

Equilibrium structure and dynamics in organic crystals by Monte Carlo simulation. Critical assessment of force fields and comparison with static packing analysis

Angelo Gavezzotti

Supporting Information

List of parameters of the AA-CLP force field

Refer to A. Gavezzotti, New J. Chem. 2011, 35, 1360 for the description of the force field, and to the document CLPmanual.doc available at <http://users.unimi.it/gavezzot> or from the author upon request at angelo.gavezzotti@unimi.it

Atomic species considered in the CLP intermolecular energy scheme. See A.Gavezzotti, New J. Chem. 2011, 35, 1360 for all detail and for the explanation of symbols.

	indicator	atomic polarizability, Å ³	ionization potential, a.u.	space diffusion parameter	H-bond propensity factor
hydrogen radius 1.10		0.39	0.500		
acetylene CH	1			0.60	0.20
=CH ₂ , arom.CH	2			0.62	0.10
aliphatic CH, CH ₂ , CH ₃	3			0.64	0.05
R-OH, R-SH alcohol, thiol	5			0.75	0.99
COO-H acid	6			0.80	0.99
CON)-H amide	7			0.80	0.90
R ₂ NH, RNH ₂ , (R ₃ N ⁺)H	8			0.80	0.99
H ₂ O (water)	9			0.80	0.99
unnormalized hydrogen atom from Cambridge files	99				
carbon 1.77			0.414	1.00	0.00
carbonyl C=(O)	10	1.05			
≡C-	11	1.35			
sp ² or allene C	12	1.35			
sp ³ C	13	1.05			
aromatic core C	14	1.90			
nitrogen 1.64		0.95	0.534		
(R _n H _{4-n})N ⁺	16			0.63	0.00
(R _n H _{3-n})N	17			0.63	-0.97
arom.N, R=N(H)	18			0.58	-0.99
-C≡N, -N=N	19			0.70	-0.70
nitro N	20			0.63	0.00
amide N (CONH, CONH ₂)	21			0.63	-0.85
oxygen 1.58		0.75	0.500		
-O-	23			0.45	-0.90
H ₂ O (water)	24			0.70	-0.99
C=O, COO ⁻	27			0.50	-0.99
(C=O)-OH	28			0.50	-0.90
R-OH	29			0.45	-0.99
N=O	30			0.50	-0.95
S=O	31			0.75	-0.90
P=O	32			0.75	-0.90
sulfur 1.81		3.00	0.381		

-S-	34			2.00	-0.5
(C)=S	35			2.00	-0.5
(O)=S	36			2.50	0.0
R-S(H)	37			2.00	-0.5
heteroatoms					
P 1.9	38	1.54	0.386	3.0	0
AS 1.8	39	3.5	0.400	5.0	0
Se 1.8	40	3.5	0.400	6.0	0
F 1.46	41	0.40	0.640	0.20	0.00
Cl 1.76	42	2.50	0.477	2.40	-0.20
Br 1.87	43	3.27	0.434	1.50	0.00
I 2.03	44	5.00	0.384	5.00	0.00
B 1.70	46	1.60	0.305	1.00	0.00
Si 2.00	47	2.00	0.280	1.00	0.00

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c -----
  data symbol/
1 ' H', ' H', ' H', ' H', ' H', ' H', ' H', ' H', ' H', ' C',      1-10
2 ' C', ' C', ' C', ' C', ' ', ' N', ' N', ' N', ' N', ' N',      11-20
3 ' N', ' ', ' O', ' O', ' ', ' ', ' O', ' O', ' O', ' O',      21-30
4 ' O', ' O', ' ', ' S', ' S', ' S', ' S', ' P', 'AS', 'SE',      31-40
5 ' F', 'CL', 'BR', ' I', 'AL', ' B', 'SI', ' ', ' ', ' ', ' '/      41-50
c   average bonding radii version of 8.2011
  data ravrg/
1 0.30,0.30,0.30,0.30,0.30,0.30,0.30,0.30,0.30,0.70,
2 0.60,0.70,0.77,0.70,0.00,0.75,0.75,0.65,0.55,0.72,
3 0.70,0.00,0.68,0.68,0.00,0.00,0.55,0.68,0.68,0.50,
4 0.40,0.40,0.00,1.05,1.05,1.05,1.05,1.05,1.2,1.2,
5 0.65,1.00,1.20,1.35,0.00,0.90,1.17,0.0,0.0,0.0/
c   non-bonded radii
  data ravidw/
1 1.10,1.10,1.10,0.00,1.10,1.10,1.10,1.10,1.10,1.77,
2 1.77,1.77,1.77,1.77,0.00,1.64,1.64,1.64,1.64,1.64,
3 1.64,0.00,1.58,1.58,0.00,0.00,1.58,1.58,1.58,1.58,
4 1.58,1.58,0.00,1.81,1.81,1.81,1.81,1.90,1.80,1.80,
5 1.46,1.76,1.87,2.03,0.00,1.70,2.00,0.00,1.70,1.50/
c   AA-clp and PIXEL atomic polarizabilities
c   adapted from Miller JACS 112,8573,1990
  data polat/
1 0.39,0.39,0.39,0.00,0.39,0.39,0.39,0.39,0.39,1.05,
2 1.35,1.35,1.05,1.90,0.00,1.00,1.00,1.05,1.00,1.00,
3 1.00,0.00,0.75,0.75,0.00,0.00,0.75,0.75,0.75,0.75,
4 0.75,0.75,0.00,3.00,3.00,3.00,3.00,1.54,3.50,3.50,
5 0.40,2.50,3.27,5.00,0.00,1.60,2.00,0.00,2.30,0.40/
c   AA-clp diffuseness factors
  data diffu/
1 0.60,0.62,0.64,0.00,0.75,0.80,0.80,0.80,0.80,1.00,
2 1.00,1.00,1.00,1.00,0.00,0.63,0.63,0.58,0.70,0.63,
3 0.63,0.00,0.45,0.70,0.00,0.00,0.50,0.50,0.45,0.50,
4 0.75,0.75,0.00,2.00,2.00,2.50,2.00,3.00,5.00,6.00,
5 0.20,2.40,1.50,5.00,0.00,1.00,1.00,0.00,1.00,1.00/
c   AA-clp acceptor-donor index
  data acdo/
1 0.20,0.10,0.05,0.00,0.99,0.99,0.90,0.99,0.99,0.00,
2 0.00,0.00,0.00,0.00,0.00,0.00,-0.97,-0.99,-0.70,0.00,
3 -0.85,0.00,-0.90,-0.99,0.00,0.00,-0.99,-0.90,-0.99,-0.95,
4 -0.90,-0.90,0.00,-0.50,-0.50,0.00,-0.50,0.00,0.00,0.00,
5 0.00,-0.20,0.00,0.00,0.00,0.00,0.00,0.00,0.00,0.00/
c   Pauling electronegativities
  data elneg/
1 2.10,2.10,2.10,2.10,2.10,2.10,2.10,2.10,2.50,
2 2.50,2.50,2.50,2.50,0.00,3.00,3.00,3.00,3.00,
3 3.00,0.00,3.50,3.50,0.00,0.00,3.50,3.50,3.50,
4 3.50,3.50,0.00,2.50,2.50,2.50,2.50,2.10,2.20,2.60,
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5 4.00,3.00,2.80,2.50,0.00,2.00,1.80,0.00,1.80,0.90/
c  ionization potentials
   data potio/
1 0.500,0.500,0.500,0.000,0.500,0.500,0.500,0.500,0.500,0.414,
2 0.414,0.414,0.414,0.414,0.000,0.534,0.534,0.534,0.534,0.534,
3 0.534,0.000,0.500,0.500,0.000,0.000,0.500,0.500,0.500,0.500,
4 0.500,0.500,0.000,0.381,0.381,0.381,0.381,0.386,0.400,0.400,
5 0.640,0.477,0.434,0.384,0.000,0.305,0.280,0.000,0.400,0.200/
c  alpha(s) for Extended Huckel
   data alphas/
1 -10.0,-10.0,-10.0,-10.0,-10.0,-10.0,-10.0,-10.0,-10.0,-21.4,
2 -21.4,-21.4,-21.4,-21.4,0.000,-26.0,-26.0,-26.0,-26.0,-26.0,
3 -26.0,0.000,-32.3,-32.3,0.000,0.000,-32.3,-32.3,-32.3,-32.3,
4 -32.3,-32.3,0.000,-20.0,-20.0,-20.0,-20.0,-18.6,-17.0,-20.5,
5 -40.0,-26.3,-22.1,-18.0,-12.3,-15.2,-17.3,0.000,-7.80,0.000/
c  alpha(p) for Extended Huckel
   data alphap/
1 0.000,0.000,0.000,0.000,0.000,0.000,0.000,0.000,0.000,-11.4,
2 -11.4,-11.4,-11.4,-11.4,0.000,-13.4,-13.4,-13.4,-13.4,-13.4,
3 -13.4,0.000,-14.8,-14.8,0.000,0.000,-14.8,-14.8,-14.8,-14.8,
4 -14.8,-14.8,0.000,-11.0,-11.0,-11.0,-11.0,-14.0,-14.0,-14.4,
5 -18.1,-14.2,-13.1,-12.7,-6.50,-8.50,-9.20,0.000,-3.80,0.000/
c  s slater coeff's for eht H,C,N,O,S,P,As,Se,F,Cl,Br,I,Si
   data slats/
1 1.300,1.300,1.300,1.300,1.300,1.300,1.300,1.300,1.300,1.625,
2 1.625,1.625,1.625,1.625,0.000,1.950,1.950,1.950,1.950,1.950,
3 1.950,0.000,2.275,2.275,0.000,0.000,2.275,2.275,2.275,2.275,
4 2.275,2.275,0.000,2.122,2.122,2.122,2.122,1.600,2.230,2.750,
5 2.425,2.356,2.588,2.679,0.000,1.300,1.200,0.000,0.000,0.000/
c  p slater coeff's for eht H,C,N,O,S,P,As,Se,F,Cl,Br,I,Si
   data slatp/
1 0.000,0.000,0.000,0.000,0.000,0.000,0.000,0.000,0.000,1.625,
2 1.625,1.625,1.625,1.625,0.000,1.950,1.950,1.950,1.950,1.950,
3 1.950,0.000,2.275,2.275,0.000,0.000,2.275,2.275,2.275,2.275,
4 2.275,2.275,0.000,1.827,1.827,1.827,1.827,1.600,1.890,2.290,
5 2.425,2.033,2.131,2.322,0.000,1.300,0.900,0.000,0.000,0.000/
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Supporting Information

CSD Refcode, space group, density, temperature of the Xray determination,
year, crystallographic R-factor
Atom-Atom CLP lattice energies from the static original crystal structure:
Coulombic, polarization, dispersion repulsion cell-dipole Kroon-van Eick term, total

#ABUMIT	'P 21/n'						
cell	3.9495	10.6260	15.2700	90.00	97.00	90.00	
crystal density	1.535		T(K)	223.0	year	2001.	R = 4.86
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-2.7	-6.0	-77.9	21.5	-0.0	-65.1
#ACANIL01	'P b c a'						
cell	19.5090	9.3640	7.7780	90.00	90.00	90.00	
crystal density	1.264		T(K)	113.0	year	1985.	R = 3.30
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-38.3	-25.8	-95.2	48.8	-0.0	-110.5
#ADIPAC07	'P 21/c'						
cell	7.1870	5.1626	10.0150	90.00	110.86	90.00	
crystal density	1.398		T(K)	130.0	year	2000.	R = 6.83
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-47.4	-58.1	-121.2	95.8	-0.0	-131.0
#ARCLAM01	'P 21/n'						
cell	8.2062	5.7480	9.0527	90.00	111.37	90.00	
crystal density	1.187		T(K)	113.0	year	2007.	R = 4.15
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-39.8	-23.3	-60.8	48.7	-0.0	-75.2
#AYOJED	'P 21/n'						
cell	5.9008	10.0652	11.6577	90.00	102.92	90.00	
crystal density	1.143		T(K)	120.0	year	2004.	R = 4.65
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-5.3	-10.1	-79.8	25.7	-0.0	-69.6
#BENZAC07	'P 21/c'						
cell	5.3930	5.0030	21.6890	90.00	98.51	90.00	
crystal density	1.402		T(K)	20.0	year	1996.	R = 6.90
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-29.1	-23.1	-100.3	67.8	-0.0	-84.7
#BENZEN07	'P b c a'						
cell	7.3980	9.4350	6.7780	90.00	90.00	90.00	
crystal density	1.097		T(K)	123.0	year	1987.	R = 4.60
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-7.3	-6.2	-55.5	17.5	-0.0	-51.5
#BILNOZ01	'P 21/c'						
cell	10.0180	6.8230	13.1470	90.00	90.04	90.00	
crystal density	1.262		T(K)	210.0	year	1989.	R = 3.40
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-3.3	-18.5	-81.1	28.7	-0.0	-74.2
#BIPHEN04	'P 21/a'						
cell	8.1200	5.6300	9.5100	90.00	95.10	90.00	
crystal density	1.183		T(K)	295.0	year	1977.	R = 6.30
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-10.7	-9.5	-91.8	22.9	-0.0	-89.1
#BNZQUI03	'P 21/c'						
cell	5.7430	6.7710	6.8670	90.00	100.14	90.00	
crystal density	1.366		T(K)	173.0	year	2002.	R = 4.29
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-31.9	-18.9	-62.0	45.3	-0.0	-67.4
#BULVAL03	'B 21/c'						
cell	6.4800	20.5840	10.3700	90.00	90.17	90.00	
crystal density	1.250		T(K)	110.0	year	1996.	R = 2.40
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-6.0	-11.8	-86.8	32.7	-0.0	-71.9
#BZAMID01	'P 21/c'						
cell	5.6070	5.0460	22.0530	90.00	90.66	90.00	
crystal density	1.290		T(K)	295.0	year	1972.	R = 6.80
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-36.0	-21.0	-85.5	43.8	-0.0	-98.8
#CAXNUL05	'P 21/n'						
cell	7.5997	8.1079	12.9590	90.00	91.33	90.00	
crystal density	1.665		T(K)	295.0	year	2007.	R = 3.84
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-10.8	-11.0	-94.2	34.3	-0.0	-81.7
#CECGEX	'P 21'						
cell	4.7167	7.4607	11.2850	90.00	96.95	90.00	
crystal density	1.349		T(K)	200.0	year	2006.	R = 3.10
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-34.3	-22.4	-88.3	47.0	-0.0	-98.0
#CTCYDD	'P 21/c'						
cell	7.5560	18.5450	8.4960	90.00	113.73	90.00	
crystal density	1.645		T(K)	295.0	year	1976.	R = 4.50
AA-CLP	Ec,Ep,Ed,Er,Ecd,Et	-2.5	-9.5	-111.1	33.3	-0.0	-89.9
#DAZNAP	'P b c a'						

cell	13.6950	10.5570	9.2850	90.00	90.00	90.00		
crystal density	1.288		T(K)	295.0	year	1972.	R =	3.90
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-21.5	-7.5	-81.8	24.7	-0.0	-86.1
#DCBDOX10 'P n a m'								
cell	5.9830	7.1140	24.6370	90.00	90.00	90.00		
crystal density	1.603		T(K)	295.0	year	1973.	R =	6.40
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			0.3	-20.4	-134.0	41.1	-0.0	-112.9
#DCLBEN01 'P 21/n '								
cell	14.762	5.832	4.039	90.00	112.-78	90.00		
crystal density	1.523		T(K)	295.0	year	1997.	R =	4.95
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-3.1	-6.9	-79.6	22.9	-0.0	-66.7
#DCLBEN02 'P -1'								
cell	7.3200	5.9500	3.9800	93.17	113.58	93.50		
crystal density	1.545		T(K)	295.0	year	1957.	R =	6.00
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-3.1	-6.9	-79.6	22.9	-0.0	-66.7
#DEZDUH 'P n a 21'								
cell	14.9630	5.6710	9.5590	90.00	90.00	90.00		
crystal density	1.770		T(K)	173.0	year	1984.	R =	4.50
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-16.9	-18.8	-69.0	37.4	-1.3	-68.6
#DEZXEL 'P c a 21'								
cell	11.8810	9.8180	7.4400	90.00	90.00	90.00		
crystal density	1.669		T(K)	295.0	year	1984.	R =	3.70
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-17.3	-18.6	-107.9	46.3	-2.6	-99.9
#DITBOX 'P 21'								
cell	7.7330	6.2450	10.8150	90.00	108.34	90.00		
crystal density	1.208		T(K)	295.0	year	1986.	R =	3.80
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-8.0	-11.9	-102.6	29.7	-0.1	-92.9
#DNBENZ14 'P n a 21'								
cell	14.0690	13.2450	3.7380	90.00	90.00	90.00		
crystal density	1.603		T(K)	200.0	year	2002.	R =	5.40
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-18.3	-23.7	-92.4	48.8	-1.2	-86.8
#DNITBZ11 'P 21/n'								
cell	11.1340	5.4590	5.6810	90.00	92.26	90.00		
crystal density	1.618		T(K)	295.0	year	1980.	R =	4.08
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-22.3	-25.1	-91.4	49.7	-0.0	-89.2
#EXODAW 'P -1'								
cell	5.6040	6.1169	7.8400	92.97	91.55	109.32		
crystal density	1.530		T(K)	294.0	year	2003.	R =	5.00
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-29.2	-28.3	-109.7	51.1	-0.0	-116.2
#EZURUM 'P 21/c'								
cell	10.1739	6.5823	12.4662	90.00	94.07	90.00		
crystal density	1.385		T(K)	173.0	year	2004.	R =	2.48
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-24.0	-23.4	-97.5	50.1	-0.0	-94.8
#FACFOE 'P 21/n'								
cell	7.4806	5.9608	11.7250	90.00	103.82	90.00		
crystal density	1.493		T(K)	123.0	year	1998.	R =	3.44
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-5.6	-9.6	-61.4	24.9	-0.0	-51.6
#FACGEV 'P 21/c'								
cell	5.8090	6.5300	7.1900	90.00	101.89	90.00		
crystal density	1.420		T(K)	215.0	year	1998.	R =	4.43
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-6.4	-9.2	-53.8	20.6	-0.0	-48.8
#FACJAU 'P 21/c'								
cell	4.4719	10.2850	6.3420	90.00	107.97	90.00		
crystal density	1.796		T(K)	135.0	year	1998.	R =	4.24
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-11.3	-12.0	-66.5	36.8	-0.0	-53.1
#FAXTUU01 'P 21 21 21'								
cell	6.0396	10.1568	15.5495	90.00	90.00	90.00		
crystal density	1.800		T(K)	183.0	year	2007.	R =	2.87
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-29.2	-31.9	-118.2	62.6	-0.0	-116.8
#FMANUL01 'P n a 21'								
cell	9.1110	13.2030	6.9810	90.00	90.00	90.00		
crystal density	1.409		T(K)	173.0	year	1976.	R =	4.80
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-10.5	-13.5	-87.4	31.9	-2.3	-81.8
#FOVNIN 'P 21 c n'								
cell	7.7210	11.3790	18.5070	90.00	90.00	90.00		
crystal density	1.815		T(K)	295.0	year	1985.	R =	3.00
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-3.2	-7.0	-132.4	39.1	-0.2	-103.7
#FOVQOX 'P n a 21'								
cell	9.5240	11.0060	5.9420	90.00	90.00	90.00		
crystal density	1.324		T(K)	298.0	year	2009.	R =	3.52
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-60.5	-29.3	-103.3	56.6	-3.3	-139.8
#GLURAC03 'C 2/c'								
cell	12.9769	4.7484	9.6955	90.00	98.30	90.00		
crystal density	1.484		T(K)	130.0	year	2000.	R =	4.64
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-63.1	-57.2	-116.1	94.3	-0.0	-142.2
#HAYYAH 'P 21/n'								
cell	7.9180	14.1090	8.1930	90.00	111.46	90.00		
crystal density	1.218		T(K)	295.0	year	1994.	R =	4.55

AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-7.0	-12.9	-98.2	34.2	-0.0	-83.9
#HCLBNZ11 'P 21/n'						
cell 8.0476 3.8363	14.8208	90.00	92.13	90.00		
crystal density 2.069	T(K)	295.0	year 1974.	R =	4.60	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	7.3	-4.0	-135.7	38.6	-0.0	-93.7
#HCLHEP 'C 2/c'						
cell 12.5990 10.3200	9.9940	90.00	107.02	90.00		
crystal density 1.641						
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-9.6	-10.5	-129.4	42.4	-0.0	-107.1
#HEPTAN02 'P -1'						
cell 4.1160 4.6860	20.3480	78.11	81.79	74.25		
crystal density 0.904	T(K)	90.0	year 1999.	R =	7.02	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	0.5	-22.8	-70.6	26.8	-0.0	-66.1
#HEXANE01 'P -1'						
cell 4.1309 4.6963	8.5390	83.40	87.26	75.17		
crystal density 0.900	T(K)	90.0	year 1999.	R =	3.42	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	0.6	-20.6	-62.2	23.0	-0.0	-59.1
#HITMUS 'P 21/c'						
cell 7.0290 8.5860	7.7730	90.00	114.34	90.00		
crystal density 1.353	T(K)	295.0	year 1998.	R =	5.47	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-34.3	-31.9	-84.5	45.5	-0.0	-105.1
#HOWBAW 'P -1'						
cell 5.4500 5.4490	7.6780	93.27	94.10	108.93		
crystal density 1.303	T(K)	153.0	year 1999.	R =	6.32	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-10.8	-17.1	-112.1	45.9	-0.0	-94.0
#JOHBUD 'C c'						
cell 11.4210 6.0190	10.1770	90.00	104.62	90.00		
crystal density 1.551	T(K)	295.0	year 1991.	R =	5.20	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-29.6	-27.4	-84.9	62.0	-0.3	-80.1
#MCINAM10 'A b a 2'						
cell 11.2890 17.1750	9.5280	90.00	90.00	90.00		
crystal density 1.159	T(K)	295.0	year 1978.	R =	5.00	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-27.5	-20.2	-96.8	53.6	-8.9	-99.9
#NAPHTA10 'P 21/a'						
cell 8.2128 5.9727	8.6745	90.00	123.39	90.00		
crystal density 1.198	T(K)	239.0	year 1982.	R =	3.50	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-7.6	-7.9	-85.3	23.2	-0.0	-77.6
#NBORAN02 'P 21 21 21'						
cell 5.9260 9.4890	13.4520	90.00	90.00	90.00		
crystal density 1.442	T(K)	173.0	year 2000.	R =	4.10	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-35.8	-29.7	-82.0	45.0	-0.0	-102.5
#NITRBE01 'P 21/c'						
cell 3.8014 11.6153	12.9843	90.00	94.98	90.00		
crystal density 1.432	T(K)	103.0	year 1992.	R =	2.20	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-12.5	-14.4	-76.7	32.4	-0.0	-71.1
#OCTANE01 'P -1'						
cell 4.1947 4.7518	10.9980	85.11	83.77	74.26		
crystal density 0.906	T(K)	90.0	year 1999.	R =	4.64	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	0.9	-24.7	-74.8	24.4	-0.0	-74.2
#PHBALD11 'P 21/c'						
cell 6.6992 13.5550	7.1441	90.00	112.87	90.00		
crystal density 1.357	T(K)	296.0	year 2008.	R =	3.81	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-43.2	-23.4	-85.8	45.3	-0.0	-107.0
#PUGDEB 'C 2/c'						
cell 7.4238 11.5900	7.0473	90.00	112.78	90.00		
crystal density 1.569	T(K)	233.0	year 2009.	R =	6.13	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-6.7	-10.1	-56.3	22.4	-0.0	-50.7
#PVVAWA01 'I 2/a'						
cell 6.1600 11.9090	7.5040	90.00	95.47	90.00		
crystal density 1.601	T(K)	130.0	year 1998.	R =	4.19	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-6.4	-13.5	-60.0	30.4	-0.0	-49.5
#QATTIO 'P 21/n'						
cell 5.0140 13.7880	7.4640	90.00	107.27	90.00		
crystal density 1.215	T(K)	130.0	year 2000.	R =	6.32	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-58.6	-30.8	-89.8	55.6	-0.0	-123.6
#QATTOU 'P 21 21 21'						
cell 5.3234 6.6991	17.0400	90.00	90.00	90.00		
crystal density 1.138	T(K)	130.0	year 2000.	R =	3.10	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-60.7	-32.6	-96.2	64.5	-0.0	-125.1
#TCHLBZ03 'P 21 21 21'						
cell 3.8422 13.0973	13.7984	90.00	90.00	90.00		
crystal density 1.736	T(K)	120.0	year 2003.	R =	3.01	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	1.0	-8.3	-100.7	31.0	-0.0	-77.0
#TEPPTH06 'P -1'						
cell 7.7017 6.3457	3.6679	92.92	107.91	94.64		
crystal density 1.628	T(K)	82.0	year 1986.	R =	6.90	
AA-CLP Ec,Ep,Ed,Er,Ecd,Et	-62.1	-44.5	-145.0	107.3	-0.0	-144.4
#TEPNIT11 'P -1'						

cell	3.8430	6.5750	7.3130	114.50	93.53	96.99			
crystal density	1.285			T(K)	295.0	year	1984.	R =	4.26
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-29.9	-17.0	-75.6	28.1	-0.0	-94.3	
#VACCEH 'P b c a'									
cell	7.0700	7.1690	9.9090	90.00	90.00	90.00			
crystal density	1.060			T(K)	153.0	year	1988.	R =	3.40
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-4.8	-10.3	-55.1	17.1	-0.0	-53.2	
#XAYMEP 'P -1'									
cell	3.6860	5.2900	9.4700	102.43	92.78	100.93			
crystal density	1.490			T(K)	150.0	year	2000.	R =	4.05
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-10.1	-13.5	-117.2	43.6	-0.0	-97.2	
#XAYMIT 'P 21 21 21'									
cell	3.7611	8.2710	26.1100	90.00	90.00	90.00			
crystal density	1.490			T(K)	150.0	year	2000.	R =	4.85
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-16.8	-18.0	-121.7	44.3	-0.0	-112.2	
#XOZBUK 'P 21/n'									
cell	9.0374	5.2012	13.0270	90.00	97.58	90.00			
crystal density	1.522			T(K)	100.0	year	2009.	R =	4.06
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-27.0	-19.4	-92.5	50.7	-0.0	-88.2	
#YUYPU01 'P 21/c'									
cell	3.7848	11.9274	14.5974	90.00	91.62	90.00			
crystal density	1.292			T(K)	153.0	year	2002.	R =	5.89
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-27.9	-16.9	-76.0	27.5	-0.0	-93.3	
#ZIVKOE 'P -1'									
cell	6.5470	7.0570	9.6870	107.48	102.07	102.23			
crystal density	1.450			T(K)	155.0	year	1996.	R =	4.90
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-35.0	-26.5	-100.0	52.0	-0.0	-109.6	
#ZZZITY01 'P 21/n'									
cell	5.8060	5.0230	11.2150	90.00	100.48	90.00			
crystal density	1.096			T(K)	180.0	year	1986.	R =	4.50
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-6.1	-13.6	-73.3	24.0	-0.0	-69.1	
#ZZZSPY01 'P b c a'									
cell	10.5160	7.5960	16.8680	90.00	90.00	90.00			
crystal density	1.047			T(K)	200.0	year	2000.	R =	5.29
AA-CLP Ec,Ep,Ed,Er,Ecd,Et			-4.5	-13.1	-65.1	18.2	-0.0	-64.6	

Equilibrium structure and dynamics in organic crystals by Monte Carlo simulation. Critical assessment of force fields and comparison with static packing analysis

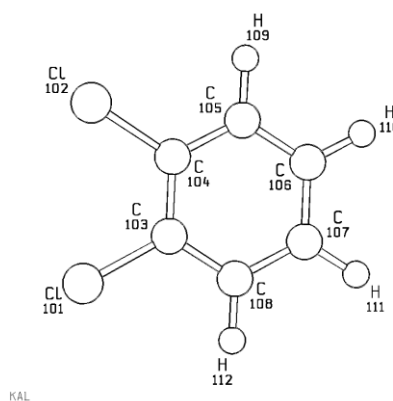
Angelo Gavezzotti

Supporting Information

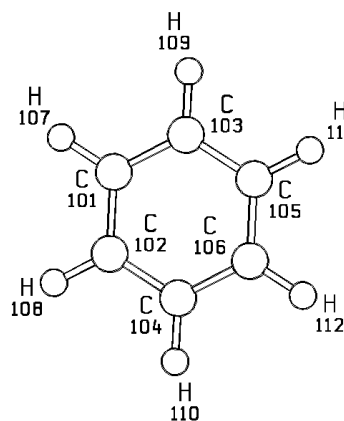
"Topology" (force field) files, atom numbering, x,y,z atomic coordinates, raw atomic charges to be rescaled by a factor of 0.41 rigid molecules

Refer to A. Gavezzotti, New J. Chem. 2011, 35, 1360 for the description of the force field, and to the document CLPmanual.doc available at <http://users.unimi.it/gavezzot> or from the author upon request at angelo.gavezzotti@unimi.it

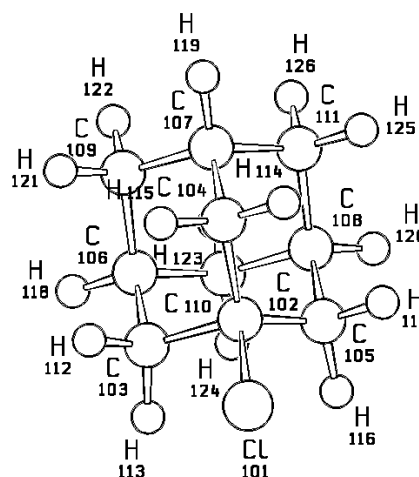
#ABUMIT	'P 21/n'	topology			
12					
1	-0.00297	1.58605	-1.41325	42	-0.2317
2	0.00635	-1.57767	-1.42712	42	-0.2284
3	-0.00339	0.69215	0.07133	12	0.3068
4	-0.01034	-0.69624	0.06331	12	0.3055
5	-0.01074	-1.38881	1.26777	12	-0.3348
6	-0.00080	-0.70129	2.45782	12	-0.3166
7	0.00736	0.68523	2.46844	12	-0.3214
8	0.00703	1.38659	1.27136	12	-0.3378
9	-0.01889	-2.46873	1.26889	2	0.2923
10	0.00065	-1.24475	3.39116	2	0.2860
11	0.01396	1.21868	3.40745	2	0.2868
12	0.01487	2.46651	1.27429	2	0.2933



#BENZEN07	'P b c a'	topology			
12					
1	0.00142	0.94794	1.02091	12	-0.2879
2	-0.00142	-0.41000	1.33501	12	-0.2889
3	-0.00142	1.35749	-0.30985	12	-0.2886
4	0.00142	-1.35749	0.30985	12	-0.2886
5	0.00142	0.41000	-1.33501	12	-0.2889
6	-0.00142	-0.94794	-1.02091	12	-0.2879
7	0.00586	1.68389	1.81129	2	0.2883
8	-0.00581	-0.72785	2.36712	2	0.2888
9	-0.00586	2.41057	-0.54951	2	0.2883
10	0.00586	-2.41057	0.54951	2	0.2883
11	0.00581	0.72785	-2.36712	2	0.2888
12	-0.00586	-1.68389	-1.81129	2	0.2883



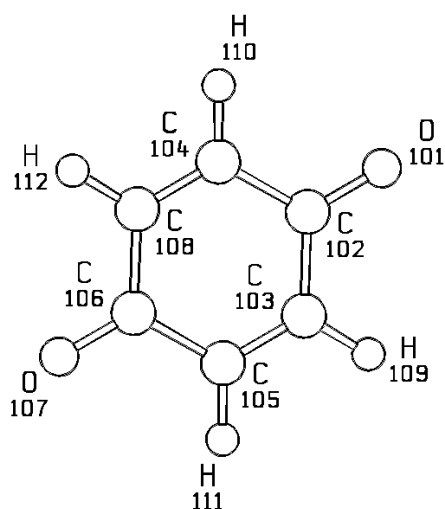
#BILNOZ01	'P 21/c'	topology			
26					
1	0.02176	0.00450	-2.66944	42	-0.4825
2	-0.15278	-0.00037	-0.70951	13	0.4558
3	0.01464	-1.44155	-0.35769	13	-0.5815
4	1.24394	0.73774	-0.34487	13	-0.6225
5	-1.24531	0.71670	-0.34358	13	-0.5492
6	0.01644	-1.44588	1.16312	13	-0.2238
7	1.24460	0.72670	1.18289	13	-0.2287
8	-1.23412	0.70828	1.18189	13	-0.2099
9	1.25839	-0.71683	1.67847	13	-0.5805
10	-1.22912	-0.73353	1.68297	13	-0.5821
11	-0.00198	1.43462	1.69720	13	-0.5794
12	0.93964	-1.83600	-0.75158	3	0.2829



13	-0.79621	-2.03735	-0.75014	3	0.2828
14	1.27276	1.74494	-0.73353	3	0.2839
15	2.09150	0.20122	-0.74507	3	0.2839
16	-2.14904	0.26506	-0.72543	3	0.2852
17	-1.18990	1.72584	-0.72434	3	0.2855
18	0.02025	-2.46962	1.50703	3	0.2655
19	2.12022	1.24110	1.55048	3	0.2662
20	-2.11441	1.21598	1.54748	3	0.2646
21	2.14882	-1.21647	1.32652	3	0.2800
22	1.27112	-0.73333	2.75827	3	0.2810
23	-1.23559	-0.74676	2.76287	3	0.2815
24	-2.11536	-1.24505	1.33764	3	0.2801
25	-0.00986	2.45983	1.35760	3	0.2800
26	-0.00287	1.44080	2.77719	3	0.2814

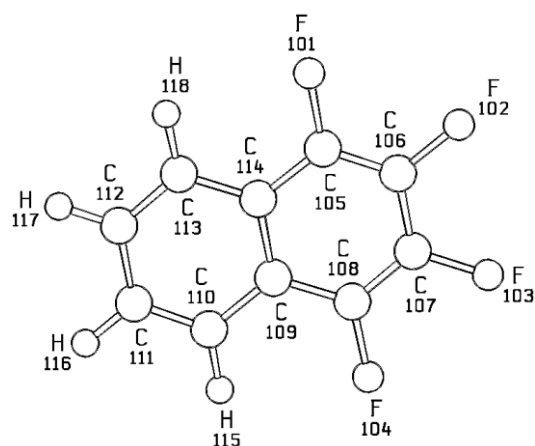
#BNZQUI03 'P 21/c' topology

12					
1	-0.00559	-0.00010	2.64911	27	-1.1217
2	0.00407	0.00315	1.42705	10	0.9741
3	0.00723	1.25938	0.66500	12	-0.2253
4	0.00722	-1.26461	0.66525	12	-0.2219
5	-0.00722	1.26461	-0.66525	12	-0.2219
6	-0.00407	-0.00315	-1.42705	10	0.9741
7	0.00559	0.00010	-2.64911	27	-1.1217
8	-0.00723	-1.25938	-0.66500	12	-0.2253
9	0.02159	2.19938	1.19660	2	0.2971
10	0.02143	-2.20561	1.19512	2	0.2977
11	-0.02143	2.20561	-1.19512	2	0.2977
12	-0.02159	-2.19938	-1.19660	2	0.2971

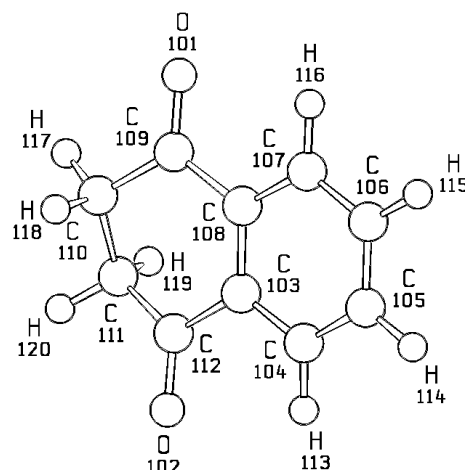


#CAXNUL05 'P 21/n' topology

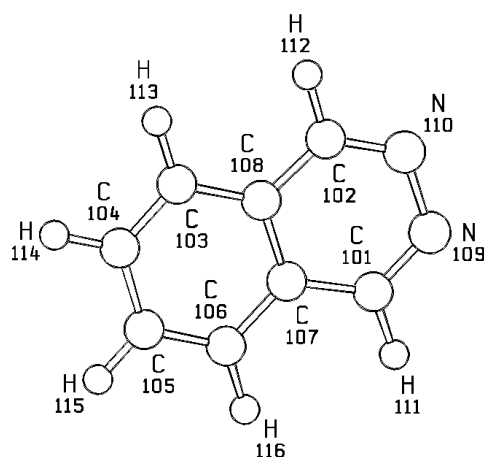
18					
1	-0.00803	2.71503	0.38185	41	-0.4988
2	-0.00849	1.34485	2.70903	41	-0.4935
3	0.00689	-1.34577	2.70796	41	-0.4954
4	-0.02883	-2.71010	0.38654	41	-0.4957
5	0.00490	1.36841	0.36701	12	0.5071
6	0.01008	0.69549	1.53821	12	0.5241
7	0.01380	-0.69495	1.53340	12	0.5202
8	0.00612	-1.37144	0.36425	12	0.5115
9	0.01395	-0.70689	-0.87606	14	0.0053
10	0.01578	-1.39066	-2.10988	12	-0.3085
11	0.00412	-0.69753	-3.27690	12	-0.3084
12	-0.01356	0.69430	-3.27570	12	-0.3071
13	-0.00246	1.39139	-2.11099	12	-0.3110
14	0.00843	0.70583	-0.87337	14	0.0054
15	0.02650	-2.47045	-2.12603	2	0.2872
16	0.00864	-1.23129	-4.21580	2	0.2850
17	-0.03646	1.22718	-4.21476	2	0.2848
18	-0.00194	2.47122	-2.12909	2	0.2877



