Electronic Supplementary Information for

o-Carborane derivatives for probing molecular polarity effects on liquid crystal phase stability and dielectric behavior

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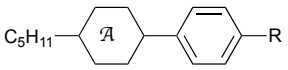
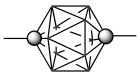
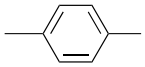
1. Thermal analysis

Table S1. Transition temperatures and enthalpies for compounds in series **1**.[a]

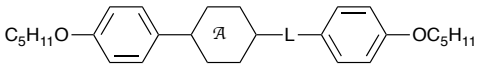


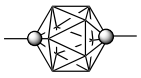
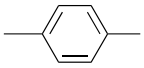
1

	R	 **A**	 **B**	 **Ph**
a	–C_6H_4-OC_8H_{17}	Cr 71 (SmA 45) N 149 I [b] *20.1* *1.3*	Cr 58 (SmC 38) SmA 121 N 144 I [c] *37.8* *0.7* *1.0*	Cr 97 E 194 SmB 211 SmA 222 I [b] *12.6* *5.0* *6.7* *11.3*
b	–C≡CC_6H_4-OC_8H_{17}	Cr 90 N 176 I *28.6* *1.5*	Cr 114 SmA 140 N 168 I *27.9* *0.2* *0.7*	Cr 96 Cr 156 B 177 N 206 I *10.3* *4.4* *11.0* *2.0*
c	–N=CHC_6H_4-OC_8H_{17}	Cr 111 N 177 I *33.8* *1.2*	Cr 101 SmA 157 N 171 I *51.7* *0.7* *0.9*	Cr 95 (H? 90) G 139 [d] SmF 150 [d] SmI *23.8* *0.5* *~0* *~0* 166 SmC 191 SmA 198 N 214 I *3.6* *0.1* *0.7* *1.8*
d	–N=NC_6H_4-$COOC_5H_{11}$ [*]	Cr 72 Cr 94 N* 160 I *5.6* *18.6* *0.6*	Cr 124 N* 151 I *17.0* *0.3*	E 115 SmB 136 SmA* 193 I *2.4* *2.1* *6.2*

[a] Cr-crystal, N-nematic, Sm-smectic, soft-crystalline phases B, E, G and possibly H. [b] Ref [1]. [c] Ref. [2] [d] From XRD measurement.

Table S2. Transition temperatures and enthalpies for for compounds in series **2**.[a]



	L	 **A**	 **B**	 **Ph**
e	–CH=CH–	Cr 124 N 135 I [b] *54.3* *2.1*	Cr 121 N (101) I [c,d] *46.3* *1.2*	Cr 72 X 209 G 254 SmC 258 SmA 281 N 285 I [b] *7.7* *5.4* *11.8* *0.0* *4.4* *1.4*
f	–CH_2CH_2–	Cr 94 N 123 I [b] *30.6* *2.4*	Cr 81 (N 78) I [e] *27.0* *1.6*	Cr 118 B[f] 173 I [b] *30.6* *21.1*

[a] Cr-crystal, N-nematic, Sm-smectic, soft-crystalline phases E and G, X-unidentified phase. [b] Ref [3]. [c] Ref. [2]. [d] Second heating: Cr 63 (*19.4*) N 101 (*1.2*) I. [e] Second heating: Cr 69 (*17.8*) N 77 (*1.1*) I.[f] Previously an E phase reported. Ref [3]

2. Powder XRD measurements

X-ray diffraction experiments in broad angle range were performed with Bruker D8 GADDS system (Cu K_α radiation, Göbel mirror, point collimator, Vantec 2000 area detector) equipped with a modified Linkam heating stage. For small angle diffraction experiments Bruker Nanostar system was used (Cu K_α radiation, cross-coupled Göbel mirrors, three pinhole collimation, Vantec 2000 area detector). Samples were prepared in a form of a thin film / droplet on heated surface or in thin-walled glass capillaries. Results are shown in Figures S1 – S4.

