



Correction: A new potential for methylammonium lead iodide

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Correction for 'A new potential for methylammonium lead iodide' by C. M. Handley *et al.*, *Phys. Chem. Chem. Phys.*, 2017, **19**, 2313–2321.

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A correction has been made to the table of parameters, Table 1, where unfortunately, a redundant line of parameters, remained within the text. This line “I H2 1142.79 0.025” is not part of this parameter set. The removal of this line of parameters has no impact on the results present within this paper, as this error is only with respect to the parameters as printed within this paper, and not within the input files of the simulations used to generate the results of this paper. We apologise for any confusion this may have incurred.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.



Table 1 Parameterisation

Buckingham potentials ($A \exp(-\rho/r) - C/r^6$)						
		A (eV)	ρ (Å)	C (eV Å ⁻⁶)		
Pb	I	6876.2	0.32367	510.0		
Pb	Pb	17032.7	0.285	1100.19		
I	I	1791.81	0.46529	470		
Lennard-Jones 12-6 potential ($X/r^{12} - Y/r^6$)						
		X (eV Å ¹²)	Y (eV Å ⁶)			
Pb	C	100000.89	121.072			
Pb	N	90000.60	131.856			
Pb	H1	1435.31	8.789			
Pb	H2	3590.72	16.445			
I	C	15180.13	0.743			
I	N	40465.16	0.809			
I	H1	1134.51	0.054			
I	H2	942.79	0.025			
C	C	45262.52	29.32			
C	N	43197.02	31.98			
N	N	40975.84	34.77			
C	H1	986.76	2.66			
C	H2	111.38	0.90			
N	H1	875.63	2.80			
N	H2	92.25	0.91			
H1	H1	8.76	0.15			
H1	H2	0.40	0.033			
H2	H2	0.006	0.004			
Two body potentials ($\frac{1}{2}k(r - r_0)^2$)						
		k (eV Å ⁻²)	r ₀ (Å)			
C	N	25.480	1.499			
C	H1	29.395	1.091			
N	H2	32.024	1.033			
Three body potentials ($((k/2)(\theta - \theta_0)^2)$)						
			k (eV)	θ ₀ (°)		
N	C	H1	4.254	108.0		
C	N	H2	4.009	110.11		
H1	C	H1	3.388	110.74		
H2	N	H2	3.517	108.11		
4 body potentials ($A[1 + \cos(m\phi - \delta)]$)						
				A (eV)	δ (°)	m
H1	C	N	H2	0.00675	0.0	3
Charges						
				q		
Pb				1.263		
I				-0.632		
C				0.072		
N				-0.832		
H1				0.058		
H2				0.405		

