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Molecular Second Moments and Diamagnetic Susceptibilities. Reparametrization of the Independent Atom Model Formulas

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The independent atom model (IAM) is applied to the calculation of molecular second moments and diamagnetic susceptibilities. The earlier formulas are generalized and better agrement with experimental data and ab initio results is achieved.

INTRODUCTION

We have shown that molecular second moments and the related diamagnetic susceptibilities exhibit atomic additivity[1], thus offering a support to the concept of modified atoms in molecules[2–4]. Although in some extreme cases[5], like e. g. in alkali-halides[6], intramolecular charge transfer is important, generally, the model of neutral and spherical atoms placed at the equilibrium positions is sufficient. This model of independent atoms (IAM) has a surprisingly good performance as far as second moments and molecular diamagnetic susceptibilities are concerned[1–4]. Recently, we found that the IAM model provides good results for Van der Waals complexes too[7]. The applied formulas employ very few empirical parameters — one per period of the Mendeleev table of elements. In the present paper we show that an improved performance of the IAM model is achieved if each atom is characterized by a separate adjustable additive constant.

THEORY AND RESULTS

The temperature independent part of the magnetic susceptibility has two contributions:

$$\chi_{aa} = \chi_{aa}{}^{d} + \chi_{aa}{}^{p} \tag{1}$$

where the first term refers to Langevin's diamagnetism, whereas the second represents Van Vleck's high frequency paramagnetic term[9]. Langevin's term can be expressed by molecular second moments:

$$\chi_{aa}{}^{d} = K\,[\langle b^2\rangle_e + \langle c^2\rangle_e] \tag{2}$$

where a, b and c denote inertial coordinates. The abbreviation K signifies a combination of fundamental constants $K = Ne^2/4mc^2$, which have their usual meaning. The second moments are easily decomposed into three contributions within the one electron MO-LCAO picture:

$$\langle r_a^2\rangle = \sum_{A}\sum_{\mu}^{A} P_{\mu\mu}\,\langle \Phi_\mu \,|\, r_a^2 \,|\, \Phi_\mu\rangle + 2 \sum_{\mu<\nu}^{A\;A}\sum P_{\mu\nu}\,\langle \Phi_\mu \,|\, r_a^2 \,|\, \Phi_\nu\rangle + 2 \sum\sum_{A<B}^{A\;B}\sum\sum_{\mu<\nu}\sum P_{\mu\nu}\,\langle \Phi_\mu \,|\, r_a^2 \,|\, \Phi_\nu\rangle \tag{3}$$

with an analogous expression for coordinates *b* and *c*. Atomic orbitals are denoted by Φ, whilst summations with capital letters are extended over all atoms in a molecule. A series of consecutive coordinative translations $r_a = R_{Aa} + r_{Aa}(i)$ brings formula (3) to single center contributions:

$$\langle r_a^2\rangle \cong \sum_{A} \Big[Q_A\, R_{Aa}^2 + \sum_{\mu}^{A} Q_\mu\,\langle \Phi_\mu(i) \,|\, r_{Aa}^2(i) \,|\, \Phi_\mu(i)\rangle\Big] \tag{4}$$

Here, R_{Aa} and $r_{Aa}(i)$ denote the a-th coordinate of nucleus A from the center of mass and the corresponding coordinate of the i-th electron relative to the host nucleus A, respectively. The total number of electrons apportioned to atom A is given by Q_A, whilst Q_μ denotes the orbital population. It was tacitly assumed in the course of derivation of formula (4) that the Mulliken approximation $\Phi_\mu\Phi_\nu = (1/2)S_{\mu\nu}\,[\Phi_\mu^2 + \Phi_\nu^2]$ for two center mixed densities holds to a good approximation. It appears that the second moment is given by two contributions. The first term in (4) represents the second moment in the monopole approximation. The second term is a correction of the first and arises from the spatial extension of the AOs. The monopole term dominates due to the squares of atomic coordinates. Careful scrutiny of theoretical results has shown that the spatial term is approximately isotropic and constant for each atom belonging to the same row of the periodic table of elements[1]. Thus, the approximate expression takes a succint form:

$$\langle r_a^2\rangle \cong \sum_{A} Q_A\, R_{Aa}^2 + \sum_{p} n_p\, k_p \tag{5}$$