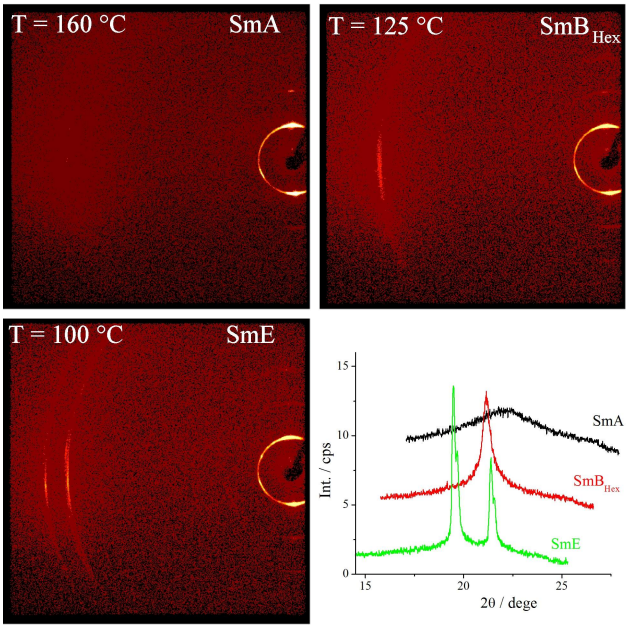


Fig. S1. Wide angle data for azo ester **1[Ph]d**.

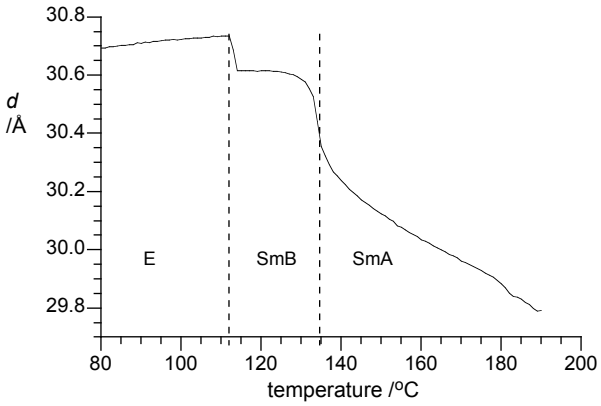


Fig. S2. Layer spacing *d* as a function of temperature for **1[Ph]d**.

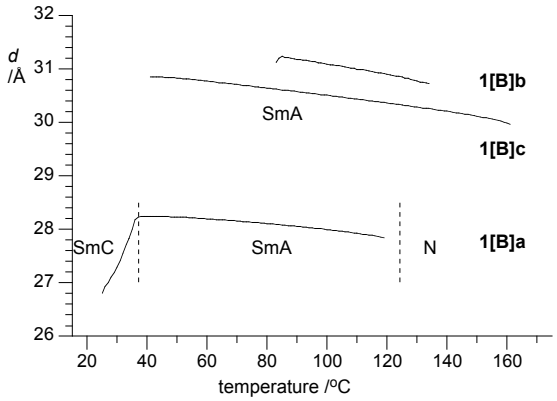


Fig. S3. Layer spacing *d* as a function of temperature for selected compounds.

Thermal expansion coefficients of the SmA phase:

1[B]a $\kappa = -5.11 \pm 0.06$ pm K^{-1} (95 – 130 °C)

1[B]b $\kappa = -9.65 \pm 0.08$ pm K^{-1} (70 – 95 °C)

1[B]c $\kappa = -7.00 \pm 0.02$ pm K^{-1} (60 – 140 °C)

