

Melting points of potential liquid organic hydrogen carrier systems consisting of N-alkylcarbazoles

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A. Conditions of the DSC measurements

components/mixtures with $T_m < 60^\circ\text{C}$:

1. Constant cooling rate with $dT/dt = +40 \text{ K/min}$ to the desired temperature
2. Isotherm segment for at least $t=5 \text{ min}$
3. Constant heating rate with $dT/dt = +10 \text{ K/min}$ to the desired temperature
4. Isotherm segment for $t=5 \text{ min}$
5. Steps 1-4 were repeated 2 times

components/mixtures with $T_m > 60^\circ\text{C}$

1. Constant heating rate with $dT/dt = +10 \text{ K/min}$ to the desired temperature
2. Isotherm segment for $t=5 \text{ min}$
3. Constant cooling rate with $dT/dt = +40 \text{ K/min}$ to the desired temperature
4. Isotherm segment for least $t=5 \text{ min}$
5. Steps 1-4 were repeated 2 times

If necessary the measurements were repeated with a lower heating rate (3 or 5 K/min) to obtain a higher resolution of the solid-liquid transition. Samples which did not crystallize during the DSC cooling segment, were only heated up once.

B. Experimental Data

Table 1. Experimental SLE Data for the System N-ethylcarbazole (1) – N-ethyl-dodecahydro-carbazole (2) at Liquid Mole fraction x, Temperature T, and Pressure p = 0.1 MPa^a

x ₁	T/K	Solid Phase
0.10	285.6	N-ethylcarbazole
0.12	290.0	N-ethylcarbazole
0.14	294.6	N-ethylcarbazole
0.18	299.0	N-ethylcarbazole
0.23	303.3	N-ethylcarbazole
0.28	307.3	N-ethylcarbazole
0.35	312.7	N-ethylcarbazole
0.44	316.7	N-ethylcarbazole
0.53	321.7	N-ethylcarbazole
0.66	325.0	N-ethylcarbazole
0.76	328.5	N-ethylcarbazole
0.88	334.3	N-ethylcarbazole
1	342.4	N-ethylcarbazole

^aStandard uncertainties u are u(T_m) = 1 K, u(x) = 0.02, u(p) = 5 kPa

Table 2. Experimental SLE Data for the System N-ethylcarbazole (1) – carbazole (2) at Liquid Mole fraction x, Melting Temperature T_m, Eutectic Temperature T_{eu}, and Pressure p = 0.1 MPa^a

x1	T _m /K	T _{eu} /K	Solid Phase
0	517.1	-	Carbazole
0.1	512.0	339.9	Carbazole
0.2	500.9	340.1	Carbazole
0.3	487.0	339.7	Carbazole
0.4	477.5	340.0	Carbazole
0.5	468.7	340.2	Carbazole
0.6	457.1	340.0	Carbazole
0.7	440.1	340.9	Carbazole
0.8	418.7	340.6	Carbazole
0.9	386.9	340.4	Carbazole
1	342.4	-	N-ethylcarbazole

^aStandard uncertainties u are u(T_m) = 1 K, u(T_{eu}) = 2 K u(x) = 0.001, u(p) = 5 kPa

Table 3. Experimental SLE Data for the System N-ethylcarbazole (1) – N-methylcarbazole (2) at Liquid Mole fraction x, Melting Temperature T_m , Eutectic Temperature T_{eu} , and Pressure $p = 0.1 \text{ MPa}^a$

x1	T_m/K	T_{eu}/K	Solid Phase
0	361	-	N-methylcarbazole
0.249	344.1	315.9	N-methylcarbazole
0.4	330.6	313.8	N-methylcarbazole
0.5	321.4	314.1	N-methylcarbazole
0.7	323.9	315.7	N-ethylcarbazole
0.892	336.4	315.1	N-ethylcarbazole
1	342.4	-	N-ethylcarbazole

^aStandard uncertainties u are $u(T_m) = 1 \text{ K}$, $u(T_{eu}) = 2 \text{ K}$, $u(x) = 0.001$, $u(p) = 5 \text{ kPa}$

Table 4. Experimental SLE Data for the System N-ethylcarbazole (1) – N-propylcarbazole (2) at Liquid Mole fraction x, Melting Temperature T_m , Eutectic Temperature T_{eu} , and Pressure $p = 0.1 \text{ MPa}^a$

x1	T_m/K	T_{eu}/K	Solid Phase
0	320.3	-	N-propylcarbazole
0.052	319.9	-	N-propylcarbazole
0.1	318	294.7	N-propylcarbazole
0.2	312.8	295.9	N-propylcarbazole
0.3	306.8	291.9	N-propylcarbazole
0.4		291.9	N-propylcarbazole
0.494		296.1	N-ethylcarbazole
0.498		294.5	N-ethylcarbazole
0.548		298.0	N-ethylcarbazole
0.601	316.8	299.9	N-ethylcarbazole
0.7	321.3	299.6	N-ethylcarbazole
0.8	329.1	298.9	N-ethylcarbazole
0.899	336.4	297.3	N-ethylcarbazole
1	342.4	-	N-ethylcarbazole

