

CORRECTION

[View Article Online](#)
[View Journal](#) | [View Issue](#)


Cite this: *Phys. Chem. Chem. Phys.*,
2018, **20**, 695

DOI: 10.1039/c7cp90269g

rsc.li/pccp

The authors would like to make a correction to Table 6 in the published article where the data reported do not correspond to the legend.

The reported basis set in Table 6 is not the “Set of coefficients and exponents corresponding to **oxygen core ionized** optimized unrestricted HartreeFock (UHF) configurations for 6-31G basis set as calculated in ref. 54” as indicated in the caption, but is actually the **ground state basis set of oxygen atom...**

The corrected Table 6 is shown below.

Table 6 Set of coefficients and exponents corresponding to oxygen core ionized optimized unrestricted HartreeFock (UHF) configurations for 6-31G basis set as calculated in ref. 54

O-631G*+(3s,3p,2d)	Exponents	(s) Coefficients	(p) Coefficients	(d) Coefficients
S	5964.6252793	0.001710342000		
S	895.5465891	0.013114581001		
S	203.7560106	0.065221864006		
S	57.5539866	0.228700142019		
S	18.4231966	0.476898256040		
S	6.4949949	0.354239792030		
L	21.8822316	-0.116752153036	0.065285646026	
L	5.1691771	-0.308316030094	0.335628169132	
L	1.4954882	1.232400167378	0.729263460286	
L	0.4392245	1.00	1.00	
D	1.50			1.00
L	0.1464000	1.00	1.00	
L	0.0487000	1.00	1.00	
L	0.0162000	1.00	1.00	
D	0.50			1.00
D	0.16			1.00

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

^a Sorbonne Universités, UPMC Univ Paris 06, UMR 7614, Laboratoire de Chimie Physique Matière et Rayonnement, F-75005, Paris, France.

E-mail: Nicolas.Sisourat@upmc.fr

^b CNRS, UMR 7614, Laboratoire de Chimie Physique Matière et Rayonnement, F-75005, Paris, France

^c Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden

