

## Preface.

Energy of covalent interaction is taken in standard form:

$$U_{\text{cov}} = \sum_i K_b^{(i)} (b_i - b_i^{(0)})^2 + \sum_j K_\theta^{(j)} (\theta_j - \theta_j^{(0)})^2 + \sum_k K_\phi^{(k)} (1 - \cos(n_k (\phi_k - \phi_k^{(0)}))),$$

where summation is taken by  $i$  for all covalent bonds, by  $j$  for all covalent angles, by  $k$  for all torsion and out-of-plane quasi-torsion angles (see below), and  $b_i \equiv b_i\{\mathbf{r}\}$ ,  $\theta_j \equiv \theta_j\{\mathbf{r}\}$ ,  $\phi_k \equiv \phi_k\{\mathbf{r}\}$  – values of covalent bond length, covalent angles and covalent torsion (and out-of-plane) angles correspondingly.  $b_i\{\mathbf{r}\}$ ,  $\theta_j\{\mathbf{r}\}$ ,  $\phi_k\{\mathbf{r}\}$  are function of atomic coordinates  $\{\mathbf{r}\}$ .

Fixed covalent parameters  $K_b^{(i)}$ ,  $b_i^{(0)}$ ;  $K_\theta^{(j)}$ ,  $\theta_j^{(0)}$ ;  $K_\phi^{(k)}$ ,  $n_k$ ,  $\phi_k^{(0)}$  determined by involved in corresponded bond or angle atoms ( $i'$ ,  $i''$ ;  $j'$ ,  $j''$ ,  $j'''$ ;  $k'$ ,  $k''$ ,  $k'''$ ,  $k''''$ , correspondingly) accordingly their “atomic codes for covalent interactions”; these “codes” (see Table A1.1) take into account not only atoms, but also their covalent surroundings. There is a symmetry for all these types interactions: parameters for bond  $i'-i''$  and  $i''-i'$  are equal, for bonds  $j'-j''-j'''$  and  $j'''-j''-j'$  are equal, and for torsion angles  $k'-k''-k'''-k''''$  and  $k''''-k'''-k''-k'$  are also equal. Majority of covalent parameters were taken from ENCAD force field[1]. If ENCAD parameterization not have certain parameters for considered in this work molecules, then we add insufficient covalent parameters by similarity with existing in ENCAD, with taking into account values in the experimental crystal structure, see below Tables A1.2 – A1.5.

Covalent bond length definition is  $b_i\{\mathbf{r}\} = |\mathbf{r}_{i'} - \mathbf{r}_{i''}|$ , where  $i'$ ,  $i''$  – atoms, involved in  $i$ -bond, and  $\mathbf{r}_{i'}$ ,  $\mathbf{r}_{i''}$  – coordinates of these atoms.

Covalent angle definition is  $\theta_j\{\mathbf{r}\} = \arccos((\mathbf{r}_{j''} - \mathbf{r}_{j'''}) \cdot (\mathbf{r}_{j'} - \mathbf{r}_{j''})) / (|\mathbf{r}_{j''} - \mathbf{r}_{j'''}| \cdot |\mathbf{r}_{j'} - \mathbf{r}_{j''}|)$ , where  $j'$ ,  $j''$ ,  $j'''$  – atoms, involved in  $j$ -angle, with middle atom  $j''$ .

Covalent torsion angle  $\phi_k\{\mathbf{r}\}$ , where  $-180^\circ \leq \phi_k \leq 180^\circ$ , is defined by four involved atoms ( $k'$ ,  $k''$ ,  $k'''$ ,  $k''''$ ), where none of these points not coincide with other in space, and three of them not belong one straight line; see. Fig. A1.1a):  $\phi_k\{\mathbf{r}\} = \arccos(\mathbf{n}_{123} \cdot \mathbf{n}_{234}) \cdot \text{sign}([\mathbf{n}_{123} \times \mathbf{n}_{234}] \cdot \mathbf{r}_{23})$ , where  $\text{sign}(x)$  function definition is little different from common one:  $\text{sign}(x \geq 0) = 1$ ,  $\text{sign}(x < 0) = -1$ ; it need to be mentioned that corresponded vectors are defined as follows  $\mathbf{r}_{12} = \mathbf{r}_{k''} - \mathbf{r}_{k'}$ ,  $\mathbf{r}_{23} = \mathbf{r}_{k'''} - \mathbf{r}_{k''}$ ,  $\mathbf{r}_{34} = \mathbf{r}_{k''''} - \mathbf{r}_{k'''}$ , and  $\mathbf{n}_{123} = [\mathbf{r}_{12} \times \mathbf{r}_{23}] / |\mathbf{r}_{12} \times \mathbf{r}_{23}|$ ,  $\mathbf{n}_{234} = [\mathbf{r}_{23} \times \mathbf{r}_{34}] / |\mathbf{r}_{23} \times \mathbf{r}_{34}|$ .

Out-of-plane or quasi-torsion angle  $\phi_k\{\mathbf{r}\}$ , i.e. angle plane atom distortions, where three “boundary” atoms covalently bounded with “central” one, defined in the same way as torsion angle, but in opposite to previous, where all “bonds”  $k'-k''$ ,  $k''-k'''$ ,  $k'''-k''''$  are equal real covalent bonds (Fig. A1.1a), the first “bond” not correspond,  $k'-k''$ , any real covalent bond (Fig. A1.1b).

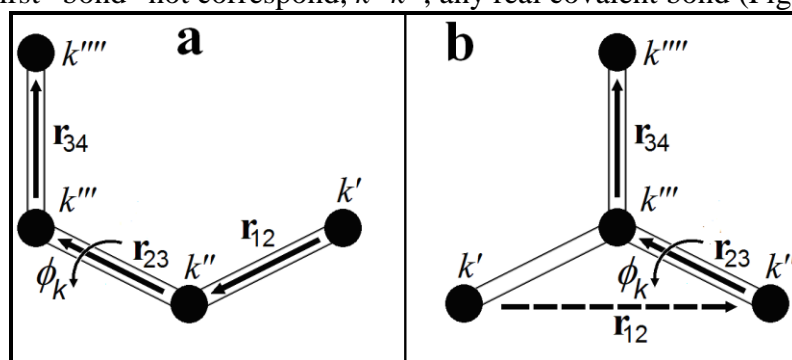


Figure A1.1. Definition of torsion angle (a) and out-of-plane quasi-torsion angle (b).

## List of atomic and covalent parameters of ENCAD and their modifications

Table A1.1. Covalent and nonvalent atomic typification

Atom and atomic code for covalent interactions	Atomic symbol for nonvalent interactions	Description
<i>Hydrogen</i>		
H	H	Nonpolar hydrogen
HN	D	Hydrogen, connected to oxygen
HO	D	Hydrogen, connected to nitrogen
HW	D	Hydrogen in water
<i>Oxygen</i>		
O	O	Oxygen in carbonyl C=O group
OR	O	Divalent oxygen in the ring
OH	V	Oxygen in hydroxyl OH group
O2	V	Divalent oxygen in ether -O- group
O"	Q	Oxygen in carboxylate ion COO <sup>-</sup> group
OP	Q	Oxygen in phosphate ion POO <sup>-</sup> group
OW	W	Oxygen in water
<i>Nitrogen</i>		
N	N	Trivalent nitrogen
N1	N	Nitrogen in >NH group
N2	N	Nitrogen in -NH <sub>2</sub> group
M1	M	Nitrogen in >NH <sup>+</sup> group
M2	M	Nitrogen in -NH <sub>2</sub> <sup>+</sup> group
M3	M	Nitrogen in -NH <sub>3</sub> <sup>+</sup> group
L5	L	Divalent nitrogen in 5-membered ring
L6	L	Divalent nitrogen in 6-membered ring
<i>Carbon</i>		
C1	C	Tetravalent sp <sup>3</sup> carbon in CH group
C2	C	Tetravalent sp <sup>3</sup> carbon in CH <sub>2</sub> group
C3	C	Tetravalent sp <sup>3</sup> carbon in CH <sub>3</sub> group
CP	C	Tetravalent sp <sup>3</sup> carbon in proline, in >CH <sub>2</sub> group
A'	A	Trivalent sp <sup>2</sup> carbon in carbonyl >CO group
A6	A	Trivalent sp <sup>2</sup> carbon in >CH group in 6-membered ring
A5	A	Trivalent sp <sup>2</sup> carbon in >CH group in 5-membered ring
A7	A	Trivalent sp <sup>2</sup> carbon >C- at the junction of 5- and 6-membered rings
A"	A	Trivalent sp <sup>2</sup> carbon in -COO <sup>-</sup> group
<i>Other</i>		
S	S	Divalent sulfur in thioether -S- group
SH	S	Divalent sulfur in thiol -SH group
P	P	Tetravalent phosphorus

To find in Tables S1.2-S1.5 sought-for covalent parameters one need to identify covalent atomic codes in the table S1.1. Then the needed combination of atomic codes has to be tried to find in the cells of tables without question signs, then (if such combination doesn't exist) for search one should try by changing second code character to question sign "?" and after this if even such combination doesn't exist all atomic code character set to be "??"

