Adducts of Carbon Black with a Biosourced Janus Molecule for Elastomeric Composites with Lower Dissipation of Energy

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Supplementary material

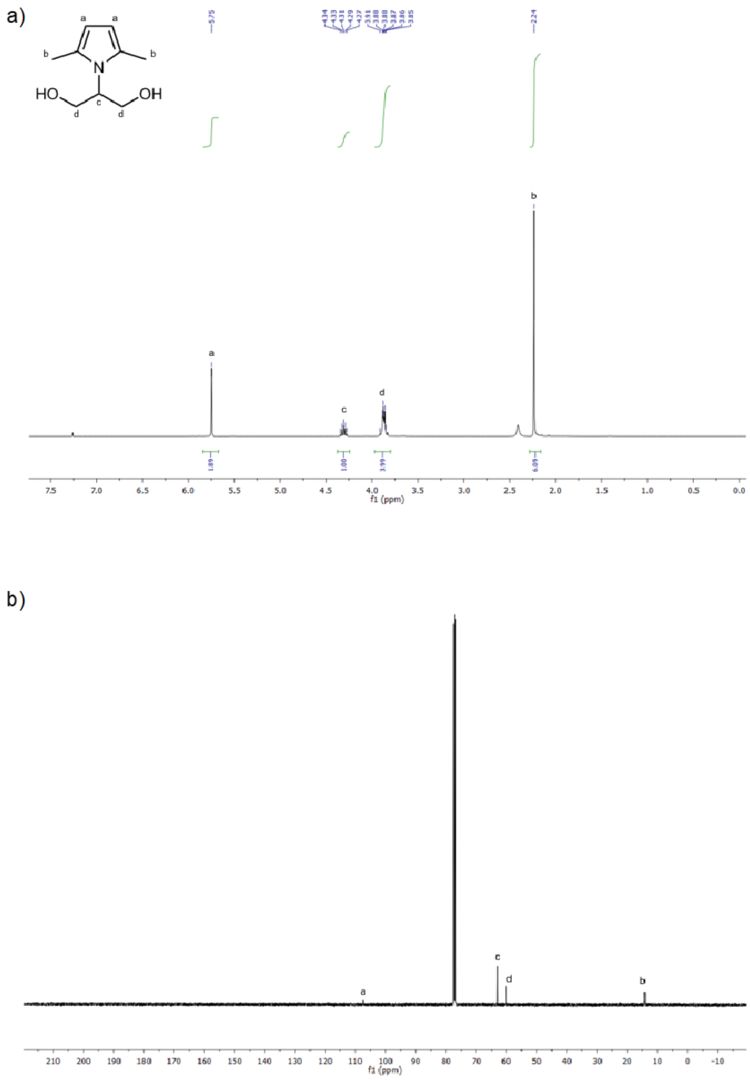

Figure S1. ^{1}H (a, $CDCl_3$, 400 MHz) and ^{13}C (b, $CDCl_3$, 100 MHz) NMR spectra of 2-(2,5-dimethyl-1*H*-pyrrol-1-yl)-1,3-propanediol (serinol pyrrole, SP).

