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Short Communication

Transport properties of argon and krypton according to L-J (12-6) potential in the temperature range 90-270 K

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Abstract

New values of the potential parameters of the Lennard-Jones (12-6) model derived for argon and krypton in the temperature range 400-2500 K are found useful in describing the transport properties in the low temperature range 90-270 K as well. The agreement of the predicted values with the sophisticated potentials as well as with the recent experimental data is found to be very good.

Key words : Transport coefficients, Lennard-Jones potential, argon, krypton, low temperatures.

Lennard-Jones (12-6) potential with modified parameters has been found[1,2] to be capable of reproducing the transport properties of rare gases with accuracies comparable to those of the sophisticated potentials in the temperature range 400-2500 K. Recently, Shashkov *et al*[3] have reported new experimental data on thermal conductivity of argon and krypton in the temperature range 90-270 K. It is, therefore, appropriate to examine the suitability of the L-J (12-6) potential for predicting the transport properties of argon and krypton in the temperature range 90-270 K.

The modified potential parameters suggested for argon[1] are :

$\epsilon/k = 135$ K, $\sigma = 3 \cdot 345$ Å and those for krypton[2] are :

$\epsilon/k = 193$ K, $\sigma = 3 \cdot 566$ Å.

The transport properties of argon and krypton calculated on the basis of these modified parameter values in conjunction with the kinetic theory expressions[4] are given in Tables I and II respectively in the temperature range 90–270 K. The collision integrals and the higher approximation correction factors suggested by Klein and Smith[5] were used for the calculations.

Table I

Predicted values of transport properties of argon based on L–J (12–6) potential

Temperature K	Thermal conductivity $mWm^{-1} K^{-1}$	Viscosity $\mu g/cm. s$	Self-diffusion coefficient cm^2/s
90	5·66	72·5	0·0179
100	6·31	80·8	0·0221
120	7·62	97·5	0·0320
140	8·90	114·0	0·0428
150	9·55	122·3	0·0498
160	10·18	130·3	0·0566
180	11·40	146·0	0·0712
200	12·60	161·3	0·0873
220	13·76	176·1	0·1046
240	14·88	190·4	0·1232
250	15·42	197·4	0·1330
260	15·96	204·3	0·1431
270	16·49	211·1	0·1535

Table II

Predicted values of transport properties of krypton based on L–J (12–6) potential

Temperature K	Thermal conductivity $mWm^{-1} K^{-1}$	Viscosity $\mu g/cm. s$	Self-diffusion coefficient cm^2/s
90	2·83	76·1	0·0090
100	3·13	84·2	0·0111
120	3·77	101·2	0·0161
140	4·41	118·5	0·0220
150	4·74	127·3	0·0253
160	5·07	136·2	0·0288
180	5·72	153·5	0·0366
200	6·46	173·6	0·0451
220	7·11	191·0	0·0544
240	7·74	208·0	0·0645
250	8·06	216·5	0·0699
260	8·36	224·7	0·0754
270	8·68	233·0	0·0812

These calculated transport coefficients have been compared with the values based on the sophisticated potentials ESBFW for argon[6] and BDVKS for krypton[7] in fig. 1 (thermal conductivity), fig. 2 (viscosity) and fig. 3 (self-diffusion coefficients). ESBFW and BDVKS potentials have been found by Nain *et al*[8] to be the best models for describing the transport properties of argon and krypton respectively. The agreement in the case of thermal conductivity of argon is very good (curve 1, fig. 1), the average absolute and maximum deviations being 1·5 and 2·0 per cent respectively, whereas in the case of krypton (curve 2, fig. 1) the agreement below 150 K is not at all good. The average absolute and maximum deviations in the case of viscosity of argon (curve 1, fig. 2) are 1·6 and 2·0 per cent respectively, but like thermal conductivity the agreement for viscosity of krypton (curve 2, fig. 2) is not satisfactory below 150 K. Similarly, the agreement for self-diffusion coefficient of argon (curve 1, fig. 3) is excellent (the average absolute and maximum deviations are 0·9 and 1·3 per cent respectively), but for krypton the same trend is observed as in thermal conductivity and viscosity.