Due to abovementioned in preface potential symmetry, one should search one of the reflection symmetric combination for bonds (combination for *i'-i''* is also valid for *i''-i'*), for angles (combination for *j'-j''-j'''* is also valid for *j'''-j''-j'*) and for torsion and out-of-plane angles (combination for *k'-k''-k'''-k''''* is also valid for *k''''-k'''-k''-k'*).

$$\text{Energy of covalent bonds: } U_{\text{cov.bonds}} = \sum_i K_b^{(i)} (b_i - b_i^{(0)})^2$$

Table A1.2. Covalent bonds parameters

Bond	$K_b$ kcal/mol/Å <sup>2</sup>	$b^{(0)}$ (Å)	Molecule for which the parameters set has been extended or corrected
O?-H?	250	1	
N?-H?	250	1	
C?-H?	250	1.09	
C?-O?	250	1.437	
C?-OH	250	1.439	
C?-N?	250	1.467	
C?-M?	250	1.472	
C?-C?	250	1.525	
CP-CP	250	1.519	
C1-CP	250	1.498	
A?-H?	250	1.09	
A?-C?	250	1.526	
A'-O?	500	1.236	
A"-O"	500	1.223	
A'-N?	500	1.322	
A5-N?	500	1.334	
A5-C?	250	1.516	
A5-A5	500	1.376	Misprint in [1] was corrected for pyrrole molecule (AL45 instead A5-A5)
A5-A7	500	1.451	
A5-L?	500	1.334	
A6-O?	500	1.228	
A6-OH	250	1.378	
A6-A6	500	1.389	
A6-A7	500	1.411	
A6-M?	500	1.335	
A7-N?	500	1.367	
A7-N1	500	1.343	
A7-A7	500	1.364	
S?-H?	250	1.33	
S?-C?	250	1.808	
S?-S?	250	2.015	
M?-H?	250	1	
A6-N?	500	1.355	
A6-L?	500	1.355	
A7-L?	500	1.367	
P?-OP	500	1.48	
P?-O2	250	1.594	
Added to ENCAD set bonds parameters <sup>a</sup>			Molecule <sup>b</sup>
N-O	500	1.22	Nitrobenzene
N1-L5	250	1.382	Indazole
A'-A6	250	1.494	Acetophenone
OR-A5	250	1.386	Succinic anhydride
O-A5	500	1.193	
A7-S	250	1.741	Dibenzothiophene
A6-S	250	1.763	Phenothiazine
A'-A'	250	1.534	Dimethyl oxalate

<sup>a</sup> All these bonds are single or  $\pi$ -resonance bonds, and we assign them a constants  $K_b=250$  or, correspondently,  $K_b=500$ . (For similarity to the examples above)

<sup>b</sup> We took this molecule from crystal from CSD [2] database to measure distance to assign the length of bond.

$$\text{Energy of covalent angles: } U_{\text{cov.angles}} = \sum_j K_{\theta}^{(j)} (\theta_j - \theta_j^{(0)})^2$$