where n_p is the number of atoms of the p-th row in a molecule, whilst k_p is the corresponding adjustable parameter. It was observed[1] that k_p approaches very closely the *ab initio* $(1/3)\,\langle\, 0 \,|\, (r^2) \,|\, 0 \,\rangle$ values for free atoms averaged over the p-th period of the Mendeleev table of elements. Hence, $\langle r_a^2\rangle$ can be given in an approximate but parameter free form. It follows that the second moments and diamagnetic susceptibilities are given in a very simple and transparent form. Extensive studies have shown that intramolecular charge migration can be usually disregarded. Therefore, one can put $Q_A = Z_A$ which leads to the IAM formula:

$$\langle r_a^2\rangle \cong \sum_{A} Z_A\, R_{Aa}^2 + \sum_{p} n_p\, k_p \tag{6}$$

which requires a knowledge of molecular geometry only. Formula (6) gives results which can be favourably compared with experimental and *ab initio* values[1–4]. It proved useful in rationalizing[4] the Pascal rules[11] for molecular magnetic susceptibility. However, one can further improve its performance by introducing spatial constant k_A for each atom:

$$\langle r_a^2\rangle = \sum_{A} [Z_A\, R_{Aa}^2 + k_A] \tag{7}$$

TABLE I

*Comparison of the performance of the previous IAM model and the present reoptimized IAM model in estimating molecular second moments (in 10^{-16} cm^2)**

Molecule	IAM model		Reoptimized IAM model		Exptl.	Ref.
	$\langle a^2\rangle$ $\langle b^2\rangle$ $\langle c^2\rangle$	$\Delta(\langle a^2\rangle)$ $\Delta(\langle b^2\rangle)$ $\Delta(\langle c^2\rangle)$	$\langle a^2\rangle$ $\langle b^2\rangle$ $\langle c^2\rangle$	$\Delta(\langle a^2\rangle)$ $\Delta(\langle b^2\rangle)$ $\Delta(\langle c^2\rangle)$		
3-methylfurane	94.4	0.4	94.4	0.4	94.0	12
	42.0	0.5	42.0	0.5	41.5	
	8.8	0.7	8.8	0.7	9.5	
		0.53		0.53		
$CH_3OCH=CH_2$	52.66	0.56	52.66	0.56	52.1	13
	22.06	0.36	22.06	0.36	21.7	
	6.76	0.3	6.76	0.3	7.06	
		0.41		0.41		
CH_4	5.4	0.47	5.2	0.27	4.93	14, 23
	5.4	0.47	5.2	0.27	4.93	
	7.7	3.37	7.5	3.57	11.07	
		1.44		1.37		
$CH_3OCH=CH_2$	52.6	0.5	52.6	0.5	52.1	14, 24
	22.0	0.3	22.0	0.3	21.7	
	6.8	0.27	6.8	0.27	7.07	
		0.36		0.36		
H_3SiBr	68.1	0.8	68.8	0.1	68.9	14, 25
	9.6	0.7	10.3	0	10.3	
	9.6	0.7	10.3	0	10.3	
		0.73		0.03		
$CH_3CHCHCHO$ (trans)	134.7	1.7	134.7	1.7	136.4	14, 26
	15.7	0.2	15.7	0.2	15.9	
	7.8	1.1	7.8	1.1	8.9	
		1.0		1.0		
$HC=N=NH$	4.26	0.22	4.46	0.02	4.48	15, 27
	4.43	0.37	4.63	0.17	4.8	
	32.34	0.84	32.54	0.64	33.18	
		0.98		0.28		
$NH=C=NH$	4.22	0.21	4.42	0.01	4.43	15, 27
	4.22	0.21	4.42	0.01	4.43	
	33.05	0.54	33.25	0.34	33.59	
		0.32		0.12		
$HCNNH_2$	3.65	0.5	3.85	0.3	4.15	15, 27
	5.09	0.31	5.29	0.51	4.78	
	31.24	0.66	31.44	0.46	31.9	
		0.49		0.42		
1-Si-3-cyclopentene	48.2	0.35	48.6	0.05	48.55	15, 28
	63.5	0.27	63.9	0.13	63.77	
	10.2	1.51	10.6	1.11	11.71	
		0.71		0.43		
XeF_6	75.8	2.45	77.9	0.35	78.25	15, 29
	75.8	2.45	77.9	0.35	78.25	
	75.8	2.45	77.9	0.35	78.25	
		2.45		0.35		

