Accurate measurements of hyperfine structure (HFS) in atoms can provide important information about the coupling of the nucleus with its electronic environment. Therefore, the purpose of this study was to calculate the HFS constants (A) by applying the multiconfiguration Dirac–Hartree–Fock method. The General-purpose relativistic atomic structure package Grasp2K [1], which was used to execute the calculations, is based on this method.

With the help of the MDHF method 51 states were computed from $5p^6, 5p^5\{6s, 6p, 5d, 4f, 5g\}$ configuration list. Configuration state functions were generated by using the active space method. The active space is formed by selecting an orbital set, which is considered to be active. Then every possible configuration formed from this set of orbitals with corresponding space and spin symmetry forms the active space.

To compute the HFS constants, 5 different active space generation strategies were applied during the study. It was discovered that the most accurate strategy was the one where single and double substitutions were allowed from $5s, 5p, nl$, in this case $nl$: $6s, 6p, 5d, 4f, 5g$, shells into the active space [2]. The active space was increased by adding 3 additional sets of virtual orbitals (layers). These layers had the orbital symmetry $l = s - g$ and total angular momentum $j = 0 - 6$. In order to examine, whether it is possible to achieve even more accurate results, relativistic configuration interaction calculation including Breit interaction and quantum electrodynamics effects was performed.

The interaction between electrons and nucleus in the atom is described by the total momentum $F = l + J$, which couples the nuclear $l$ and electronic $J$ total angular momenta. Therefore, the HFS of Xe I atom can be examined and the accuracy of generated radial wave and atomic state functions can be evaluated in layers, which are close to the nucleus. The HFS of atomic energy levels is the result of interaction between electrons and electromagnetic multipole moments of the nucleus. The Hamiltonian of this can be expressed as [3]:

$$\hat{H}_{hfs} = \sum_{k=1}^{\infty} \hat{T}^{(k)} \cdot \hat{M}^{(k)},$$

(1)

where $\hat{T}^{(k)}$ and $\hat{M}^{(k)}$ are spherical tensor operators of rank $k$ in the electronic and nuclear spaces, respectively. The nuclear tensor operator is related to the usual nuclear magnetic dipole moment $\mu_l$ by relation:

$$\mu_l = \langle \Psi(vIM_l) | \hat{M}_0^{(1)} | \Psi(vIM_l) \rangle, \quad M_l = 1.$$  

(2)

The calculated A constants were evaluated by comparing them with experimental results computed by other authors. Constants of levels $6s^2[1/2]_1$ and $6s^2[3/2]_1$ are listed in a table below and compared with the results of other authors [4, 5].

<table>
<thead>
<tr>
<th></th>
<th>[4]</th>
<th>[5]</th>
<th>a6</th>
<th>b6</th>
<th>c4</th>
<th>d5</th>
<th>f3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$6s^2[1/2]_1$</td>
<td>-5788(5)</td>
<td>-5808(2)</td>
<td>-5373</td>
<td>-5372</td>
<td>-5469</td>
<td>-5654</td>
<td>-6119</td>
</tr>
<tr>
<td>$6s^2[3/2]_1$</td>
<td>-956(1)</td>
<td>-959.1</td>
<td>-951</td>
<td>-951</td>
<td>-940</td>
<td>-990</td>
<td>-901</td>
</tr>
</tbody>
</table>

The first two columns present the experimental values of A constants calculated by other authors. The 1st column represents the best and the 2nd column represents the worst match of experimental values with theoretical results computed when applying the 4th strategy. The other 5 columns represent A constants computed by applying different strategies to generate the active space. The strategy $S\{5s\}[5p, nl]$, where single substitutions were allowed from $5s, 5p, nl$ shells into the active space, is marked as a6. The second strategy $5h\{5s\}[5p, nl]$, when the active space was increased by adding the h orbital symmetry, is marked as b6. The strategies, where $4d$ and $\{4p, 4d\}$ shells were move to the active set of orbitals from the core, are marked as c4 and d5 accordingly. The most accurate $SD\{5s\}[5p, nl]$ strategy is marked as f3. The hyperfine structure for the rest of the states of Xe will be presented during the conference.


