This journal is © The Owner Societies 2011

Table A-1 Multipole moments and static polarizabilities (in a.u.) of the FOX-7 monomer in Cartesian form. Only low order moments are shown however contributions through L=7 were used in computation of the asymptotic energies.

FOX-7 monomer coordinates in atomic units (center of mass at origin) corresponding to moments presented below :

C	-0.05429	0.02885	-0.04153
C	-2.44240	-0.86246	0.98948
N	0.41496	0.33671	-2.62400
N	2.00944	0.54773	1.61696
O	2.39533	1.40802	-3.35334
O	-1.22121	-0.36840	-4.17201
O	1.54626	1.41298	3.74813
O	4.21094	0.06732	0.95781
N	-4.28576	-1.60356	-0.51621
H	-5.73892	-2.13239	0.10629
H	-4.10208	-1.58619	-2.15189
N	-2.78399	-1.03253	3.46495
H	-4.15580	-1.58619	4.02571
H	-1.74212	-0.41929	4.49441

Dipole:

$\mu_z =$ 1.431031459

$\mu_x =$ -3.232299188

$\mu_y =$ -1.200439329

Quadrupole:

$\Theta_{xx} =$ 7.089181685

$\Theta_{yy} =$ -0.026275395

$\Theta_{zz} =$ -7.062906290

$\Theta_{xy} =$ 4.461641208

$\Theta_{xz} =$ -6.449349686

$\Theta_{yz} =$ -2.396866480

This journal is © The Owner Societies 2011

Static polarizabilities

Dipole-dipole:

x x	94.842290
x y	14.666980
x z	-3.549274
y y	51.919650
y z	0.372805
z z	94.329090

Dipole-quadrupole:

x xx	-25.421340
x xy	-43.771720
x xz	7.077876
x yy	13.097790
x yz	-24.523518
x zz	12.323550
y xx	-38.161159
y xy	-33.500910
y xz	-11.839840
y yy	-8.265131
y yz	11.442672
y zz	46.426290
z xx	-5.321900
z xy	7.718745
z xz	-43.223267
z yy	2.901502

z yz	13.021558
z zz	2.420398

Quadrupole-quadrupole:

xx xx	2939.828600
xx xy	197.319712
xx xz	30.898974
xx yy	-653.207000
xx yz	-82.076733
xx zz	-2286.621600
xy xy	1191.406500
xy xz	-83.816550
xy yy	220.883602
xy yz	-51.762007
xy zz	-418.203314
xz xz	2412.473250
xz yy	27.840003
xz yz	585.509850
xz zz	-58.738977
yy yy	1184.852400
yy yz	7.635147
yy zz	-531.645400
yz yz	1300.629750
yz zz	74.441585
zz zz	2818.267000

This journal is © The Owner Societies 2011

Table A-2. Coordinates (Angstroms) of the FOX-7 monomer (R enantiomer) used in potential fitting and simulation. The S configuration is generated by reflection of the atomic coordinates below through the *xz* plane.

C1	-0.02155	0.01502	0.02857
C2	0.53064	-0.45663	1.29036
N3	-1.38939	0.17793	-0.21164
N4	0.85035	0.2896	-1.06713
N5	-0.26101	-0.8488	2.26997
N6	1.84152	-0.54663	1.46426
O7	-1.78082	0.74484	-1.25755
O8	-2.20401	-0.19519	0.65844
O9	1.97937	0.74746	-0.82794
O10	0.49545	0.03538	-2.23025
H11	0.07243	-1.12864	3.0372
H12	-1.12705	-0.83961	2.1773
H13	2.14205	-0.83961	2.18861
H14	2.38338	-0.22212	0.91008

Table A-3. Atomic charges corresponding to atom labeling in Table A-2.

