Prospective candidates for the EDM experiments of new type: calculations of enhancement of P,T-odd effects in HI^+ and liquid Xe.

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Abstract. The search for the P,T-parity non-conservation (PNC) effects is of fundamental importance in physics. Experiments are performed on TlF and YbF, and are prepared on PbO and HgH molecules. Recently some new approaches were suggested, such as the search for P,T-odd effects in liquid xenon and on HI^+ molecular ion. For preparation and interpretation of these experiments high-precision calculations of the electronic structure are required. Recently developed theoretical methods allow one to analyze the atomic-molecular systems from the point of enhancement of P,T-odd effects and recommend such or another system as a prospective candidate. We calculated enhancement factor for electron EDM in the ground state of HI^+ molecular ion, required for experiment of new type on electron EDM search. The results of calculations of P,T-odd effects in liquid xenon are also discussed.

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Prospective systems for EDM search. It is known that existence of the permanent electric dipole moments (EDM) of the elementary particles violate two fundamental symmetries: space parity (P) and time reversal (T). Considerable experimental efforts invested recently to the search for the electron and proton EDMs are primarily connected with the high sensitivity of EDM to the "new physics" beyond the Standard Model (see [1] and references). In heavy atoms and heavy atom compounds the EDM of the constituent particles is greatly enhanced due to relativistic effects, as for electron EDM, or due to nucleus finite size, as for proton EDM. The main goal of theoretical investigation is the calculation of the EDM enhancement factor, but modern theoretical methods also allow reliable calculating the molecular spectroscopic parameters needed for more effective experimental design.

Some new approaches were recently suggested for electron and proton EDM search. First of all experiment in rotating electric field was suggested by R.Stutz and E.Cornell with molecular diatomic cations, like HI^+ (the initial choice), PtH^+ and HfH^+. Second, experiments on liquid Xe was suggested by M. Romalis and in [2]. All mentioned experiments are unified by complicated electronic structure of the experimental "working bodies".

Methods of calculations. EDM enhancement in heavy atom compounds strongly depend on relativistic and correlation effects, thus relativistic correlation treatment of the electronic structure is required. In group of quantum chemistry in PNPI

TABLE 1. Calculated $E_{\rm eff}$ (in $\times 10^{24}$ Hz/(e·cm)), $A_{||}$ (in MHz) and quadrupole interaction value eQq_0 (in MHz) for the ground state $X^2\Pi_{3/2}$ of ^{127}IH$^+$. Experimental values for $A_{||}$ is 1021 MHz and for quadrupole coupling constant eQq_0 is -712.6 MHz.

Method		$E_{\rm eff}$	$A_{\parallel}$	eQq_0
AGRECP/SCF calculations				
restricted SCF	*7 electrons*	0.008	949	-647
GRECP/RCC calculations				
RCC-S	*7 electrons*	0.206	863	-719
RCC-S	*25 electrons*	0.226	906	-807
RCC-SD	*25 electrons*	0.345	962	-752
GRECP/SODCI calculations				
Thresh.(mHartree)	SAF number			
	25 electrons			
0.0003	12 678 133	0.336	968	-745
a(1) metastable state in PbO molecule				
		-6.1		

(`http://qchem.pnpi.spb.ru`) a number of theoretical methods were suggested and developed which allow one to calculate required properties with necessary for experiment high accuracy. The new approaches are applied in:

1. proper choice of spin-dependent Hamiltonian — generalized relativistic effective core potential method, GRECP; [3]
2. restoration of proper shape of wavefunction in the core of heavy atom — non-variational one-center restoration scheme, NOCR [4];
3. generation of optimal basis set [5, 6];
4. development of correlation methods jointly with the leading quantum chemistry groups — group of prof. U.Kaldor (Tel-Aviv University) and group of R.Buenker (Wuppertal University).

HI$^+$ calculations. The results of calculated parameters are presented in Table 1. The value of $E_{\rm eff}$ characterizes the strength of interaction of electron EDM to inner molecular field, $A_{||}$ is z-component of hyperfine coupling tensor of electronic to nuclear spins. Inclusion of polarization and correlation effects (compare spin-averaged self-consistent field **AGRECP/SCF** results with **GRECP/RCC** and **GRECP/SODCI** ones) changes considerably the value of $E_{\rm eff}$, while $A_{||}$ is little changed. That fact shows that the structure of correlation contributions to the calculated parameters is considerably different. Another important point is that our final value of $E_{\rm eff}$ (**GRECP/SODCI** result) is much lower than $E_{\rm eff}$ for a(1) metastable state of PbO molecule.

TABLE 2. SCF values of parameter X (see [8]) for different model of liquid Xe.

Model	Free atom	Cavity	Lattice-1	Lattice-2
X (MHz)	238	$\sim 183^*$	196	278

* The numerical values for cavity model is not given explicitly in [7], thus we restored that from graphical representation given in the article. Such approximation doesn't influence our conclusions.

Lattice model of liquid Xe and calculated parameters. In liquid xenon calculations we used *lattice model*, in which single Xe atom is surrounded by six Xe atoms according to the cubic close-packed crystalline lattice. This model is more realistic, than *spherical cavity model* (see [7]), where single atom is confined to spherical cavity with certain boundary conditions on atomic Xe wavefunction. As our calculations show (see Table 2) enhancement of P,T-odd effects in liquid Xe crucially depend on inter-atomic interactions in liquid and, unlike cavity model, no suppression of enhancement takes place. In our calculations we choose the direction of electric field along z-axis. The strength of the field was 0.012 a.u. In "Lattice-1" model electrons of surrounded atoms are frozen (that simulates cavity model), in "Lattice-2" model electrons are included in SCF procedure for atoms on z-axis.

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