Rounding and Uncertainties in Determining Parameters and Properties from Fits to Experimental Data

or

A Failure to Round Data-Analysis Parameters Appropriately May Make them Useless!

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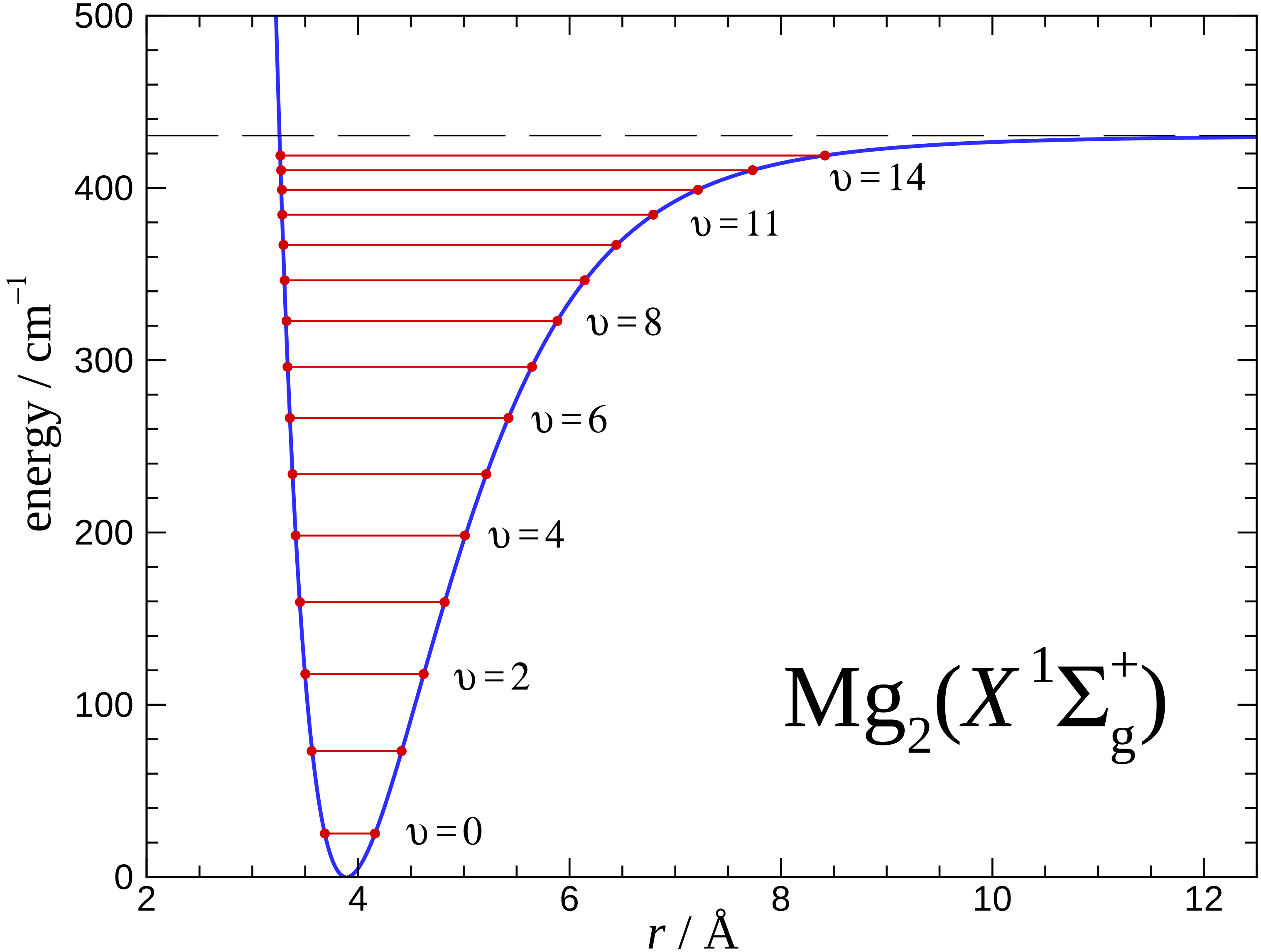
Research supported by the Natural Sciences and Engineering Research Council of Canada.

Consider a recent analysis of extensive high-quality data for the ground state of Mg_2



A direct fit to 4741 data with accuracies in the range $0.005 - 0.05$ cm^{-1} yielded an analytic potential defined by the parameters . . .

Table I. Parameters of "X-representation" potential energy function from fit to $Mg_2(X\,^1\Sigma_g^+)$ data.[a]

$$V(r) \;=\; \sum_{i=1}^{n} a_i \xi(r)^i \qquad \text{with} \qquad \xi(r) \;=\; \frac{r - R_m}{r + b\,R_m}$$

	parameter	
R_m	[3.89039]	
a_1	$-0.770548964164001222\times10^{-2}$	
a_2	$0.705289125191954554\times10^{4}$	
a_3	$-0.179327568767261764\times10^{5}$	
a_4	$0.228278059421389626\times10^{5}$	
a_5	$-0.144881409083685430\times10^{5}$	
a_6	$-0.638841357804591826\times10^{5}$	
a_7	$0.201722011755478365\times10^{6}$	
a_8	$-0.286947115902508434\times10^{6}$	
a_9	$0.528096212291666190\times10^{6}$	
a_{10}	$-0.841629359994647559\times10^{6}$	
a_{11}	$0.510277917592615297\times10^{6}$	
$\overline{dd}$	1.46224	*is the dimensionless RMS Deviation* $\equiv \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i^{\rm calc}-y_i^{\rm obs}}{unc(y_i)}\right)^2$

[a] H. Knöckel and S. Rühmann and E. Tiemann, *J. Chem. Phys.* **138**, 94303 (2013).