^aStandard uncertainties u are $u(T_m) = 1 \text{ K}$, $u(T_{eu}) = 2 \text{ K}$, $u(x) = 0.001$, $u(p) = 5 \text{ kPa}$

Table 5. Experimental SLE Data for the System N-ethylcarbazole (1) – N-isopropylcarbazole (2) at Liquid Mole fraction x, Melting Temperature T_m , Eutectic Temperature T_{eu} , and Pressure $p = 0.1 \text{ MPa}^a$

x1	T_m/K	T_{eu}/K	Solid Phase
0	393.9	-	N-isopropylcarbazole
0.1	393.2	373.2	N-isopropylcarbazole
0.2	393.2	370.2	N-isopropylcarbazole
0.3	391.3	370.2	N-isopropylcarbazole
0.4	387.3	367.4	N-isopropylcarbazole
0.45	384.2	366.4	N-isopropylcarbazole
0.5	382.2	355.5	N-isopropylcarbazole
0.55	378.8	333.1	1:1- compound
0.6	378.2	334.1	1:1- compound
0.7	371.9	337.2	1:1- compound
0.8	364.3	337.9	1:1- compound
0.9	351.6	338.1	1:1- compound
0.95	342	338.2	1:1- compound
1	342.4	-	N-ethylcarbazole

^aStandard uncertainties u are $u(T_m) = 1 \text{ K}$, $u(T_{eu}) = 2 \text{ K}$, $u(x) = 0.001$, $u(p) = 5 \text{ kPa}$

Table 6. Experimental SLE Data for the System N-ethylcarbazole (1) – N-butylcarbazole (2) at Liquid Mole fraction x, Melting Temperature T_m , Eutectic Temperature T_{eu} , and Pressure $p = 0.1 \text{ MPa}^a$

x1	T_m/K	T_{eu}/K	Solid Phase
0	330.6	-	N-butylcarbazole
0.2	322.2	303.9	N-butylcarbazole
0.325	316.2	302.3	N-butylcarbazole
0.51		304.2	N-ethylcarbazole
0.66	319.8	303.9	N-ethylcarbazole
0.91	338	304.5	N-ethylcarbazole
1	342.4	-	N-ethylcarbazole

^aStandard uncertainties u are $u(T_m) = 1 \text{ K}$, $u(T_{eu}) = 2 \text{ K}$, $u(x) = 0.001$, $u(p) = 5 \text{ kPa}$

Table 7. Experimental SLE Data for the System N-propylcarbazole (1) – N-butylcarbazole (2) at Liquid Mole fraction x, Melting Temperature T_m , Eutectic Temperature T_{eu} , Temperature of Transition T_{tr} and Pressure $p = 0.1 \text{ MPa}^a$

x1	T_m/K	T_{eu}/K	T_{tr}/s	Solid Phase
0	330.6			N-butylcarbazole
0.1	328.1	295.7		N-butylcarbazole
0.2	324.6	296.5		N-butylcarbazole
0.3	318.1	299.9		N-butylcarbazole
0.4	311	297.5		N-butylcarbazole
0.48	306	297.8	284.3	N-butylcarbazole
0.50	305.3	297.2	285.6	N-butylcarbazole
0.53	303.9	297.9	284.9	N-butylcarbazole
0.56	300.1	-	285.3	N-butylcarbazole
0.6	299.7	296.5	284.8	N-propylcarbazole
0.7	308.5	298.4	283.2	N-propylcarbazole
0.8	314.1	299.5	282.8	N-propylcarbazole
0.9	317.8	298.2	281.9	N-propylcarbazole
1	320.3			N-propylcarbazole

^aStandard uncertainties u are $u(T_m) = 1 \text{ K}$, $u(T_{eu}) = 2 \text{ K}$, $u(T_{TR}) = 2 \text{ K}$, $u(x) = 0.001$, $u(p) = 5 \text{ kPa}$

