Erratum: "Monte Carlo study of liquid crystal phases of hard and soft spherocylinders" [J. Chem. Phys. 117, 2934 (2002)]

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The Monte Carlo NPT simulations for the repulsive soft spherocylinder model (SRS) presented in the paper were performed at a reduced temperature of $T^*=20$, instead of $T^*=5$ as stated throughout the article, due to an incorrect input factor in the numerical routine.

The correct simulation for the SRS model at $T^*=5$ has been newly performed, following the methodology described in the article. The thermodynamic data resulting from the expansion of the SRS fluid along the $T^*=5$ isotherm are given in Table I of this Erratum. Hence, this table is the counterpart to Table IV of the original paper actually showing data from an expansion run of the SRS fluid at $T^*=20$. Furthermore, it can also be directly compared to Table II for the expansion of the SWSC fluid at $T^*=5$. As can be seen, the pressures and coexistence densities for the isotropic–nematic and nematic–smectic A transitions for the SRS fluid at $T^*=5$, as obtained by averaging the pressures of the two boundary states of each phase transition and from their individual densities, are $P^*_{\mathrm{I-N}}=1.175$; $\rho^*_{\mathrm{I}}=0.0990$, $\rho^*_{\mathrm{N}}=0.1027$, and $P^*_{\mathrm{N-SmA}}=1.625$; $\rho^*_{\mathrm{N}}=0.1191$, $\rho^*_{\mathrm{SmA}}=0.125$, respectively. Even though these coexistence densities are significantly smaller than the ones found at $T^*=20$, the same qualitative shift of both the I–N and the N–Sm A transitions toward higher densities with respect to the HSC and SWSC fluids is still observed. Thus, the justification for such shift given in the paper in terms of the smaller magnitude in the SRS fluid of entropic excluded volume effects in comparison to its hard core counterparts, actually based on results at $T^*=20$ for the SRS model, indeed stays valid at $T^*=5$. As discussed in the paper, this trend is expected to reverse at lower temperatures as a consequence of the longer range of the repulsive wall of the SRS, in consonance with the findings of Earl *et al.* [Mol. Phys. **99**, 1719 (2001)].

TABLE I. Isothermal–isobaric Monte Carlo (MC-NPT) simulation results from the expansion of the SRS fluid of molecular elongation $L^*=L/\sigma=5$, at temperature $T^*=kT/\varepsilon=5$. This table is the counterpart to Table IV of the original paper, actually showing data from an expansion run of the SRS fluid at a greater temperature, $T^*=20$.

$P^*=P\cdot\sigma^3/kT$	$P^*\cdot v_{\mathrm{HSC}}/\sigma^3$	$\rho^*=\rho\cdot\sigma^3$	$\eta=\rho\cdot v_{\mathrm{HSC}}$	$U^*=U/\varepsilon$	S	Phase
1.00	4.45	0.0930(6)	0.414(3)	4.6(2)	0.127(5)	I
1.10	4.90	0.0968(6)	0.431(3)	4.9(2)	0.135(4)	I
1.15	5.12	0.0990(6)	0.440(3)	5.1(2)	0.209(5)	I
1.20	5.34	0.1027(6)	0.457(3)	5.2(2)	0.566(4)	N
1.25	5.56	0.1049(6)	0.467(3)	5.4(2)	0.623(4)	N
1.30	5.79	0.1078(6)	0.480(3)	5.6(2)	0.731(4)	N
1.35	6.01	0.1092(6)	0.486(3)	5.7(2)	0.739(4)	N
1.40	6.23	0.1114(6)	0.496(3)	5.9(2)	0.776(3)	N
1.50	6.68	0.1150(6)	0.512(3)	6.2(2)	0.821(3)	N
1.60	7.12	0.1191(8)	0.530(4)	6.5(2)	0.862(3)	N
1.65	7.34	0.125(1)	0.558(5)	6.4(2)	0.908(3)	Sm A
1.70	7.57	0.1281(8)	0.570(4)	6.5(2)	0.924(3)	Sm A
1.75	7.79	0.1303(8)	0.580(4)	6.6(2)	0.929(3)	Sm A
1.80	8.01	0.1328(8)	0.591(4)	6.7(2)	0.936(3)	Sm A
1.85	8.23	0.1346(8)	0.599(4)	6.8(2)	0.942(3)	Sm A
1.90	8.46	0.1366(8)	0.608(4)	6.9(2)	0.933(3)	Sm A
2.00	8.90	0.1393(8)	0.620(4)	7.2(2)	0.862(3)	Sm A
2.10	9.35	0.1418(8)	0.631(4)	7.5(2)	0.942(3)	Sm A

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