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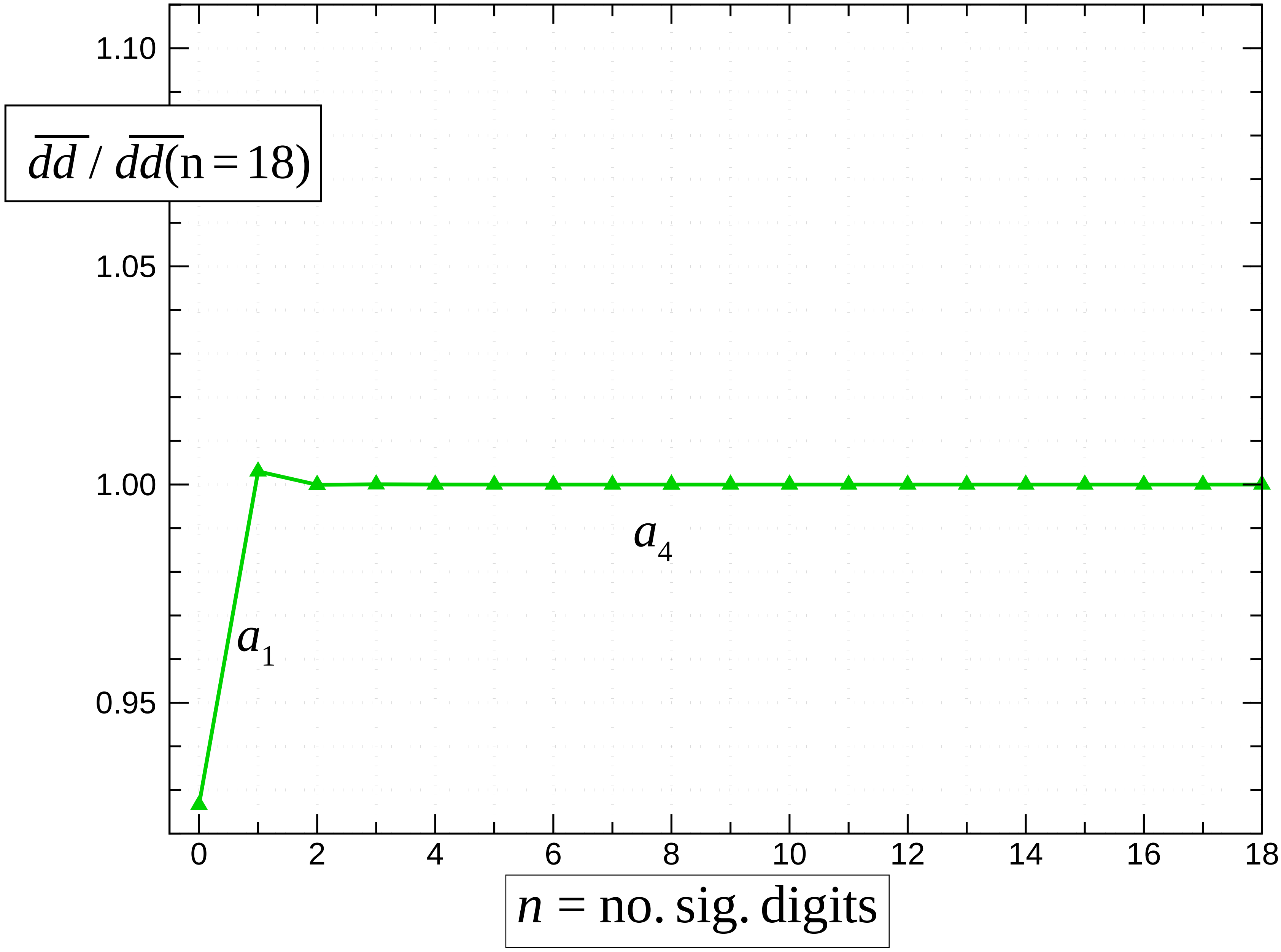
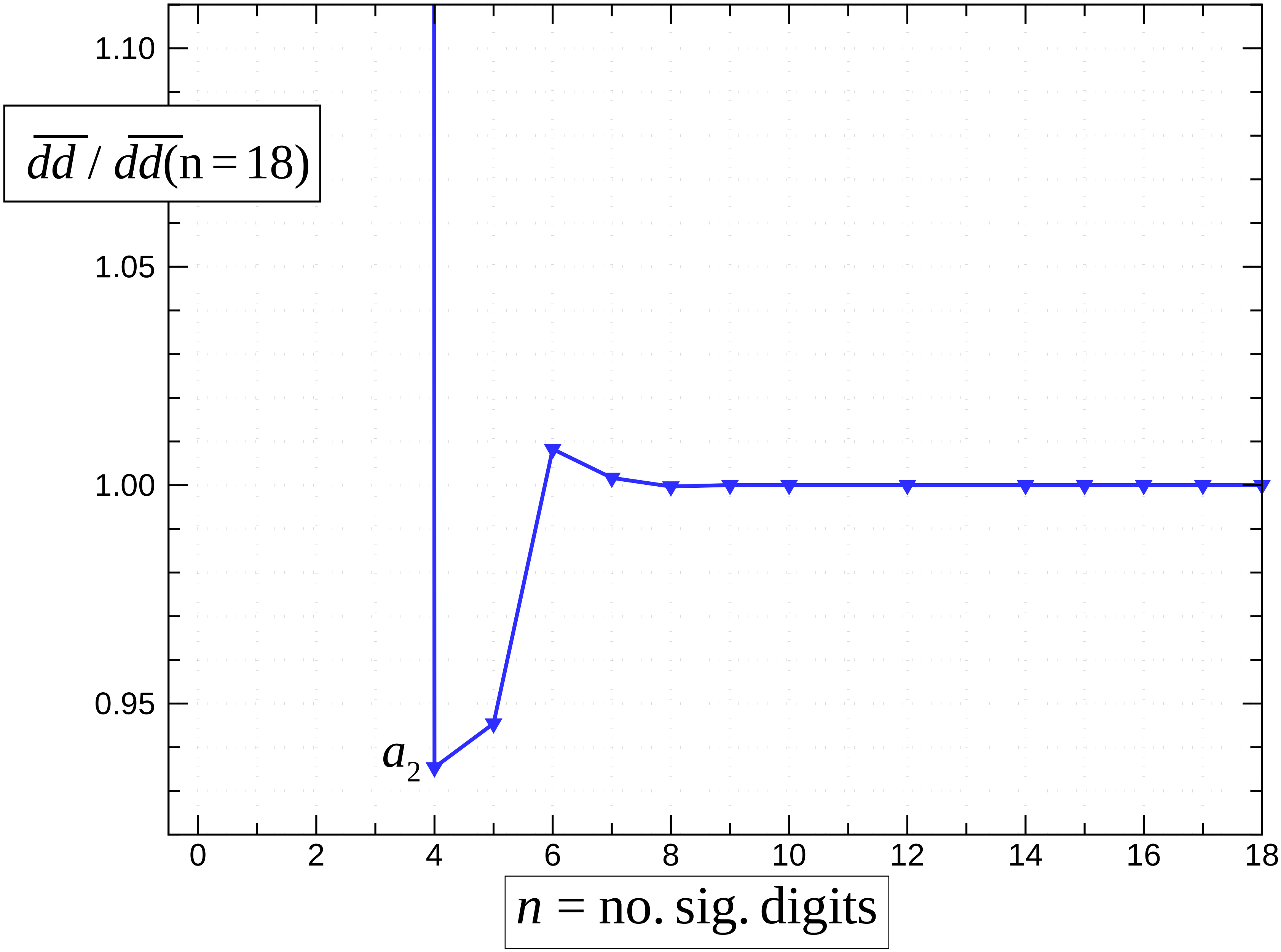
But 18 digits is an awful lot! ***Can we round them off in a sensible way ?***

