استمارة قبول بحث للنشر

الجامعة المستنصرية
كلية العلوم
مجلة علوم المستنصرية
(هيئة التحرير)

**AL-MUSTANSIRIYAH
JOURNAL OF SCIENCE
(Editorial Board)
College of Science
Al-Mustansiriyah University
Baghdad - Iraq**

الرقم : ف - 63
التاريخ : 18 / 6 /2008

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تهديكم هيئة تحرير مجلة علوم المستنصرية أطيب تحياتها و تود بعد أن تدارست وأطلعت على آراء المقيمين بخصوص بحثكم الموسوم :

Triple – Dipole Dispersion Coefficient for H and Alkali Atoms in Ground and Excited S – State

ان تعلمكم بقرارها الذي اتخذته باجتماعها المنعقد في **18/ 6 / 2008** بقبول البحث للنشر في المجلد (التاسع عشر) العدد (السادس) من المجلة .

مع التقديـــــر

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رئيس التحرير
2008/ 6 /18

نسخة منه إلى /
ملفات المجلة

ABSTRACT

In this study, we calculated the dipole – dipole – dipole dispersion interaction coefficient (the triple - dipole dispersion interaction coefficient υ_{abc}) for three atomic systems of a single valence electron (H and alkali - metal atoms) in the ground and first excited energy S-states, where this coefficient enters in the principle equation of the dispersion potential for three atoms in homonuclear or hetronuclear systems interactions. Furthermore , we computed the υ_{abc} coefficient by using the approximate formula which is depends on the static dipole polarizabilities $\alpha_2(0)$ at $w=0$ and the dominant dispersion forces coefficient C_6 for dipole – dipole interaction. Alkali atoms were described by using the frozen core approximation (FCA) ,where, we used the developed formula of the model potential which is describing the motion of the valence electron in the presence of a frozen core . Our results which were evaluated by calculating the effective transition frequencies ω_i and the effective oscillator strengths f_i, in a good agreement with the approximate values and comparable with the results of other researchers .

Triple – Dipole Dispersion Coefficient for H and Alkali Atoms in Ground and Excited S-State

INTRODUCTION

The four fundamental forces known to physics – strong, electromagnetic, weak and gravitation are believed to explain all physical processes and structures observed in nature. In atoms and molecules , electromagnetic force account for chemical bonds and intermolecular interactions such as ionic and hydrogen bonds , also these force is responsible for the long-range attractive interactions between atoms and molecules . In the region where the retardation effects can be neglected, these are collectively known as van der Waals forces, which are arise from induction and orientation effects. The strength of dispersion forces (van der Waals) depends on the electric dipole polarizability of the interacting atoms or molecules , in other words , these forces increase with the polarizability of interacting atoms [1] .

Three different types of forces constitute the van der Waals force: the induction force between one permanent and one induced dipole, the orientation force between a pair of permanent dipoles, and the dispersion force between a pair of instantaneous induced dipoles. Each of these forces has an interaction energy proportional to the inverse sixth power of the separation R^6 [1,2]. Knowledge of the dispersion potential forces for interaction among atoms plays an important role in the study of cold atom collision processes, which have applications to laser cooling and trapping of atoms[2]. The long-range limit of the dispersion potential interactions may be expressed in a power series in the inverses of the internuclear separations R. The algebraic coefficient of each power combination in this series is a dispersion coefficient [3] . The dispersion series includes, in addition to the well-known pair-interaction coefficients C_6, C_8, and C_{10} (which result from second-order perturbation theory), a coefficient υ_{abc} related to the electric dipole momentum interactions among all three atoms. The υ_{abc} coefficient results from third-order perturbation theory and describes the strength of the non additive, three-atom interaction , also , may be result by the variational method , or by the classical Drude model [3,4]. There is great current interest in forming diatomic molecules in cold gases of alkali metal atoms, by photoassociation spectroscopy by magnetic tuning through atom-atom Feshbach resonances and through 3-body recombination [4,5,6]. The successful achievement of Bose – Einstein condensation has triggered a large interest in interacting Bose gases .One importance factor limiting the achievable density in Bose – Einstein condensates of trapped atoms is the loss of atoms through 3-body recombination .This process provides a unique windows on three – body dynamic of cold atoms [6,7].It has recently been shown that the three – body recombination rate also depends not only on the atom – atom scattering length but on three – body forces [5].