A comparison of the thermal conductivity values calculated on the basis of L–J (12–6) potential with the experimental data of Shashkov *et al*[3], shown in fig. 1, reveals that

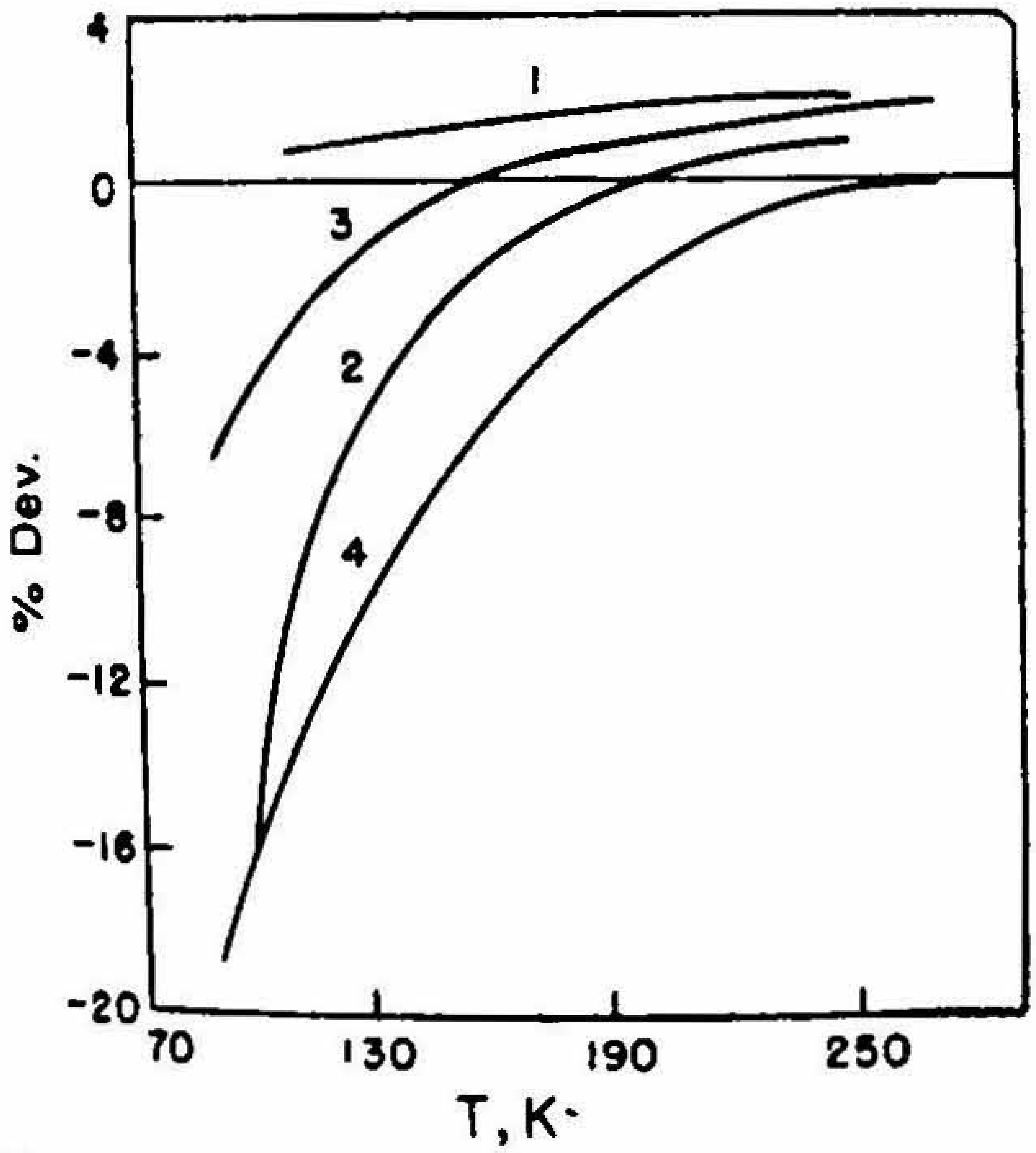

FIG. 1. Comparison of the thermal conductivity based on the predictions of L–J (12–6) potential with the predictions of sophisticated potentials and experimental data.