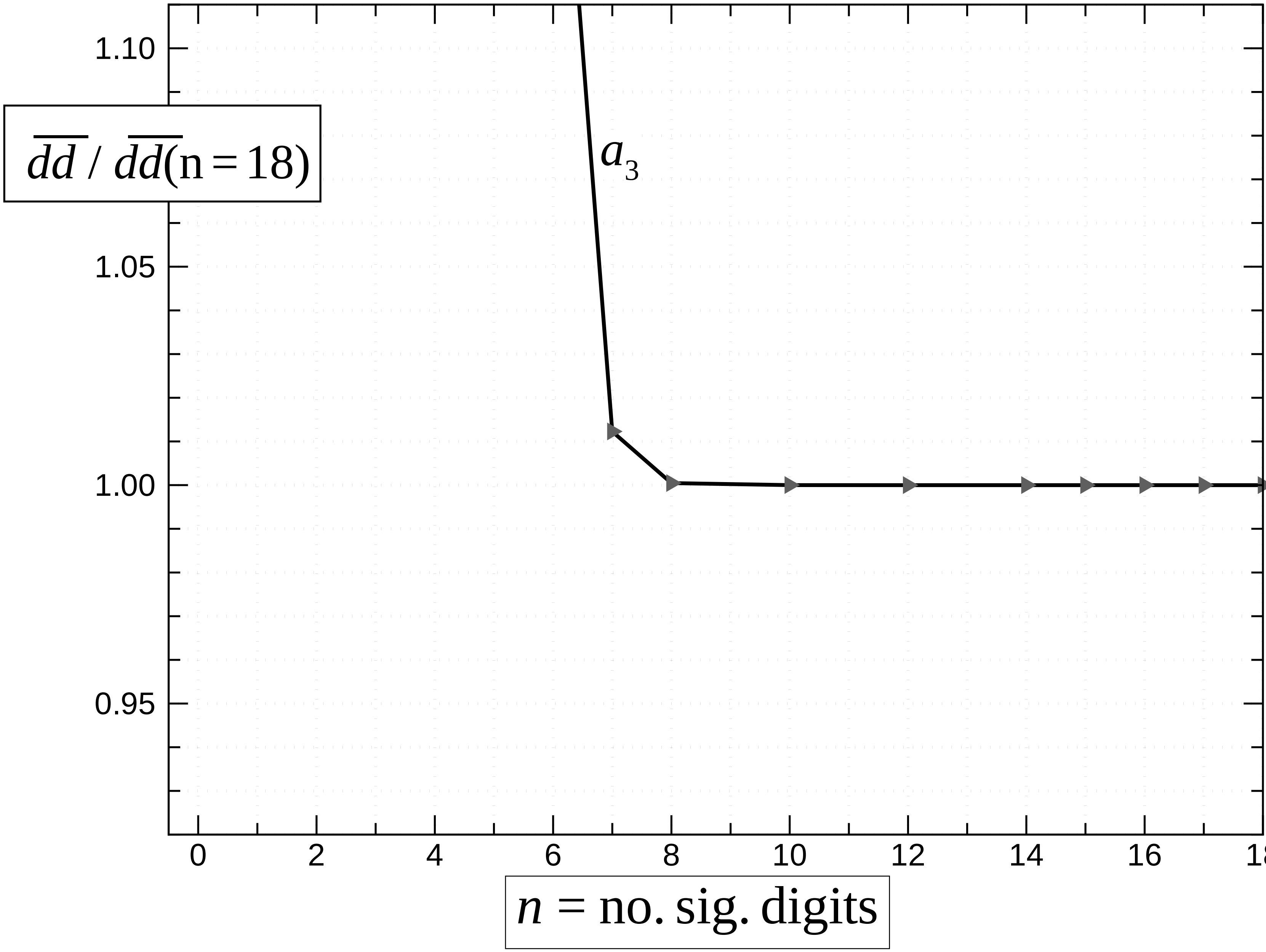
What happens to $\overline{dd}$ if we round parameter a_1 at its n^{th} significant digit ?



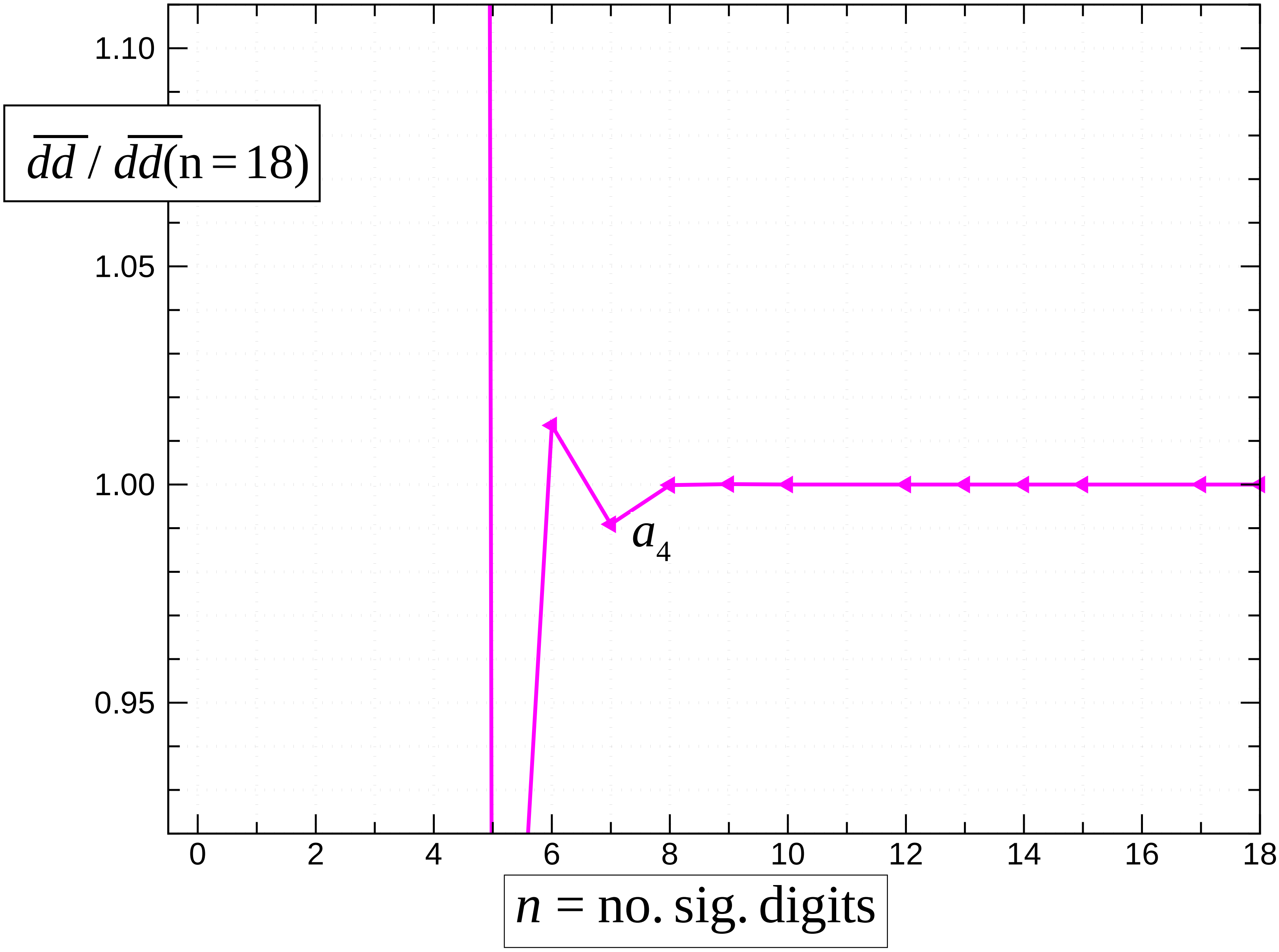
What happens to $\overline{dd}$ if we round parameter a_2 at its n^{th} significant digit?