C. NMR spectra of synthesized compounds

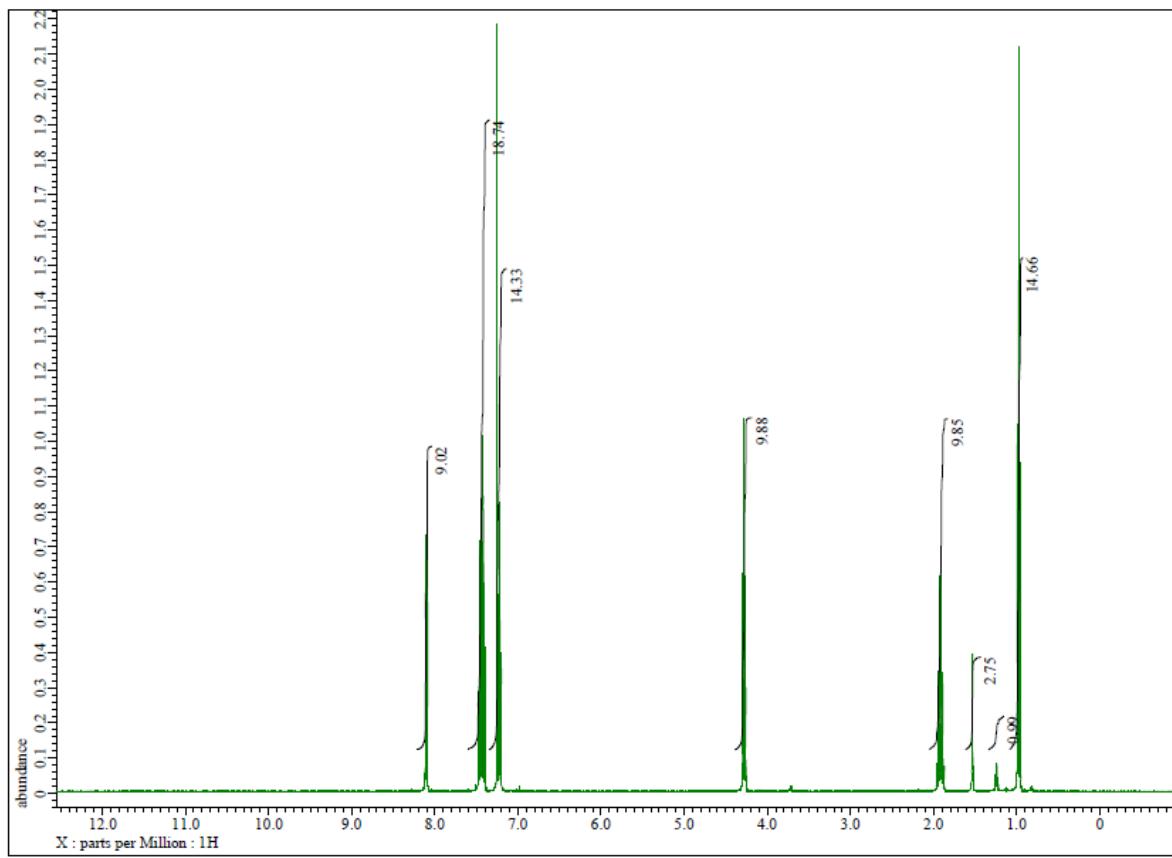


Figure 1: ¹H NMR spectrum of N-propylcarbazole