Curve 1 : Ar (ESBFW potential, Aziz[6])

Curve 2 : Kr (BDVKS potential, Buck *et al*[7]) (Common for figs. 2 and 3 too)

Curve 3 : data on Ar (Shashkov *et al*[3])

Curve 4 : data on Kr (Shashkov *et al*[3])

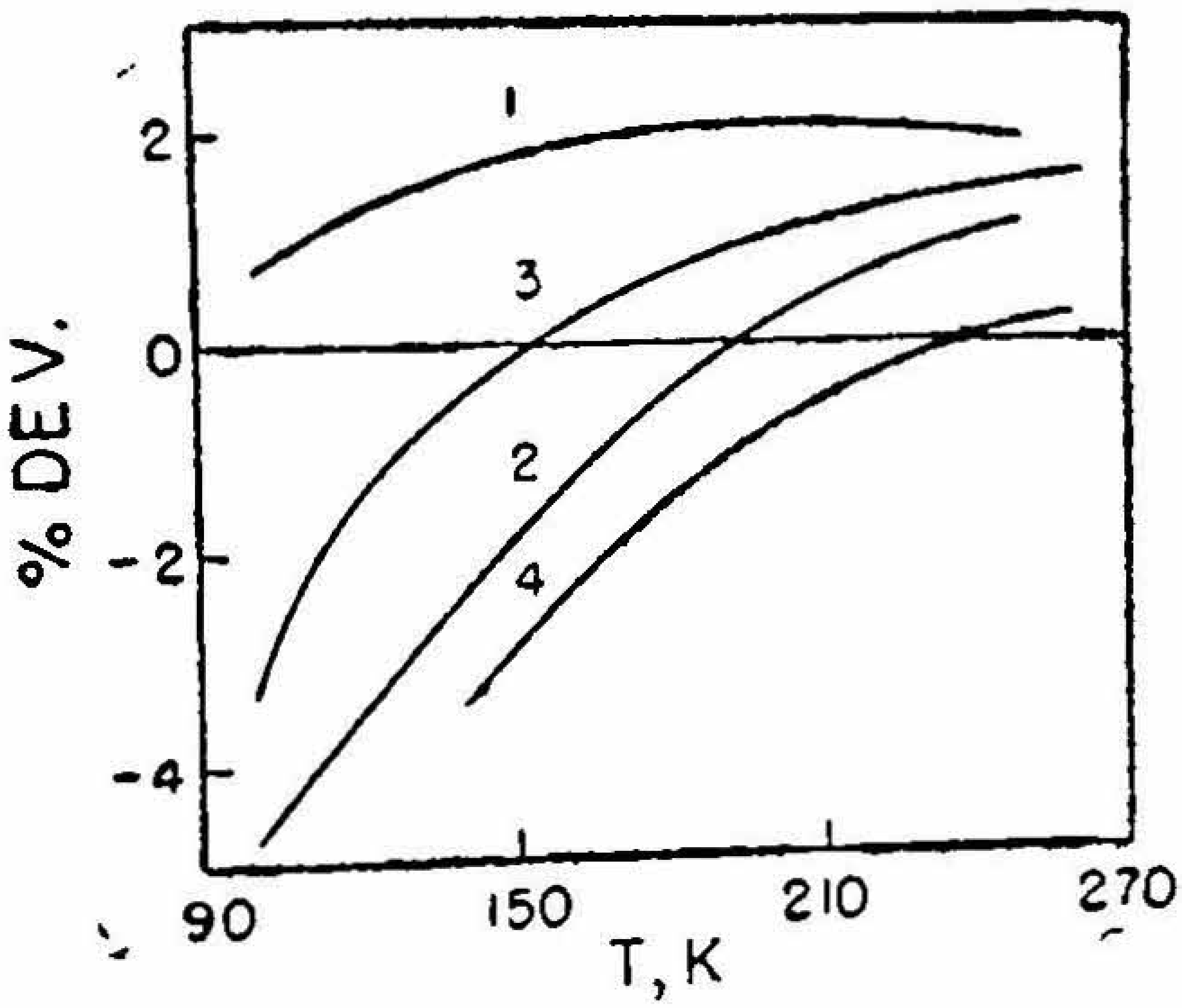

FIG. 2. Comparison of viscosity based on the predictions of L–J (12–6) potential with the predictions of sophisticated potentials and recommended data.