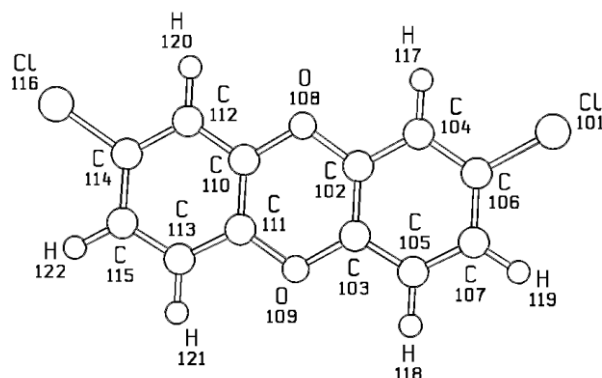
#CECGEX	'P 21'	topology		
20				
1	-0.10292	-2.67383	-1.00333	27 -1.1776
2	0.09077	2.67930	-0.97593	27 -1.1800
3	-0.01673	0.69335	0.30707	12 0.0343
4	-0.01241	1.37531	1.52352	12 -0.2477
5	0.02406	0.68620	2.70765	12 -0.2455
6	0.00999	-0.69027	2.71504	12 -0.2514
7	-0.01451	-1.38645	1.51680	12 -0.2471
8	-0.01174	-0.71108	0.30168	12 0.0368
9	0.04850	-1.46252	-0.97895	10 0.9045
10	0.33532	-0.67620	-2.21657	13 -0.5080
11	-0.30662	0.69710	-2.22400	13 -0.5032
12	-0.04734	1.46399	-0.97784	10 0.9020
13	-0.03799	2.45494	1.53258	2 0.2867
14	0.06410	1.22700	3.64163	2 0.2853
15	0.01798	-1.22650	3.65245	2 0.2864
16	-0.03600	-2.46615	1.52722	2 0.2868
17	-0.02099	-1.23131	-3.07173	3 0.3032
18	1.40457	-0.56085	-2.31540	3 0.3639
19	-1.37318	0.58496	-2.35133	3 0.3663
20	0.07296	1.25709	-3.06585	3 0.3044



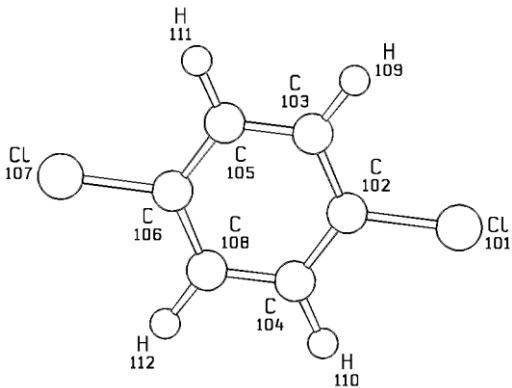
#DAZNAP	'P b c a'	topology		
16				
1	-0.00902	-1.30207	1.23362	12 0.1735
2	0.01014	1.29890	1.23086	12 0.1722
3	-0.00968	1.38042	-1.24990	12 -0.2705
4	-0.00401	0.69371	-2.41787	12 -0.2449
5	0.00490	-0.69180	-2.42892	12 -0.2492
6	0.00999	-1.37834	-1.26084	12 -0.2701
7	-0.00299	-0.69066	-0.03346	14 0.0865
8	-0.00077	0.68866	-0.04076	14 0.0909
9	-0.00576	-0.68619	2.37542	18 -0.5900
10	0.00626	0.68662	2.36872	18 -0.5839
11	-0.01713	-2.38175	1.25801	2 0.2740
12	0.02297	2.37851	1.25580	2 0.2732
13	-0.02104	2.46037	-1.25627	2 0.2852
14	-0.00650	1.23370	-3.35318	2 0.2832
15	0.00780	-1.22434	-3.36843	2 0.2847
16	0.02407	-2.45818	-1.27194	2 0.2851



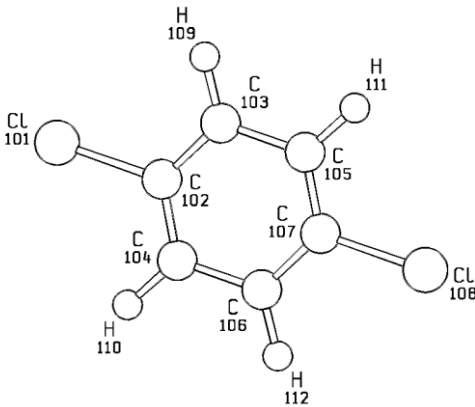
#DCBDOX10	'P n a m'	topology		
22				
1	-0.08557	1.15999	-5.02841	42 -0.2457
2	0.09082	0.25396	-1.15548	12 0.4844
3	0.04690	-1.14543	-1.16040	12 0.4352
4	0.07073	0.96850	-2.33805	12 -0.4098
5	-0.04141	-1.80345	-2.36515	12 -0.3259
6	-0.01566	0.24126	-3.54034	12 0.3222
7	-0.04305	-1.14603	-3.55758	12 -0.3658
8	0.18651	1.00324	-0.00000	23 -0.7944
9	0.03729	-1.87562	0.00000	23 -0.7807
10	0.09082	0.25396	1.15548	12 0.4844
11	0.04690	-1.14543	1.16040	12 0.4352
12	0.07073	0.96850	2.33805	12 -0.4098
13	-0.04141	-1.80345	2.36515	12 -0.3259
14	-0.01566	0.24126	3.54034	12 0.3222
15	-0.04305	-1.14603	3.55758	12 -0.3658
16	-0.08557	1.15999	5.02841	42 -0.2457
17	0.11959	2.04738	-2.34002	2 0.3060
18	-0.11206	-2.88112	-2.36515	2 0.2929
19	-0.06502	-1.68915	-4.49083	2 0.2941
20	0.11959	2.04738	2.34002	2 0.3060
21	-0.11206	-2.88112	2.36515	2 0.2929
22	-0.06502	-1.68915	4.49083	2 0.2941



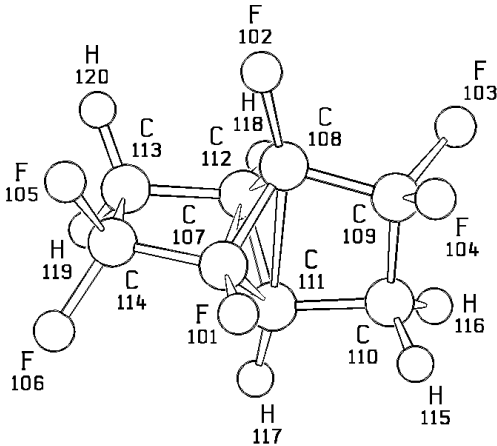
#DCLBEN01	'P 21/a'	topology			
12					
1	0.00063	0.00019	-3.10432	42	-0.2487
2	-0.00509	0.00159	-1.36075	12	0.3204
3	0.00015	1.19581	-0.68187	12	-0.3276
4	0.00015	-1.18849	-0.68841	12	-0.3254
5	-0.00015	1.18849	0.68841	12	-0.3254
6	0.00509	-0.00159	1.36075	12	0.3204
7	-0.00063	-0.00019	3.10432	42	-0.2487
8	-0.00015	-1.19581	0.68187	12	-0.3276
9	0.00444	2.13075	-1.22247	2	0.2908
10	0.00446	-2.11977	-1.23533	2	0.2904
11	-0.00446	2.11977	1.23533	2	0.2904
12	-0.00444	-2.13075	1.22247	2	0.2908



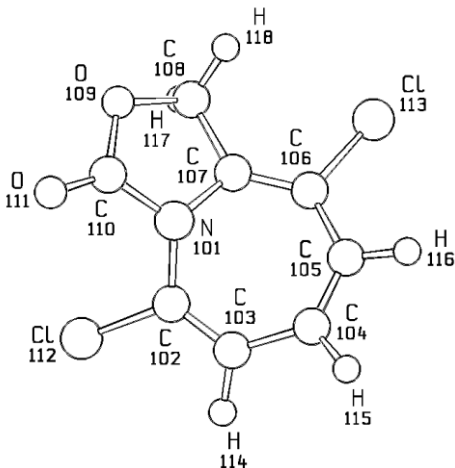
#DCLBEN02	'P -1'	topology			
12					
1	-0.00112	0.00610	3.14556	42	-0.2880
2	-0.01956	-0.00497	1.35794	12	0.3447
3	0.01568	1.16233	0.69626	12	-0.3278
4	0.01586	-1.15169	0.73891	12	-0.3133
5	-0.01586	1.15169	-0.73891	12	-0.3133
6	-0.01568	-1.16233	-0.69626	12	-0.3278
7	0.01956	0.00497	-1.35794	12	0.3447
8	0.00112	-0.00610	-3.14556	42	-0.2880
9	0.06705	2.09643	1.23597	2	0.2921
10	0.06794	-2.07600	1.29507	2	0.2923
11	-0.06794	2.07600	-1.29507	2	0.2923
12	-0.06705	-2.09643	-1.23597	2	0.2921



#DEZDUH	'P n a 21'	topology			
20					
1	1.04508	1.57754	-0.52586	41	-0.5145
2	1.07473	-1.54706	0.50613	41	-0.5149
3	-0.42975	-0.74203	2.82422	41	-0.5245
4	1.12098	0.68380	2.29362	41	-0.5314
5	1.11886	-0.68046	-2.28913	41	-0.5264
6	-0.43957	0.72950	-2.82821	41	-0.5267
7	0.11810	0.57292	-0.52878	13	0.5247
8	0.13326	-0.55577	0.53280	13	0.5250
9	-0.06188	0.13442	1.84728	13	1.0720
10	-1.11928	1.14373	1.48518	13	-0.6248
11	-1.31959	0.77226	0.01774	13	-0.2553
12	-1.29838	-0.79243	-0.01442	13	-0.2552
13	-1.10681	-1.16563	-1.47169	13	-0.6289
14	-0.05319	-0.13529	-1.84052	13	1.0710
15	-0.77702	2.16050	1.60906	3	0.2930
16	-2.02088	1.02181	2.06713	3	0.2916
17	-2.08490	1.41455	-0.39226	3	0.2708
18	-2.04456	-1.45760	0.39443	3	0.2706
19	-2.01285	-1.05446	-2.04896	3	0.2914
20	-0.75447	-2.17898	-1.59550	3	0.2923

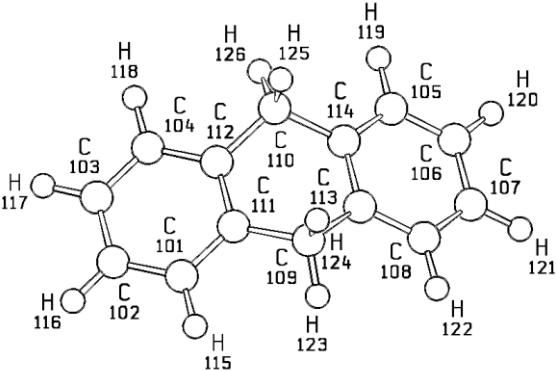


#DEZXEL	'P c a 21'	topology			
18					
1	-0.32880	0.23550	-0.58141	17	-0.3662
2	0.01904	-0.98284	-1.23790	12	0.6067
3	-0.16737	-2.16050	-0.71447	12	-0.4751
4	-0.73780	-2.43971	0.60097	12	-0.3250
5	-0.65316	-1.66672	1.67663	12	-0.3395
6	-0.06296	-0.35784	1.74568	12	0.1821
7	0.10254	0.51052	0.74780	12	0.2419
8	0.48754	1.94771	0.75783	13	-0.0713
9	-0.13033	2.46230	-0.46291	23	-0.7965

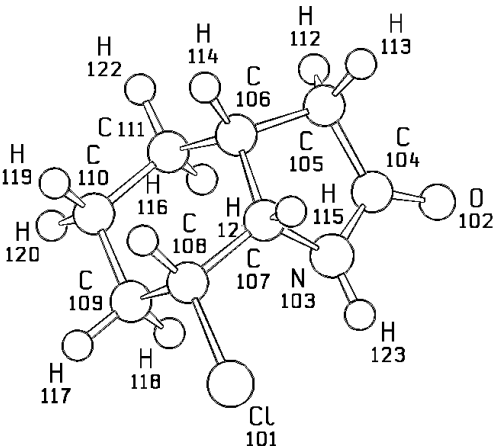


10	-0.52659	1.44095	-1.24608	10	1.4783
11	-1.01765	1.60695	-2.32554	27	-1.1677
12	0.80368	-0.78373	-2.76071	42	-0.2112
13	0.38136	0.22197	3.33521	42	-0.2571
14	0.12790	-3.01197	-1.30968	2	0.3095
15	-1.28195	-3.36633	0.70891	2	0.2879
16	-1.06954	-2.06072	2.59195	2	0.2963
17	1.56049	2.06954	0.73928	3	0.3057
18	0.10953	2.45192	1.63489	3	0.3014

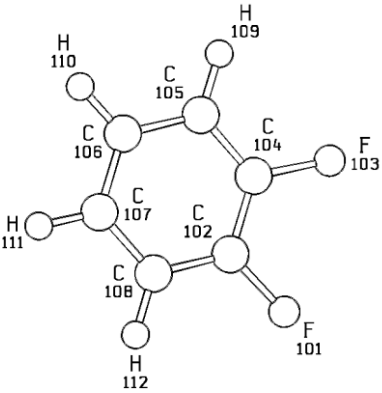
#DITBOX	'P 21'	topology			
26					
1	-0.11481	-1.37671	2.40064	12	-0.3290
2	-0.48301	-0.69853	3.54995	12	-0.3170
3	-0.47772	0.68343	3.54583	12	-0.3138
4	-0.12643	1.38077	2.40931	12	-0.3277
5	-0.11764	1.37613	-2.41327	12	-0.3246
6	-0.47403	0.68564	-3.54814	12	-0.3145
7	-0.48794	-0.69674	-3.54547	12	-0.3171
8	-0.12447	-1.38873	-2.40018	12	-0.3345
9	0.69208	-1.41201	0.00398	13	-0.5433
10	0.67632	1.42751	-0.00441	13	-0.5495
11	0.25621	-0.68662	1.25507	12	0.0339
12	0.23850	0.70110	1.25626	12	0.0317
13	0.25386	-0.69843	-1.24598	12	0.0307
14	0.24786	0.70355	-1.26322	12	0.0295
15	-0.11625	-2.45668	2.39535	2	0.2863
16	-0.77047	-1.24206	4.43778	2	0.2876
17	-0.75120	1.22219	4.44099	2	0.2857
18	-0.13539	2.46073	2.41680	2	0.2871
19	-0.12361	2.45607	-2.42129	2	0.2865
20	-0.74377	1.22502	-4.44406	2	0.2860
21	-0.78128	-1.23661	-4.43364	2	0.2871
22	-0.13389	-2.46869	-2.40036	2	0.2877
23	0.27491	-2.40815	0.00826	3	0.2921
24	1.76844	-1.50096	0.00252	3	0.3343
25	1.75189	1.52446	-0.00106	3	0.3328
26	0.25173	2.42057	-0.00579	3	0.2918



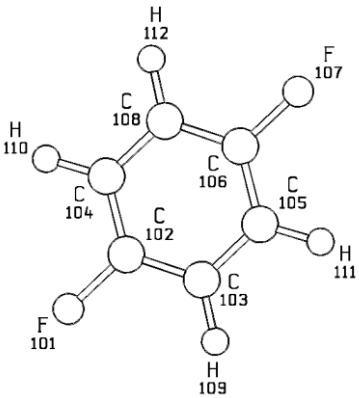
#EZURUM	'P 21/c'	topology			
23					
1	-0.07339	-1.25321	-2.44131	42	-0.3139
2	0.81217	-1.57784	2.81341	27	-1.2231
3	0.22333	-1.05510	0.65515	21	-0.6477
4	0.19495	-0.89403	1.99524	10	1.0408
5	-0.74184	0.25554	2.31061	13	-0.5743
6	-0.90046	0.96985	0.96216	13	-0.2519
7	-0.75996	-0.21116	-0.02819	13	-0.0086
8	-0.35567	0.22430	-1.42417	13	0.0179
9	0.83829	1.15334	-1.46402	13	-0.5726
10	0.49894	2.39700	-0.64335	13	-0.5565
11	0.20473	2.02425	0.80057	13	-0.5695
12	-0.31974	0.91304	3.05626	3	0.3096
13	-1.69176	-0.10174	2.68002	3	0.3327
14	-1.82040	1.52078	0.83347	3	0.2740
15	-1.66199	-0.76996	-0.22907	3	0.2709
16	-1.13061	0.93552	-1.66920	3	0.2947
17	1.06206	1.42934	-2.48394	3	0.2826
18	1.70746	0.66120	-1.05308	3	0.2809
19	-0.36214	2.88830	-1.07189	3	0.2818
20	1.32811	3.08817	-0.67588	3	0.2810
21	1.11071	1.64707	1.25151	3	0.2811
22	-0.08775	2.91603	1.33491	3	0.2829
23	0.61852	-1.87258	0.23611	7	0.4872



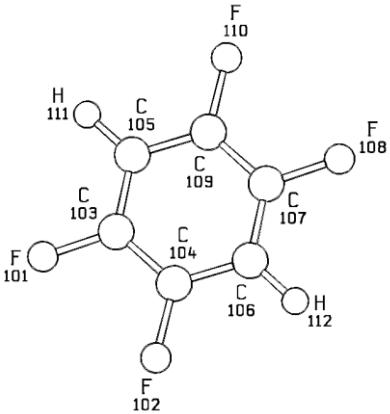
#FACFOE	'P 21/n'		topology		
12					
1	-0.00634	-1.33739	-1.60997	41	-0.4653
2	0.00978	-0.69151	-0.42995	12	0.5345
3	-0.00481	1.32436	-1.62921	41	-0.4674
4	0.00995	0.68642	-0.43766	12	0.5307
5	0.00517	1.39841	0.73952	12	-0.3367
6	-0.00789	0.70091	1.93988	12	-0.3138
7	-0.00334	-0.68389	1.94945	12	-0.3136
8	0.00476	-1.39254	0.75449	12	-0.3386
9	0.01143	2.47836	0.73008	2	0.2989
10	-0.02176	1.24281	2.87398	2	0.2859
11	-0.00612	-1.21515	2.88976	2	0.2863
12	0.00707	-2.47255	0.75498	2	0.2989



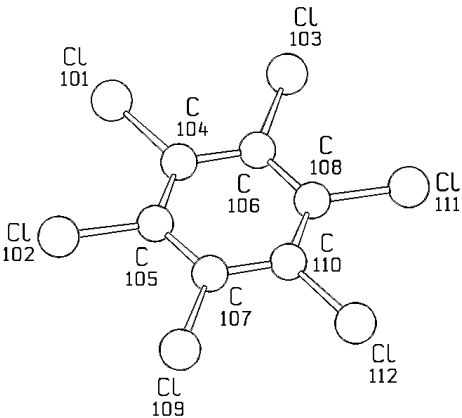
#FACGEV	'P 21/c'		topology		
12					
1	-0.00119	-0.00614	-2.70609	41	-0.4746
2	0.00252	-0.00117	-1.34453	12	0.5415
3	0.00102	1.20196	-0.69847	12	-0.3296
4	0.00103	-1.20216	-0.67872	12	-0.3316
5	-0.00103	1.20216	0.67872	12	-0.3316
6	-0.00252	0.00117	1.34453	12	0.5415
7	0.00119	0.00614	2.70609	41	-0.4746
8	-0.00102	-1.20196	0.69847	12	-0.3296
9	0.00146	2.12878	-1.25287	2	0.2976
10	0.00147	-2.13280	-1.22675	2	0.2968
11	-0.00147	2.13280	1.22675	2	0.2968
12	-0.00146	-2.12878	1.25287	2	0.2976