The first investigations of the triple-dipole interaction were by Axilrod and Teller and by Muto in 1943. Axilrod and Teller give the order of magnitude of the constant υ_{abc} and Muto estimated its value using a simple atomic model. Axilrod later also employed a simplified atomic model to derive the constant υ_{abc}, obtaining a value in agreement with that of Muto. Midzuno and Kihara used a variational method to find an approximate expression for the coefficient υ_{abc} in terms of the reduced masses and polarizabilities of the three interacting atoms . Aub and Zienau derived the three-body interaction energy for three neutral atoms by the methods of quantum electrodynamics. In the region in which the distances between atoms is small compared to the wavelengths corresponding to typical atomic excitations, their results agree with those obtained by Axilrod (and also with those of Muto). A compact expression for the υ_{abc} coefficient (in terms of an integral over the product of the dynamic atomic dipole polarizabilities of imaginary frequencies) was established by McLachlan . The first accurate evaluation of the υ_{abc} coefficient was given by Chan and Dalgarno for three hydrogen atoms in 1965 using a double integral representation for the υ_{abc} coefficient [2].

THEORETICAL FORMULATIONS

In a Born-Oppenheimer picture , the electronic Hamiltonian of the triple interacting atoms is given by [2] :

$$H = H_1 + H_2 + H_3 + V_{12} + V_{23} + V_{31} \qquad \text{............................(1)}$$

where H_j , for j=1,2,3, is the Hamiltonian of the j th atom and V_{ij} for i=1,2,3 , j=3,2,1 is the Coulomb interaction between the atomic charge distributions of the i th and j th atoms. The eigenvalue of the equation (1) as a function of the internuclear distances which is represent the potential energy describing the interactions among the three atoms. We are concerned with the long-range behavior of the dispersion potential , for the case in which, in the dissociation limit, the atoms are in their ground state. Thus, in this limit, the eigenvalue problem may be solved using perturbation theory, where the unperturbed state is described by the sum of the atomic Hamiltonians, (i.e. H_1,H_2,H_3), and the perturbation by the sum of the Coulomb interactions between the atomic charge distributions. The perturbation parameters are proportional to the inverses of the internuclear distances.

The long-range part of the interaction between three atoms is not exactly equal to the interaction energies taken in pairs. There is a nonadditive term which comes from the third – order perturbation theory . The leading term in the expression energy of the triple –atoms system are [8] :

$$V_{abc} = -\frac{C_6^{ab}}{r_{ab}^6} - \frac{C_8^{bc}}{r_{bc}^8} - \frac{C_{10}^{ca}}{r_{ca}^{10}} - \frac{\upsilon_{abc}(1+3\cos\vartheta_a\cos\vartheta_b\cos\vartheta_c)}{(r_{ab}\,r_{bc}\,r_{ca})^3} \qquad \text{..................(2)}$$

where C_6^{ab} , C_8^{cb} , C_{10}^{ca} the dispersion forces coefficients for the interaction [(dipole - dipole),(dipole - quadrupole) and (dipole - octupole)+(quadrupole - quadrupole)] respectively. $\cos\vartheta_a$, $\cos\vartheta_b$ and $\cos\vartheta_c$ are the internal angles of the triangle formed by r_{ab} ,r_{bc} and r_{ca} respectively , υ_{abc} is the triple-dipole dispersion coefficient defined by [8] :

$$\upsilon_{abc} = \frac{3}{\pi}\int_0^{\infty} \alpha_2^a(iw)\, \alpha_2^b(iw)\, \alpha_2^c(iw)\, dw \qquad \text{.........................(3)}$$

where $\alpha_2^a(iw)$, $\alpha_2^b(iw)$ *and* $\alpha_2^c(iw)$ are the dynamic dipole polarizabilities at imaginary frequencies for three interacting systems *a,b,* and *c* respectively.

Our study includes an alkali – metal atoms , therefore , in multielectron atomic systems, the problem is very complex because of the potential energy changes when we take into account the effect of other electrons in atom . By using the approximation methods in quantum mechanic such as Frozen Core Approximation (FCA), which leads to transforming the multielectron system to single electron system .Where, we ignore the effect of all orbits in atom except that which involves the valence electron. In Frozen Core Approximation (FCA),the atoms are treated as a hydrogenic system and can be described by a single valence electron , the core acts as unit monopole .The Frozen Core Approximation(FCA)is applicable to all wave functions calculations [9].

For alkali – metal atoms ,the approximation can be made from taking explicitly into account only the valence electron contribution . That, can be done by introducing a model potential describing the motion of the valence electron in the presence of frozen core [10] .This model potential developed by Marinescu , Sadeghpour ,et. al. [3] ,which is depend on the orbital angular momentum *l* of the valence electron, and given as :

$$V_l(r) = -\frac{z_l(r)}{r} - \frac{\alpha_c}{2r^4}\left[1 - e^{-(r/r_c)^6}\right] \qquad \text{..................................(4)}$$

where α_c is the static dipole polarizability of the positive ion core ,r_c is the cutoff radius , $z_l(r)$ is the radial charge given in detail in the reference [3] .

Al-Samer and Easa [9] used the above formula of the potential to describe the radial wave functions for single valence electron atoms(alkali – metal atoms), where they have been used Numerov method to calculate these functions numerically [9].The radial wave functions is useful to evaluate the dynamic dipole polarizabilities at imaginary frequencies for ground and excited energy states.

In this study , we concerned to derive special expression for the dynamic dipole polarizability $\alpha_2(iw)$ from the generalized formula of the dynamic multipole polarizability $\alpha_{2^L}(w)$ (i.e. L=1),where L degree of polarity .The value of the multipole polarizability $\alpha_{2^L}(w)$ was obtained by analytically from a very precise variational calculation in terms of a set of N effective transition frequencies w_i and N effective oscillator strengths f_i [11] :

$$\alpha_{2^L}(w) = \sum_{i}^{N} \frac{f_i}{w_i^2 - w^2} \tag{5}$$

where N denotes to the number of the variational constants in the variational function (in our study N=5) . Equation (5) allow us to find the effective transition frequencies w_i ,which represents the singular points at multipole polarizability, where ,the transition process of the dipole polarizabiliy require to an infinity value for polarization (i.e. the perturbed function approach to infinity). Then ,the computer program was designed to solve the matrix equation for the dynamic dipole polarizability, hereby, we computed five values of the effective transition frequencies w_i .

The final equation can be used to evaluate the corresponding values of the effective oscillator strengths f_i which represents the residuals at the singular points for the dynamic multipole polarizabilities , there is another program used to find these parameters ,where :

$$f_{iL} = \lim_{w \to w_{iL}} (w_{iL}^2 - w^2)\, \alpha_{2^L}(w) \tag{6}$$

In this study , we interested to calculate the triple-dipole dispersion coefficient υ_{abc} which is given in equation (3) for single valence electron atomic systems, by substituting equation (5) for (L=1) in equation(3) , we get :

$$\upsilon_{abc} = \frac{3}{\pi} \sum_{i} \sum_{j} \sum_{k} f_i\, f_j\, f_k \int_0^\infty \frac{dw}{(w_{ia}^2 + w^2)(w_{jb}^2 + w^2)(w_{kc}^2 + w^2)} \tag{7}$$

But, by using the following integral representation [2] :

$$\frac{1}{(b+a)(c+a)} + \frac{1}{(a+b)(c+b)} + \frac{1}{(a+c)(b+c)} = \frac{4}{\pi} \int_0^\infty \mathrm{Re}\left(\frac{1}{a - iw}\right) \mathrm{Re}\left(\frac{1}{b - iw}\right) \mathrm{Re}\left(\frac{1}{c - iw}\right) dw \tag{8}$$

where

$$\mathrm{Re}\left(\frac{1}{a - iw}\right) \equiv \frac{a}{(a^2 + w^2)}$$

Finally, from the above mathematics substitutions ,we found the expression of the triple – dipole dispersion coefficient υ_{abc} in term of the calculated values of the effective transition frequencies w_i and the effective oscillator strengths f_i :

$$\upsilon_{abc} = \frac{3}{\pi}\sum_{i}\sum_{j}\sum_{k}\frac{f_i\, f_j\, f_k\,(w_{ia}+w_{jb}+w_{kc})}{w_{ia}w_{jb}w_{kc}\,(w_{ia}+w_{jb})(w_{jb}+w_{kc})(w_{kc}+w_{ia})} \qquad \ldots\ldots\ldots\ldots\ldots(9)$$

this expression used in our numerical computations (for *i,j,k,* =5) .