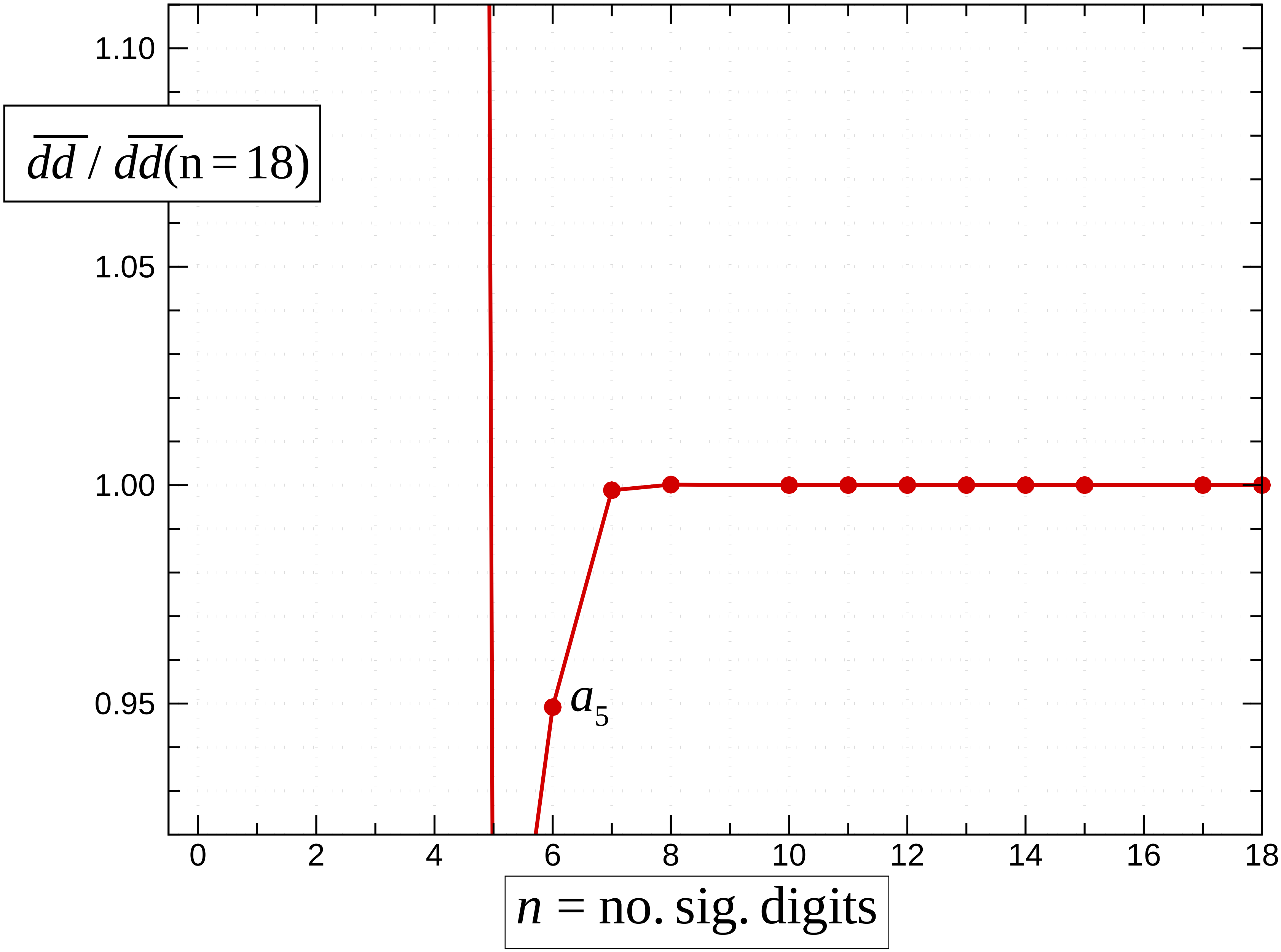
What happens to $\overline{dd}$ if we round parameter a_3 at its n^{th} significant digit ?



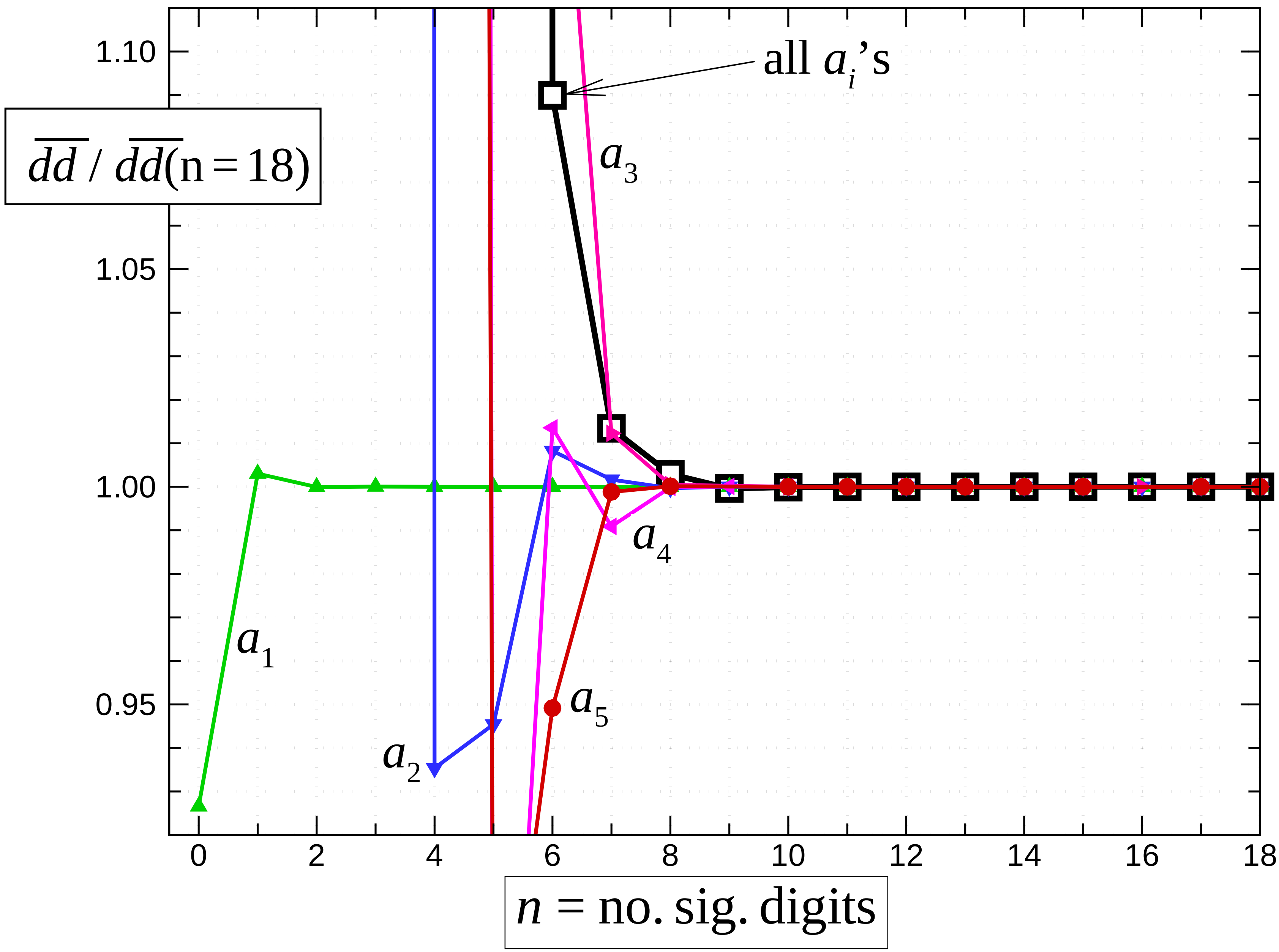
What happens to $\overline{dd}$ if we round parameter a_4 at its n^{th} significant digit ?