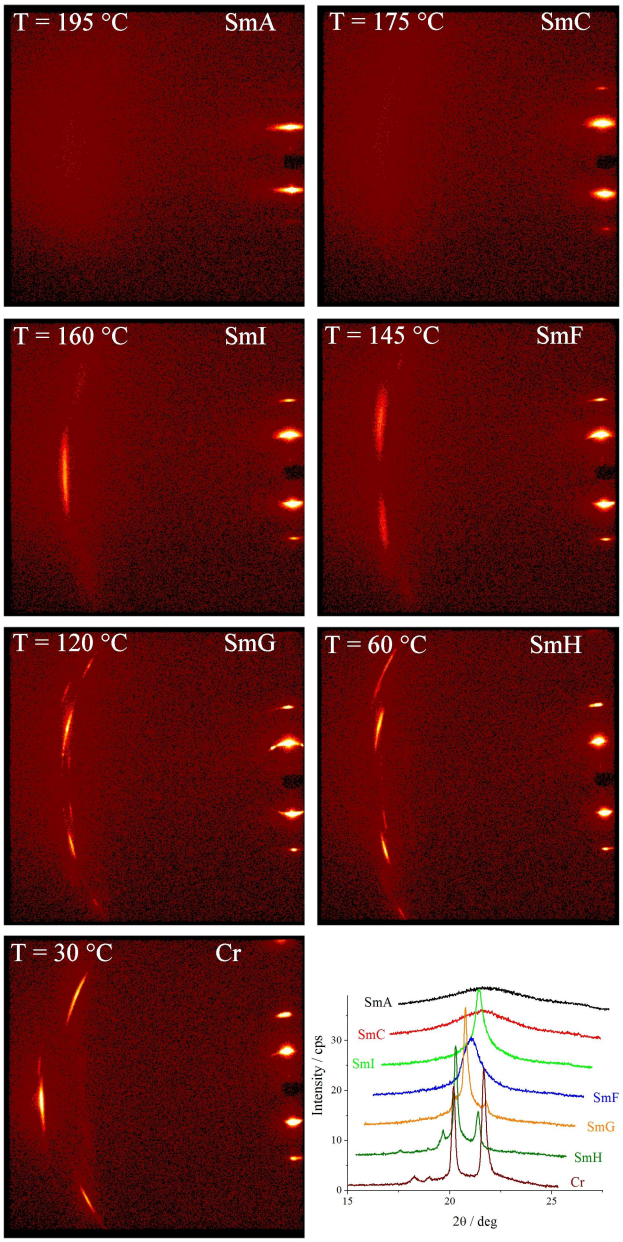


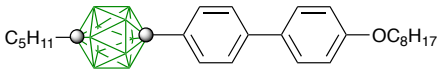
Fig. S4. Wide angle XRD data for Schiff base **1[Ph]c**.

3. Binary mixtures

Preparation of binary mixtures for dielectric studies. Solutions of compounds **1[A]a** or **1[B]a** in host **6CHBT** (15-20 mg) in dry CH_2Cl_2 (~0.5 mL) were heated at ~60 ^oC for 2 hr in an open vial to enssure homogeneity of the sample. The sample was degassed under vacuum (0.2 mmHg), left at ambient temperature for 2 hr and analyzed by polarized optical microscopy (POM). After a minimum of several days, the mixtures were inspected again and no inhomogeneity or partial crystallization was found.

Thermal analysis Virtual N-I transition temperatures [T_{NI}] were determined for selected compounds in **6CHBT** host. The clearing temperature for each homogenous mixture, prepared as above, was determined by DSC as the peak of the transition using small samples (~0.5 mg) and a heating rate of 5 $K \cdot min^{-1}$. The results are shown in Tables S3 and S4. The virtual N-I transition temperatures, [T_{NI}], were determined by linear extrapolation of the data for peak of the transition to pure substance (x = 1). To minimize the error, the intercept in the fitting function was set as the peak T_{NI} for the pure host.

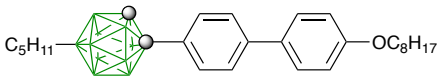
Table S3. T_{NI} for solutions of **1[A]a** in **6CHBT**.



T_{NI}/°C	**Mole fraction, x**			
	0.00 (host)	0.0413	0.0751	0.1774
Onset	43.59	47.83	52.94	67.85
Peak	43.76	48.51	54.47	69.36

[T_{NI}] = 187±3 °C, r^2 = 0.996

Table S4. T_{NI} for solutions of **1[B]a** in **6CHBT**.

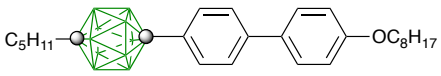


T_{NI}/°C	**Mole fraction, *x***				
	0.00 (host)	0.0549	0.0977	0.1411	0.1545
Onset	43.59	49.26	52.33	59.39	63.48
Peak	43.76	49.86	53.75	60.49	64.47

