

# The Structure of Pb(II) Ion in Hyper-Alkaline Aqueous Solution

Éva G. Bajnóczi,<sup>a,f</sup> István Pálinkó,<sup>b,f</sup> Tamás Körtvélyesi,<sup>c</sup> Szabolcs Bálint,<sup>d</sup> Imre Bakó,<sup>d</sup> Pál Sipos,<sup>a,f,\*</sup> and Ingmar Persson<sup>e,\*</sup>

<sup>a</sup> Department of Inorganic and Analytical Chemistry, University of Szeged, H-6720 Dóm tér 7., Szeged, Hungary.

<sup>b</sup> Department of Organic Chemistry, University of Szeged, H-6720 Dóm tér 8., Szeged, Hungary.

<sup>c</sup> Department of Physical Chemistry and Materials Science, University of Szeged, H-6720 Aradi vértanúk tere 1., Szeged, Hungary

<sup>d</sup> Institute of Molecular Pharmacology, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Pusztaszeri út 59-67, H-1025 Budapest, Hungary

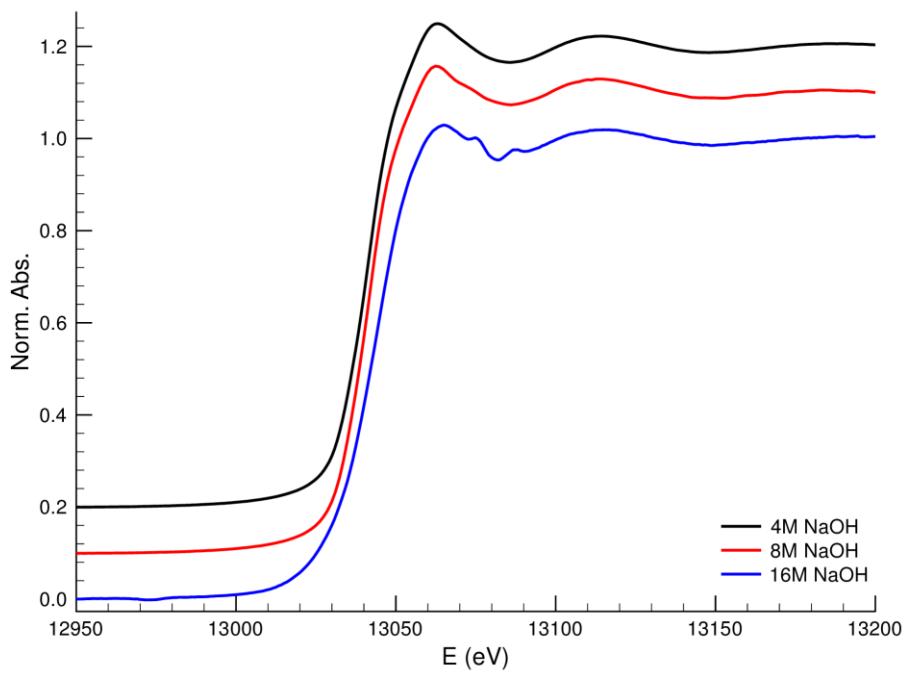
<sup>e</sup> Department of Chemistry and Biotechnology, Swedish University of Agricultural Sciences, SE-750 07, Uppsala, Sweden

<sup>f</sup> Materials and Solution Structure Research Group, Institute of Chemistry, University of Szeged H-6720 Aradi vértanúk tere 1., Szeged, Hungary

## Electronic Supplementary Information

**Table S1** The oxygen coordinated lead(II) structures used for determine the coordination number – Pb-O distance relationship for coordination number = 2, 3, 4, 5, 6, 8. The list is based on the data collected from the Inorganic Crystal Structure Database (ICSD) and the Cambridge Structural Database (CSD);  $N$  = coordination number; references marked in red text are omitted from the mean bond distance and angle. All the other structural data are listed in reference 4.

