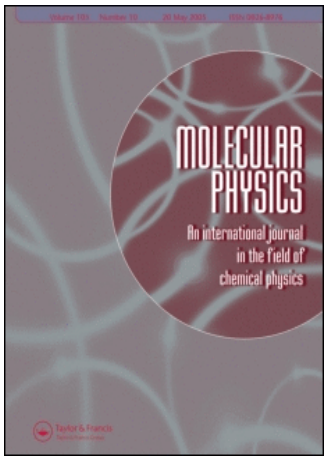

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Excess free energy of different water models computed by Monte Carlo methods

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Excess free energy of different water models computed by Monte Carlo methods

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(*Molecular Physics*, 1982, **47**, 1307)

Hermans, Pathiaseril and Anderson [1] have pointed out an error in the calculation of the free energy of SPC water. Thermodynamic integration over the path

$$E(\lambda, X^N) = \lambda^{k*} E_1(X^N) + (1 - \lambda)^{k*} E_0(X^N) \quad (1)$$

with $k = 4$, as described in [2] and tested in [3], for the SPC and MCY models of water confirmed their results for the SPC water and also verified the MCY result. The source of the error in the SPC result was traced down to a programming error in the calculation of the free energy difference between the SPC and MCY models. The table gives the results of these new thermodynamic integration calculations. In addition, they demonstrate the efficiency of the path of equation (1) for the calculation of liquid free energies.

Free energy differences calculated with thermodynamic integration.

Ref.	Syst.	R_c	N_w	n_q	k_λ	PBC	ΔA (100 K)	ΔA (300 K)	ΔA (600 K)	ΔA (1000 K)
IG	SPC	7·0	64	5	4	FCC	−23·66	−23·70 ± 0·23	−23·66 ± 0·15	−23·63 ± 0·19
IG	SPC	7·0	64	8	4	FCC	−23·53	−23·75 ± 0·25	−23·74 ± 0·20	−23·81 ± 0·13
IG	SPC	6·0	80	5	4	SC	−24·20	−24·16 ± 0·36	−24·11 ± 0·36	−24·11 ± 0·30
IG	MCY	7·0	64	5	4	FCC	−16·71	−16·86 ± 0·19	−16·86 ± 0·15	−16·90 ± 0·13
MCY	SPC	7·0	64	3	1	FCC	−6·93	−6·93 ± 0·16	−6·82 ± 0·16	

ΔA is the free energy difference between systems labelled Syst. and Ref. in kJ mol^{-1}. K refers to 1000 Monte Carlo steps. IG, SPC and MCY stand for ideal gas, SPC water and MCY water, respectively. N_w is the number of water molecules in the simulation cell. n_q is the number of thermodynamic integration quadrature points. SC and FCC stand for simple cubic and face-centred cubic (truncated octahedron) periodic boundary conditions respectively. k_λ is the exponent in equation (1). R_c is the potential cut off radius. Error estimates represent 2 S.D.

A typographical error on p. 1311 gave the temperature at which the calculations were run as 250°C. It was 25°C.

The author is grateful to Professor J. Hermans for communicating their results before publication.

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