What happens to $\overline{dd}$ if we round parameter a_5 at its n^{th} significant digit ?



And what happens if we round ***all*** a_i parameters at their n^{th} significant digit ?



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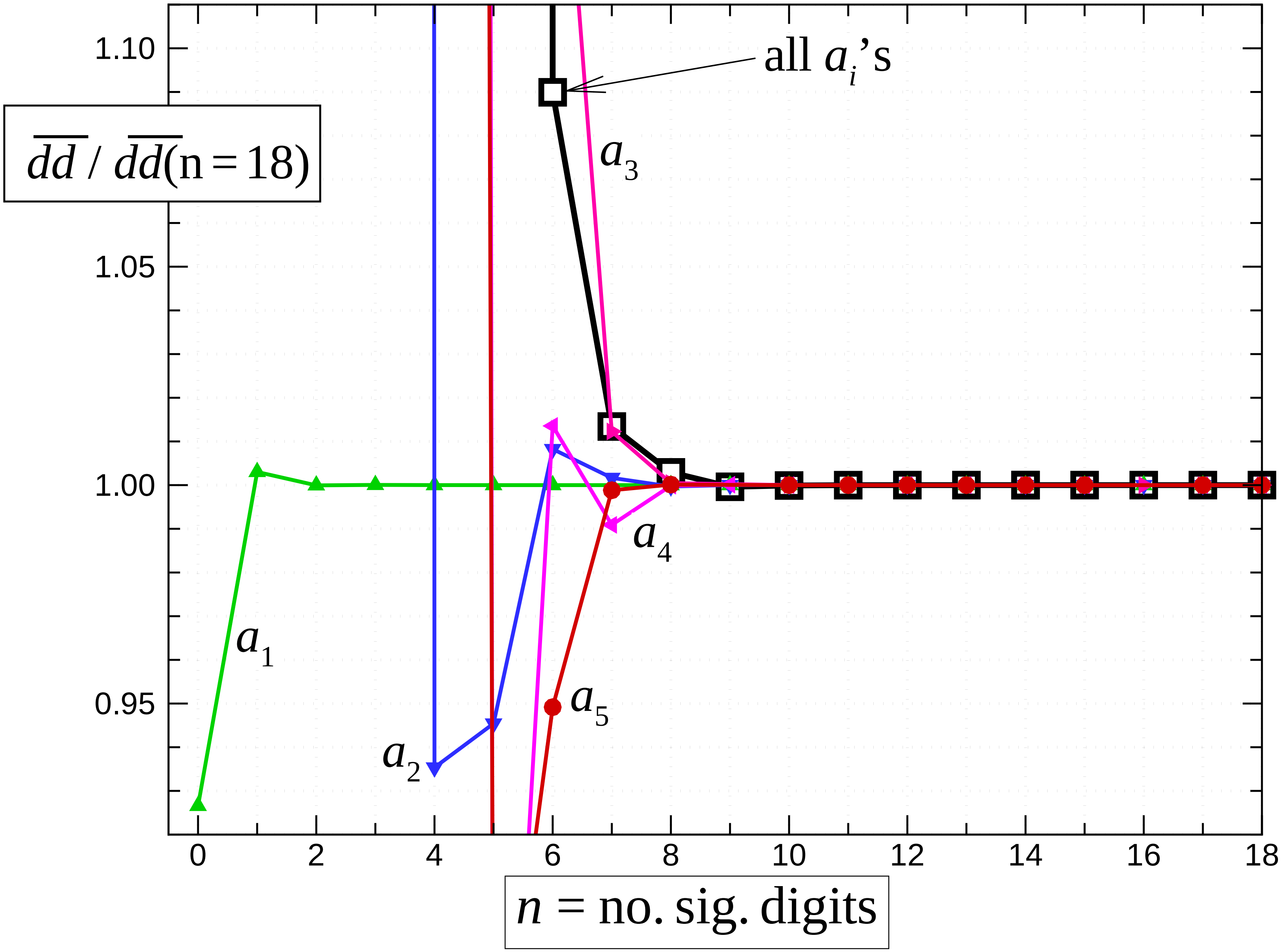

This is silly ! There must be a better way of rounding !

Do the statistical uncertainties in the fitted parameters provide any guidance ?

Table II. Parameters of "X-representation" potential energy function from fit to $Mg_2(X\,^1\Sigma_g^+)$ data

$$V(r) \;=\; \sum_{i=1}^{n} a_i \xi(r)^i \qquad \text{with} \qquad \xi(r) \;=\; \frac{r - R_m}{r + b\,R_m}$$

	parameter	**uncertainty**	
R_m	[3.89039]	$\pm\, 0.000040$	
a_1	$-0.770548964164001222 \times 10^{-2}$	± 0.0	
a_2	$0.705289125191954554 \times 10^{4}$	± 0.00038	$\times 10^4$
a_3	$-0.179327568767261764 \times 10^{5}$	± 0.0040	$\times 10^4$
a_4	$0.228278059421389626 \times 10^{5}$	± 0.045	$\times 10^5$
a_5	$-0.144881409083685430 \times 10^{5}$	± 0.046	$\times 10^5$
a_6	$-0.638841357804591826 \times 10^{5}$	± 0.11	$\times 10^5$
a_7	$0.201722011755478365 \times 10^{6}$	± 0.12	$\times 10^6$
a_8	$-0.286947115902508434 \times 10^{6}$	± 0.66★	$\times 10^6$
a_9	$0.528096212291666190 \times 10^{6}$	$\pm 0.5(160)$★	$\times 10^6$
a_{10}	$-0.841629359994647559 \times 10^{6}$	± 1.8★	$\times 10^6$
a_{11}	$0.510277917592615297 \times 10^{6}$	± 0.83★	$\times 10^6$
$\overline{dd}$	1.46224	*is the dimensionless RMS Deviation*	

★ the 95% confidence limit uncertainty in this parameter is greater than 100% of its value.

Some years ago we examined the effect of rounding off fitted parameters at the n^{th} digit of the uncertainty in each parameter.[1]

For three fitting functions applied to two different data sets we found ...

model	Dunham fit to HF	Potential fit to HF	Dunham fit to I_2	NDE fit to I_2
# data	326	326	9552	9552
# param.	28	14	47	26
$\overline{dd}(n=1)$	10.20	7959.	$> 10^5$	$> 10^5$
$\overline{dd}(n=2)$	2.541	835.4	$> 10^5$	97135.
$\overline{dd}(n=3)$	0.996	78.82	17966.	$> 10^5$
$\overline{dd}(n=4)$	0.904	14.99	2668.	41868.
$\overline{dd}(n=6)$	0.903	1.058	3.111	351.9
$\overline{dd}(n=8)$	0.903	1.051	1.369	4.067
$\overline{dd}(n=10)$	0.903	1.051	1.347	1.422
$\overline{dd}(n=12)$	0.903	1.051	1.329	1.383

[1] R.J. Le Roy, *J. Mol. Spectrosc.* **191**, 223 (1998).