Molecule	IAM model		Reoptimized IAM model		Exptl.	Ref.
	$\langle c^2\rangle$ $\langle a^2\rangle$ $\langle b^2\rangle$	$\Delta(\langle c^2\rangle)$ $\Delta(\langle a^2\rangle)$ $\Delta(\langle b^2\rangle)$	$\langle a^2\rangle$ $\langle b^2\rangle$ $\langle c^2\rangle$	$\Delta(\langle a^2\rangle)$ $\Delta(\langle b^2\rangle)$ $\Delta(\langle c^2\rangle)$		
B_2H_6	7.5	0.5	7.9	0.1	8.0	16, 30
	5.2	0	5.6	0.4	5.2	
	20.0	0.92	20.4	0.52	20.92	
		0.47		0.34		
SOF_2	13.2	1.3	13.9	2.0	11.9	17
	27.5	0.9	28.2	0.2	28.4	
	29.2	0.4	29.9	0.3	29.6	
		0.87		0.83		
oxacyclobutane	10.0	0.2	9.7	0.1	9.8	18, 31
	29.2	1.4	28.9	1.1	27.8	
	27.3	0.8	27.0	1.1	28.1	
		0.8		0.77		
cyclobutanone	11.1	0.3	10.8	0	10.8	19
	33.1	0.3	32.8	0	32.8	
	61.5	1.7	61.2	2.0	63.2	
		0.77		0.67		
cyclopentadiene	7.8	0.8	7.6	1.0	8.6	19
	42.6	0.1	42.4	0.1	42.5	
	42.5	0.4	42.3	0.2	42.1	
		0.43		0.43		
methylenecyclopropane	47.9	0.3	47.9	0.3	48.2	20, 32
	18.5	0	18.8	0	18.8	
	8.3	0.2	8.3	0.2	8.5	
		0.17		0.17		
propene	37.72	0.22	37.42	0.08	37.5	20, 33
	11.78	0.58	11.48	0.28	11.2	
	5.74	0.36	5.44	0.66	6.1	
		0.39		0.34		
cyclopentadiene	45.4	3.1	44.8	2.5	42.3	20, 34
	45.3	3.5	44.7	2.9	41.8	
	10.6	2.2	10.0	1.6	8.4	
		2.93		2.33		
CH_3F	13.14	0.14	12.94	0.06	13.0	14, 35
	4.26	0.36	4.06	0.16	3.9	
	4.26	0.36	4.06	0.16	3.9	
		0.29		0.13		
ethanal	32.7	0.4	32.7	0.4	32.3	21
	9.3	0.3	9.3	0.3	9.6	
	5.3	0.3	5.3	0.3	5.6	
		0.33		0.33		
NH_3	2.94	0.34	2.74	0.14	2.6	21
	2.94	0.34	2.74	0.14	2.6	
	2.94	1.04	2.74	0.84	1.9	
		0.57		0.37		
2-oxacyclobutanone	56.57	0.63	56.77	0.43	57.2	21
	28.31	0.49	28.51	0.29	28.8	
	9.04	0.44	9.24	0.64	8.6	
		0.52		0.45		

3-methyl-2-oxacyclobutanone	106.8	0.8	107.2	0.4	107.6	21
	31.8	0.3	32.2	0.1	32.1	
	8.4	0.3	8.8	0.1	8.7	
		0.47		0.2		
cyclopropene	17.71	0.09	17.51	0.29	17.8	20, 36
	13.83	0.33	13.63	0.13	13.5	
	5.47	0.33	5.27	0.53	5.8	
		0.25		0.32		
ethyleneoxide	16.69	0.39	16.59	0.29	16.3	21
	12.87	0.43	12.77	0.53	13.3	
	7.18	0.38	7.08	0.28	6.8	
		0.4		0.37		
CH_2F_2	25.19	0.61	25.19	0.61	25.8	18, 37
	9.01	0.01	9.01	0.01	9.0	
	5.04	0.04	5.04	0.04	5.0	
		0.22		0.22		
2-methylfurane	92.8	2.0	92.8	2.0	90.8	15, 38
	40.3	0.6	40.3	0.6	39.7	
	8.8	0.3	8.8	0.3	9.1	
		0.97		0.97		
BH_3NH_3	6.53	0.21	6.53	0.21	6.74	22
	6.53	0.21	6.53	0.21	6.74	
	21.81	0.02	21.81	0.02	21.79	
		0.15		0.15		
propene	37.72	0.22	37.42	0.08	37.5	21
	11.78	0.58	11.48	0.28	11.2	
	5.74	0.36	5.44	0.66	6.1	
		0.39		0.34		
CH_3COOH	45.2	0.4	45.4	0.2	45.6	18, 39
	18.8	0.2	19.0	0	19.0	
	6.4	0.1	6.6	0.1	6.5	
		0.23		0.1		
1,2-diaza-1-cyclopropene	15.4	0.09	15.4	0.09	15.49	18, 40
	8.63	1.03	8.63	1.03	9.66	
	5.09	0.01	5.09	0.01	5.08	
		0.38		0.38		
1,2-diaza-3,3-difluoro-1,1-cyclopropene	36.88	1.26	37.28	0.86	38.14	18, 40
	10.85	0.75	11.25	0.35	11.6	
	27.52	0.28	27.92	0.68	27.24	
		0.76		0.63		
thiirene	32.02	3.02	31.82	2.82	29.0	18, 41
	18.22	1.22	18.02	1.02	17.0	
	8.64	0.64	8.44	0.44	8.0	
		1.63		1.43		
PF_3	10.0	1.5	10.7	2.2	8.5	14, 27
	31.6	3.5	32.3	2.8	35.1	
	31.6	3.5	32.3	2.8	35.1	
		2.83		2.6		
OPF_3	34.34	1.34	35.34	2.34	33.0	17
	31.79	2.91	32.79	1.91	34.7	
	31.79	2.91	32.79	1.91	34.7	
		2.39		2.05		

Molecule	IAM model		Reoptimized IAM model		Exptl.	Ref.
	$\langle c^2\rangle$ $\langle a^2\rangle$ $\langle b^2\rangle$	$\Delta(\langle c^2\rangle)$ $\Delta(\langle a^2\rangle)$ $\Delta(\langle b^2\rangle)$	$\langle a^2\rangle$ $\langle b^2\rangle$ $\langle c^2\rangle$	$\Delta(\langle a^2\rangle)$ $\Delta(\langle b^2\rangle)$ $\Delta(\langle c^2\rangle)$		
H_3CSiH_3	9.24	0.18	9.44	0.02	9.42	18, 42
	9.24	0.18	9.44	0.02	9.42	
	31.24	0.3	31.44	0.1	31.54	
		0.22		0.05		
FNO	23.9	0.1	24.4	0.4	24.0	16, 43
	3.0	0.4	3.5	0.9	2.6	
	3.0	0.1	3.5	0.4	3.1	
		0.2		0.57		
HBS	18.9	0.2	19.6	0.5	19.1	15, 44
	3.7	0.8	4.4	0.1	4.5	
	3.7	0.8	4.4	0.1	4.5	
		0.6		0.23		
CS	13.8	0.2	14.0	0	14.0	15, 44
	3.5	0.4	3.7	0.2	3.9	
	3.5	0.4	3.7	0.2	3.9	
		0.33		0.13		
HOCl	21.1	0.2	21.4	0.1	21.3	15, 44
	4.5	0.3	4.8	0	4.8	
	3.7	0.2	4.0	0.1	3.9	
		0.23		0.07		
cyclopropenone	39.2	1.0	39.5	0.7	40.2	15, 44
	14.3	0.1	14.6	0.4	14.2	
	4.4	0.7	4.7	0.4	5.1	
		0.6		0.5		
4-oxa-2,5-cyclohexadienone	104.2	1.2	104.8	0.6	105.4	15, 44
	59.2	1.3	59.8	1.9	57.9	
	7.8	0.6	8.4	0	8.4	
		1.03		0.83		
2-oxa-3,5-cyclohexadienone	102.3	0.9	102.9	0.3	103.2	15, 44
	59.5	0.4	60.1	1.0	59.1	
	7.8	0.4	8.4	0.2	8.2	
		0.57		0.5		
1,2-difluorobenzene	128.3	0.7	128.5	0.5	129.0	15, 44
	92.0	0.8	92.2	1.0	91.2	
	8.8	0.7	9.0	0.5	9.5	
		0.73		0.67		
1,4-diaza-1,3,5-cyclohexatriene	57.47	3.07	57.67	3.27	54.4	15, 44
	50.82	2.18	51.02	1.98	53.0	
	6.8	1.6	7.0	1.4	8.4	
		2.28		2.22		
XeF_4	77.9	3.27	79.8	1.37	81.17	15, 29
	77.9	3.27	79.8	1.37	81.17	
	9.5	0.67	11.4	2.57	8.83	
		2.4		1.77		
HCP	18.5	1.1	18.9	1.5	17.4	14, 45
	3.7	0.6	4.1	0.2	4.3	
	3.7	0.6	4.1	0.2	4.3	
		0.77		0.63		