Midzuno and Kihara derived the approximate expression for the atomic triple-dipole dispersion coefficient υ_{abc} which depends directly on the static dipole polarizability $\alpha_2(0)$ and the dominant dispersion coefficient (for dipole – dipole interaction) C_6 . For the case of the three similar atoms, they obtain [2] :

$$\upsilon_{abc} = \frac{3}{4}\alpha_2(0)\, C_6 \qquad \ldots\ldots\ldots\ldots\ldots(10)$$

and , in the general case of the three different atoms :

$$\upsilon_{abc} = \frac{2\,Q_1\,Q_2\,Q_3\,(Q_1+Q_2+Q_3)}{(Q_1+Q_2)(Q_2+Q_3)(Q_3+Q_1)} \qquad \ldots\ldots\ldots\ldots\ldots(11)$$

where :

$$Q_i = \frac{\alpha_2^{(j)}(o)\,\alpha_2^{(k)}(o)}{\alpha_2^{(i)}(o)}\;C_6^{ii} \qquad \ldots\ldots\ldots\ldots\ldots(12)$$

In the above formulas, we used the results of the previous calculations of static dipole polarizabilities $\alpha_2(0)$ and dipole – dipole dispersion forces coefficient C_6 which were presented by Al-samer and Easa [9] , and the obtained results of the υ_{abc} coefficient were used for comparing with the results achieved numerically in our work .

RESULTS , DISCUSSION AND CONCLUSIONS

In this work, we interested to calculate the triple – dipole dispersion coefficient υ_{abc} for the interaction of three atoms in single valence electron (H and Alkali –metal atoms). The υ_{abc} coefficient which is given by Eq. (9) consists primarily calculation of the effective transition frequencies w_i and effective oscillator strengths f_i .This study includes the ground and first excited S-state for all possible systems combinations .

Table(1) represents the calculated values of the υ_{abc} coefficient for three homonuclear systems (identical atoms) in the ground and first excited S-state .Our results were compared with others such as Marinescu M. et. al. [2] , Yan Z.C. et. al. [8] and Khalaf S.K.[12] for ground state interactions. Firstly , the calculations have been tested numerically by comparing our results for the interaction of three H- atoms with the results of Refs. [8,12]. We found that the υ_{abc} coefficient was equal to 21.64253 , which is in excellent agreement with the value 21.64246 and 21.64243 of Refs.[8,12] respectively .

Table(1):The Values of υ_{abc} for Homonuclear Interactions-Ground & First Excited S-State

Homonuclear - Ground State			
Interactions	**Present Work**	**Previous Work**	**Approximate Values**
H-H-H	21.64253	21.64246 [8]	21.93416
		21.64243 [12]	
Li-Li-Li	125519.16357	170100 [2]	125512.16918
		170595 [12]	
Na-Na-Na	216620.21692	175800 [2]	216631.52920
K-K-K	1323660.8603	837500 [2]	1323893.8600
Rb-Rb-Rb	2116409.5607	1060000 [2]	2116041.9452
Cs-Cs-Cs	4708879.4155	1910000 [2]	4712792.7057
Homonuclear – First S-Excited State			
H-H-H	1.06485 E7	---------------	1.06547 E7
Li-Li-Li	1.94492 E9	---------------	1.92853 E9
Na-Na-Na	2.83240 E9	---------------	2.83346 E9
K-K-K	9.25260 E9	---------------	9.25949 E9
Rb-Rb-Rb	1.2784 E10	---------------	1.2769 E10
Cs-Cs-Cs	2.1677 E10	---------------	2.1737 E10

Furthermore, this table involves our calculations of the υ_{abc} coefficient (Approximate Values) which were evaluated by using approximate formulas giving by Midzuno and Kihara ,as mentioned in detail by Ref. [2] . These formulas depend upon the values of the static dipole polarizabilities $\alpha_2(0)$ and the dominant dispersion forces coefficient C_6 for atom-atom interaction ,we used the results obtained previously by Al-Samer and Easa [12] as an input data.

