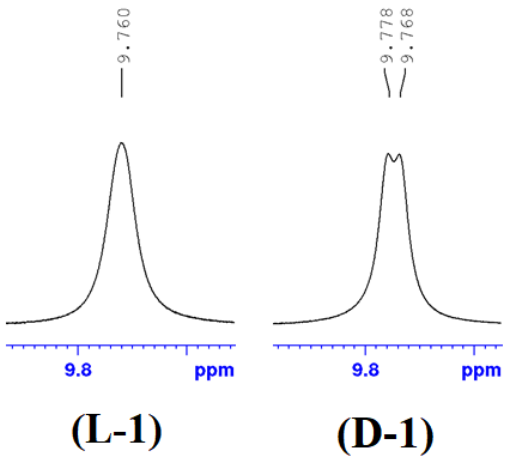

Figure S1 The signal of $N_{CP}H$ proton for compounds L-1 and D-1.

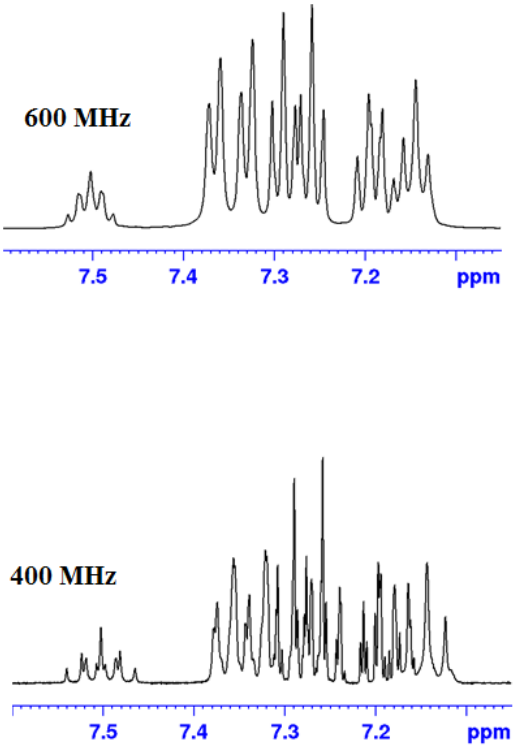

Figure S2 Selected region of ^{1}HNMR spectra at two different frequencies, for L-1 in DMSO-d_6.