HBS	18.9	0.2	19.6	0.5	19.1	14, 45
	3.7	0.8	4.4	0.1	4.5	
	3.7	0.8	4.4	0.1	4.5	
		0.6		0.23		
CF_2	5.8	0.57	6.0	0.37	6.37	14, 46
	22.1	0.43	22.3	0.23	22.53	
	3.0	0.12	3.2	0.32	2.88	
		0.37		0.31		
HCOSH	46.7	1.0	47.2	0.5	47.7	14, 47
	11.1	0.6	11.6	1.1	10.5	
	4.9	0.4	5.4	0.1	5.3	
		0.67		0.57		
1,3-difluorobenzene	152.8	1.0	152.4	0.8	153.2	12
	80.1	0.7	80.3	0.9	79.4	
	8.8	0.7	9.0	0.5	9.5	
		0.8		0.73		
HCCF	31.54	0.04	31.44	0.14	31.5	21
	3.2	0.3	3.3	0.2	3.5	
	3.2	0.3	3.3	0.2	3.5	
		0.21		0.18		
OCO	24.64	0.86	25.24	0.26	25.5	21
	3.0	0.1	3.6	0.7	2.9	
	3.0	0.1	3.6	0.7	2.9	
		0.35		0.55		
CH_3F	13.14	0.14	12.94	0.06	13.0	21
	4.26	0.36	4.06	0.16	3.9	
	4.26	0.36	4.06	0.16	3.9	
		0.29		0.13		
benzene	60.8	0.7	60.8	0.7	60.1	20, 32
	60.8	0.7	60.8	0.7	60.1	
	7.2	0.5	7.2	0.5	7.7	
		0.63		0.63		
fluorobenzene	111.6	0.2	111.7	0.1	111.8	21
	61.6	0.8	61.7	0.9	60.8	
	8.0	0.4	8.1	0.3	8.4	
		0.47		0.43		
N=N	6.22	0.38	6.42	0.18	6.6	18, 48
	2.0	0.1	2.2	0.1	2.1	
	2.0	0.1	2.2	0.1	2.1	
		0.19		0.13		
O=O	7.83	0.37	8.43	0.23	8.2	18, 48
	2.0	0.3	2.6	0.3	2.3	
	2.0	0.3	2.6	0.3	2.3	
		0.32		0.28		
N=N=O	23.08	1.02	23.58	0.52	24.1	18, 48
	3.0	0	3.5	0.5	3.0	
	3.0	0	3.5	0.5	3.0	
		0.34		0.51		
HCN	12.69	0.4	12.79	0.3	13.09	18, 48
	2.2	0.24	2.3	0.14	2.44	
	2.2	0.24	2.3	0.14	2.44	
		0.29		0.19		

Molecule	IAM model		Reoptimized IAM model		Exptl.	Ref.
	$\langle c^2\rangle$ $\langle a^2\rangle$ $\langle b^2\rangle$	$\Delta(\langle c^2\rangle)$ $\Delta(\langle a^2\rangle)$ $\Delta(\langle b^2\rangle)$	$\langle a^2\rangle$ $\langle b^2\rangle$ $\langle c^2\rangle$	$\Delta(\langle a^2\rangle)$ $\Delta(\langle b^2\rangle)$ $\Delta(\langle c^2\rangle)$		
furane	36.0	0.2	36.3	0.1	36.2	18, 48
	38.42	0.62	38.72	0.92	37.8	
	5.8	1.0	6.1	0.7	6.8	
		0.61		0.57		
$O=CF_2$	25.13	0.97	25.63	0.47	26.1	18, 48
	24.26	0.54	24.76	0.04	24.8	
	4.0	0	4.5	0.5	4.0	
		0.5		0.34		
cis-1,2-difluorethene	46.05	0.65	46.25	0.45	46.7	18, 48
	18.43	0.33	18.63	0.53	18.1	
	4.4	0.1	4.6	0.1	4.5	
		0.36		0.36		
CH_3Cl	25.53	0.53	25.23	0.23	25.0	18, 49
	5.73	0.2	5.43	0.1	5.53	
	5.73	0.2	5.43	0.1	5.53	
		0.31		0.14		
CH_3I	46.9	1.1	46.8	1.0	45.8	18, 49
	8.74	0.04	8.64	0.06	8.7	
	8.74	0.04	8.64	0.06	8.7	
		0.39		0.37		
ClF	19.1	0.1	19.2	0	19.2	18, 50
	3.5	0.1	3.6	0	3.6	
	3.5	0.1	3.6	0	3.6	
		0.1		0		
BrF	26.74	0.04	27.04	0.34	26.7	18, 50
	4.5	0.1	4.8	0.2	4.6	
	4.5	0.1	4.8	0.2	4.6	
		0.08		0.25		
ClCN	46.31	0.39	46.41	0.29	46.7	14, 54
	4.5	0.4	4.6	0.3	4.9	
	4.5	0.4	4.6	0.3	4.9	
		0.4		0.3		
BrCN	65.18	0.42	65.48	0.12	65.6	18, 50
	5.5	0.4	5.8	0.1	5.9	
	5.5	0.4	5.8	0.1	5.9	
		0.41		0.11		
ICN	83.61	0.39	83.91	0.09	84.0	18, 50
	7.5	0.4	7.8	0.1	7.9	
	7.5	0.4	7.8	0.1	7.9	
		0.4		0.1		
HCl	4.26	0.58	4.26	0.58	3.68	18, 51
	2.7	0.23	2.7	0.23	2.93	
	2.7	0.23	2.7	0.23	2.93	
		0.35		0.35		
SO_2	29.11	0.89	29.91	0.09	30.0	18, 51
	8.6	0.1	9.4	0.7	8.7	
	4.5	0.3	5.3	1.1	4.2	
		0.43		0.63		