Table A1.3. Covalent angles parameters\*

Angle	$K_{\theta}$ (kcal/mol)	$\theta^{(0)}$ (degrees)	Molecule for which the parameters set has been extended or corrected
H?-O?-H?	60	109.47	
A?-O?-H?	60	110	
C?-O?-H?	60	110	
H?-N?-H?	60	120	
C?-N?-H?	60	119.5	
A?-N?-H?	60	119.6	
C?-N?-C?	60	112.4	
A?-N?-C?	60	121.3	
A5-N?-A5	120	108	
A5-N1-A7	120	108	
H?-C?-H?	60	109.5	
O?-C?-H?	60	109	
O?-C?-C?	60	109.5	
C?-C?-H?	60	109.5	
N?-C?-H?	60	109.5	
M?-C?-H?	60	109.5	
M?-C?-C?	60	111	
A?-C?-H?	60	109.5	
C?-C?-N?	60	109.1	
A?-C?-N?	60	111.3	
A5-A5-N?	120	108	
A5-A5-L?	120	108	
N1-A5-L5	120	108	
C2-A5-N1	60	126	
A7-A5-A5	120	108	
??-A6-??	120	120	
M?-A6-M?	120	120	
H -A6-??	60	120	
A6-A6-C?	60	120.1	
A6-A6-A6	120	120	
A5-A6-A6	120	120.2	
OH-A6-A6	60	118.4	
A7-A6-A6	120	120	
A5-A7-A7	120	108	
A7-A7-A6	120	120	
A5-A7-A6	120	132	
N?-A7-A6	60	132	
N1-A7-A6	120	132	
N1-A7-A7	120	108	
L?-A7-A6	60	132	
C?-S?-H?	60	110	
C?-S?-C?	60	99.1	
S?-S?-C?	60	104.3	
H?-M?-H?	60	120	
C?-M?-H?	60	119.5	
A?-M?-H?	60	119.6	
A6-M?-C?	60	123.2	
A7-A7-A6	120	120	
N -A7-A7	60	108	
N -A7-L6	60	126	
L5-A7-A7	60	108	

A7-A7-L6	60	120	
OP-P -OP	60	120	
A?-C?-M?	60	111.3	
C?-C?-C?	60	111.4	
A?-C?-C?	60	110.1	
S?-C?-C?	60	115.5	
S?-C?-H	60	110	
A6-C?-C?	60	114.1	
A5-C?-C?	60	113.9	
OH-C?-C?	60	107.9	
H?-A?-H?	60	120	
A?-A?-H?	60	120	
O?-A?-O	60	120	
N?-A?-H?	60	120	
H?-A'-O?	60	121	
N?-A'-O?	120	123.5	
C?-A'-O?	60	121	
C?-A'-N?	60	115.5	
O"-A"-C?	60	117.7	
O"-A"-O"	120	124.6	
H -A5-??	60	126	
C2-A5-A?	60	126	
H?-M3-H?	60	109.5	
C?-M3-H?	60	109.5	
A5-L?-A5	120	108	
A'-N -CP	60	125.8	
N -C1-CP	60	104	
A'-C1-CP	60	111.9	
N -CP-CP	60	105.1	
C1-CP-CP	60	107.2	
CP-CP-CP	60	103.9	
C1-OR-C1	60	108.16	
P -O2-A?	60	120	
P -O2-C2	60	120	
C1-OR-C?	60	109.5	
C1-O2-P	60	120	
A7-N -A5	60	108	
A6-N -A6	60	120	
A6-N1-A6	60	120	
OH-C1-N?	60	109.5	
OR-C1-N	60	107.97	
OR-C1-A6	60	107.97	
A5-C3-A7	60	109	
N -A5-N	60	107.78	
N -A5-C3	60	126	
N -A5-L5	60	108	
N -A7-L5	60	133.61	
C3-A7-A6	60	108.86	
C3-A7-A7	60	132.53	
OP-P -O2	60	109.5	
O2-P -O2	60	101.5	
A5-L5-A7	60	108	
A6-L5-A7	60	119.34	
??-L6-??	120	120	
N1-A5-N1	120	108	