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$\overline{dd}(n=12)$	0.903	1.051	1.329	1.383

Clearly, ***no useful criterion here !***

This led us to develop the ***S****equential* ***R****ounding and* ***R****efitting procedure*

[2] R.J. Le Roy, *J. Mol. Spectrosc.* **191**, 223 (1998).

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- With that second parameter *also fixed* at its rounded value, repeat the fit to optimize the remaining parameters

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- With that second parameter *also fixed* at its rounded value, repeat the fit to optimize the remaining parameters
- iterate this procedure until the last parameter is rounded.
- The final $\overline{dd}$ and final total # sig. digits are *in*sensitive to the order in which the parameters are rounded!

Our experience indicates that, the cumulative effect of applying the the ***SRR*** procedure with each stage of ***R**ounding* being being performed at the first digit of the parameter uncertainty, usually only increases $\overline{dd}$ in its 3^{rd} or 4^{th} significant digit.

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Now apply it to our Mg_2 data analysis !

Table IV. Parameters of "X-representation" potential energy function from fit to $Mg_2(X\,^1\Sigma_g^+)$

$$V(r) \;=\; \sum_{i=1}^{n} a_i\,\xi(r)^i \qquad \text{with} \qquad \xi(r) \;=\; \frac{r - R_m}{r + b\,R_m}$$

	parameter	uncertainty		after S.R.R.	
R_m	[3.89039]	$\pm$ 0.000040		3.890423(40)	
a_1	$-0.770548964164001222\times 10^{-2}$	$\pm$0.0		[0.0]	
a_2	$0.705289125191954554\times 10^{4}$	$\pm$0.00038	$\times 10^4$	7.053263(3800)	$\times 10^3$
a_3	$-0.179327568767261764\times 10^{5}$	$\pm$0.0040	$\times 10^4$	$-$ 1.78875(400)	$\times 10^4$
a_4	$0.228278059421389626\times 10^{5}$	$\pm$0.045	$\times 10^5$	2.2467(450)	$\times 10^4$
a_5	$-0.144881409083685430\times 10^{5}$	$\pm$0.046	$\times 10^5$	$-$1.501(460)	$\times 10^4$
a_6	$-0.638841357804591826\times 10^{5}$	$\pm$0.11	$\times 10^5$	$-$5.196(1100)	$\times 10^4$
a_7	$0.201722011755478365\times 10^{6}$	$\pm$0.12	$\times 10^6$	1.696(1200)	$\times 10^5$
a_8	$-0.286947115902508434\times 10^{6}$	$\pm$0.66★	$\times 10^6$	$-$3.07(66)★	$\times 10^5$
a_9	$0.528096212291666190\times 10^{6}$	$\pm$0.5(160)★	$\times 10^6$	7.5(160)★	$\times 10^6$
a_{10}	$-0.841629359994647559\times 10^{6}$	$\pm$1.8★	$\times 10^6$	$-$1.2(18)★	$\times 10^6$
a_{11}	$0.510277917592615297\times 10^{6}$	$\pm$0.83★	$\times 10^6$	7.(83)★	$\times 10^5$
$\overline{dd}$	1.46224			1.11932	
#digits	198			38	

★ the 95% confidence limit uncertainty in this parameter is greater than 100% of its value.

Table I Parameters of "X-representation" potential energy function from fit to $Mg_2(X\,^1\Sigma_g^+)$ data

$$V(r) \;=\; \sum_{i=1}^{n} a_i\, \xi(r)^i \qquad \text{with} \qquad \xi(r) \;=\; \frac{r - R_m}{r + b\,R_m}$$

	parameter			***after S.R.R.***	
R_m	[3.89039]	3.890423(40)		3.890398(40)	
a_1	$-0.770548964164001222\times10^{-2}$	[0.0]		0.0	
a_2	$0.705289125191954554\times10^{4}$	7.053263(3800)	$\times10^3$	7.056201(2100)	$\times10^3$
a_3	$-0.179327568767261764\times10^{5}$	− 1.78875(400)	$\times10^4$	−1.79298(290)	$\times10^4$
a_4	$0.228278059421389626\times10^{5}$	2.2467(450)	$\times10^4$	2.2331(310)	$\times10^4$
a_5	$-0.144881409083685430\times10^{5}$	−1.501(460)	$\times10^4$	−1.108(140)	$\times10^4$
a_6	$-0.638841357804591826\times10^{5}$	−5.196(1100)	$\times10^4$	−6.446(910)	$\times10^4$
a_7	$0.201722011755478365\times10^{6}$	1.696(1200)	$\times10^5$	1.133(580)	$\times10^5$
a_8	$-0.286947115902508434\times10^{6}$	−3.07(66)★	$\times10^5$	1.6(16)★	$\times10^5$
a_9	$0.528096212291666190\times10^{6}$	7.5(160)★	$\times10^6$	−4.9(21)	$\times10^5$
a_{10}	$-0.841629359994647559\times10^{6}$	−1.2(18)★	$\times10^6$	3.(1)	$\times10^5$
a_{11}	$0.510277917592615297\times10^{6}$	7.(83)★	$\times10^5$		
$\overline{dd}$	1.46224	1.11932		1.11968(+0.03%)	
#digits	180	38		36	

★ the 95% confidence limit uncertainty in this parameter is greater than 100% of its value.

Table V. Parameters of "X-representation" potential energy function from fit to $Mg_2(X\,^1\Sigma_g^+)$ data

$$V(r) \;=\; \sum_{i=1}^{n} a_i \xi(r)^i \qquad \text{with} \qquad \xi(r) \;=\; \frac{r - R_m}{r + b\,R_m}$$

	parameter	*after S.R.R.*			
R_m	[3.89039]	3.890398(40)		3.890356(35)	
a_1	$-0.770548964164001222\times10^{-2}$	0.0		0.0	
a_2	$0.705289125191954554\times10^{4}$	7.056201(2100)	$\times10^3$	7.051573(160)	$\times10^3$
a_3	$-0.179327568767261764\times10^{5}$	$-1.79298(290)$	$\times10^4$	$-1.79357(280)$	$\times10^4$
a_4	$0.228278059421389626\times10^{5}$	2.2331(310)	$\times10^4$	2.3059(120)	$\times10^4$
a_5	$-0.144881409083685430\times10^{5}$	$-1.108(140)$	$\times10^4$	$-1.481(90)$	$\times10^4$
a_6	$-0.638841357804591826\times10^{5}$	$-6.446(910)$	$\times10^4$	$-7.429(700)$	$\times10^4$
a_7	$0.201722011755478365\times10^{6}$	1.133(580)	$\times10^5$	2.453(240)	$\times10^5$
a_8	$-0.286947115902508434\times10^{6}$	1.6(16)★	$\times10^5$	$-2.61(31)$	$\times10^5$
a_9	$0.528096212291666190\times10^{6}$	$-4.9(21)$	$\times10^5$	9.(2)	$\times10^4$
a_{10}	$-0.841629359994647559\times10^{6}$	3.(1)	$\times10^5$		
a_{11}	$0.510277917592615297\times10^{6}$				
10^5					
$\overline{dd}$	1.46224	1.11968(+0.03%)		1.12387(+0.38%)	
#digits	198	36		35	

★ the 95% confidence limit uncertainty in this parameter is greater than 100% of its value.