$S{=}CH_2$	20.9	0.2	21.1	0	21.1	18, 52
	5.6	1.0	5.8	0.8	6.6	
	3.9	0.7	4.1	0.5	4.6	
		0.63		0.43		

* Difference between the calculated and experimental (or ab initio) second moment is denoted by Δ. Each triplet of Δ values is followed by the average error. Heading exptl. refers to either experimental or *ab initio* data.

where summation embraces all atoms in a molecule. Empirical parameters k_A are determined here by the least-squares fitting of available experimental and *ab initio* data. The results are presented in Table I.

DISCUSSION

Perusal of the data presented in Table 1 shows that formula (7) is improvement over the earlier expression (6). This is evidenced by a decreased sum of absolute errors of 117.8 relative to the earlier value of 147.0 (in 10^{-16} cm^2). The average absolute value for the reparametrized IAM model (7) is 0.5 10^{-16} cm^2, which is close to the usual experimental errors. Of course, our empirical constants k_A are »contaminated« by inaccuracies of the used experimental data and/or *ab initio* results, but this is unavoidable. The »optimal« adjustable parametres are given in Table II. Comparison with earlier values reveals similarity, but there are some differences. In the first place H-atom values for sp^3 and sp^2 nearest neighbours are clearly distinguished, although the difference is only 0.1. Somewhat higher values have been found for the second row atoms. The most notable increase takes place in boron (1.5). Similar situation if found in the third row atoms, but this time a significantly higher value for k_a constant is estimated for silicon. As general conclusion, we can say that further experimental measurements and *ab initio* calculations on molecules involving other atoms not included in Table II are highly desirable. They will enable determination of the corresponding k_A constants, thus extending the field of application of formula (7). We are, namely, quite confident that additivity of the molecular second moments is generally valid.

TABLE II

Comparison of empirical parameters for the two IAM parametrizations (in 10^{-16} cm^2)

Atom	H	B	C	N	O	F
Orginal IAM	0.2	1.0	1.0	1.0	1.0	1.0
Reparametrized IAM	0.1[a]; 0.2[b]	1.5	1.0	1.1	1.3	1.1
Atom	**Si**	**P**	**S**	**C**	**Br**	**I**
Orginal IAM	2.5	2.5	2.5	2.5	3.5	5.5
Reparametrized IAM	3.3	2.9	2.7	2.5	3.7	5.7

[a] H-atom value for sp^3 neighboring atom.

[b] H-atom value for sp^2 neighboring atom.

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SAŽETAK

Molekularni drugi momenti i dijamagnetska susceptibilnost. Reparametrizacija formula u okviru modela nezavisnih atoma.

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Primijenjen je model nezavisnih atoma na računanje drugih momenata raspodjele elektronske gustoće u molekulama i srodne im dijamagnetske susceptibilnosti. Prijašnje formule su poopćene i postignuto je bolje slaganje s eksperimentalnim podacima i *ab initio* vrijednostima.