#FACJAU	'P 21/c'		topology		
12					
1	-0.00509	-1.34816	2.36230	41	-0.4659
2	0.00236	1.34977	2.36205	41	-0.4680
3	0.00677	-0.69374	1.18576	12	0.5065
4	0.00155	0.68972	1.18314	12	0.5042
5	0.00713	-1.40896	-0.00040	12	-0.3886
6	-0.00700	1.40888	0.00044	12	-0.3886
7	-0.00664	0.69367	-1.18573	12	0.5065
8	0.00522	1.34808	-2.36226	41	-0.4659
9	-0.00142	-0.68980	-1.18310	12	0.5042
10	-0.00276	-1.34954	-2.36215	41	-0.4680
11	0.01382	-2.48896	-0.00246	2	0.3118
12	-0.01368	2.48888	0.00250	2	0.3118

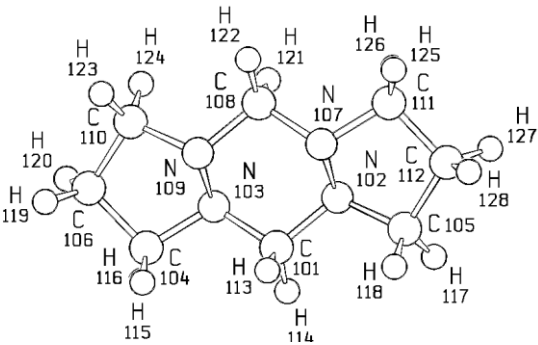


#HCLBNZ11	'P 21/n'		topology		
12					
1	-0.01620	2.31239	-2.07728	42	-0.2254
2	0.01664	2.95182	0.96441	42	-0.2222
3	0.01632	-0.64297	-3.04196	42	-0.2237
4	-0.00186	1.03722	-0.92804	12	0.2236
5	-0.00086	1.32302	0.43695	12	0.2236
6	0.00110	-0.28339	-1.36561	12	0.2241
7	-0.00110	0.28339	1.36561	12	0.2242
8	0.00086	-1.32302	-0.43695	12	0.2236
9	-0.01632	0.64297	3.04196	42	-0.2237
10	0.00186	-1.03722	0.92804	12	0.2236

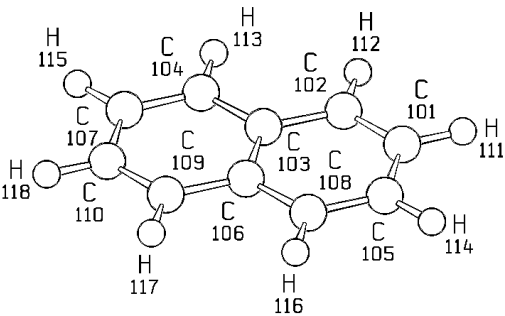


11	-0.01664	-2.95182	-0.96441	42	-0.2222
12	0.01620	-2.31239	2.07728	42	-0.2254

#HOWBAW	'P -1'			topology	
28					
1	-0.09277	-1.38897	-0.00126	13	-0.0384
2	0.36977	-0.64722	1.17813	17	-0.4842
3	0.35183	-0.64322	-1.17579	17	-0.4798
4	-0.11060	-1.20479	-2.45829	13	-0.2967
5	-0.08204	-1.20924	2.46655	13	-0.2995
6	0.02636	-0.00754	-3.41982	13	-0.5931
7	-0.35215	0.64300	1.17599	17	-0.4800
8	0.09289	1.38893	0.00119	13	-0.0385
9	-0.36965	0.64718	-1.17820	17	-0.4842
10	0.08216	1.20920	-2.46662	13	-0.2995
11	0.11072	1.20475	2.45822	13	-0.2966
12	-0.02654	0.00792	3.41991	13	-0.5932
13	-1.16925	-1.47605	0.00559	3	0.2513
14	0.32266	-2.38585	-0.00730	3	0.2738
15	-1.13260	-1.54829	-2.39543	3	0.2681
16	0.50256	-2.03701	-2.77109	3	0.2755
17	0.56980	-2.00265	2.80123	3	0.2761
18	-1.08305	-1.60809	2.39370	3	0.2690
19	-0.81683	0.05666	-4.09158	3	0.2889
20	0.92352	-0.08206	-4.01649	3	0.2892
21	1.16937	1.47583	-0.00556	3	0.2513
22	-0.32241	2.38586	0.00715	3	0.2738
23	-0.56957	2.00278	-2.80120	3	0.2761
24	1.08325	1.60786	-2.39381	3	0.2690
25	-0.50207	2.03728	2.77087	3	0.2755
26	1.13283	1.54784	2.39514	3	0.2681
27	0.81639	-0.05614	4.09199	3	0.2889
28	-0.92391	0.08256	4.01625	3	0.2892

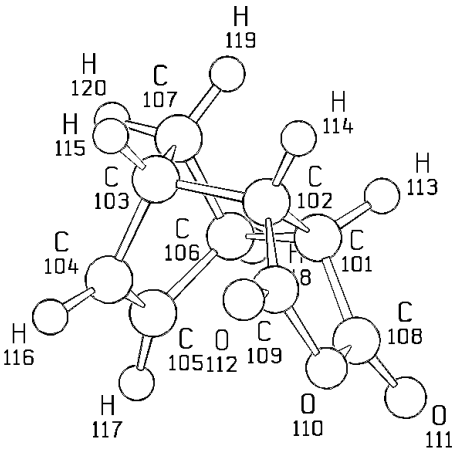


#NAPHTA10	'P 21/a'			topology	
18					
1	-0.00281	0.70317	2.42029	12	-0.2921
2	0.00463	1.40150	1.24364	12	-0.3088
3	-0.00053	0.70988	-0.00165	14	0.0502
4	-0.00360	1.40072	-1.24119	12	-0.3076
5	-0.00091	-0.70365	2.42437	12	-0.2938
6	0.00053	-0.70988	0.00165	14	0.0502
7	0.00091	0.70365	-2.42437	12	-0.2938
8	0.00360	-1.40072	1.24119	12	-0.3076
9	-0.00463	-1.40150	-1.24364	12	-0.3088
10	0.00281	-0.70317	-2.42029	12	-0.2921
11	-0.01023	1.23893	3.35799	2	0.2870
12	0.01443	2.48136	1.25907	2	0.2888
13	-0.00953	2.48060	-1.25414	2	0.2887
14	-0.00303	-1.23817	3.36279	2	0.2876
15	0.00303	1.23817	-3.36279	2	0.2876
16	0.00953	-2.48060	1.25414	2	0.2887
17	-0.01443	-2.48136	-1.25907	2	0.2888
18	0.01023	-1.23893	-3.35799	2	0.2870



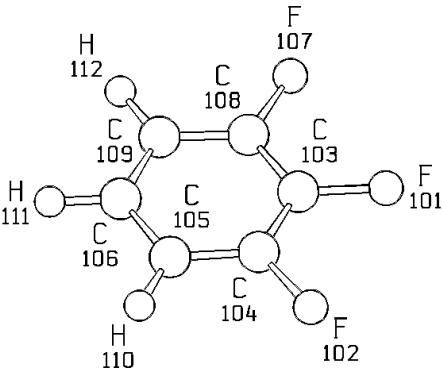
#NBORAN02 'P 21 21 2 topology

20					
1	0.86461	-0.81103	-0.03780	13	-0.2314
2	0.92859	0.71995	-0.14323	13	-0.2304
3	0.22963	1.01989	-1.52248	13	-0.1818
4	-1.23512	0.66145	-1.34971	12	-0.3614
5	-1.32220	-0.66324	-1.23777	12	-0.3723
6	0.08199	-1.23108	-1.34059	13	-0.1775
7	0.72332	-0.21593	-2.31398	13	-0.5433
8	0.12468	-1.07261	1.24356	10	1.3505
9	0.15738	1.21129	1.04822	10	1.3502
10	-0.29954	0.12516	1.80303	23	-0.7237
11	-0.12755	-2.10784	1.79175	27	-1.1226
12	-0.11259	2.32411	1.38324	27	-1.1134
13	1.79527	-1.35298	0.04309	3	0.3254
14	1.90029	1.18846	-0.09106	3	0.3302
15	0.37236	2.01329	-1.92135	3	0.2719
16	-2.06068	1.35719	-1.32233	2	0.3007
17	-2.22986	-1.23180	-1.09872	2	0.3009
18	0.07155	-2.28672	-1.56840	3	0.2725
19	1.79914	-0.29162	-2.37155	3	0.2747
20	0.33059	-0.27182	-3.31843	3	0.2809



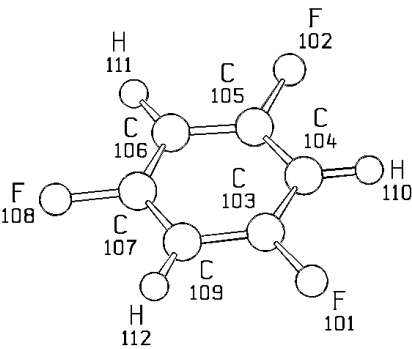
#PUGDEB 'C 2/c' topology

12					
1	0.00000	-1.94879	0.00000	41	-0.4650
2	-0.00159	-0.64260	2.30261	41	-0.4675
3	0.00000	-0.60783	0.00000	12	0.4803
4	0.00263	0.07598	1.16904	12	0.5421
5	0.00186	1.43201	1.19863	12	-0.3686
6	-0.00000	2.11002	-0.00000	12	-0.3040
7	0.00159	-0.64260	-2.30261	41	-0.4675
8	-0.00263	0.07598	-1.16904	12	0.5421
9	-0.00186	1.43201	-1.19864	12	-0.3686
10	0.00270	1.96596	2.13742	2	0.2973
11	-0.00000	3.18998	-0.00000	2	0.2822
12	-0.00270	1.96596	-2.13743	2	0.2973



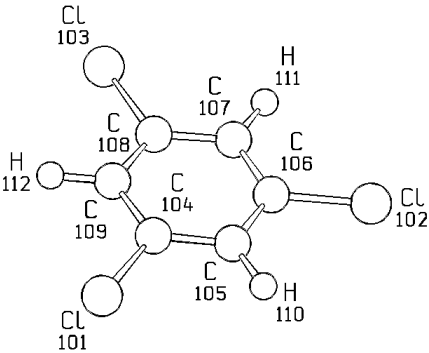
#PVVAWA01 'I 2/a' topology

12					
1	0.00000	-2.70212	0.00008	41	-0.4685
2	0.00548	1.35282	-2.35071	41	-0.4720
3	0.00000	-1.35164	0.00004	12	0.5995
4	-0.01041	-0.70145	-1.22069	12	-0.4388
5	-0.00288	0.67285	-1.17397	12	0.5961
6	-0.00000	1.40291	-0.00004	12	-0.4416
7	0.00288	0.67292	1.17392	12	0.5961
8	-0.00548	1.35296	2.35062	41	-0.4720
9	0.01041	-0.70137	1.22074	12	-0.4388
10	-0.02364	-1.24155	-2.15586	2	0.3134
11	-0.00000	2.48294	-0.00008	2	0.3132
12	0.02364	-1.24142	2.15593	2	0.3134



#TCHLBZ03 'P 21 21 2 topology

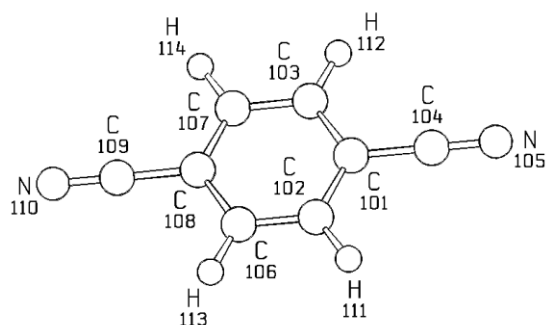
12					
1	-0.00439	-3.10180	0.21985	42	-0.2393
2	-0.00291	1.35829	-2.79443	42	-0.2381
3	-0.00706	1.73435	2.58005	42	-0.2408
4	0.00579	-1.36513	0.08602	12	0.3716
5	-0.00269	-0.77605	-1.16226	12	-0.4317



6	0.00575	0.60462	-1.23029	12	0.3746
7	0.00766	1.40213	-0.09803	12	-0.4354
8	0.00944	0.76856	1.13244	12	0.3731
9	0.01491	-0.60883	1.25642	12	-0.4389
10	-0.01554	-1.37653	-2.05986	2	0.3013
11	0.00775	2.47953	-0.17264	2	0.3017
12	0.02588	-1.08214	2.22714	2	0.3017

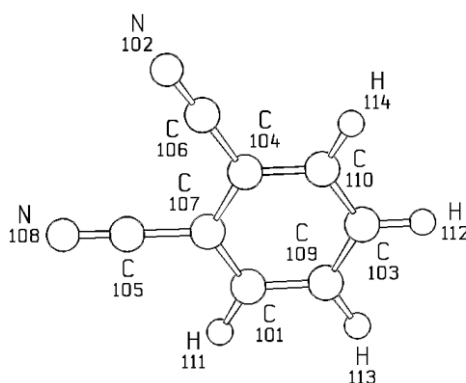
#TEPNIT11 'P -1' topology

14					
1	-0.00623	-0.00501	1.37398	12	0.1323
2	-0.00349	-1.21331	0.68967	12	-0.2351
3	-0.00355	1.20880	0.69223	12	-0.2357
4	-0.00403	-0.00377	2.81508	11	0.7778
5	0.00567	0.00367	3.95954	19	-1.0177
6	0.00355	-1.20880	-0.69223	12	-0.2357
7	0.00349	1.21331	-0.68967	12	-0.2351
8	0.00623	0.00501	-1.37398	12	0.1323
9	0.00403	0.00377	-2.81508	11	0.7778
10	-0.00567	-0.00367	-3.95954	19	-1.0177
11	-0.00682	-2.14722	1.23199	2	0.2893
12	-0.00695	2.14001	1.23924	2	0.2890
13	0.00695	-2.14001	-1.23924	2	0.2890
14	0.00682	2.14722	-1.23199	2	0.2893



#YUYPUD01 'P 21/c' topology

14					
1	-0.00797	-1.39261	-1.19095	12	-0.2317
2	-0.01130	1.94547	2.28522	19	-1.0229
3	0.00041	0.69140	-2.38043	12	-0.2559
4	0.00607	0.70519	0.01382	12	0.1512
5	0.00349	-1.40854	1.27138	11	0.7804
6	0.00441	1.40886	1.27074	11	0.7816
7	0.00508	-0.70286	0.01175	12	0.1504
8	0.00188	-1.94951	2.28375	19	-1.0216
9	-0.00416	-0.68863	-2.38296	12	-0.2550
10	0.00511	1.39146	-1.18424	12	-0.2302
11	-0.02103	-2.47245	-1.19780	2	0.2895
12	0.00030	1.22948	-3.31691	2	0.2876
13	-0.00475	-1.22312	-3.32135	2	0.2876
14	0.00800	2.47140	-1.18927	2	0.2889



Equilibrium structure and dynamics in organic crystals by Monte Carlo simulation. Critical assessment of force fields and comparison with static packing analysis

Angelo Gavezzotti

Supporting Information

Topology" (force field) files,

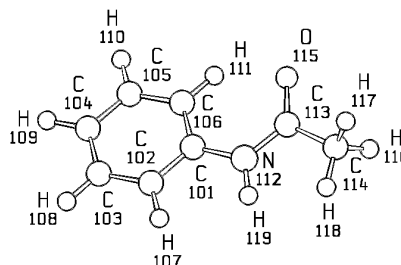
See description in Suppl_Tables4.doc

Refer to A. Gavezzotti, New J. Chem. 2011, 35, 1360 for the description of the force field, and to the document CLPmanual.doc available at <http://users.unimi.it/gavezzot> or from the author upon request at angelo.gavezzotti@unimi.it.

#ACANIL01 'P b c a'R topology

12					
1	-0.10849	-0.30876	0.28472	12	0.3119
2	0.03337	-1.33436	1.22518	12	-0.3517
3	0.13947	-1.03324	2.57459	12	-0.2826
4	0.09887	0.28877	3.00096	12	-0.3300
5	-0.08583	1.29802	2.07407	12	-0.2802
6	-0.19517	1.01416	0.71709	12	-0.3548
7	0.06036	-2.36369	0.89939	2	0.2924
8	0.25400	-1.82842	3.29633	2	0.2871
9	0.21077	0.52613	4.04851	2	0.2879
10	-0.14616	2.32295	2.40923	2	0.2863
11	-0.34595	1.81139	0.00420	2	0.2981
12	-0.16130	-0.69629	-1.07717	21	-0.5677

*atomic coordinates, atom type, raw charge
(to be rescaled by factor 0.41)*



5 ncard slave

13	-1	0	12	1	6	10	1.0587
14	-1	0	13	12	1	13	-0.8973
15	-1	0	13	14	12	27	-1.2314
16	17	18	14	13	12	3	0.32897
19	-1	0	12	13	14	7	0.4864

*"slave atom" construction codes
see Suppl:TableS4.doc*

0 ncard-v

0 nstr-u

1 nbend-u

13 12 19 122.5 0.22 *bending energy parameters; atoms, eq.angle, force constant*

3 ntors-u

13	12	1	6	0.0	0	-2.2407E-06	3.6303E-04	-1.1094E-02	-0.4742	20.136	<i>torsion energy</i>	
14	13	12	19	0.0	0	0.00	0.00	5.1375E-03	0.00	-0.0844	<i>specification</i>	
16	14	13	15	0.0	0.8	3	0.00	0.00000	0.00	0.0000	<i>see Supp_TableS4</i>	

#ADIPAC07 'P 21/c'RE topology

5					
1	0.10791	0.61784	-1.83738	13	-0.5561
2	0.01853	-0.37763	-0.67412	13	-0.5600
3	-0.01853	0.37763	0.67412	13	-0.5600
4	-0.87269	-0.97864	-0.77825	3	0.2841
5	0.87171	-1.03939	-0.69622	3	0.2846

12 ncard slave

6	-1	0	3	2	1	13	-0.5561
13	-1	0	6	3	2	10	1.3355
14	-1	0	13	6	3	28	-0.9622
15	-1	0	13	6	14	27	-1.1809
16	-1	0	14	13	15	6	0.6825
17	-1	0	1	2	3	10	1.3355
18	-1	0	17	1	2	28	-0.9622
19	-1	0	17	1	18	27	-1.1809
20	-1	0	18	17	19	6	0.6825
7	8	0	1	2	17	3	0.33625
9	10	0	3	2	6	3	0.28435
11	12	0	6	3	13	3	0.33625

0 ncard-v

0 nstr-u

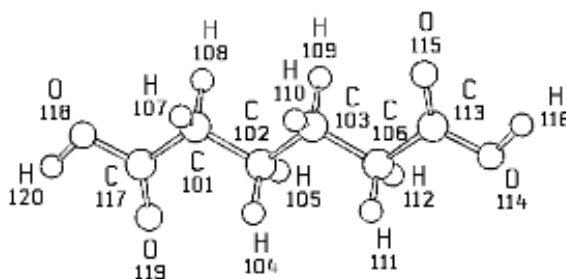
2 nbend-u

20 18 17 104.0 0.1333

16 14 13 104.0 0.1333

7 ntors-u

20	18	17	19	0.0	0.0	0	-1.6863E-06	1.0417E-07	2.0280E-02	-3.4524E-04	0.000
19	17	1	2	0.0	0.0	0	5.6222E-08	-1.6317E-05	1.2839E-03	2.3332E-02	-0.2539
17	1	2	3	0.0	0.0	0	-1.5501E-06	1.1161E-03	-2.9199E-01	3.2793E+01	-1.3241E+03
1	2	3	6	0.0	0.0	0	-1.5501E-06	1.1161E-03	-2.9199E-01	3.2793E+01	-1.3241E+03
2	3	6	13	0.0	0.0	0	-1.5501E-06	1.1161E-03	-2.9199E-01	3.2793E+01	-1.3241E+03



```

16 14 13 15 0.0 0.0 0 -1.6863E-06 1.0417E-07 2.0280E-02 -3.4524E-04 0.000
15 13 6 3 0.0 0.0 0 5.6222E-08 -1.6317E-05 1.2839E-03 2.3332E-02 -0.2539