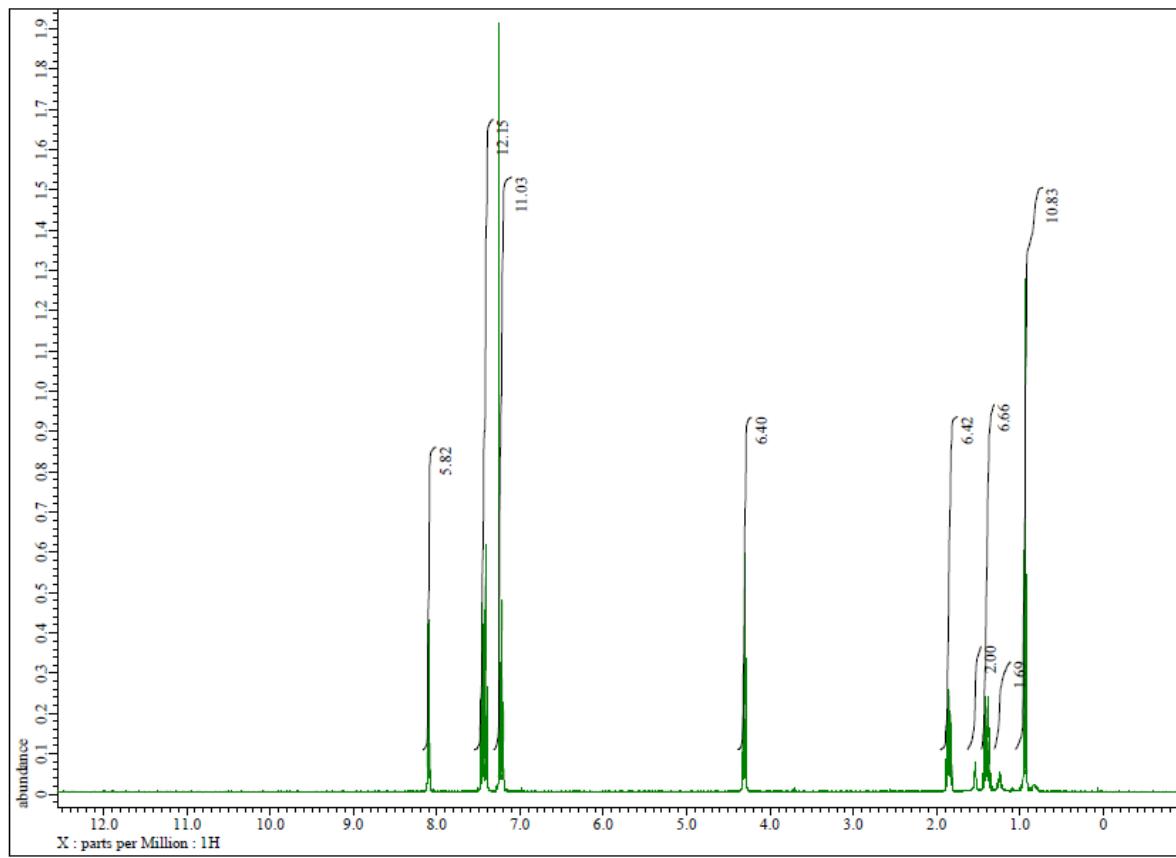


Figure 2. ¹H NMR spectrum of N-butylcarbazole

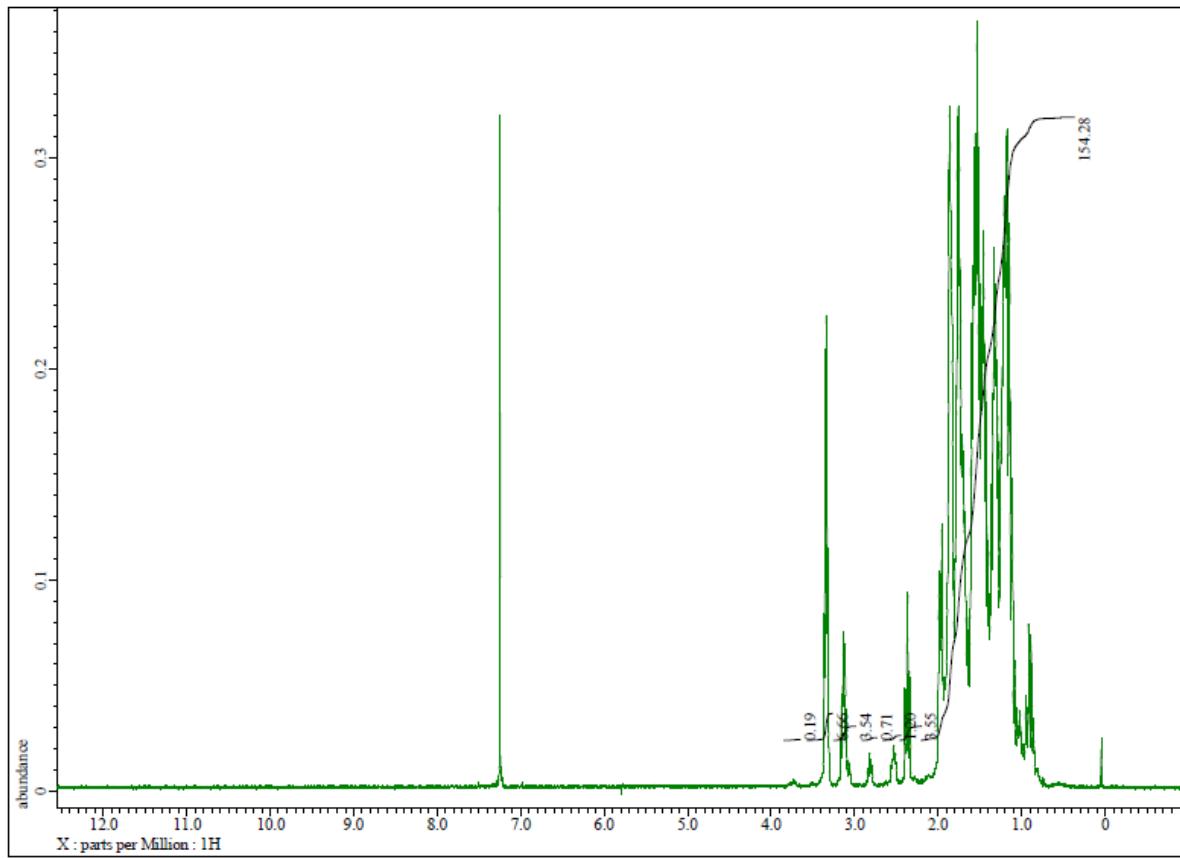


Figure 3. ¹H NMR spectrum of 12H-carbazole