Added to ENCAD set angles parameters <sup>a</sup>			Molecule <sup>b</sup>
A6-C2-A6	60	109.5	Fluorene
C3-A'-C3	60	116	Acetone
C2-OR-C2	60	110.11	Trioxane, 1,4-dioxane, tetrahydrofuran
OR-C2-OR	60	109.57	Trioxane
A6-O2-A6	120	110.6	Succinic anhydride
OR-A5-C2	120	110.1	Succinic anhydride
O -A6-C2	120	130.53	Succinic anhydride
A5-OR-A5	120	110.63	Succinic anhydride
A6-N -O	120	118.8	Nitrobenzene
O -N -O	120	123.2	Nitrobenzene
A6-OR-A6	120	103	Dibenzofuran
A6-A'-C3	60	119	Acetophenone
A6-A'-O	120	120	Acetophenone
A6-A7-C2	60	120	Acenaphthene
A6-A7-A6	120	118.31	Acenaphthene
A6-L5-A6	120	104.13	Benzimidazole
L5-A5-N1	120	114.06	Benzimidazole
A7-A7-N1	120	105.39	Benzimidazole
A7-N1-A5	120	106.67	Benzimidazole
A7-A5-L5	120	113.83	Indazole
N1-L5-A?	120	105.74	Indazole
L5-N1-A?	120	110.15	Indazole
HN-N1-L?	60	128.14	Indazole
A5-A7-A6	120	138.13	Indazole
A5-A7-A7	120	102.28	Indazole
A5-A5-A5	120	107.05	Pyrrole
A7-A7-A7	120	106.67	Carbazole
A7-N1-A7	120	109.2	Carbazole
A6-A7-S	120	126.1	Dibenzothiophene
A7-S -A7	120	91.53	Dibenzothiophene
A7-A7-S	120	112.3	Dibenzothiophene
A6-S -A6	120	100.86	Phenothiazine
A6-N1-A6	120	124.44	Phenothiazine
A'-O2-C3	60	108.16	Dimethyl oxalate
A'-A'-O	60	124.15	Dimethyl oxalate
A'-A'-O2	60	109.58	Dimethyl oxalate

\* All  $(\theta_j - \theta_j^{(0)})$  are measured in radians, not in degrees!

<sup>a</sup> All these angles are formed by single bonds or situated in rings, or formed by  $\pi$ -resonance bonds, and we assign them a constants  $K_\theta=60$  or, correspondently,  $K_\theta=120$ . (For similarity to the examples above)

<sup>b</sup> We took this molecule from crystal from CSD [2] database to measure covalent angle to assign the angle magnitude.

$$\text{Energy of covalent torsion angles: } U_{\text{cov.torsion}} = \sum_k K_{\phi}^{(k)} \left( 1 - \cos \left( n_k \left( \phi_k - \phi_k^{(0)} \right) \right) \right)$$

Table A1.4. Torsion angles parameters

Torsion angle	$K_{\phi}$ kcal/mol	$n$ (see. <sup>a</sup> )	$\phi^{(0)}$ degree	Molecule for which the parameters set has been extended or corrected
??-A?-A?-??	10	2	0	
C?-A?-A?-??	10	2	180	
C?-A?-A?-H?	10	2	0	
C?-A5-A7-A6	10	2	0	
??-A5-N?-??	80	2	0	
??-A5-N?-C?	10	2	180	
C?-A5-N?-??	10	2	180	
??-A5-L?-??	10	2	0	
N -A5-L?-A7	10	2	0	
H?-A5-L5-A5	10	2	180	
A6-N1-A6-N2	20	2	0	
??-A6-N?-??	10	2	0	
O -A6-N1-A6	20	2	0	
??-A6-N -C?	10	2	180	
H -A6-N -C1	10	2	0	
??-A6-L?-??	10	2	0	
A6-L6-A6-N2	20	2	0	
A6-L6-A6-H?	20	2	0	
C?-A'-N?-C?	10	2	180	
C?-A'-N?-H?	10	2	0	
C?-A6-A6-A6	20	2	180	
C?-A6-A6-H?	20	2	0	
A6-A6-A6-A6	20	2	0	
??-A6-M?-??	10	2	0	
L?-A7-A6-L?	10	2	180	
L?-A7-A6-N1	10	2	180	
L?-A7-A7-L?	10	2	180	
N?-A7-A6-A6	10	2	180	
N?-A7-A7-A6	10	2	180	
??-A7-L?-??	10	2	0	
A6-A7-L5-A5	20	2	0	
N?-A7-L6-A6	10	2	180	
A7-A7-N?-A5	10	2	0	
??-A7-N?-C?	10	2	0	
??-P?-O?-??	2	3	60	
??-N?-C?-??	0	6	0	
A'-N?-C?-A'	0	6	0	
C?-N?-A'-H?	10	2	0	
??-C?-O?-??	0.6	3	60	
??-C?-C?-??	1.4	3	60	
??-C?-A?-??	0.1	6	30	
??-C?-A'-??	0	6	0	
??-C?-M3-??	1.4	3	60	
??-S?-C?-??	1	3	60	
S?-S?-C?-??	0	1	0	
??-S?-S?-??	6	2	90	
??-M?-C?-??	0	6	0	
A'-N -CP-CP	10	1	180	
??-C?-CP-??	1.4	3	0	
N -C1-CP-CP	10	1	0	