```

#ARCLAM01 'P 21/n'RE topology

```

6
1 0.02328 0.65179 0.84069 12 -0.3113
2 -0.01998 0.00395 1.97948 12 -0.5419
3 0.07423 1.73053 0.85307 2 0.3008
4 -0.07111 -1.07482 1.98544 2 0.3084
5 -0.00452 0.54898 2.91168 2 0.3040
6 0.00436 -0.05188 -0.46255 10 1.0695

```

4 ncard slave

```

7 -1 0 6 1 2 21 -0.8601
8 -1 0 6 1 7 27 -1.2482
9 -1 0 7 6 1 7 0.4890
10 -1 0 7 6 8 7 0.4898

```

0 ncard-v

0 nstr-u

2 nbend-u

```

9 7 6 122.5 0.22000

```

```

10 7 6 118.0 0.2000

```

3 ntors-u

```

8 6 1 2 0.0 0 7.6392E-07 -2.3582E-04 2.0827E-02 -0.30358 0.7917
10 7 6 8 0.0 0 0.00 0.00 9.5944E-03 0.00 0.053
9 7 6 1 0.0 0 0.00 0.00 5.1373E-03 0.00 0.084

```

#AYOJED 'P 21/n' topology

```

14
1 0.01063 0.00292 1.77928 12 0.0779
2 -0.01202 1.18973 1.05365 12 -0.3288
3 -0.02926 1.20186 -0.32860 12 -0.2805
4 -0.02725 -0.00773 -1.03647 14 0.0750
5 -0.03190 -1.20314 -0.32051 12 -0.2793
6 -0.00849 -1.19660 1.06251 12 -0.3324
7 0.03975 0.00851 3.28343 13 -0.8847
8 -0.00287 -0.00558 -2.47614 11 0.0277
9 0.05124 0.00673 -3.66015 11 -0.5341
10 -0.01621 2.12940 1.58600 2 0.2873
11 -0.04428 2.14107 -0.86162 2 0.2880
12 -0.05403 -2.14386 -0.85056 2 0.2872
13 -0.00491 -2.13471 1.59766 2 0.2879
17 0.10053 0.01797 -4.73891 1 0.3738

```

1 ncard slave

```

14 15 16 7 1 2 3 0.3116

```

0 ncard-v

0 nstr-u

0 nbend-u

1 ntors-u

```

14 7 1 2 0.0 0.08 3 0.0 0.0 0.0 0.0 0.0

```

#BENZAC07 'P 21/c' topology

```

12
1 -0.00283 0.02399 -0.18205 12 -0.0035
2 -0.00353 1.21624 0.53886 12 -0.2456
3 -0.00242 1.18769 1.92373 12 -0.2908
4 0.00181 -0.03321 2.59205 12 -0.2465
5 0.01035 -1.22628 1.87375 12 -0.2918
6 -0.00864 -1.19641 0.48524 12 -0.2453
7 -0.00434 0.05819 -1.65870 10 1.3340
8 -0.00498 2.16244 0.01805 2 0.2880
9 -0.00488 2.11116 2.48383 2 0.2879
10 -0.00156 -0.05539 3.67179 2 0.2872
11 0.03162 -2.17197 2.39480 2 0.2882
12 -0.02787 -2.11932 -0.07534 2 0.2886

```

3 ncard slave

```

14 -1 0 7 1 6 28 -0.9151
13 -1 0 7 1 14 27 -1.2026
15 -1 0 14 7 13 6 0.6672

```

0 ncard-v

0 nstr-u

1 nbend-u

```

15 14 7 104.00 0.133

```

2 ntors-u

```

13 7 1 8 0.0 0.0 0 0.000 0.000 4.9191E-03 0.000 -0.01
13 7 14 15 0.0 0.0 0 -1.5443E-06 0.000 1.7163E-02 0.000 0.005

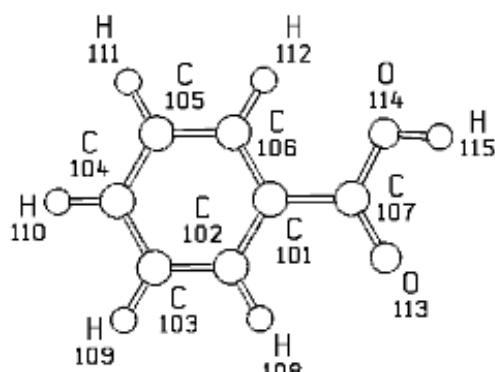
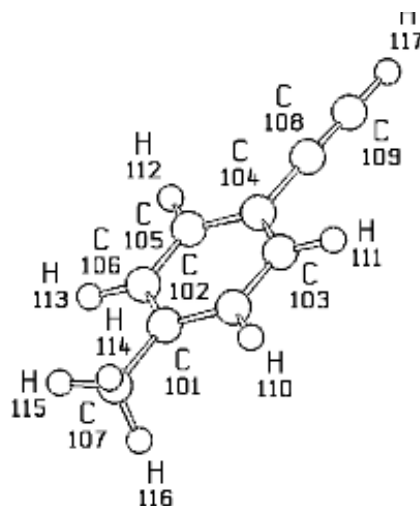
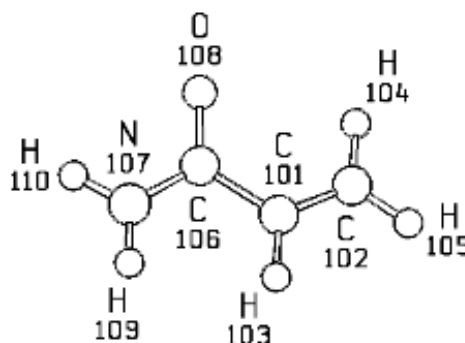
```

#BIPHEN04 'P 21/a' topology

```

12
1 0.00801 0.00221 0.74600 12 0.0476
2 0.00810 1.19182 1.47301 12 -0.3083
3 -0.00182 1.19583 2.86346 12 -0.2898
4 -0.00679 -0.00073 3.56383 12 -0.2929

```



5	0.00441	-1.19617	2.86150	12	-0.2897		
6	0.00189	-1.19321	1.47165	12	-0.3094		
7	-0.00801	-0.00221	-0.74600	12	0.0476		
8	0.01609	2.13302	0.94339	2	0.2898		
9	-0.00567	2.13349	3.39926	2	0.2875		
10	-0.01926	-0.00160	4.64378	2	0.2877		
11	0.01515	-2.13402	3.39697	2	0.2874		
12	-0.00490	-2.13384	0.94097	2	0.2901		
10	ncard slave						
13	-1	0	7	1	6	12	-0.3083
14	-1	0	13	7	1	12	-0.2898
15	-1	0	14	13	7	12	-0.2929
16	-1	0	15	14	13	12	-0.3094
17	-1	0	16	15	14	12	-0.2897
18	0	0	13	7	14	2	0.2898
19	0	0	14	13	15	2	0.2875
20	0	0	15	14	16	2	0.2877
21	0	0	16	15	17	2	0.2874
22	0	0	17	16	7	2	0.2901

H₂O
120

0 ncard-v
0 nstr-u
0 nbend-u
1 ntors-u
6 1 7 13 45.0 3.0 4 0. 0. 0. 0. 0.
#BZAMID01 'P 21/c'RE topology

12					
1	-0.02519	-0.00678	2.56733	12	-0.2541
2	-0.19768	-1.19249	1.88262	12	-0.2980
3	-0.17931	-1.18339	0.48589	12	-0.2584
4	-0.00854	0.00061	-0.19875	12	0.0147
5	0.15072	1.18236	0.50110	12	-0.2725
6	0.23364	1.20528	1.97343	12	-0.3097
7	0.02777	-0.04211	-1.69398	10	1.0730
8	0.21604	2.11223	-0.04420	2	0.2899
9	0.47618	2.09536	2.53493	2	0.2986
10	-0.09866	-0.03316	3.64445	2	0.2832
11	-0.34518	-2.11715	2.42063	2	0.2891
12	-0.29937	-2.10769	-0.05964	2	0.2861

	4	ncard		slave			
13	-1	0	7	4	5	21	-0.8853
14	-1	0	7	4	13	27	-1.2415
15	-1	0	13	7	14	7	0.4911
16	-1	0	13	7	4	7	0.4940

0 ncard-v
0 nstr-u
2 nbend-u
15 13 7 118.0 0.2000
16 13 7 122.5 0.2200

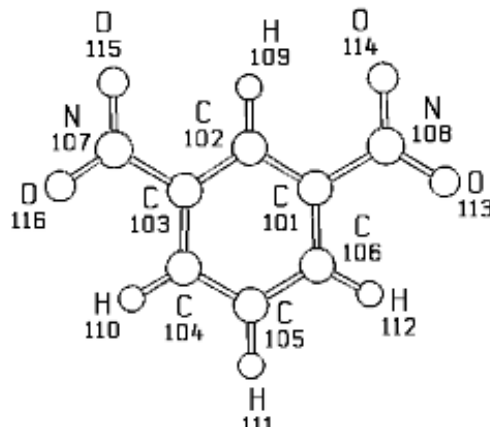
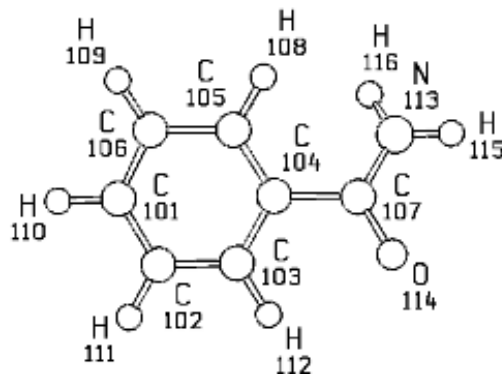
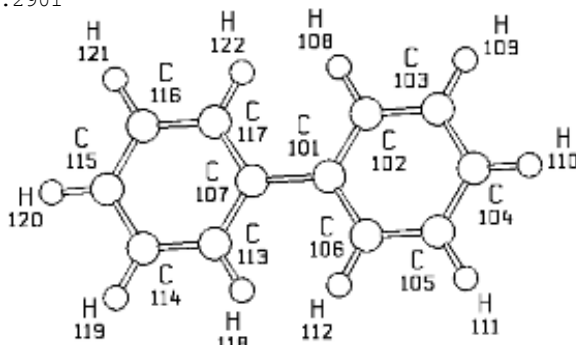
3 ntors-u											
14	7	4	3	0.	0.	0	7.6392E-07	-2.3582E-04	2.0827E-02	-0.30358	0.7917
15	13	7	14	0.	0.	0	0.00	0.00	9.5944E-03	0.00	0.053
16	13	7	4	0.	0.	0	0.00	0.00	5.1373E-03	0.00	0.084

#DNBENZ14 'P n a 21' topology

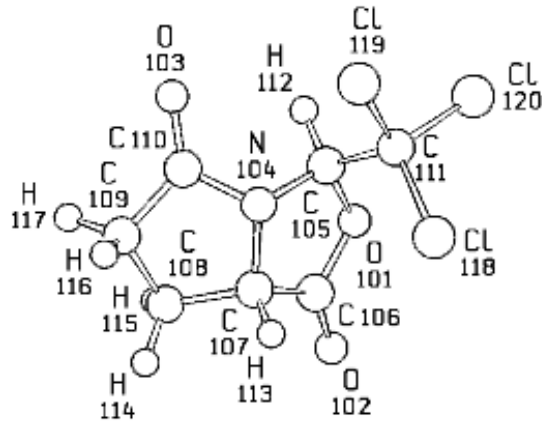
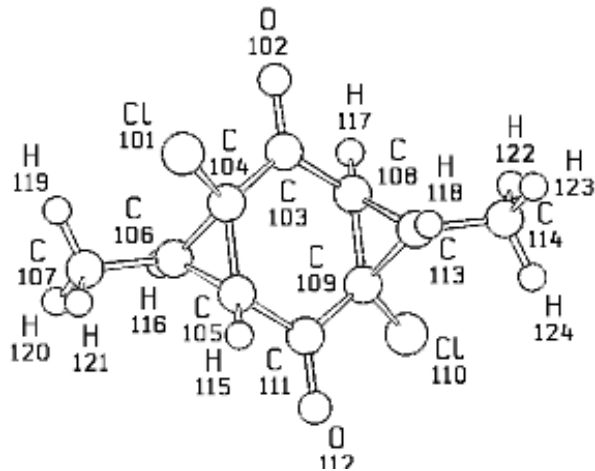
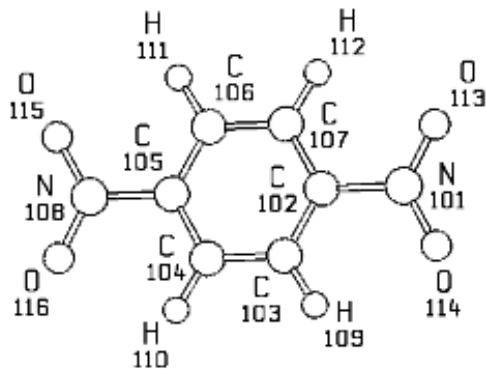
12					
1	-0.01337	0.18309	1.16524	12	0.2328
2	0.00803	-0.54771	-0.00785	12	-0.1934
3	-0.01739	0.19604	-1.17693	12	0.2289
4	-0.09233	1.57572	-1.19528	12	-0.1947
5	-0.13311	2.25556	0.01180	12	-0.2760
6	-0.08250	1.55934	1.20676	12	-0.1957
7	0.02285	-0.54692	-2.44984	20	1.2047
8	0.03733	-0.55128	2.44070	20	1.2030
9	0.04231	-1.62716	-0.01305	2	0.3042
10	-0.11860	2.11350	-2.13145	2	0.2950
11	-0.20469	3.33315	0.01990	2	0.2861
12	-0.09682	2.08276	2.15136	2	0.2951

	4	ncard slave					
13	-1	0	8	1	6	30	-0.8054
14	-1	0	8	1	13	30	-0.7943
15	-1	0	7	3	2	30	-0.7870
16	-1	0	7	3	15	30	-0.8036

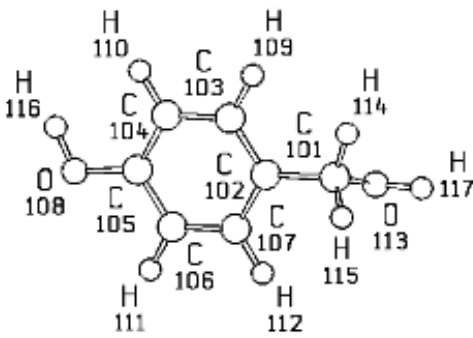
0 ncard-v
0 nstr-u
0 nbend-u
2 ntors-u
13 8 1 6 0.0 0.0 0 7.5175E-07 0.00 1.1649E-03 0.00 -0.1575
15 7 3 2 0.0 0.0 0 7.5175E-07 0.00 1.1649E-03 0.00 -0.1575
#DNITBZ11 'P 21/n' topology



```
12
1 -0.00712 0.00118 -2.82366 20 1.2081
2 -0.00392 -0.00096 -1.34544 12 0.2616
3 -0.09931 1.20663 -0.69269 12 -0.2412
4 -0.09443 1.20941 0.69345 12 -0.2413
5 0.00392 0.00096 1.34544 12 0.2616
6 0.09931 -1.20663 0.69269 12 -0.2412
7 0.09443 -1.20941 -0.69345 12 -0.2413
8 0.00712 -0.00118 2.82366 20 1.2081
9 -0.17613 2.13025 -1.24716 2 0.2943
10 -0.16582 2.13417 1.24671 2 0.2945
11 0.17613 -2.13025 1.24716 2 0.2943
12 0.16582 -2.13417 -1.24671 2 0.2945
4 ncard slave
13 -1 0 1 2 7 30 -0.7898
14 -1 0 1 2 13 30 -0.7862
16 -1 0 8 5 4 30 -0.7862
15 -1 0 8 5 16 30 -0.7898
0 ncard-v
0 nstr-u
0 nbend-u
2 ntors-u
13 1 2 7 0.0 0.0 0 7.5175E-07 0.00 1.1649E-03 0.00 -0.1575
16 8 5 4 0.0 0.0 0 7.5175E-07 0.00 1.1649E-03 0.00 -0.1575
#EXODAW methyl ren topology
18
1 -0.71498 0.60266 -2.98634 42 -0.2691
2 1.13371 2.16930 -1.25228 27 -1.1718
3 0.62283 1.22865 -0.70250 10 0.8847
4 0.00538 0.10438 -1.47193 13 0.3534
5 -0.59873 -1.10843 -0.77780 13 -0.3202
6 0.77354 -1.20698 -1.42923 13 -0.1752
7 0.94781 -2.04445 -2.68308 13 -0.8854
8 0.59873 1.10843 0.77780 13 -0.3202
9 -0.00538 -0.10438 1.47193 13 0.3534
10 0.71498 -0.60266 2.98634 42 -0.2691
11 -0.62283 -1.22865 0.70250 10 0.8847
12 -1.13371 -2.16930 1.25228 27 -1.1718
13 -0.77354 1.20698 1.42923 13 -0.1753
14 -0.94781 2.04445 2.68308 13 -0.8854
15 -1.55936 -1.59755 -0.84407 3 0.3512
16 1.76257 -1.49491 -1.10477 3 0.3295
17 1.55936 1.59755 0.84407 3 0.3512
18 -1.76257 1.49491 1.10477 3 0.3296
2 ncard slave
19 20 21 7 6 16 3 0.3009
22 23 24 14 13 18 3 0.3009
0 ncard-v
0 nstr-u
0 nbend-u
2 ntors-u
22 14 13 18 60. 7.7 3 0. 0. 0. 0. 0.
20 7 6 16 60. 7.7 3 0. 0. 0. 0. 0.
#FAXTUU01 renumbered topology
17
1 -0.96618 1.35606 -0.23466 23 -0.7918
2 -0.34419 2.90174 -1.71771 27 -1.1213
3 -0.87227 -2.52601 -1.37271 27 -1.1865
4 0.12867 -0.48098 -1.04486 17 -0.4660
5 -0.67666 -0.01661 0.05271 13 0.4461
6 -0.27041 1.77922 -1.33164 10 1.3318
7 0.56893 0.63861 -1.87014 13 0.0093
8 0.31192 0.19364 -3.32426 13 -0.5360
9 0.25532 -1.33350 -3.20695 13 -0.5577
10 -0.25244 -1.57805 -1.80867 10 1.0693
11 0.04636 -0.08864 1.41243 13 0.9020
12 -1.57166 -0.62075 0.07097 3 0.2617
13 1.60837 0.92541 -1.80904 3 0.3226
14 1.10749 0.51108 -3.98206 3 0.2838
15 -0.61562 0.59639 -3.70368 3 0.2854
16 1.23190 -1.77209 -3.34959 3 0.3371
17 -0.41138 -1.75684 -3.94360 3 0.3060
1 ncard slave
18 19 20 11 5 4 42 -0.29867
0 ncard-v
0 nstr-u
0 nbend-u
1 ntors-u
```

