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CORRECTION

Cite this: *Phys. Chem. Chem. Phys.*, 2017, **19**, 14185

Correction: A new potential for methylammonium lead iodide

C. M. Handley and C. L. Freeman*

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

DOI: 10.1039/c7cp90104f

rsc.li/pccp

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.

Department of Materials Science and Engineering, University of Sheffield, Mappin Street, Sheffield, S1 3JD, UK. E-mail: c.l.freeman@sheffield.ac.uk

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