C?-A'-N-CP	10	2	0	
Corrected <sup>b,c</sup> or added <sup>d</sup> to ENCAD set torsion angles parameters <sup>a</sup>				Molecule
A6-A6-A6-H?	10	2	0	see. <sup>b</sup>
??-A?-OH-??	1.65	2	0	Phenol group <sup>c</sup>
??-A?-O2-??	1.8	2	0	Oxy-phenoles <sup>c</sup>
A5-N1-A5-A5	10	2	0	Pyrrole <sup>d</sup>
A5-N1-A5-H	10	2	0	Pyrrole <sup>d</sup>
A5-A5-N1-HN	10	2	0	Pyrrole <sup>d</sup>
H -A5-N1-HN	10	2	0	Pyrrole <sup>d</sup>
A6-A6-OR-A6	1.8	2	0	Dibenzofuran <sup>e</sup>
O-A5-OR-A5	1.8	2	0	Succinic anhydride <sup>e</sup>
C2-A5-OR-A5	1.8	2	0	Succinic anhydride <sup>e</sup>
A6-A7-N1-HN	10	2	0	Carbazole <sup>d</sup>
A6-A7-N1-A7	10	2	0	Carbazole <sup>d</sup>
A5-L5-N1-A7	10	2	0	Indazole <sup>d</sup>
A5-L5-N1-HN	10	2	0	Indazole <sup>d</sup>
A6-A7-N1-L5	10	2	0	Indazole <sup>d</sup>
A7-A7-N1-L5	10	2	0	Indazole <sup>d</sup>
A6-A7-N1-A5	10	2	0	Benzimidazole <sup>d</sup>
A7-A7-N1-HN	10	2	0	Benzimidazole <sup>d</sup>
A7-A7-N1-A7	10	2	0	Benzimidazole <sup>d</sup>
A6-A7-S -A7	10	2	0	Dibenzothiophene
A7-S -A7-A7	10	2	0	Dibenzothiophene
A6-S-A6-A6	10	2	0	Phenothiazine

<sup>a</sup> For all rotational angles around sp<sup>2</sup>-sp<sup>2</sup> bonds,  $n_k=1$ , given in ENCAD, was changed to  $n_k=2$ , so energy minimums can occur, according symmetry, in both planar arrangements of atomic chain. For preserving the initial slope, given in ENCAD  $K_\phi^{(k)}$  was decreased by factor  $2^2=4$ .

<sup>b</sup> In original parameters tables ENCAD this row occurs 2 times with the different  $K_\phi$ :  $K_\phi=40$  and  $K_\phi=80$ ; so we left  $K_\phi=40$ .

<sup>c</sup> For phenol group values  $n_k=2$ ,  $K_\phi^{(k)}$  и  $\phi_k^{(0)}$  was taken from the experimental data, given in [3]

<sup>d</sup> All added angles have  $K_\phi^{(k)}=10$  – by analogy with many angles of rotation in sp<sup>2</sup>-sp<sup>2</sup> bonds, given above.

<sup>e</sup> Lower bound estimate – by very distant analogy with oxy-phenols.

Additional comment.

If the bond  $k''-k'''$ , where rotation occurs, have some extensions from atoms  $k''$  и/или  $k'''$ , i.e. if first and/or last atom of torsion angle can be chosen ambiguously ( $k' = k^{(1)}, -k^{(2)}, \dots, k''' = k'''^{(1)}, k'''^{(2)}, \dots$ ), then one should choose the most heaviest atoms to continue extensions [1].



$$\text{Out-of-plane torsion angles: } U_{\text{covalent}} = \sum_k K_{\phi}^{(k)} (1 - \cos(n_k (\phi_k - \phi_k^{(0)})))$$