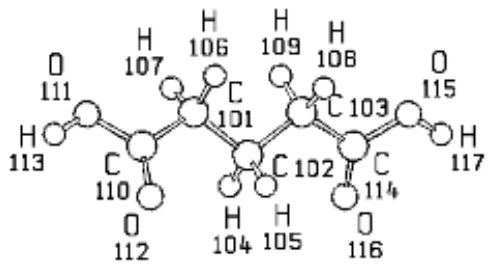


```
18 11 5 4 60.0 26.55 3 0. 0. 0. 0. 0.
#FOVQOX 'P n a 21' topology
12
1 0.45550 -0.23705 2.43180 13 0.1116
2 0.28251 -0.14394 0.94702 12 0.0025
3 0.10395 -1.28256 0.16872 12 -0.2999
4 -0.07224 -1.19431 -1.20493 12 -0.3520
5 -0.06244 0.04122 -1.81864 12 0.6994
6 0.11221 1.19340 -1.05825 12 -0.3567
7 0.28386 1.08830 0.30765 12 -0.2979
8 -0.21438 0.20457 -3.17099 29 -1.3730
9 0.10236 -2.25326 0.64206 2 0.2856
10 -0.21655 -2.08962 -1.79145 2 0.2960
11 0.11345 2.16331 -1.53331 2 0.2969
12 0.42248 1.98568 0.89234 2 0.2851
```



```
4 ncard slave
13 -1 0 1 2 7 29 -1.4520
14 15 0 1 2 13 3 0.2741
16 -1 0 8 5 4 5 0.80315
17 -1 0 13 1 2 5 0.80315
0 ncard-v
0 nstr-u
2 nbend-u
16 8 5 109.0 0.16
17 13 1 107.0 0.14
3 ntors-u
13 1 2 7 0.0 2.5 2 0.0 0.0 0.0 0.0 0.0
16 8 5 4 0.0 0.0 0 -2.8027E-07 0.00 4.1124E-03 0.00 0.13364
17 13 1 2 0.0 0.0 0 3.3904E-09 -9.0072E-06 2.2680E-03 -1.9463E-01 10.704
```

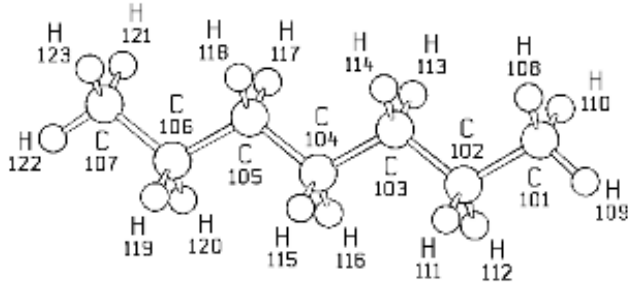
```
#GLURAC03 'C 2/c'REN topology
5
1 -0.08793 0.64867 1.23739 13 -0.5524
2 0.00000 -0.23453 0.00000 13 -0.5355
3 0.08793 0.64867 -1.23739 13 -0.5524
4 -0.87153 -0.86934 -0.06197 3 0.2843
5 0.87153 -0.86934 0.06197 3 0.2843
```



```
10 ncard slave
10 -1 0 1 2 3 10 1.3300
11 -1 0 10 1 2 28 -0.9456
12 -1 0 10 1 11 27 -1.1834
6 7 0 1 10 2 3 0.3338
13 -1 0 11 10 12 6 0.6671
14 -1 0 3 2 1 10 1.3300
15 -1 0 14 3 2 28 -0.9456
16 -1 0 14 3 15 27 -1.1834
17 -1 0 15 14 16 6 0.6671
8 9 0 3 2 14 3 0.3380
0 ncard-v
0 nstr-u
2 nbend-u
13 11 10 104.0 0.1333
17 15 14 104.0 0.1333
6 ntors u
13 11 10 12 0.0 0.0 0 -1.6863E-06 1.0417E-07 2.0280E-02 -3.4524E-04 0.000
12 10 1 2 0.0 0.0 0 5.6222E-08 -1.6317E-05 1.2839E-03 2.3332E-02 -0.2539
10 1 2 3 0.0 0.0 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
1 2 3 14 0.0 0.0 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
17 15 14 16 0.0 0.0 0 -1.6863E-06 1.0417E-07 2.0280E-02 -3.4524E-04 0.000
16 14 3 2 0.0 0.0 0 5.6222E-08 -1.6317E-05 1.2839E-03 2.3332E-02 -0.2539
```

```
#HEPTAN02 'P -1' topology
3
1 -0.00068 0.36581 3.80442 13 -0.9000
2 -0.00901 -0.48730 2.54789 13 -0.5600
3 0.00682 0.34306 1.27075 13 -0.5600
```

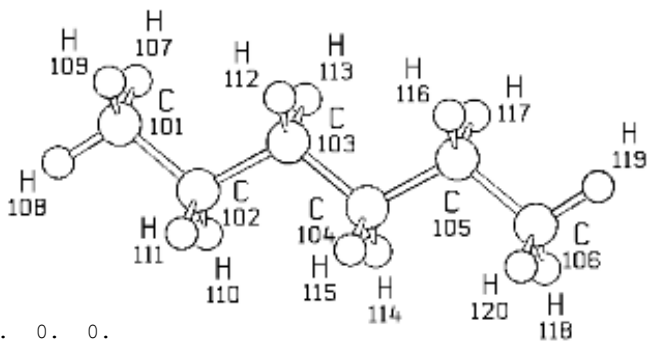
```
11 ncard slave
4 -1 0 3 2 1 13 -0.5600
5 -1 0 4 3 2 13 -0.5600
6 -1 0 5 4 3 13 -0.5600
7 -1 0 6 5 4 13 -0.9000
8 9 10 1 2 3 3 0.3000
11 12 0 2 1 3 3 0.2800
13 14 0 3 2 4 3 0.2800
15 16 0 4 3 5 3 0.2800
17 18 0 5 4 6 3 0.2800
19 20 0 6 5 7 3 0.2800
21 22 23 7 6 5 3 0.3000
0 ncard-v
0 nstr-u
```



```
0 nbend-u
6 ntors-u
8 1 2 3 60. 7.7 3 0. 0. 0. 0. 0.
1 2 3 4 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
2 3 4 5 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
3 4 5 6 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
4 5 6 7 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
21 7 6 5 60. 7.7 3 0. 0. 0. 0. 0.
```

#HEXANE01 'P -1' topology

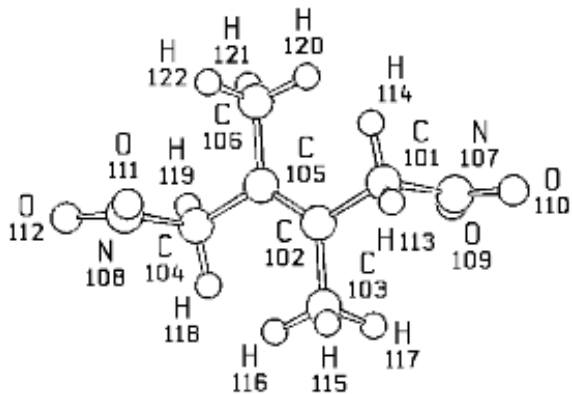
```
3
1 -0.00257 0.22175 -3.19145 13 -0.9000
2 0.00280 -0.53915 -1.87575 13 -0.5600
3 0.00542 0.37513 -0.66190 13 -0.5600
9 ncard slave
4 -1 0 3 2 1 13 -0.5600
5 -1 0 4 3 2 13 -0.5600
6 -1 0 5 4 3 13 -0.9000
7 8 9 1 2 3 3 0.3000
10 11 0 2 1 3 3 0.2800
12 13 0 3 2 4 3 0.2800
14 15 0 4 3 5 3 0.2800
16 17 0 5 4 6 3 0.2800
18 19 20 6 5 4 3 0.3000
```



```
0 ncard-v
0 nstr-u
0 nbend-u
5 ntors-u
7 1 2 3 60. 7.7 3 0. 0. 0. 0. 0.
1 2 3 4 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
2 3 4 5 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
3 4 5 6 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
18 6 5 4 60. 7.7 3 0. 0. 0. 0. 0.
```

#HITMUS 'P 21/c' topology

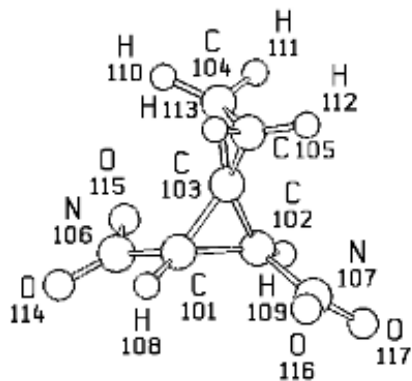
```
6
1 0.83384 0.17988 -1.71795 13 -0.3213
2 0.16338 -0.38659 -0.51138 12 -0.0347
3 -0.04199 -1.86647 -0.57416 13 -0.8772
4 -0.83384 -0.17988 1.71795 13 -0.3212
5 -0.16339 0.38659 0.51138 12 -0.0349
6 0.04199 1.86647 0.57416 13 -0.8774
10 ncard slave
7 -1 0 1 2 3 20 1.2104
9 -1 0 7 1 2 30 -0.7905
10 -1 0 7 1 9 30 -0.8036
8 -1 0 4 5 6 20 1.2099
11 -1 0 8 4 5 30 -0.7908
12 -1 0 8 4 11 30 -0.8039
13 14 0 1 2 7 3 0.3437
18 19 0 4 5 8 3 0.3437
15 16 17 3 2 5 3 0.3100
20 21 22 6 5 2 3 0.3100
```



```
0 ncard-v
0 nstr-u
0 nbend-u
6 ntors-u
9 7 1 2 0.0 0.0 0 -4.3269E-07 7.5651E-05 -3.3830E-03 2.7094E-02 0.600
11 8 4 5 0.0 0.0 0 -4.3269E-07 7.5651E-05 -3.3830E-03 2.7094E-02 0.600
15 3 2 5 0.0 3.7 3 0.0 0.0 0.0 0.0 0.0
20 6 5 2 0.0 3.7 3 0.0 0.0 0.0 0.0 0.0
7 1 2 5 0.0 3.7 3 0.0 0.0 0.0 0.0 0.0
8 4 5 2 0.0 3.7 3 0.0 0.0 0.0 0.0 0.0
```

#JOHBUD 'C c' topology

```
13
1 0.51905 -0.21122 0.54456 13 -0.0224
2 -0.54668 -0.19295 -0.54711 13 -0.0022
3 -0.02271 1.04639 -0.01825 13 0.2596
4 -0.55184 2.31744 0.51109 13 -0.5826
5 0.56748 2.31369 -0.50510 13 -0.5853
6 0.08661 -0.68178 1.85241 20 1.1820
7 -0.03968 -0.64515 -1.87409 20 1.1905
8 1.51129 -0.60294 0.71316 3 0.3269
9 -1.55197 -0.56162 -0.68788 3 0.3152
10 -0.36644 2.60830 1.53454 3 0.2985
11 -1.54046 2.65816 0.24115 3 0.2970
12 0.39600 2.65003 -1.51700 3 0.2986
13 1.57002 2.60017 -0.22362 3 0.2969
4 ncard slave
14 -1 0 6 1 8 30 -0.7809
```



```
17 -1 0 7 2 9 30 -0.8623
15 -1 0 6 1 14 30 -0.8848
16 -1 0 7 2 17 30 -0.7446
0 ncard-v
0 nstr-u
0 nbend-u
2 ntors-u
14 6 1 8 0.0 0.0 0 -4.3269E-07 7.5651E-05 -3.3830E-03 2.7094E-02 0.600
17 7 2 9 0.0 0.0 0 -4.3269E-07 7.5651E-05 -3.3830E-03 2.7094E-02 0.600
#MCINAM10 'A b a 2'R topology
```

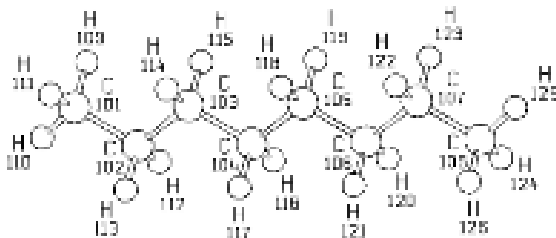
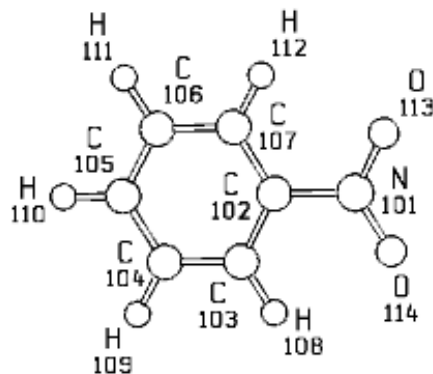
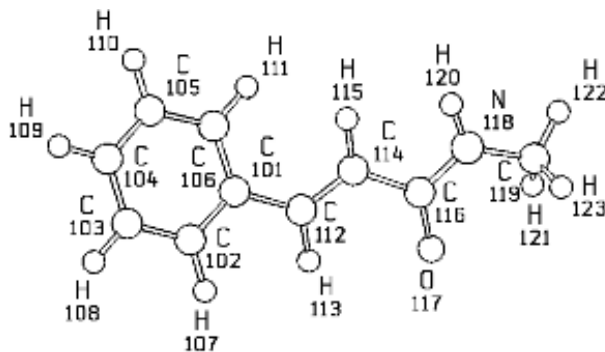
```
12
1 -0.07641 0.22787 -1.37484 12 0.0608
2 0.15472 1.21486 -2.32633 12 -0.2943
3 0.25309 0.90104 -3.68953 12 -0.2905
4 0.09628 -0.39548 -4.11017 12 -0.2743
5 -0.17010 -1.37140 -3.18783 12 -0.2873
6 -0.23010 -1.07798 -1.82464 12 -0.2952
7 0.26048 2.24206 -2.00979 2 0.2861
8 0.45260 1.68105 -4.40939 2 0.2870
9 0.18206 -0.64352 -5.15775 2 0.2864
10 -0.33659 -2.38526 -3.52058 2 0.2856
11 -0.39749 -1.87290 -1.11297 2 0.2883
12 -0.12204 0.58658 0.05311 12 -0.2063
9 ncard slave
14 -1 0 12 1 6 12 -0.3692
13 0 0 12 1 14 2 0.2926
16 -1 0 14 12 1 10 1.0138
15 0 0 14 12 16 2 0.3028
18 -1 0 16 14 12 21 -0.5574
17 -1 0 16 14 18 27 -1.2600
19 -1 0 18 16 14 13 -0.6364
20 -1 0 18 16 14 7 0.4879
21 22 23 19 18 16 3 0.2932
```

```
0 ncard-v
0 nstr-u
1 nbend-u
20 18 16 122.50 0.2200
5 ntors-u
14 12 1 6 0.0 0 -2.3529E-06 3.9583E-04 -1.5811E-02 -9.8980E-02 10.186
16 14 12 1 0.0 0 -4.1935E-06 3.0193E-03 -7.8639E-01 87.450 -3468.4
12 14 16 17 0.0 0 7.6392E-07 -2.3582E-04 2.0827E-02 -0.30358 0.7916
20 18 16 14 0.0 0 0.00 0.00 5.1375E-03 0.00 -0.0844
21 19 18 16 0.25 3 0.00 0.00 0.00000 0.00 0.00
```

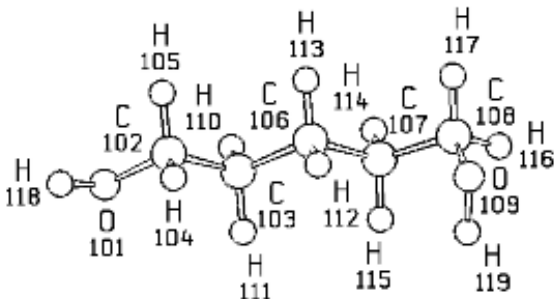
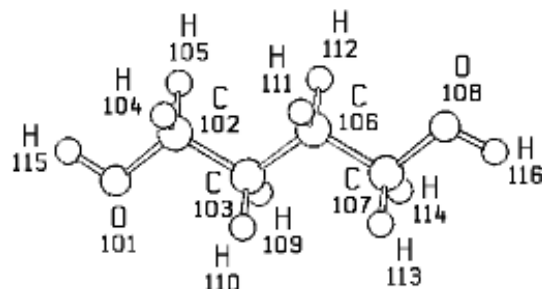
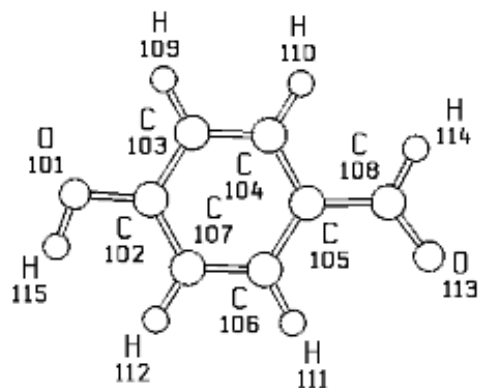
```
#NITRBE01 'P 21/c'RE topology
12
1 -0.00108 0.00218 -1.63730 20 1.2002
2 -0.00252 0.00296 -0.17234 12 0.2277
3 0.01919 -1.21571 0.48630 12 -0.2362
4 0.01365 -1.20799 1.86881 12 -0.2818
5 -0.00649 -0.00549 2.56262 12 -0.2274
6 -0.01154 1.20159 1.88010 12 -0.2813
7 -0.00843 1.21805 0.49632 12 -0.2362
8 0.03984 -2.14458 -0.06417 2 0.2955
9 0.02506 -2.14163 2.41161 2 0.2863
10 -0.01829 -0.01032 3.64255 2 0.2868
11 -0.01790 2.13115 2.42986 2 0.2865
12 -0.01055 2.15106 -0.04775 2 0.2954
2 ncard slave
13 -1 0 1 2 7 30 -0.8031
14 -1 0 1 2 13 30 -0.8122
0 ncard-v
0 nstr-u
0 nbend-u
1 ntors-u
```

```
13 1 2 7 0.0 0.0 0 7.5175E-07 0.00 1.1649E-03 0.00 -0.1575
#OCTANE01 'P -1' topology
```

```
3
1 -0.00416 0.26722 -4.45025 13 -0.9000
2 0.00308 -0.52847 -3.16019 13 -0.5600
3 0.00566 0.34663 -1.92012 13 -0.5600
13 ncard slave
4 -1 0 3 2 1 13 -0.5600
5 -1 0 4 3 2 13 -0.5600
6 -1 0 5 4 3 13 -0.5600
7 -1 0 6 5 4 13 -0.5600
8 -1 0 7 6 5 13 -0.9000
9 10 11 1 2 3 3 0.3000
12 13 0 2 1 3 3 0.2800
```