Use of a different analytic model can lead to fits requiring fewer parameters/digits.

For example, rather than using a simple "X-representation" polynomial expansion to represent the potential:

$$V(r) = \sum_{i=1}^{n} a_i\, \xi(r)^i \qquad \text{with} \qquad \xi(r) = \frac{r - R_m}{r + b\, R_m}$$

★ Use a "Morse/Lennard-Jones" (MLR) function that has explicit parameters to define the well depth and equilibrium distance, and an algebraic form that incorporates the correct theoretical inverse-power-sum long-range tail.

If we define $\quad u_{\rm LR}(r) = \dfrac{C_{m_1}}{r^{m_1}} + \dfrac{C_{m_2}}{r^{m_2}} + \ldots \quad$ we can write

$$V_{\rm MLR}(r) = \mathfrak{D}_e \left\{ 1 - \frac{u_{\rm LR}(r)}{u_{\rm LR}(r_e)}\, e^{-\beta(r)\, y_p^{\rm eq}(r)} \right\}^2$$

$$\xrightarrow{r \,\gg\, r_e} \mathfrak{D}_e - \left[\frac{2\,\mathfrak{D}_e\, e^{-\beta_\infty}}{u_{\rm LR}(r_e)}\right] u_{\rm LR}(r) = \mathfrak{D}_e - \frac{C_{m_1}}{r^{m_1}} - \frac{C_{m_2}}{r^{m_2}} - \ldots$$

in which $\quad \beta(r) = \beta_\infty\, y_p^{\rm ref}(r) + [1 - y_p^{\rm ref}(r)] \sum_{i=0}^{N_\beta} \beta_i\, y_q^{\rm ref}(r)^i$

and $\quad \beta_\infty = \ln\{2\,\mathfrak{D}_e / u_{\rm LR}(r_e)\}$, where $\; y_q^{\rm ref}(r) \equiv \dfrac{r^q - {r_{\rm ref}}^q}{r^q + {r_{\rm ref}}^q}$

Fitted MLR potentials require fewer expansion parameters to attain a good fit.

Table VI. Parameters for the "X-representation" (column 1) and MLR (others) potentials for $Mg_2(X\,^1\Sigma_g^+)$ reported by Knöckel *et al.* (2013) (columns 1 and 2), and those determined here following application of our ***SRR*** procedure (columns 2 …).

	"X − representation" potentials	Morse/Long − Range (MLR) potentials			
	Knöckel *et al.*(2013)	Knöckel *et al.*(2013)	*present work*		
$\mathfrak{D}_e$	[430.472]	430.369	430.393(5	430.394(5)	
r_e	[3.89039]	3.89039	3.890359(62)	3.890416(34)	
$a_0\,/\,\beta_0$	[0.0]	− 166551033592512887	−1.66525(43)	−1.58978(10)	−
$a_1\,/\,\beta_1$	$-0.770548964164001222\times10^{-2}$	−00294159018281270335	−0.0314(42)	−2.105(1)	−
$a_2\,/\,\beta_2$	$0.705289125191954554\times10^{4}$	−104633090905496307	−1.0413(290)	−7.983(7)	−
$a_3\,/\,\beta_3$	$-0.179327568767261764\times10^{5}$	−0324453179411172965	−0.24(11)	−1.20(3)	−
$a_4\,/\,\beta_4$	$0.228278059421389626\times10^{5}$	−184420236755870848	−2.35(70)	−4.5(1)	−
$a_5\,/\,\beta_5$	$-0.144881409083685430\times10^{5}$	114228141585836918	1.0(11)★	5.3(3)	
$a_6\,/\,\beta_6$	$-0.638841357804591826\times10^{5}$	119434493806085307	6.0(48)	−0.2(3)★	
$a_0\,/\,\beta_7$	$0.201722011755478365\times10^{6}$	−773024102172378935	−16.45(110)	0.6(7)★	
$a_8\,/\,\beta_8$	$-0.286947115902508434\times10^{6}$	753234036484323610	12.0(68)		
$a_9\,/$	$0.528096212291666190\times10^{6}$				
$a_{10}\,/$	$-0.841629359994647559\times10^{6}$				
$a_{11},\,/$	$0.510277917592615297\times10^{6}$				
$\overline{dd}$	1.46224	1.21346	1.11822	1.11930(+0.01%)	1.
#digits	180	174	43	37	

Table VII. Parameters for the "X-representation" (column 1) and MLR (others) potentials for $Mg_2(X\,^1\Sigma_g^+)$ reported by Knöckel *et al.* (2013) (columns 1 and 2), and those determined here following application of our ***SRR*** procedure (columns ...).

	"X – representation" potentials	Morse/Long – Range (MLR) potentials			
	Knöckel *et al.*(2013)		*present work*		
$\mathfrak{D}_e$	[430.472]	430.393(5)	430.394(5)	430.396(4)	430.396(4)
r_e	[3.89039]	3.890359(62)	3.890416(34)	3.89042(34)	3.89042(31)
$a_0\,/\,\beta_0$	[0.0]	−166525(43)	−1.58978(10)	−1.58977(10)	−1.58977(9)
$a_1\,/\,\beta_1$	$-0.770548964164001222\times10^{-2}$	−00314(42)	−2.105(1)	−0.2104(7)	−0.2104(6)
$a_2\,/\,\beta_2$	$0.705289125191954554\times10^{4}$	−10413(290)	−7.983(7)	−0.794(5)	−0.794(3)
$a_3\,/\,\beta_3$	$-0.179327568767261764\times10^{5}$	−024(11)	−1.20(3)	−0.14(1)	−0.14(1)
$a_4\,/\,\beta_4$	$0.228278059421389626\times10^{5}$	−235(70)	−4.5(1)	−0.51(1)	−0.51(1)
$a_5\,/\,\beta_5$	$-0.144881409083685430\times10^{5}$	10(11)*	5.3(3)	0.75(6)	0.75(5)
$a_6\,/\,\beta_6$	$-0.638841357804591826\times10^{5}$	60(48)	−0.2(3)*	0.0(2)*	
$a_0\,/\,\beta_7$	$0.201722011755478365\times10^{6}$	−1645(110)	0.6(7)*		
$a_8\,/\,\beta_8$	$-0.286947115902508434\times10^{6}$	120(68)			
$a_9\,/$	$0.528096212291666190\times10^{6}$				
$a_{10}\,/$	$-0.841629359994647559\times10^{6}$				
$a_{11},\,/$	$0.510277917592615297\times10^{6}$				
$\overline{dd}$	1.46224	1.11822	1.11930(+0.01%)	1.11973(+0.04%)	1.11973(+0.0
#digits	180	43	37	33	32

Table VIII. Parameters for the "X-representation" (column 1) and MLR (others) potentials for $Mg_2(X\,^1\Sigma_g^+)$ reported by Knöckel *et al.* (2013) (columns 1 and 2), and those determined here following application of our ***SRR*** procedure (columns ...).