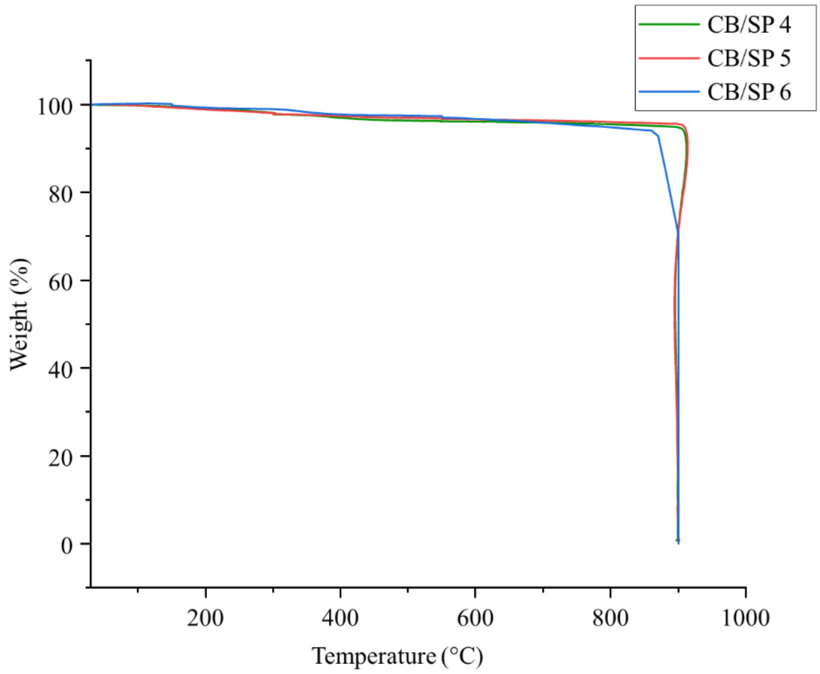

Figure S2 Thermograph from TGA analysis of CB/SP-4, CB/SP-5 and CB/SP-6.

Table S1 Structural parameters from X-ray analysis for pristine CB N326 and CB/SP-6 adduct

Sample	d_{002} (nm)	$D_\perp$ (nm)	$D_\parallel$ (nm)	$D_\parallel / D_\perp$	$D_\perp / d_{002}s$
CB N326	0.34	1.51	1.54	1.02	4.4
CB – SP 4	0.34	1.54	2.12	1.38	4.5
CB – SP 5	0.34	1.62	2.03	1.25	4.7

The Bragg's law was used to determine the interlayer distance and the Scherrer equation to estimate the size of the crystallites, orthogonal ($D_\perp$), and parallel ($D_\parallel$) to the structural layers, through the peak shape analysis of the (002) reflection ($D_\perp$) and the (100) reflection. The ratio ($D_\parallel$) / ($D_\perp$) gives the shape anisotropy.

Table S2 Data from the crosslinking of composites of Table 1[a,b]

	Silica	**CB/SP-6**
M_L [dNm]	1.95	2.07
M_H [dNm]	15.4	19.74
M_H-M_L [dNm]	13.45	17.67
t_{S1} [min]	2.44	2.12
t_{90} [min]	4.02	3.43
Curing rate [dNm/min][c]	8.51	13.48

[a] For experimental details see the experimental part

[b] M_L: minimum modulus, M_H: maximum modulus, t_{s1}: induction crosslinking time, t_{90}: optimum crosslinking time,

[c] the curing rate was calculated by means of the following equation:

$$Curing\ Rate = \frac{M_H - M_L}{t_{90} - t_{s1}}$$

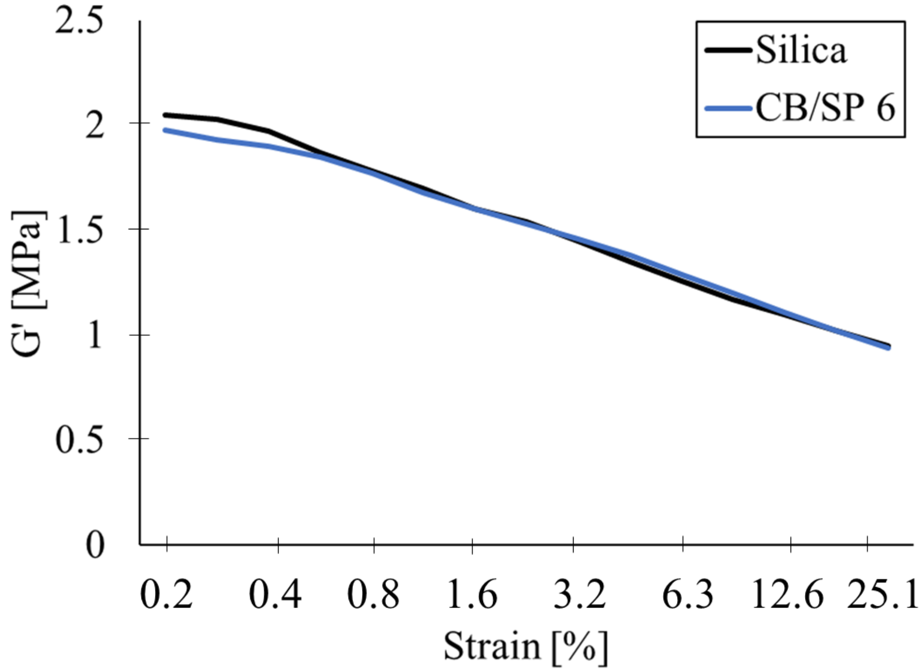

Figure S3. G’ vs strain for composites of **Table 1**

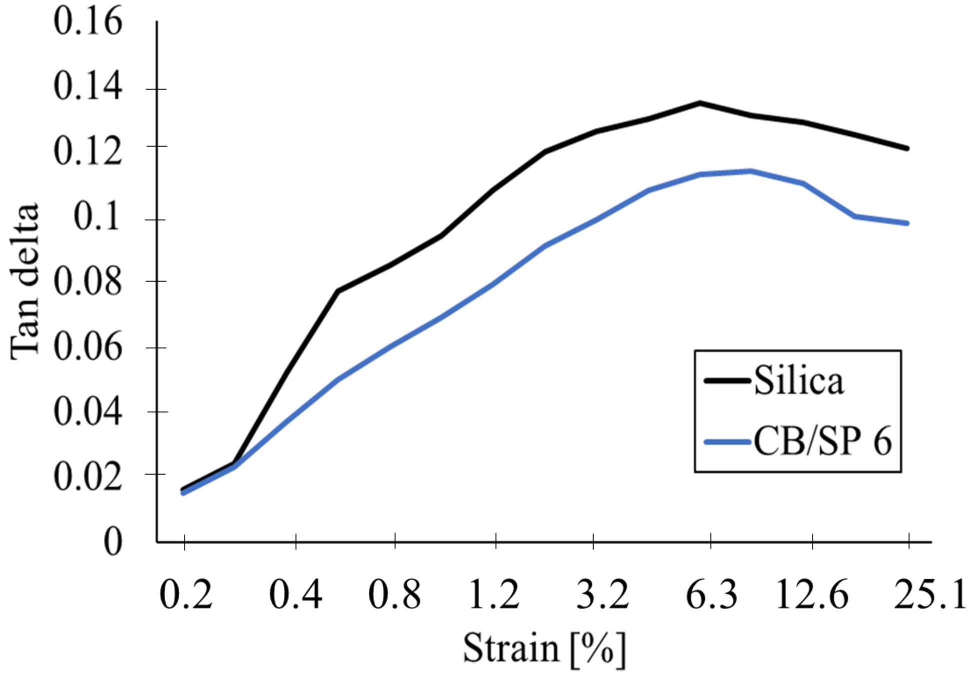

Figure S4. Tan delta vs strain for composites of **Table 1**

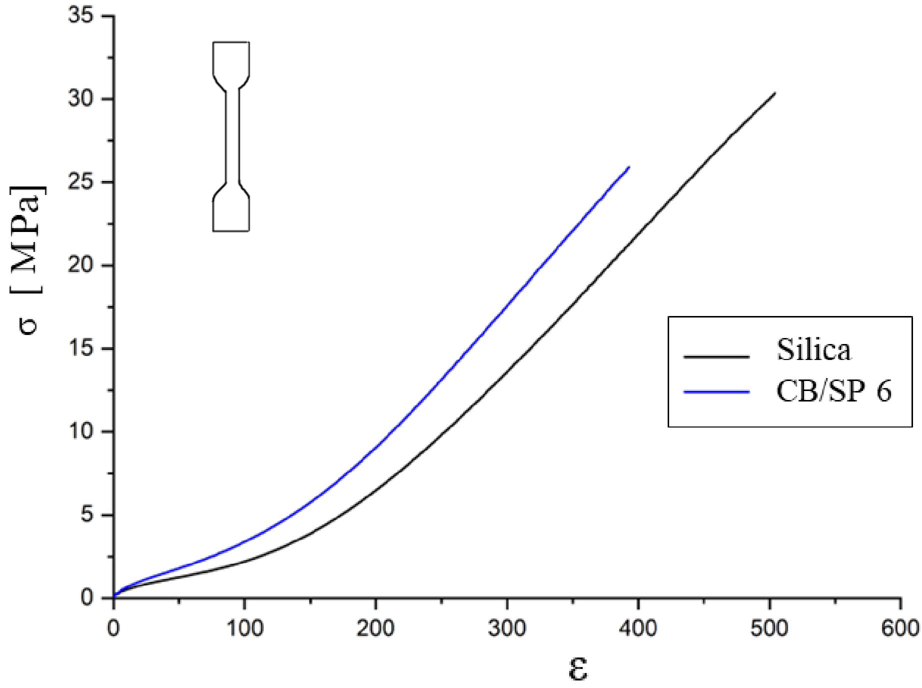

Figure S5. Tensile properties for composites of **Table 1**

Table S3 Data from the crosslinking reaction of composites of Table 2[a,b]

	Silica	CB/SP-4	CB/SP-5
M_L [dNm]	3.6	2.75	3.01
M_H [dNm]	22.42	21.21	23.29
t_{90} [min]	4.26	4.35	4.21
t_{s1} [min]	2.33	2.50	2.38
Curing rate [dNm/min] [c]	9.75	9.98	11.08

[a] For experimental details see the experimental part [b] M_L: minimum modulus, M_H: maximum modulus, t_{s1}: induction crosslinking time, t_{90}: optimum crosslinking time,

[c] the curing rate was calculated by means of the following equation:

$$Curing\ Rate = \frac{M_H - M_L}{t_{90} - t_{s1}}$$

Table S4. Dynamic-mechanical properties from shear tests of the uncured composites of Table 2.

	Silica	CB/SP-4	CB/SP-5
$G'_{0.2\%}$ [MPa]	1.43	1.16	1.15
$G'_{25\%}$ [MPa]	0.35	0.30	0.31
$\Delta G'$ [MPa]	1.08	0.86	0.84
$\Delta G'/G'_{0.2\%}$	0.76	0.74	0.73
G''_{max} [MPa]	0.42	0.33	0.31
$Tan(\delta)_{max}$	0.45	0.44	0.42

Table S5. Dynamic-mechanical properties from shear tests of the cured composites of Table 2

	Silica	CB/SP-4	CB/SP-5
$G'_{0.2\%}$ [MPa]	4.03	3.47	3.84
$G'_{25\%}$ [MPa]	1.25	1.18	1.30
$\Delta G'$ [MPa]	3.09	2.54	2.74
$\Delta G'/G'_{0.2\%}$	0.77	0.73	0.71
G''_{max} [MPa]	0.47	0.38	0.41
$Tan(\delta)_{max}$	0.21	0.19	0.19