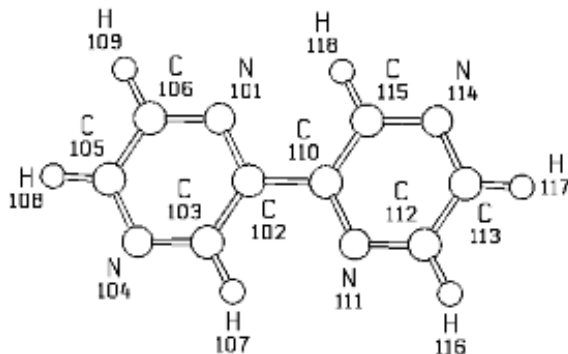
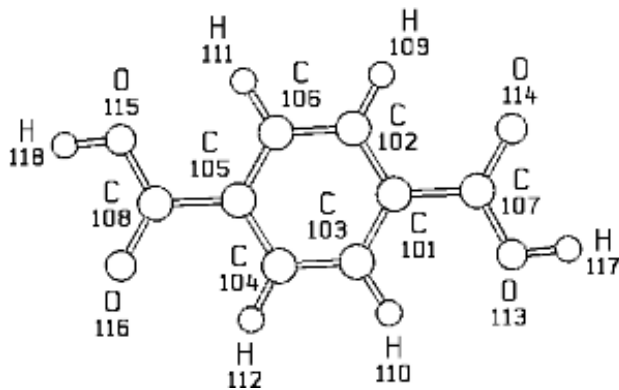
```
14 15 0 3 2 4 3 0.2800
16 17 0 4 3 5 3 0.2800
18 19 0 5 4 6 3 0.2800
20 21 0 6 5 7 3 0.2800
22 23 0 7 6 8 3 0.2800
24 25 26 8 7 6 3 0.3000
0 ncard-v
0 nstr-u
0 nbend-u
7 ntors-u
9 1 2 3 60. 7.7 3 0. 0. 0. 0. 0.
1 2 3 4 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
2 3 4 5 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
3 4 5 6 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
4 5 6 7 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
5 6 7 8 0. 0. 0 -1.5501E-06 1.1161E-03 -2.9199E-01 3.2793E+01 -1.3241E+03
24 8 7 6 60. 7.7 3 0. 0. 0. 0. 0.
#PHBALD11 'P 21/c'RE topology
12
1 -0.01044 -0.15852 3.13648 29 -1.3472
2 0.00067 -0.07962 1.78479 12 0.7870
3 -0.00394 1.19505 1.21784 12 -0.3605
4 0.00384 1.32418 -0.15039 12 -0.2112
5 0.00185 0.20805 -0.98833 12 -0.0176
6 0.00752 -1.06746 -0.40059 12 -0.2130
7 0.01955 -1.20803 0.96426 12 -0.3502
8 0.01516 0.40724 -2.42254 10 0.6178
9 -0.01352 2.07199 1.84814 2 0.2972
10 0.01163 2.31188 -0.58720 2 0.2846
11 0.00238 -1.94594 -1.02875 2 0.2864
12 0.04370 -2.19403 1.40434 2 0.2957
3 ncard slave
13 -1 0 8 5 6 27 -1.1412
14 -1 0 8 5 13 2 0.2586
15 -1 0 1 2 7 5 0.8135
0 ncard-v
0 nstr-u
1 nbend-u
15 1 2 109.00 0.16
2 ntors-u
6 5 8 13 0.0 0.0 0 -5.5370E-07 0.00 8.5360E-03 0.00 0.092
15 1 2 7 0.0 0.0 0 -2.8027E-07 0.00 4.1124E-03 0.00 0.13364
#QATTIO 'P 21/n'RE topology
5
1 0.02860 0.26007 -3.04982 29 -1.4633
2 -0.00462 -0.52788 -1.85325 13 0.1162
3 -0.02511 0.39409 -0.65869 13 -0.5660
4 0.86360 -1.16867 -1.80959 3 0.2691
5 -0.88334 -1.15574 -1.84953 3 0.2693
8 ncard slave
6 -1 0 3 2 1 13 -0.5662
7 -1 0 6 3 2 13 0.1153
8 -1 0 7 6 3 29 -1.4624
9 10 0 3 2 6 3 0.2858
11 12 0 6 3 7 3 0.28585
13 14 0 7 6 8 3 0.2695
15 -1 0 1 2 3 5 0.8032
16 -1 0 8 7 6 5 0.8024
0 ncard-v
0 nstr-u
2 nbend-u
15 1 2 107.0 0.14
16 8 7 107.0 0.14
5 ntors-u
2 3 6 7 0.0 0.0 0 -1.5501E-06 1.1161E-03 -2.9199E-01 32.793 -1324.1
1 2 3 9 60.0 8.0 3 0.00 0.00 0.00 0.00 0.00
8 7 6 11 60.0 8.0 3 0.00 0.00 0.00 0.00 0.00
15 1 2 3 0.0 0.0 0 3.3904E-09 -9.0072E-06 2.2680E-03 -1.9463E-01 10.704
16 8 7 6 0.0 0.0 0 3.3904E-09 -9.0072E-06 2.2680E-03 -1.9463E-01 10.704
#QATTOU 'P 21 21 2 topology
5
1 -0.26010 -0.00398 3.54971 29 -1.4626
2 0.33301 -0.47025 2.33334 13 0.1149
3 -0.19268 0.36692 1.18884 13 -0.5734
4 0.08647 -1.50986 2.17564 3 0.2693
5 1.40834 -0.38707 2.38988 3 0.2692
10 ncard slave
6 -1 0 3 2 1 13 -0.5558
```



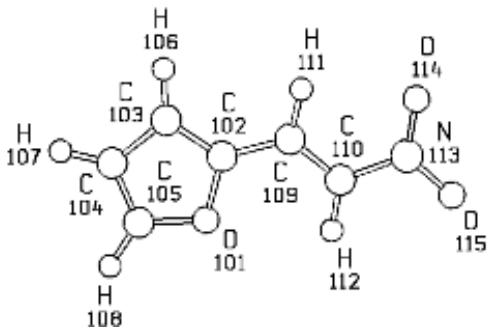
```
7 -1 0 6 3 2 13 -0.5749
8 -1 0 7 6 3 13 0.1096
9 -1 0 8 7 6 29 -1.4634
10 11 0 3 2 6 3 0.2859
12 13 0 6 7 3 3 0.28205
14 15 0 7 6 8 3 0.2902
16 17 0 8 9 7 3 0.27085
18 -1 0 1 2 3 5 0.8039
19 -1 0 9 8 7 5 0.8053
0 ncard-v
0 nstr-u
2 nbend-u
18 1 2 107.0 0.14
19 9 8 107.0 0.14
6 ntors-u
2 3 6 7 0.0 0.0 0 -1.5501E-06 1.1161E-03 -2.9199E-01 32.793 -1324.1
3 6 7 8 0.0 0.0 0 -1.5501E-06 1.1161E-03 -2.9199E-01 32.793 -1324.1
1 2 3 10 60.0 8.0 3 0.00 0.00 0.00 0.00 0.00
9 8 7 14 60.0 8.0 3 0.00 0.00 0.00 0.00 0.00
18 1 2 3 0.0 0.0 0 3.3904E-09 -9.0072E-06 2.2680E-03 -1.9463E-01 10.704
19 9 8 7 0.0 0.0 0 3.3904E-09 -9.0072E-06 2.2680E-03 -1.9463E-01 10.704
```

```
#TEPHTH06 'P -1'RENU topology
12
1 0.04735 0.01865 -1.38326 12 0.0412
2 0.07953 1.20677 -0.68850 12 -0.2491
3 -0.03755 -1.16749 -0.69071 12 -0.2485
4 -0.07953 -1.20677 0.68850 12 -0.2491
5 -0.04735 -0.01865 1.38326 12 0.0412
6 0.03755 1.16749 0.69071 12 -0.2485
7 0.01487 0.04201 -2.86268 10 1.3473
8 -0.01487 -0.04201 2.86268 10 1.3473
9 0.13642 2.14987 -1.21167 2 0.2874
10 -0.07238 -2.09517 -1.24261 2 0.2842
11 0.07238 2.09517 1.24261 2 0.2842
12 -0.13642 -2.14987 1.21167 2 0.2874
6 ncard slave
13 -1 0 7 1 3 28 -0.8966
14 -1 0 7 1 13 27 -1.2317
17 -1 0 13 7 14 6 0.6657
15 -1 0 8 5 6 28 -0.8966
16 -1 0 8 5 15 27 -1.2317
18 -1 0 15 8 16 6 0.6657
0 -lcard-v
0 nstr-u
2 nbend-u
17 13 7 104.00 0.1333
18 15 8 104.00 0.1333
4 ntors-u
14 7 1 9 0.0 0.0 0 0.000 0.000 4.9191E-03 0.000 -0.01
17 13 7 14 0.0 0.0 0 -1.5443E-06 0.000 1.7163E-02 0.000 0.005
16 8 5 4 0.0 0.0 0 0.000 0.000 4.9191E-03 0.000 -0.01
18 15 8 16 0.0 0.0 0 -1.5443E-06 0.000 1.7163E-02 0.000 0.005
```

```
#XAYMEP renumbered
10
1 0.00685 1.20842 -1.34398 18 -0.7576
2 0.00403 0.01069 -0.74184 12 0.3879
3 0.00550 -1.18045 -1.49258 12 0.0961
4 0.00132 -1.17751 -2.83012 18 -0.7245
5 -0.00625 0.02315 -3.42030 12 0.0742
6 0.00041 1.20655 -2.67905 12 0.0810
7 0.01013 -2.12677 -0.97169 2 0.2821
8 -0.01791 0.07880 -4.49875 2 0.2807
9 0.00017 2.15128 -3.20289 2 0.2800
10 -0.00407 -0.01061 0.74185 12 0.3878
8 ncard slave
11 -1 0 10 2 1 18 -0.7576
12 -1 0 11 10 2 12 0.0810
13 -1 0 12 11 10 12 0.0743
14 -1 0 13 12 11 18 -0.7243
15 -1 0 14 13 12 12 0.0960
16 0 0 12 11 13 2 0.2800
17 0 0 13 12 14 2 0.2806
18 0 0 15 14 10 2 0.2821
0 ncard-v
0 nstr-u
0 nbend-u
1 ntors-u
11 10 2 1 0.0 12.5 2 0. 0. 0. 0. 0.
```

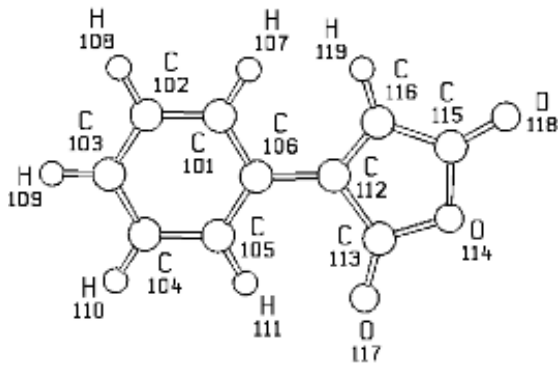


#XOZBUK	'P 21/n'	topology
9		
1	0.00578	0.99805 -1.63698 23 -0.7022
2	-0.01959	-0.29953 -1.17567 12 0.4934
3	-0.02296	-1.16734 -2.22625 12 -0.2581
4	0.00332	-0.37922 -3.40798 12 -0.3636
5	0.02616	0.91222 -3.00125 12 0.2419
6	-0.04196	-2.24575 -2.17119 2 0.3022
7	0.00474	-0.73815 -4.42658 2 0.3022
8	0.05644	1.76227 -3.66678 2 0.3026
9	-0.01389	-0.53176 0.23505 12 -0.1481
6	ncard slave	
10	-1 0	9 2 1 12 -0.1436
11	0 0	9 10 2 2 0.3093
13	-1 0	10 9 11 20 1.1153
12	0 0	10 9 13 2 0.3074
14	-1 0	13 10 9 30 -0.8735
15	-1 0	13 10 14 30 -0.8853



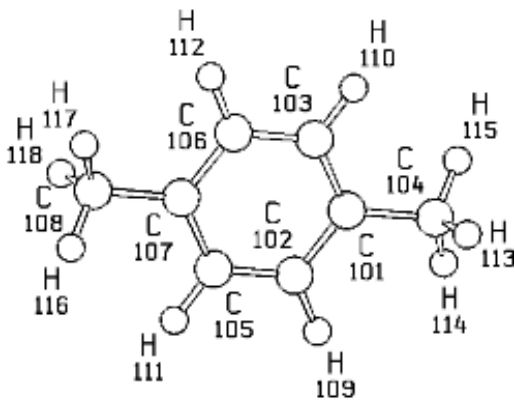
0	ncard-v	
0	nstr-u	
0	nbend-u	
3	ntors-u	
14 13 10	9 0.0 0.0	0 7.5175E-07 0.00 1.1649E-03 0.00 -0.1575
13 10	9 2 0.0 0.0	0 0.00 0.00 4.2310E-02 -15.231 1370.6
10 9 2	3 180.0 5.0 2	0.0 0.0 0.0 0.0

#ZIVKOE	'P -1'	renum topology
11		
1	-0.06950	-1.36198 1.69024 12 -0.2838
2	-0.06772	-1.39687 3.07723 12 -0.2881
3	0.00585	-0.21768 3.80030 12 -0.2667
4	0.08668	0.99321 3.13539 12 -0.2890
5	0.08218	1.03448 1.74614 12 -0.2827
6	0.00040	-0.14230 1.00815 12 0.0572
7	-0.12535	-2.28480 1.13188 2 0.2884
8	-0.12374	-2.34391 3.59339 2 0.2873
9	0.00017	-0.24326 4.87997 2 0.2869
10	0.15368	1.91182 3.69941 2 0.2869
11	0.14245	1.98487 1.23675 2 0.2911



8	ncardu	
12 -1	0 6 1	2 12 0.1240
13 -1	0 12 6 5	10 1.3793
14 -1	0 13 12 6	23 -0.7575
15 -1	0 14 13 12	10 1.3492
16 -1	0 15 14 13	12 -0.3056
17 -1	0 13 12 16	27 -1.1023
18 -1	0 15 16 12	27 -1.0791
19 0	0 16 12 15	2 0.3043
0	ncard-v	
0	nstr-u	
0	nbend-u	
1	ntors-u	
5 6 12 13	0.0 0.0 0	0. -5.3062e-05 1.0011e-02 -0.34146 3.3601

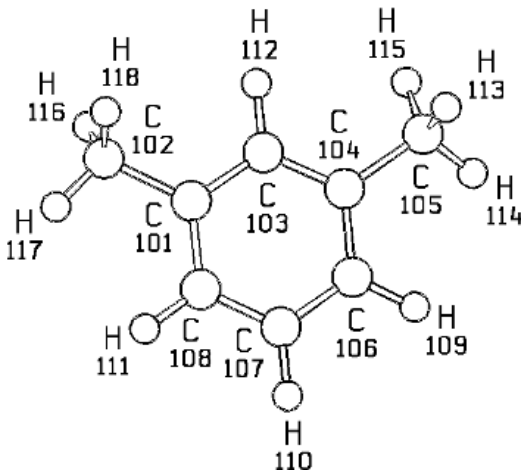
#ZZZITY01	'P 21/n'	r topology
12		
1	0.01275	-0.00174 1.41525 12 0.0467
2	0.00732	-1.19483 0.69402 12 -0.3323
3	0.00736	1.19016 0.69546 12 -0.3317
4	-0.00775	0.00094 2.91824 13 -0.8866
5	-0.00736	-1.19016 -0.69546 12 -0.3317
6	-0.00732	1.19483 -0.69402 12 -0.3323
7	-0.01275	0.00174 -1.41525 12 0.0467
8	0.00775	-0.00094 -2.91824 13 -0.8866
9	0.01461	-2.13642 1.22294 2 0.2874
10	0.01479	2.12982 1.22777 2 0.2870
11	-0.01479	-2.12982 -1.22777 2 0.2870
12	-0.01461	2.13642 -1.22294 2 0.2874



2	ncard slave	
13 14 15	4 1 2	3 0.30987
16 17 18	8 7 6	3 0.30987
0	ncard-v	
0	nstr-u	
0	nbend-u	
2	ntors-u	
13 4 1 2	30.0 0.08	6 0.0 0.0 0.0 0.0
16 8 7 6	30.0 0.08	6 0.0 0.0 0.0 0.0

#ZZZSPY01	'P b c a'	r topology
12		
1	0.00603	-0.29153 1.21302 12 0.0747

2	-0.00913	-1.05321	2.52351	13	-0.8912						
3	0.00791	-0.96643	0.01247	12	-0.3709						
4	0.01007	-0.30407	-1.20882	12	0.0733						
5	-0.00770	-1.06494	-2.51473	13	-0.8892						
6	0.00093	1.08417	-1.20380	12	-0.3591						
7	-0.00800	1.78111	-0.01113	12	-0.2857						
8	0.00611	1.09649	1.18871	12	-0.3591						
9	0.00078	1.62342	-2.13962	2	0.2862						
10	-0.02598	2.86096	-0.01664	2	0.2868						
11	0.01733	1.64706	2.11782	2	0.2858						
12	0.00772	-2.04638	0.02067	2	0.2855						
2	ncard slave										
13	14	15	5	4	6	3	0.31057				
16	17	18	2	1	8	3	0.31033				
0	ncard-v										
0	nstr-u										
0	nbend-u										
2	ntors-u										
13	5	4	6	30.0	0.08	6	0.	0.	0.	0.	0.
16	2	1	8	30.0	0.08	6	0.	0.	0.	0.	0.