For the first two points: $[T_{NI}] = 148\pm3$ °C, $r^2 = 0.996$

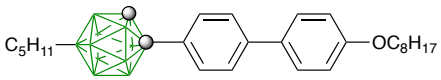
Dielectric measurements. Dielectric properties of solutions of selected esters in **6CHBT** were measured by a Liquid Crystal Analytical System (LCAS - Series II, LC Vision, Inc.) using GLCAS software version 0.13.14, which implements literature procedures for dielectric constants.[5] The instrument was calibrated using a series of capacitors (11.30 pF – 3292 pF). The homogenous binary mixtures were loaded into ITO electrooptical cells by capillary forces with moderate heating supplied by a heat gun. The cells (about 10 μm thick, electrode area 1.00 cm^2 and anti-parallel rubbed polyimide layer) were obtained from LC Vision, Inc. The filled cells were heated to an isotropic phase and cooled to room temperature before measuring of dielectric properties. Default parameters were used for measurements: triangular shaped voltage bias ranging from 0.1-20 V at 1 kHz frequency. The threshold voltage V_{th} was measured at a 5% change. For each mixture the measurement was repeated 10 times manually for two cells. The results were averaged to calculate the mixture's parameters. Results are shown in Tables S5 and S6. All measurements were run at 25 °C. Error in concentration is estimated at about 1.5%. The dielectric values obtained for each concentration were fitted to a linear function in which the intercept was set at the value extrapolated for the pure host. The resulting extrapolated values for pure additives are shown in Table 3 in the main text.

Table S5. Dielectric parameters for **1[A]a** in **6CHBT** at 25 °C.



Parameter	**Mole fraction, *x***			
	0.00 (host)	0.04135	0.0751	0.1774
$\varepsilon_{\parallel}$	12.05±0.01	11.60±0.04	11.17±0.03	9.92±0.04
$\varepsilon_{\perp}$	3.99±0.01	3.905±0.01	3.77±0.01	3.51±0.02
$\Delta\varepsilon$	8.06±0.01	7.70±0.04	7.40±0.03	6.41±0.03
K_{11}	7.0	8.6±0.8	8.89±0.04	10.7±0.1
K_{22}	4.22	5.2±0.5	5.32±0.03	6.4±0.1
γ	81	81±3.5	64±2	42±1.6

Table S6. Dielectric parameters for **1[B]a** in **6CHBT** at 25 °C.



Parameter	**Mole fraction, *x***				
	0.00 (host)	0.0549	0.0977	0.1411	0.1545
$\varepsilon_{\parallel}$	12.05±0.01	12.32±0.1	12.61±0.07	13.24±0.01	13.2±0.06
$\varepsilon_{\perp}$	3.99±0.01	4.08±0.03	4.27±0.02	4.29±0.01	4.32±0.01
$\Delta\varepsilon$	8.06±0.01	8.24±0.07	8.34±0.06	8.94±0.01	8.88±0.06
K_{11}	7.0	8.4±0.25	8.6±0.5	9.6±1.0	10.5±0.1
K_{22}	4.22	5.1±0.15	5.1±0.3	5.8±0.6	6.3±0.1
γ	81	105±1	48±1.3	53±0.6	129±4

4. Background for calculations in the nematic phase

The equations derived from the Maier-Meier theory[4] used in this work were adopted from literature[5] and had the following form:

$$\Delta\varepsilon = \frac{NFh}{\varepsilon_0}\left\{\Delta\alpha - \frac{F\mu_{eff}^2}{2k_BT}(1 - 3cos^2\beta)\right\}S \quad (1)$$

$$\varepsilon_{\parallel} = 1 + \frac{NFh}{\varepsilon_0}\left\{\bar{\alpha} + \frac{2}{3}\Delta\alpha S + \frac{F\mu_{eff}^2}{3k_BT}[1 - (1 - 3cos^2\beta)S\right\} \quad (2)$$

$$\varepsilon_{\perp} = 1 + \frac{NFh}{\varepsilon_0}\left\{\bar{\alpha} - \frac{1}{3}\Delta\alpha S + \frac{F\mu_{eff}^2}{3k_BT}[1 + \frac{1}{2}(1 - 3cos^2\beta)S\right\} \quad (3)$$

All quantities were in SI units as defined in the ESI in previous publications.[6]

- Dielectric permittivity of vacuum:

$\varepsilon = 1.114 \cdot 10^{-10} / 4\pi = 8.865 \cdot 10^{-12}$ F·m^{-1}

- The diagonalized values of the electronic polarizabilities tensors matrix α_{xx}, α_{yy}, α_{zz} expressed in a.u. units were converted to F·m^2 units by multiplying with $1.482 \cdot 4\pi\varepsilon \cdot 10^{-31} = 1.651 \cdot 10^{-41}$
- Computed dipole moments μ_x, μ_y, μ_z in Debye were converted to dipole moments in C·m units using the conversion 1D = $3.3356\ 10^{-30}$ C·m
- Number density *N* is expressed in molecules per m^3

Field parameters $F = 1.34806$ and $h = 1.394366197$ in equations 1–3 were assummed to be of pure host, **6CHBT**, and obtained from literature dielectric and optical data[7] according to equation 4 and 5. Permittivity ε_s was assumed to be experimental average permittivity ($\varepsilon = 6.70$) for the

pure host, **6CHBT**. The density of the hosts **6CHBT** at 25 °C was taken as 1.02 g/cm^3 according to a literature report.[7]

$$F = \frac{1}{1-\bar{\alpha}\cdot f} \text{ where } f = \frac{2\left(\bar{\varepsilon}_s - 1\right)}{2\bar{\varepsilon}_s + 1}\cdot\frac{N}{3\varepsilon_0} \quad (4)$$

$$h = \frac{3\varepsilon_s}{(2\varepsilon_s + 1)} \quad (5)$$

5. Procedures for Maier-Meier analysis.

The apparent order parameter S_{app} and the Kirkwood factor g for the additives were obtained by solving simultaneously equations for Δε and $\varepsilon_\parallel$ (equation 1 and 2, letting $S = S_{app}$). The unknown g from the expression for Δε (equation 1) was substituted into the expression for $\varepsilon_\parallel$ (equation 2) and solved for S_{app} (equation 6). In this form, apparent order parameter S_{app} does not depend on the dipole moment μ, but depends on the dielectric permittivity components $\varepsilon_\parallel$ and $\varepsilon_\perp$. The obtained value S_{app} was substituted to the expression for parameter g (equation 7).

$$S_{app} = \frac{2\Delta\varepsilon\varepsilon_0}{NFh[2\Delta\alpha+3\bar{\alpha}(1-3cos^2\beta)]-3(\bar{\varepsilon}-1)\varepsilon_0(1-3cos^2\beta)} \quad (6)$$

$$g = \frac{[(\varepsilon_\parallel-1)\varepsilon_0-\bar{\alpha}NFh-\frac{2}{3}\Delta\alpha NFhS_{app}]3k_BT}{NF^2h\mu^2[1-(1-3cos^2\beta)S_{app}]} \quad (7)$$

The protocol was verified by substituting the computed parameters $S = S_{app}$ and g into equation 1–3 and calculating back the dielectric parameters.

6. Quantum mechanical calculation

Quantum-mechanical calculations were carried out using Gaussian 09 suite of programs.[8] Geometry optimizations for unconstrained conformers of **1a** – **1c** with most extended molecular shapes were undertaken at the B3LYP/6-31G(2d,p) level of theory using default convergence limits. Vibrational frequencies were used to characterize the nature of the stationary points and to

obtain exact polarizabilities in vacuum. The alkyl groups were in all-*trans* conformation. No conformational search was attempted. Final coordinates for each molecular model are provided below and the calculated molecular lengths are listed in Table S7.

Table S7. Molecular length (the H···H distance) for selected compounds.[a]

	1[A]a	**1[B]a**	**1[Ph]a**	**1[A]b**	**1[B]b**	**1[Ph]b**	**1[A]c**	**1[B]c**	**1[Ph]c**
d /Å	30.74	31.01	30.13	33.27	33.28	32.60	33.05	33.01	32.38
d+*VDW*[b] /Å	33.14	33.41	32.53	35.67	35.68	35.00	35.45	35.41	34.78

[a] Measured for equilibrium geometry at the B3LYP/6-31G(2d,p) level of theory. [b] Hydrogen atom van der Waals radius of 1.20 Å.

Dipole moments and exact electronic polarizabilities of **1[A]a** and **1[B]a** used in the Maier–Meier data analysis were obtained in **6CHBT** dielectric medium using the B3LYP/6-31+G(2d,p)//B3LYP/6-31G(2d,p) method and the PCM solvation model[9] requested with SCRF(Solvent=Generic, Read) keywords and "eps=6.70" and "epsinf=2.4623" parameters (single point calculations). Exact polarizabilities were obtained with the POLAR keyword and are listed in Table S8. The reported values for dipole moment components and dielectric permittivity tensors are at Gaussian standard orientation of each molecule (charge based), which is close to the principal moment of inertia coordinates (mass based).