Table A1.5. Out-of-plane torsion angles parameters

Out-of-plane torsion angle	$K_{\phi}$ kcal/mol	$n$	$\phi^{(0)}$ degree	Shape
??-??-M2-??	2	2	0	planar –N<
??-??-N?-??	2	2	0	planar –N<
??-??-M?-??	2	2	0	planar –N<
??-??-A?-??	2	2	0	planar –C<
??-??-C?-??	2	3	0	tetrahedron center (C?) and its 3 vertices
A'-??-C1-??	2	3	0	tetrahedron center (C1) and its 3 vertices <sup>a</sup>
A'-??-C1-H?	2	3	0	tetrahedron center (C1) and its 3 vertices <sup>b</sup>
??-??-C1-A'	2	3	0	tetrahedron center (C1) and its 3 vertices <sup>a</sup>
C3-C2-C1-C3	2	3	0	tetrahedron center (C1) and its 3 vertices
C?-C1-C1-C3	2	3	0	tetrahedron center (C1) and its 3 vertices <sup>a</sup>
C3-C1-C1-OH	2	3	0	tetrahedron center (C1) and its 3 vertices <sup>b</sup>
C1-C2-C1-C3	2	3	0	tetrahedron center (C1) and its 3 vertices <sup>b</sup>
N?-A'-C1-C?	2	3	0	tetrahedron center (C1) and its 3 vertices <sup>b</sup>
M?-A'-C1-C?	2	3	0	tetrahedron center (C1) and its 3 vertices <sup>b</sup>
??-??-M3-??	2	3	0	tetrahedron center (M3) and its 3 vertices
N-C2-C1-OR	2	3	0	tetrahedron center (C1) and its 3 vertices <sup>a</sup>
??-??-P?-??	2	3	0	tetrahedron center (P?) and its 3 vertices

<sup>a</sup> In all these quasi-torsion angles, generated by  $sp^3$ -hybridized central atom,  $n_k=1$  (at  $\phi_k^{(0)} \equiv -120^0$ , accepted in ENCAD for unambiguous choosing of this atom correct chirality in proteins, DNA, RNAs, but not essentially must be the same in used by us molecules) changed to  $n_k=3$ .

<sup>b</sup> In all these quasi-torsion angles, generated by  $sp^3$ -hybridized central atom,  $n_k=1$  (at  $\phi_k^{(0)} \equiv +120^0$ , accepted in ENCAD for unambiguous choosing of this atom correct chirality in proteins, DNA, RNAs, but not essentially must be the same in used by us molecules) changed to  $n_k=3$ .

Herewith, at both cases, energy minimums of quasi-torsion angles fit to  $\phi_k^{(0)} = -120^0, 0^0, +120^0$ , as a consequence of a tetrahedron symmetry, generated by  $sp^3$ - hybridized central atom  $k'''$  (besides angle  $\phi_k^{(0)} = 0^0$  excluded – not by quasi-torsion potential, but forbidden overlapping in space of atoms  $k'$  and  $k'''$ , see. Fig. A1.2).

With the change  $n_k=1$  to  $n_k=3$ , given at ENCAD  $K_{\phi}^{(k)}$  decreased by factor  $3^2=9$  to preserving of potential well steepness.

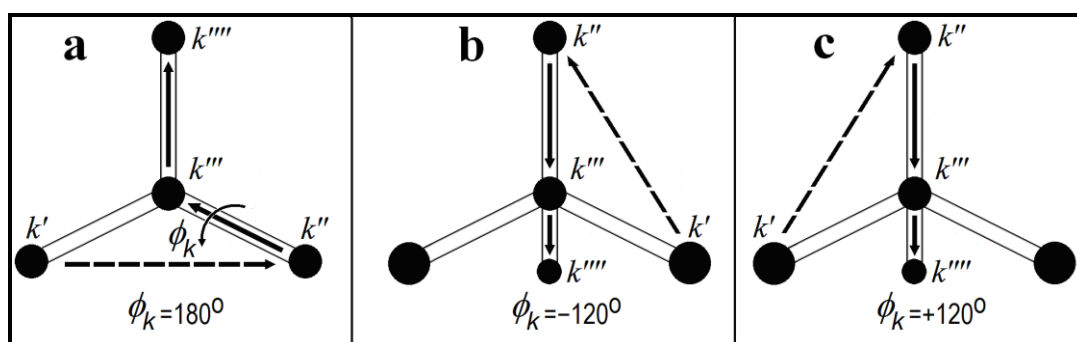


Fig. A1.2. (a) One (at fixed arrangement of atoms  $k'', k''', k''''$ ) quasi-torsion angle, generated by  $sp^2$ -hybridized central atom  $k''''$ ; (b, c) two (at fixed arrangement of atoms  $k'', k''', k''''$ ) quasi-torsion angle, generated by  $sp^3$ - hybridized central atom  $k''$ . Angle  $\phi_k^{(0)} = 0^0$  always excluded – not by quasi-torsional potential, but forbidden overlapping in space of atoms  $k'$  and  $k''''$ .

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