Table (1) , shows that our results for alkali – metal atoms were comparable with those results of Refs.[2,12], but its far from the results of these references in the case of increasing the atomic number Z , this appears especially in high alkali metal – atoms (K,Rb and Cs). The compatibility between our numerical results and the approximate values (accurate values) denotes to the accuracy in our numerical calculations of the effective transition frequencies w_i and the effective oscillator strengths f_i , consequently ,that , gives an accurate values of the dynamic dipole polarizabilities $\alpha_2(iw)$. Also, this refers to that the model potential which was developed by Marenicu M. et.al. [3] was very suitable to describe the behavior of the single valence electron in alkali – metal atoms, and ,this insures to give high accuracy in the evaluation of the wave functions .

Table (2) includes the values of the υ_{abc} coefficient for hetronuclear systems interactions in ground state ,and we took into account all possible combinations .These results are compared with others, such as Refs.[2,8,12], were it appear in a very good agreement for (H – H – Li) , (H – Li – Li) , (Li – Li – all other alkali atoms) and (Na – Na – Li) combinations . The contrast increased for K,Rb and Cs combinations gradually. This difference in our results with respect to the results of Ref. [2] due to the difference in the approximation methods which were used to describe the alkali – metal atoms, where ,we used frozen core approximation (FCA) in this study.

Our results in table (3) were compared with the approximate values for hetronuclear systems interactions , and gives a good agreement for all possible combinations . We note that there is an excess in the values of the υ_{abc} coefficient comparing with the ground state interactions. This appears explicitly in (H – H – Li) ,(Li – Li – other atoms) , (Na – Na – other alkali atoms except Cs) , (Li – Na – K) and (Li – Na – Rb) combinations , whereas , all other combinations have a numerical values less than the corresponding ground state interactions as given in table (2). This is unlike the general behavior for the long - range dispersion coefficients for two - atoms interaction C_6 , C_8 and C_{10} ,as mentioned in previous studies presented by Al-samer et.al. and Marenscu et.al.in Ref. [9,10] respectively, where ,they proved that the values of ground state interactions were less than the excited state values in all cases .

We conclude that the numerical values of the triple – dipole dispersion coefficient υ_{abc} depend strongly on the accuracy in the calculations of the dynamic dipole polarizabilities $\alpha_2(iw)$. Also the triple – dipole dispersion coefficient υ_{abc} measures the strength of the non - additive part of the long – range three atoms interaction . In all cases, we have compared our present results for the υ_{abc} coefficient with results which were computed from the approximate formulas .There is excellent agreement for all combinations of atoms . We conclude that the approximate formulas give reliable results when we use an accurate input data. The values in table (1) , (2) and (3) indicates that such three atoms non-additive dipole interaction effects are comparable in magnitude to those of the two atoms interaction effects.

Table(2):The Values of υ_{abc} for Hetronuclear Interactions-Ground State

Hetronuclear - Ground State			
Interactions	**Present Work**	**Previous Work**	**Approximate Values**
H-H-Li	269.22889	275.979 [8] 263.299 [12]	269.50630
Li-Li-H	5277.5005	6133.500 [8] 4586.320 [12]	5277.48019
Li-Li-Na	1.50319 E9	1.716 E9 [2]	1.50251 E9
Li-Li-K	2.66570 E9	2.884 E9 [2]	2.66459 E9
Li-Li-Rb	3.07330 E9	3.116 E9 [2]	3.07167 E9
Li-Li-Cs	3.88978 E9	3.768 E9 [2]	3.88863 E9
Na-Na-Li	1.80311 E9	1.735 E9 [2]	1.80270 E9
Na-Na-k	3.88508 E9	2.928 E9 [2]	3.88487 E9
Na-Na-Rb	4.49226 E9	3.161 E9 [2]	4.49165 E9
Na-Na-Cs	5.71456 E9	3.808 E9 [2]	5.71516 E9
K-K-Li	5.86070 E9	4.908 E9 [2]	5.85961 E9
K-K-Na	7.11129 E9	4.929 E9 [2]	7.11126 E9
K-K-Rb	15.4588 E9	9.057 E9 [2]	15.4575 E9
K-K-Cs	20.0147 E9	11.00 E9 [2]	19.5653 E9
Rb-Rb-Li	7.91545 E9	5.735 E9 [2]	7.91242 E9
Rb-Rb-Na	9.62636 E9	5.756 E9 [2]	9.62441 E9
Rb-Rb-K	18.0770 E9	9.796 E9 [2]	18.0739 E9
Rb-Rb-Cs	27.5235 E9	12.88 E9 [2]	27.5249 E9
Cs-Cs-Li	13.1427 E9	8.442 E9 [2]	12.7064 E9
Cs-Cs-Na	16.0421 E9	8.447 E9 [2]	15.4463 E9
Cs-Cs-K	30.5667 E9	14.48 E9 [2]	28.9390 E9
Cs-Cs-Rb	35.9355 E9	15.67 E9 [2]	33.8557 E9
Hetronuclear - Ground State			
Li-Na-K	3.21616 E9	2.904 E9 [2]	3.21548 E9
Li-Na-Rb	3.71365 E9	3.136 E9 [2]	3.71228 E9
Li-Na-Cs	4.71227 E9	3.785 E9 [2]	4.71334 E9
Li-K-Rb	6.80570 E9	5.305 E9 [2]	6.80374 E9
Li-K-Cs	8.72315 E9	6.429 E9 [2]	8.52510 E9
Li-Rb-Cs	10.1739 E9	6.925 E9 [2]	10.0262 E9
Na-K-Rb	8.26761 E9	5.327 E9 [2]	8.26672 E9
Na-K-Cs	10.6185 E9	6.444 E9 [2]	10.4764 E9
Na-Rb-Cs	12.3968 E9	6.967 E2 [2]	12.1920 E9
K-Rb-Cs	23.4578 E9	11.90 E9 [2]	22.8690 E9