Dipole moment components and polarizability tensors for selected molecules in **vacuum**
All molecules are in Gaussian standard orientation with their long molecular axes oriented along the x axis. Dipole moments in Debye and polarizability in au (1Å^3 = 0.1482 au)

1[A]a
```
X=  -1.9511    Y=  0.5738    Z=   -0.3127  Tot= 2.0576
Exact polarizability: 683.502   9.561 340.985  -2.455  -0.897 279.741
```

1[B]a
```
 X= -7.5745   Y=  -1.6777   Z=  1.1333  Tot= 7.8404
  Exact polarizability: 693.573 -12.208 338.614   4.005   9.398 283.316
```

Dipole moment components and polarizability tensors for selected molecules in **6CHBT** dielectric medium
All molecules are in Gaussian standard orientation with their long molecular axes oriented along the x axis. Dipole moments in Debye and polarizability in au (1Å^3 = 0.1482 au).

1[A]a

```
Dipole moment (field-independent basis, Debye):
X=   -1.6346    Y=  1.0371    Z=   -0.4279  Tot=  1.9826
Exact polarizability: 786.959  15.517 506.351  -2.475  -0.961 419.284
Diagonalized: 787.80   505.50   419.25
```

1[B]a

```
Dipole moment (field-independent basis, Debye):
X=  -8.2405    Y=  -2.5073    Z=  1.5168  Tot=   8.7460
Exact polarizability: 798.600 -19.533 503.265   7.500  12.271 425.370
Diagonalized: 800.00   504.04    423.19
```

Table S8. Calculated molecular parameters for selected compounds in **6CHBT** dielectric medium.[a]

	$\mu_{\|\|}$ /D	$\mu_{\perp}$ /D	μ /D	β [b] /°	$\Delta\alpha$ /Å^3	α_{avrg} /Å^3
1[A]a	1.63	1.12	1.98	34.5	48.23	84.60
1[B]a	8.24	2.93	8.75	19.6	49.85	85.33

[a] Dipole moments and polarizabilities obtained at the B3LYP/6-31+G(2d,p)// B3LYP/6-31G(2d,p) level of theory in **6CHBT** dielectric medium. Polarizability values calculated from diagonalized polarizability tensors were converted from a.u. to Å^3 using the factor 0.1482. [b] Angle between the net dipole vector μ and $\mu_{||}$.

7. Archive for DFT calculations

1[A]a

```
1\1\GINC-OCTOPUS\SP\RB3LYP\6-31+G(2d,p)\C27H46B10O1\PIOTR\02-Mar-2015\
 0\\#P B3LYP/6-31+G(2d,p) SCF=tight POLAR SCRF(Solvent=Generic,Read)\\p
 ara-C5-C2B10-PhPh-OC8,C1 at the B3LYP/6-31G(2d,p) geom in 6CHBT\\0,1\C
 ,0,-0.6418434642,0.3925341495,6.4771320524\B,0,0.6652156213,-0.4680348
 202,5.7716904055\B,0,-0.9979658179,-1.071863607,5.6460464141\B,0,0.612
 3140093,1.3071302925,5.7259785165\B,0,-1.0911990122,1.7960382736,5.596
 6760029\B,0,-2.0832077823,0.3280603481,5.537585307\B,0,-1.7173695687,1
 .2010514537,4.049792661\B,0,-0.0498135025,1.8031123646,4.1723871579\B,
 0,-1.6543518583,-0.5759081333,4.0892606742\B,0,1.0408927933,0.39842412
 59,4.2804412237\B,0,0.047723071,-1.0750292023,4.2264047578\C,0,-0.4002
 073089,0.3365587198,3.3337853314\C,0,-0.254057097,0.3213044236,1.82859
 48563\C,0,-1.0689204261,-0.477914187,1.019900374\C,0,0.7184668469,1.10
 70743788,1.1988526782\C,0,-0.9168455534,-0.4896171012,-0.3614679968\C,
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 8564,0.3991877883,-3.0665286772\C,0,1.6347246023,0.3831374784,-4.44231
 374\C,0,0.5185851554,0.2529608125,-5.2789673611\C,0,-0.752360688,0.139
 6454203,-4.7080422763\C,0,-0.8905086823,0.1559789951,-3.3214160986\O,0
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 7688736,-0.1095345825,-9.9934009447\C,0,-0.2856968005,-0.108617823,-11
 .4241630795\C,0,-1.3656666477,-0.3224839275,-12.4896449305\C,0,-0.8213
```

771452,-0.3217820069,-13.921746311\C,0,-0.813751084,0.3767478223,8.004
3318302\C,0,0.1746140839,1.2237431531,8.8125359176\C,0,-0.091078113,1.
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1[B]a

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