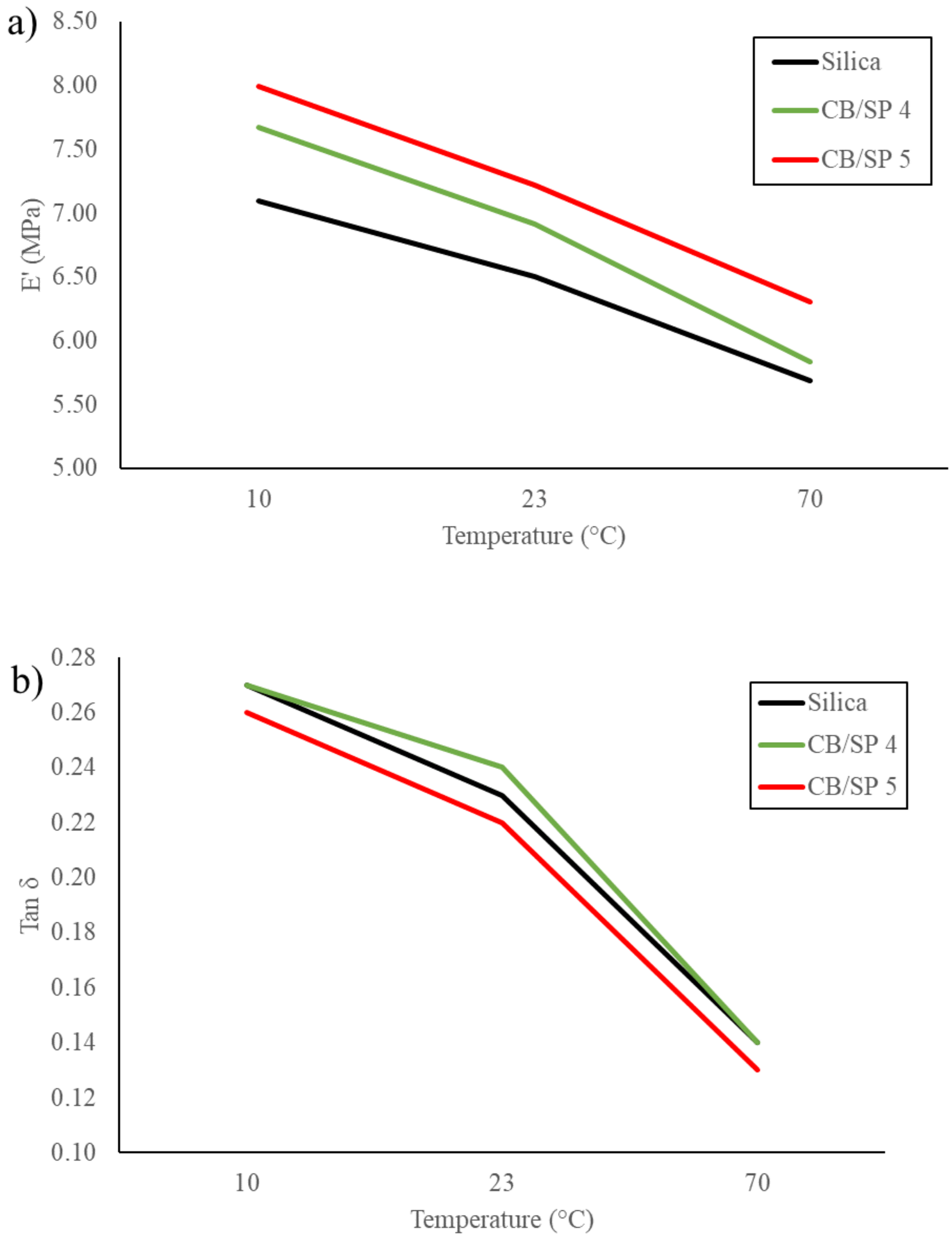

Figure S6 Storage modulus (a) and tan δ (b) curves of IR composites.

Table S6 Tensile properties of composites of **Table 2**

	Reference	**CB/SP-4**	**CB/SP-5**
σ_{50} [MPa]	1.54	1.69	1.91
σ_{100} [MPa]	2.56	2.95	3.48
σ_{300} [MPa]	12.60	14.67	16.44
σ_{300}/ σ_{100}	4.92	4.97	4.72
σ_b [MPa]	24.19	25.39	25.70
ε_b [%]	487.89	456.63	436.35
Energy [MJ/m^3]	50.18	49.66	49.84

Table S7 Optic microscopy CB dispersion results of IR-based rubber composites

	Silica	**CB/SP 4**	**CB /SP 5**
Filler	CB	CB	CB
Filler %	16	28	28
N° Aggregates	10	4	16
Average diameter [µm]	16.9	21.1	19.7
Undispersed filler %	0.27	0.16	0.32