	"X − representation" potentials	Morse/Long − Range (MLR) potentials			
	Knöckel *et al.*(2013)	*present work*			
$\mathfrak{D}_e$	[430.472]	430.394(5)	430.396(4)	430.396(4)	430.385(4
r_e	[3.89039]	3.890416(34)	3.89042(34)	3.89042(31)	3.890418(
$a_0\,/\,\beta_0$	[0.0]	−158978(10)	−1.58977(10)	−1.58977(9)	−1.71326
$a_1\,/\,\beta_1$	$-0.770548964164001222\times10^{-2}$	−2105(1)	−0.2104(7)	−0.2104(6)	0.0652(
$a_2\,/\,\beta_2$	$0.705289125191954554\times10^{4}$	−7983(7)	−0.794(5)	−0.794(3)	−1.109(6
$a_3\,/\,\beta_3$	$-0.179327568767261764\times10^{5}$	−120(3)	−0.14(1)	−0.14(1)	−0.15(3)
$a_4\,/\,\beta_4$	$0.228278059421389626\times10^{5}$	−45(1)	−0.51(1)	−0.51(1)	−2.279(2
$a_5\,/\,\beta_5$	$-0.144881409083685430\times10^{5}$	53(3)	0.75(6)	0.75(5)	
$a_6\,/\,\beta_6$	$-0.638841357804591826\times10^{5}$	−02(3)*	0.0(2)*		
$a_0\,/\,\beta_7$	$0.201722011755478365\times10^{6}$	06(7)*			
$a_8\,/\,\beta_8$	$-0.286947115902508434\times10^{6}$				
$a_9\,/$	$0.528096212291666190\times10^{6}$				
$a_{10}\,/$	$-0.841629359994647559\times10^{6}$				
$a_{11},/$	$0.510277917592615297\times10^{6}$				
$\overline{dd}$	1.46224	1.11930(+0.01%)	1.11973(+0.04%)	1.11973(+0.00%)	1.12975(−
#digits	180	37	33	32	33

Table IX. Parameters for the "X-representation" (column 1) and MLR (others) potentials for $Mg_2(X\,^1\Sigma_g^+)$ reported by Knöckel *et al.* (2013) (columns 1 and 2), and those determined here following application of our ***SRR*** procedure (columns ...).

	"X − representation" potentials	Morse/Long − Range (MLR) potentials		
	Knöckel *et al.*(2013)	*present work*		
$\mathfrak{D}_e$	[430.472]	430.396(4)	430.396(4)	430.385(4)
r_e	[3.89039]	3.89042(34)	3.89042(31)	3.890418(35)
$a_0\,/\,\beta_0$	[0.0]	−158977(10)	−1.58977(9)	−1.71326(20)
$a_1\,/\,\beta_1$	$-0.770548964164001222\times10^{-2}$	−02104(7)	−0.2104(6)	0.0652(12)
$a_2\,/\,\beta_2$	$0.705289125191954554\times10^{4}$	−0794(5)	−0.794(3)	−1.109(6)
$a_3\,/\,\beta_3$	$-0.179327568767261764\times10^{5}$	−014(1)	−0.14(1)	−0.15(3)
$a_4\,/\,\beta_4$	$0.228278059421389626\times10^{5}$	−051(1)	−0.51(1)	−2.279(26)
$a_5\,/\,\beta_5$	$-0.144881409083685430\times10^{5}$	075(6)	0.75(5)	
$a_6\,/\,\beta_6$	$-0.638841357804591826\times10^{5}$	00(2)★		
$a_0\,/\,\beta_7$	$0.201722011755478365\times10^{6}$			
$a_8\,/\,\beta_8$	$-0.286947115902508434\times10^{6}$			
$a_9\,/$	$0.528096212291666190\times10^{6}$			
$a_{10}\,/$	$-0.841629359994647559\times10^{6}$			
$a_{11},\,/$	$0.510277917592615297\times10^{6}$			
$\overline{dd}$	1.46224	1.11973(+0.04%)	1.11973(+0.00%)	1.12975(+0.61%)
#digits	180	33	32	32

Table IX. Parameters for the "X-representation" (column 1) and MLR (others) potentials for $Mg_2(X\,^1\Sigma_g^+)$ reported by Knöckel *et al.* (2013) (columns 1 and 2), and those determined here following application of our ***SRR*** procedure (columns ...).

	"X − representation" potentials	Morse/Long − Range (MLR) potentials		
	Knöckel *et al.*(2013)		*present work*	
$\mathfrak{D}_e$	[430.472]	430.396(4)	**430.396(4)**	430.385(4)
r_e	[3.89039]	3.89042(34)	**3.89042(31)**	3.890418(35)
$a_0\,/\,\beta_0$	[0.0]	−158977(10)	**−1.58977(9)**	−1.71326(20)
$a_1\,/\,\beta_1$	$-0.770548964164001222\times10^{-2}$	−02104(7)	**−0.2104(6)**	0.0652(12)
$a_2\,/\,\beta_2$	$0.705289125191954554\times10^{4}$	−0794(5)	**−0.794(3)**	−1.109(6)
$a_3\,/\,\beta_3$	$-0.179327568767261764\times10^{5}$	−014(1)	**−0.14(1)**	−0.15(3)
$a_4\,/\,\beta_4$	$0.228278059421389626\times10^{5}$	−051(1)	**−0.51(1)**	−2.279(26)
$a_5\,/\,\beta_5$	$-0.144881409083685430\times10^{5}$	075(6)	**0.75(5)**	
$a_6\,/\,\beta_6$	$-0.638841357804591826\times10^{5}$	00(2)★		
$a_0\,/\,\beta_7$	$0.201722011755478365\times10^{6}$			
$a_8\,/\,\beta_8$	$-0.286947115902508434\times10^{6}$			
$a_9\,/$	$0.528096212291666190\times10^{6}$			
$a_{10}\,/$	$-0.841629359994647559\times10^{6}$			
$a_{11},/$	$0.510277917592615297\times10^{6}$			
$\overline{dd}$	1.46224	1.11973(+0.04%)	1.11973(+0.00%)	1.12975(+0.61%)
#digits	180	33	**32**	32

Conclusions

- without some indication of uncertainties, a user cannot trust reported parameters
- parameter uncertainties alone are not a reliable guide to appropriate rounding
- reporting excessive numbers of digits greatly magnifies opportunities for transcription errors along the 'supply chain' from analysis to user
- ***S**equential **R**ounding and **R**efitting* (***SRR***) has proven to be a robust and reliable way of optimally rounding a fitted parameter set.
  - the order in which the ***S**equential **R**ounding* is performed appears not to matter
  - for higher precision, the rounding may be performed at the second or third digit of the parameter uncertainty
- ***SRR*** should be straightforward to implement with virtually *any* least-squares program
- a robust general purpose subroutine for performing linear of non-linear least-squares fits with ***SRR***, named `NLLSSRR`, for ***N**on-**L**inear **L**east-**S**quares with **S**equential **R**ounding and **R**efitting* may be downloaded freely from the URL `http://scienide2.uwaterloo.ca/~rleroy/fitting/`