Curve 3 : data on Ar (Maitland and Smith[9])

Curve 4 : data on Kr (Maitland and Smith[9])

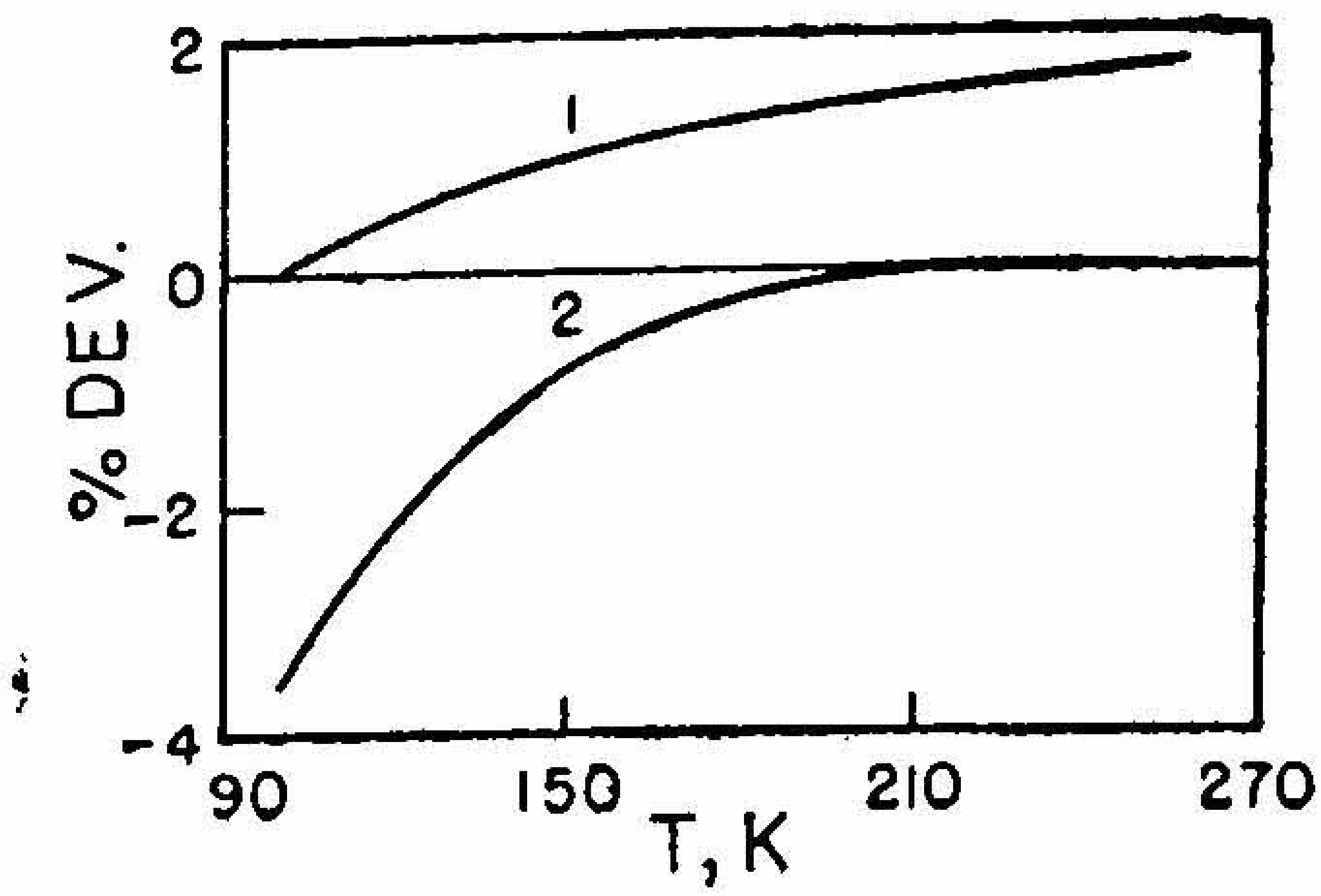

FIG. 3. Comparison of self-diffusion coefficient based on L–J (12–6) potential and the sophisticated potentials.

the agreement is very good for argon (curve 3) above 120 K, but for krypton (curve 4) it is good above 200 K only. A similar inference can be drawn if the viscosity values calculated on the basis of L–J (12–6) potential are compared with the values recommended by Maitland and Smith[9], curves 3 and 4 of fig. 2 representing argon and krypton respectively.

The new parameters of L–J (12–6) potential were earlier found satisfactory in the temperature range 400–2500 K for argon[1] and in the range 400–2000 K for krypton[2]. Thus, the simple L–J (12–6) potential with the modified parameters is capable of reproducing the transport properties in both the low- and high-temperature ranges—90–2500 K for argon and 150–2000 K for krypton—with the accuracies comparable to those of the sophisticated potentials.

This study also affirms that the measurements on thermal conductivity taken on two different apparatuses in different temperature ranges are reliable in the temperature range 120–2500 K for argon and in the range 200–2000 K for krypton and are compatible with the viscosity values as the latter were used to derive the distance parameter[1,2].

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