Atom	CHARGE (a.u.)
C1	-0.4100270
C2	0.7362470
N3	0.6745610
N4	0.7220050
N5	-0.8923120
N6	-0.9515670
O7	-0.3605990
O8	-0.4836020
O9	-0.4675610
O10	-0.3729130
H11	0.4209090
H12	0.4655270
H13	0.4564320
H14	0.4629000

This journal is © The Owner Societies 2011

Table A-4. Potential parameters for R-R interactions.

i	j	A_{ij} (kcal/mol)	B_{ij} (Ang)	C_{ij} (Ang^6 * kcal/mol)
C	C	764046.0121	0.2086	0.0801
C	N	72.8379	0.1816	19.0796
C	O	88075.9408	0.2529	250.2805
C	H	3879.6614	0.3185	204.8703
N	N	111518.8046	0.2775	822.6244
N	O	5658.5589	0.3329	645.8825
N	H	10158.7541	0.2491	0.2165
O	O	88046.0549	0.2425	129.6677
O	H	73731.6262	0.2196	278.7350
H	H	11.2533	0.7838	5.7440

Table A-5. Potential parameters for R-S interactions.

i	j	A_{ij} (kcal/mol)	B_{ij} (Ang)	C_{ij} (Ang^6 * kcal/mol)
C	C	512900.0918	0.2501	0.0732
C	N	60.4168	0.1845	12.7313
C	O	67862.0867	0.2467	169.1749
C	H	2577.8179	0.2844	204.7925
N	N	80398.8032	0.2827	1116.5450
N	O	6696.2147	0.3711	903.9598
N	H	14899.0853	0.2263	0.3438
O	O	82609.7660	0.2525	243.1237
O	H	42344.2009	0.2104	252.6077
H	H	7.4991	0.5414	8.2593

This journal is © The Owner Societies 2011

Table A-6. Energy components (kcal/mol) for minima on the RR and RS potential energy surfaces shown in Figures 5 and 6. Note that the induction energy includes the higher order induction/exchange-induction contribution extracted from the supermolecular approach. The tabulated exchange energy contains the first order exchange and second order exchange-induction and exchange-dispersion contributions.

Energy/Structure	RR1	RR2	RS1	RS2
COM distance (Å)	3.46	4.35	3.72	6.85
Electrostatic	-14.965	-13.182	-13.476	-12.672
Induction	-8.933	-6.395	-6.114	-4.500
Dispersion	-14.122	-9.022	-11.601	-5.101
Exchange	23.707	15.925	14.811	9.193
E_{int}	-14.314	-12.674	-16.379	-13.080
Fit	-16.141	-13.298	-15.328	-13.508

Table A-7. Comparison of experimental[29] and predicted molecular structural parameters[a,b] for FOX-7.

Model	Crystallographic structural parameters					
	sx	sy	sz	θ (°)	ϕ (°)	ψ (°)
Molecule 1						
Expt.	**0.76459**	**0.17122**	**0.63938**	**72.35**	**178.99**	**106.64**
Theory	**0.77744**	**0.16808**	**0.63176**	**70.91**	**179.29**	**111.12**
Ideal	***0.77744***	***0.16808***	***0.63176***	***70.91***	***179.29***	***111.12***
Molecule 2						
Expt.	**0.73541**	**0.67122**	**0.86062**	**72.35**	**1.01**	**-106.64**
Theory	**0.73344**	**0.66803**	**0.84637**	**70.91**	**0.74**	**-105.26**
Ideal	***0.72256***	***0.66808***	***0.86824***	***70.89***	***0.72***	***-111.35***
Molecule 3						
Expt.	**0.23541**	**0.82878**	**0.36062**	**72.35**	**178.99**	**106.64**
Theory	**0.23182**	**0.83532**	**0.34646**	**70.91**	**179.28**	**109.42**
Ideal	***0.22256***	***0.83192***	***0.36824***	***70.91***	***179.29***	***111.12***
Molecule 4						
Expt.	**0.26459**	**0.32878**	**0.13938**	**72.35**	**1.01**	**-106.64**
Theory	**0.27578**	**0.33542**	**0.13205**	**70.91**	**0.74**	**-104.77**
Ideal	***0.27744***	***0.33192***	***0.13176***	***70.89***	***0.72***	***-111.35***

a. Sx, Sy, Sz are center of mass fractional coordinates within the unit cell.

b. θ,ϕ ,ψ are Euler angles describing molecular orientation within the unit cell.