ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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**SUPPLEMENTARY MATERIALS TO:**

# COMPUTING OF $^{93}$Nb NMR PARAMETERS OF SOLID-STATE NIOBATES. THE GEOMETRY MATTERS

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**TABLE S1.** X-ray and DFT optimized Nb-O distances. For each compound the reference of the X-ray structure is given in brackets.

| Compound | X-ray (Å) | DFT optmized (Å) | Compound | X-ray (Å) | DFT optmized (Å) |
|---|---|---|---|---|---|
| $LaNbO_4$ [1] | 1.843 (x2)<br>1.859 (x2) | 1.866 (x2)<br>1.875 (x2) | $BiNbO_4$ [7] | 1.847 (x2)<br>1.988 (x2)<br>2.159 (x2) | 2.004 (x2)<br>1.988 (x2)<br>2.273 (x2) |
| $YNbO_4$ [2] | 1.836 (x2)<br>1.952 (x2) | 1.857 (x2)<br>1.925 (x2) | $La_3NbO_7$ [8] | 1.977 (x2)<br>2.010 (x4) | 2.004 (x4)<br>2.024 (x2) |
| $MgNb_2O_6$ [3] | 1.795 (x1)<br>1.910 (x1)<br>1.960 (x1)<br>2.071 (x1)<br>2.080 (x1)<br>2.272 (x1) | 1.809 (x1)<br>1.922 (x1)<br>1.954 (x1)<br>2.081 (x1)<br>2.100 (x1)<br>2.338 (x1) | $Mg_4Nb_2O_9$ [9] | 1.890 (x3)<br>2.120 (x3) | 1.906 (x3)<br>2.139 (x3) |
| $CaNb_2O_6$ [4] | 1.773 (x1)<br>1.918 (x1)<br>1.947 (x1)<br>2.064 (x1)<br>2.077 (x1)<br>2.320 (x1) | 1.797 (x1)<br>1.941 (x1)<br>1.944 (x1)<br>2.085 (x1)<br>2.093 (x1)<br>2.463 (x1) | $CsBiNb_2O_7$ [10] | 1.737 (x1)<br>1.964 (x1)<br>1.966 (x1)<br>2.032 (x1)<br>2.072 (x1)<br>2.405 (x1) | 1.768 (x1)<br>1.957 (x1)<br>1.972 (x1)<br>2.089 (x1)<br>2.090 (x1)<br>2.308 (x1) |
| $SnNb_2O_6$ [5] | 1.860 (x1)<br>1.879 (x1)<br>1.990 (x1)<br>2.051 (x1)<br>2.132 (x1)<br>2.173 (x1) | 1.836 (x1)<br>1.891 (x1)<br>1.853 (x1)<br>2.089 (x1)<br>2.153 (x1)<br>2.253 (x1) | $Cd_2Nb_2O_7$ (t) [11] | 1.898 (x1)<br>1.915 (x1)<br>1.931 (x1)<br>1.969 (x1)<br>2.011 (x1)<br>2.029 (x1) | 1.875 (x1)<br>1.891 (x1)<br>1.927 (x1)<br>1.980 (x1)<br>2.056 (x1)<br>2.117 (x1) |
| $Sn_2Nb_2O_7$ [6] | 2.101 (x6) | 2.007 (x6) | $Cd_2Nb_2O_7$ (c) [12] | 1.967 (x6) | 1.896 (x6) |

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