Thus, in other words , the contribution of the υ_{abc} coefficient may be comparable to the contribution of the pair – interaction dispersion coefficients C_6,C_8 and C_{10} , so , our results shows that three – body effects may not be neglected in the description of the long – range potential interaction among three alkali – metal atoms.

Table(3):The Values of υ_{abc} for Hetronuclear Interactions - First Excited S-State

Hetronuclear – First Excited S-State			
Interactions	**Present Work**	**Previous Work**	**Approximate Values**
H-H-Li	5.12928 E7	----------------	5.12105 E7
Li-Li-H	2.99076 E8	----------------	2.97708 E8
Li-Li-Na	2.20268 E9	----------------	2.19028 E9
Li-Li-K	3.22568 E9	----------------	3.20659 E9
Li-Li-Rb	3.57020 E9	----------------	3.54650 E9
Li-Li-Cs	4.20168 E9	----------------	4.17788 E9
Na-Na-Li	2.49674 E9	----------------	2.49002 E9
Na-Na-k	4.16976 E9	----------------	4.17164 E9
Na-Na-Rb	4.62177 E9	----------------	4.62094 E9
Na-Na-Cs	5.45242 E9	----------------	5.45782 E9
K-K-Li	5.42917 E9	----------------	5.41391 E9
K-K-Na	6.18899 E9	----------------	6.19259 E9
K-K-Rb	10.2996 E9	----------------	10.3007 E9
K-K-Cs	12.2391 E9	----------------	12.2559 E9
Rb-Rb-Li	6.69645 E9	----------------	6.66867 E9
Rb-Rb-Na	7.64298 E9	----------------	7.63774 E9
Rb-Rb-K	11.4716 E9	----------------	11.4655 E9
Rb-Rb-Cs	15.2204 E9	----------------	15.2219 E9
Cs-Cs-Li	9.41095 E9	----------------	9.39401 E9
Cs-Cs-Na	10.7622 E9	----------------	10.7818 E9
Cs-Cs-K	16.2572 E9	----------------	16.2905 E9
Cs-Cs-Rb	18.1502 E9	----------------	18.1759 E9
Hetronuclear - First Excited S- State			
Li-Na-K	3.66614 E9	----------------	3.65592 E9
Li-Na-Rb	4.06069 E9	----------------	4.04664 E9
Li-Na-Cs	4.78481 E9	----------------	4.77340 E9
Li-K-Rb	6.02762 E9	----------------	6.00666 E9
Li-K-Cs	7.13078 E9	----------------	7.11411 E9
Li-Rb-Cs	7.93091 E9	----------------	7.90714 E9
Na-K-Rb	6.87547 E9	----------------	6.87513 E9
Na-K-Cs	8.14234 E9	----------------	8.15190 E9
Na-Rb-Cs	9.06109 E9	----------------	9.06604 E9
K-Rb-Cs	13.6450 E9	----------------	13.6551 E9

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