$N$	CSD code	$d_{\text{Pb-O}}$	$\angle \text{O-Pb-O}$	Reference
2	VEYKUH	2.189 Å	100.6 °	Rekken, B. D.; Brown, T. M.; Olmstead, M. M.; Fettinger, J. C.; Power, P. P. <i>Inorg. Chem.</i> <b>2013</b> , 52, 3054.
	<b>Mean</b>	<b>2.189 Å/1</b>		
3	QAHVOL	2.216 Å	86.5 °	Nehete, U. N.; Chandrasekhar, V.; Jancik, V.; Roesky, H. W.; Herbst-Irmer, R. <i>Organometallics</i> <b>2004</b> , 23, 5372-5374.
3	QEXVUL	2.244 Å	77.7 °	Abakumov, G. A.; Cherkasov, V. K.; Piskunov, A.V.; Lado, A. V.; Fukin, G. K; Abakumova, L. G. <i>Izv. Akad. Nauk SSSR, Ser. Khim.</i> <b>2006</b> , 1103-1111.
3	OLAZAD	2.289 Å	82.9 °	Mauck, C. M.; van den Heuvel, T. W. P.; Hull, M. M.; Zeller, M.; Oertel, C. M. <i>Inorg. Chem.</i> <b>2010</b> , 49, 10736-10743.
3	NIPKAY	2.291 Å	78.3 °	Parr, J.; Ross, A. T.; Slawin, A. M. Z. <i>Polyhedron</i> <b>1997</b> , 16, 2765-2770.
3	MAJGOT	2.299 Å	83.2 °	van Zandt, W.; Huffman, J. C.; Stewart, J. L. <i>Main Group Met. Chem.</i> <b>1998</b> , 21, 237-240.
3	MUKYIA	2.303 Å	77.1 °	Yu-Jun Shi; Yan Xu; Xue-Tai Chen; Ziling Xue; Xiao-Zeng You <i>Eur. J. Inorg. Chem.</i> <b>2002</b> , 3210-3213.
3	QEXVUL	2.304 Å	83.9 °	Abakumov, G. A.; Cherkasov, V. K.; Piskunov, A.V.; Lado, A. V.; Fukin, G. K; Abakumova, L. G. <i>Izv. Akad. Nauk SSSR, Ser. Khim.</i> <b>2006</b> , 1103-1111.
3	QEKZAI	2.308 Å	78.5 °	Oldag, T.; Keller, H.-L. Z. <i>Anorg. Allg. Chem.</i> <b>2006</b> , 632, 1267-1272.
3	MAJGOT	2.325 Å	84.5 °	van Zandt, W.; Huffman, J. C.; Stewart, J. L. <i>Main Group Met. Chem.</i> <b>1998</b> , 21, 237-240.
3	NIPJUR	2.340 Å	75.1 °	Parr, J.; Ross, A. T.; Slawin, A. M. Z. <i>Polyhedron</i> <b>1997</b> , 16, 2765-2770.
3	NIPJOL	2.359 Å	78.4 °	Parr, J.; Ross, A. T.; Slawin, A. M. Z. <i>Polyhedron</i> <b>1997</b> , 16, 2765-2770.
3	QEKYUB01	2.361 Å	77.5 °	Oldag, T.; Keller, H.-L. Z. <i>Anorg. Allg. Chem.</i> <b>2006</b> , 632, 1267-1272.
3	BIBTIQ	2.464 Å	81.9 °	Naumov, P.; Cakir, S.; Bulut, I.; Bicer, E.; Cakir, O.; Jovanovski, G.; Ibrahim, A. R.; Usman, A.; Fun, H.-K.; Chantrapromma, S.; Ng, S. W. <i>Main Group Met. Chem.</i> <b>2002</b> , 25, 175-176.
	Average	<b>2.318 Å</b>	<b>79.9 °/10 structures</b>	



**Fig. S1.** L3 absorption edges of the trihydroxidoplumbate(II) complex in 4, 8 and 16 mol·dm<sup>-3</sup> sodium hydroxide aqueous solutions; offsets are 0.2, 0.1 and no offset, respectively.