Equilibrium structure and dynamics in organic crystals by Monte Carlo simulation. Critical assessment of force fields and comparison with static packing analysis

Angelo Gavezzotti

Supporting Information

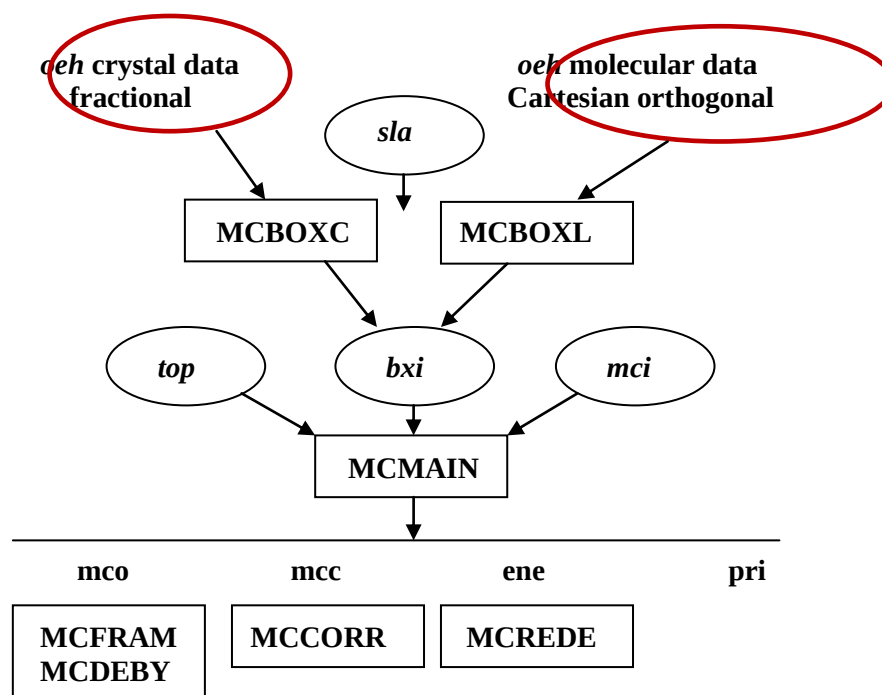
For each crystal, number of repeated cells along *a*, *b*, *c*, starting box parameters, number of molecules in box, number of atoms in box

#ABUMIT	10	4	3	39.495	42.504	45.81	480	5760
#BENZEN07	5	4	6	36.99	37.74	40.668	480	5760
#BILNOZ01	4	6	3	40.072	40.938	39.441	288	7488
#BNZQUI03	7	6	6	40.201	40.626	41.202	504	6048
#BULVAL03	6	2	4	38.88	41.168	41.48	384	7680
#CAXNUL05	5	5	3	37.9985	40.5395	38.877	300	5400
#CECGEX	7	5	3	33.0169	37.3035	33.855	210	4200
#CTCYDD	5	2	4	37.78	37.09	33.984	160	3520
#DAZNAP	3	4	4	41.085	42.228	37.14	384	6144
#DCBDOX10	7	6	2	41.881	42.684	49.274	336	7392
#DCLBEN02	6	7	10	43.92	41.65	39.8	420	5040
#DEZDUH	2	6	4	29.926	34.026	38.236	192	3840
#DEZXEL	3	4	5	35.643	39.272	37.2	240	4320
#DITBOX	5	7	4	38.665	43.715	43.26	280	7280
#EXODAW	6	6	5	33.624	36.7014	39.2	180	4320
#EZURUM	4	6	3	40.6956	39.4938	37.3986	288	6624
#FACFOE	5	7	3	37.403	41.7256	35.175	420	5040
#FACGEV	7	6	5	40.663	39.18	35.95	420	5040
#FACJAU	9	4	6	40.2471	41.14	38.052	432	5184
#FAXTUU01	7	4	3	42.2772	40.6272	46.6485	336	6720
#FMANUL01	4	3	6	36.444	39.609	41.886	288	6048
#FOVNIIN	6	4	2	46.326	45.516	37.014	192	4608
#HAYYAH	5	3	5	39.59	42.327	40.965	300	7200
#HCLBNZ11	6	12	3	48.2856	46.0356	44.4624	432	5184
#HEPTAN02	10	9	2	41.16	42.174	40.696	360	8280
#HEXANE01	10	9	5	41.309	42.2667	42.695	450	9000
#HOWBAW	6	6	5	32.7	32.694	38.39	180	5040
#NAPHTA10	5	6	4	41.064	35.8362	34.698	240	4320
#NBORAN02	6	4	3	35.556	37.956	40.356	288	5760
#OCTANE01	10	9	4	41.947	42.7662	43.992	360	9360
#PUGDEB	5	4	6	37.119	46.36	42.2838	480	5760
#PUXRAB	10	4	2	41.59	43.248	41.392	320	8000
#PVVAWA01	7	3	5	43.12	35.727	37.52	420	5040
#TCHLBZ03	11	3	3	42.2642	39.2919	41.3952	396	4752
#TEPNIT11	10	6	6	38.43	39.45	43.878	360	5040
#VACCEH	5	5	4	35.35	35.845	39.636	400	5600
#XAYMEP	10	7	4	36.86	37.03	37.88	280	5040
#XAYMIT	10	4	2	37.611	33.084	52.22	320	6400
#YUYPUD01	11	3	3	41.6328	35.7822	43.7922	396	5544
#ZIVKOE	6	6	4	39.282	42.342	38.748	288	5472
#ZZZITY01	7	8	4	40.642	40.184	44.86	448	8064
#ZZZRTI01	3	7	5	37.5339	42.4998	44.0785	420	7560
#ZZZSPY01	4	5	2	42.064	37.98	33.736	320	5760
#ACANIL01 'P	2	4	5	39.0180	37.4560	38.8900	320	6080
#ADIPAC07 'P	5	7	4	35.9350	36.1382	40.0600	280	5600
#ARCLAM01 'P	5	7	4	41.0310	40.2360	36.2108	560	5600
#AYOJED 'P	6	4	3	35.4048	40.2608	34.9731	288	4896
#BENZAC07 'P	7	8	2	37.7510	40.0240	43.3780	448	6720
#BIPHEN04 'P	5	7	4	40.6000	39.4100	38.0400	280	6160
#BZAMID01 'P	7	8	2	39.2490	40.3680	44.1060	448	7168
#DNBENZ14 'P	3	3	10	42.2070	39.7350	37.3800	360	5760
#DNITBZ11 'P	3	7	7	33.4020	38.2130	39.7670	294	4704
#FOVQOX 'P	4	4	6	38.0960	44.0240	35.6520	384	6528
#GLURAC03 'C	3	8	4	38.9307	37.9872	38.7820	384	6528
#HCLHEP 'C	3	4	4	37.7970	41.2800	39.9760	192	4416
#HITMUS 'P	5	4	5	35.1450	34.3440	38.8650	200	4400
#JOHBUD 'C	3	7	4	34.2630	42.1330	40.7080	336	5712
#MCINAM10 'A	3	2	4	33.8670	34.3500	38.1120	192	4416
#NITRBE01 'P	10	3	3	38.0140	34.8459	38.9529	360	5040
#PHBALD11 'P	6	3	5	40.1952	40.6650	35.7205	360	5400
#QATTIO 'P	7	3	5	35.0980	41.3640	37.3200	420	6720
#QATTOU 'P	7	6	2	37.2638	40.1946	34.0800	336	6384
#TEPHTH06 'P	5	6	10	38.5085	38.0742	36.6790	300	5400
#XOZBUK 'P	4	7	3	36.1496	36.4084	39.0810	336	5040

Description of essential MC procedures

Refer to A. Gavezzotti, New J. Chem. 2011, 35, 1360 to the document CLPmanual.doc available at <http://users.unimi.it/gavezzot> or from the author upon request at angelo.gavezzotti@unimi.it

Outline of the Monte Carlo modules



Block diagram of the Monte Carlo and trajectory analysis modules.

1 Introduction

The CLP package includes programs for the Monte Carlo simulation of the liquid and crystalline state of organic compounds. The package provides modules for the generation of computational boxes with liquid-like or crystalline structure, including a number of solute and solvent molecules. Periodicity can be enforced in one, two or three dimensions and pressure control is included. The main module performs a Monte Carlo simulation, and uses a structure and force field input file, 'topology' file (extension *top*), a run control file (extension *mci*), and a starting computational box file (extension *bxi*). The output consists of energies and trajectories. The package is designed to allow immediate access to a simulation of liquids and crystals with a minimum of intervention from the user.

2 Construction of molecular frameworks

Each molecular object in the computational box consists of a number of "core" atoms (≥ 3) and a number of "slave" atoms (≥ 0). The coordinates of the core atoms are given explicitly in Cartesian form, the position of slave atom *X* can be specified according to various geometrical procedures:

a) from three previously determined atoms A,B and C, on the chain A-B-C-X, by specifying the C-X distance, *R*, the BCX bond angle, α , and the ABCX torsion angle, τ .

Note: Improper dihedrals can be used to impose planarity, e.g. in a nitro group the first oxygen is obtained from a normal O-N-C-C torsional chain; the second oxygen is placed by an O-N-C...O chain setting $\tau = 180^\circ$.

b) from four known atoms in a pyramidal configuration, X-A(BCD), by specifying the XA bond distance, *R*, with three equal XAY angles;

c) from three known atoms, ABC, by specifying the BX distance, *R*, with equal ABX and XBC angles;

d) for CX₂ groups, as in c), but specifying the C-X distance, *R*, and the XCX bond angle, α ;

e) for CX_3 groups (typically, $X=H$ for a methyl group), as in a), specifying the C-X distance, the XCB bond angle, and one torsion angle τ , with the three X-atoms at τ , $\tau+120^\circ$, $\tau+240^\circ$.

These procedures are almost identical to those described in Section 2.2.2 and Figure 1. The geometry of the core-atoms fragment is unchanged during the simulation, while the R , α and τ values described above maybe either constant or variable parameters.

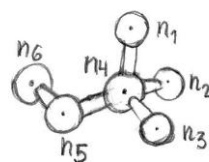
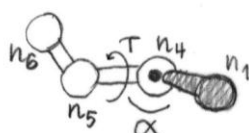
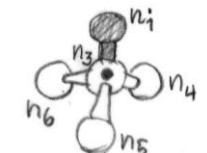
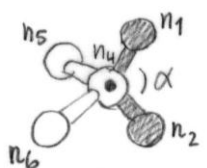
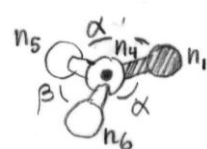
The procedure allows for two molecular species in the computational box, one formally called solute and one formally called solvent. Both can be variable-geometry species. For each molecule, solute or solvent, Cartesian coordinates are calculated for slave atoms using current values for all parameters, in a local reference frame whose origin is determined by the original specification of core atom positions; the molecular object in its current conformation is then inserted into the computational box by applying a rigid-body translation vector and a rigid-body rotation by three Euler angles. The chirality of each molecule can also be specified as previously described (§3.7 and 4.6.1). The approach provides the full range of choices between just one completely rigid molecular species and two completely flexible molecular objects.

The origin of the molecular reference system, chosen by the user, is henceforth called the “molecular center”, although it may be neither a center of mass nor a center of coordinates.

Description of the topology input file

- 1) title line
- 2) NCOREU number of core atoms, solute
ncoreu lines each with core atom number, x, y, z, atom species, raw charge
- 3) NCARDU number of slave atom lines, solute
ncardu lines each with i1, i2, i3, i4, i5, i6 integer codes, atom species, raw charge
(see Scheme for the meaning of the six codes)
- 4) NCOREV number of core atoms, solvent
ncorev lines as in 3)
- 5) NCARDV number of slave atom lines, solvent
ncardv lines, each as in 5)
- 6) NSTRU number of bond stretching functions (solute only)
nstru lines each with two atom numbers, k and R° for $E=1/2k(R-R^\circ)^2$
- 7) NBENDU number of bending functions (solute only)
nbendu lines each with three atom numbers, k and θ° for $E=1/2k(\theta-\theta^\circ)^2$
- 8) NTORSU number of torsion functions, solute
ntorsu lines each with:
four atom numbers
 τ° , k, n for $E=K\{1-\cos[n(\tau-\tau^\circ)]\}$, eq(6.4.3) zero if polynomial is used
a, b, c, d, e polynomial coefficients (eq. 6.4.2) zero if cosine function is used
- 9) NTORSV number of torsion functions, solvent
ntorsv lines as in 12)
- 10) NLISTU number of intramolecular contacts, solute
nlistu pairs of atom numbers
- 11) NLISTV number of
nlistv pairs of atom numbers
- 12) FQ, FP, FD, FR force field parameters
- 13) NPARS number of non-pairs lines each with two atomic species, and P(ij), D(ij), T(ij), eq. 3.5.1
- 14) NFNBI number of intramolecular nonbonded potentials (only if NLISTU or NLISTV ne.0):
nfnbi lines each with two atom species, and A, B, C in eq. 3.4.4 options in the Monte Carlo slave-atom file.

Trigonal



Methylene

Methine

Z-matrix

RX₃ group: three Z-matrix type atoms, n₁, n₂, n₃, with torsion angles τ , $\tau+120$, $\tau+140$, all angles equal to α .

3 Construction of computational boxes

A computational box is defined as an ensemble on N(u) solute molecules and N(v) solvent molecules, enclosed in a parallelepiped box with dimensions boxx, boxy, boxz and angles α , β and γ . Each molecule in the box is specified by three position coordinates for the molecular center, three rigid-body rotation angles, and the value of the intramolecular geometrical parameters. The **Mcboxl** module reads a file with Cartesian orthogonal coordinates of a molecular model (§.oeh format, 2.2) and prepares a cubic box containing a number of molecules, for the simulation of an isotropic liquid. The **Mcboxc** module reads a *oeh* file with crystallographic information and prepares an oblique box with multiples of the crystal unit cell in three dimensions. Any pair of boxes coming from **Mcboxl** or **Mcboxc** modules can be merged using module **Mcboxs**. This module produces a solution box by deleting solvent molecules in close contact with solute molecules.

Coordinates for the molecules in the crystal box are generated by the following procedure: a) prepare a molecular model in Cartesian orthogonal coordinates in the inertial reference frame; for non-rigid molecules, starting from a number of fixed atoms and adding a set of conformationally flexible molecular sections (the semi-rigid procedure²⁰); experimental geometries are used throughout; b) apply if necessary a symmetry-chirality operation (change of sign in one, two or three coordinates) depending on the symmetry operations of the space group; c) rotate the rigid molecule by three Euler angles calculated from the experimental crystal structure; d) translate the molecule to its location in the crystal box, using the experimental translation vector. The final computational box is then in Cartesian orthogonal coordinates.

4 Force fields

The total configurational energy is a sum of intramolecular and intermolecular terms. In general:

$$E(\text{tot}) = \sum F(\text{stretch}, \text{bend}) + \sum \phi(\tau) + \sum u(R, \text{intram}) + \sum u(R, \text{interm}) \quad (4.1)$$

where each summation runs over the appropriate degrees of freedom.

4.1 Intramolecular field. Bond stretching and bond angle bending potentials are provided in the usual quadratic form but are seldom applied in the simulation of condensed phases of organic molecules, where high-frequency vibrations can usually be ignored and bond lengths and bond angles are kept fixed. The torsional intramolecular part $\phi(\tau)$ can either be a fitted polynomial in τ or a trigonometric function in τ ($0 < \tau < 180^\circ$):

$$\phi(\tau) = a + b \tau + c \tau^2 + d \tau^3 + e \tau^4 \quad (4.2)$$

$$\begin{aligned}\phi(\tau) &= K \{1 - \cos n[\tau - \tau^\circ]\} \quad n = 1, 2, 3 \\ \phi(\tau) &= 0 \text{ for } \tau = \tau^\circ \\ \phi(\tau) &= 2K \text{ for } \cos n[\tau - \tau^\circ] = -1\end{aligned}\quad (4.3)$$

4.2. Intermolecular field. The intermolecular atom-atom non-bonded potential:

$$u(R, \text{interm}) = E(\text{CLP}) \quad (4.5)$$

where R is any intermolecular non-bonded atom-atom distance. The potentials are automatically calculated at running time from the library atomic parameters and the actual atomic point charges.

Following a well established convention, intermolecular energies are subdivided in Coulombic and non-Coulombic terms:

$$E(\text{tot}, \text{inter}) = \sum_{i, \alpha} \sum_{j, \beta} [E(\text{CLP})_{ij}] = E(\text{LP}) + E(\text{Coul}) \quad (4.6)$$

where α and β denote different molecules, and the London-Pauli and Coulombic terms include polarization+repulsion+dispersion, and Coulombic summations, respectively. The cutoff applies to centers of coordinates rather than to single atom-atom distances. In this way the summations always extend over entire molecules (neutral charge units), thus reducing if not eliminating completely the truncation effects, even if no convergence correction is applied.

5 Simulation details

5.1 Degrees of freedom (dof's). The degrees of freedom in a MC simulation are in principle the six rigid-body molecular parameters for each molecule in the box, plus the slave atom parameters. A tag specifies whether each parameter is to be altered or kept fixed during the run; the number of actual dof's is adjusted accordingly. The maximum steps for each kind of the MC move, molecular translation, rotation, or change in internal dof's, are also specified. Box periodicity can be imposed in one, two or three dimensions; each molecule in the original box has translated counterparts for a ± 1 addition of periodicity vector(s), for a maximum total of 26 repeated boxes in the three-dimensional case. Intramolecular energies are computed only for the molecules within the original box. Intermolecular energies are computed over all molecular pairs between molecules within the box or translation-repeated molecules, when the distance between centers of coordinates is below a given threshold. As soon as the center of a molecule moves outside the box boundary, the molecule is deleted and re-enters the box at the opposite end. Note that full molecules are always moved, thus avoiding problems with connectivity breaking that occur when single atoms are moved to comply with box periodicity.

5.2 MC moves. A MC move or action can be of the following types:

a) variation of molecular dof's. A random number $0 < r_1 < 1$ is generated and the number n of the parameter P to be varied is determined as $n = \text{int}(r_1 \cdot N_{\text{tot}}) + 1$ where N_{tot} is the total number of variable parameters and "int" denotes the integer part of the number. Positive or negative steps are taken by using $P' = P^\circ + (r_2 - 0.5) \cdot \text{step}$.

b) Suppression of center-of mass drift. The overall motion of the center of mass of the whole box can be stopped, at selected intervals during the simulation, by resetting all molecular position vectors to the origin in the current center of mass.

c) Box dimensions change. The box dimensions can be changed at selected intervals, with or without pressure control. Isotropic variation with cubic boxes (liquids), or anisotropic variation with oblique boxes (crystals) are possible. In detail, the box variation algorithm is as follows. The computational box is identified by three box edges, a, b, c , and three box angles, α, β, γ . Whenever one of these box dimension is changed, the positions of all molecules is undergoes a rigid-body change by the following procedure: i) calculate fractional coordinates for the centers in the old box metrics; ii) calculate new orthogonal coordinates of the centers in the new box metrics; iii) calculate the components of the displacement of each molecular center, dx, dy, dz , and apply the same displacement vector to all atoms in the computational box.

d) Pressure control. There is no temperature rescaling in MC, as temperature is a preset invariable parameter. When box periodicity is present and box dimension are allowed to vary, pressure control is possible.

Standard isothermal-isobaric ensemble (IIE) P control. The usual MC P-control based on the appropriate configurational integral for the IIE is used (as given in Allen, M.P. and Tildesley, D.J. (1989) Computer simulation of liquids, Oxford University Press, 1989, pp. 41 and 124). Pressure is set at a constant value P . Cell dimensions are varied (either isotropically or anisotropically) at preset intervals and the new total box energy U' and the new volume V' are calculated. The quantity δH is calculated:

$$\delta H = U' - U^\circ + P(V' - V^\circ) - N kT \ln(V'/V^\circ) \quad (5.9)$$

and the usual Metropolis algorithm is implemented on δH instead of ΔU . The second term is interpretable as expansion work, while the third term has no immediate interpretation. N is the number of "particles" in the system

The number of particles N is ill-defined in a simulation involving large flexible molecules (the number of molecules? the number of atoms? the number of flexible sub-molecules?)

8 Trajectory analysis

8.1 Radial density functions. Consider a pair of atomic species (atom-atom RDF), or pairs of molecular centers (center of mass RDF). N_i is the number of distances in a spherical distance bin of volume V_i , N is the total number of distance points and V is the total volume of the distance sphere, the radial density functions $g(R)$ is:

$$g(R_i) = (N_i/V_i) / (N/V) \quad (8.1)$$

N/V is the total number density of distances, corresponding to uniform and random distribution. $g(R)$ is thus normalized and $g(R_i) > 1$ indicates a significantly high frequency of distances at R_i .

8.2 Translational (diffusion) and rotational correlation. The diffusion coefficient D and rotational correlation function $\tau(\text{rot})$ are estimated as follows. The standard time-dependent formulations are:

$$\tau(t) = [\sum_k \mathbf{u}_k(t) \cdot \mathbf{u}_k(0)] / N_{\text{mol}} \quad (8.2)$$

$$D = (1/6) \langle |\mathbf{r}(t+\Delta t) - \mathbf{r}(t)|^2 \rangle / \Delta t \quad (8.3)$$

where $\mathbf{u}(t)$ is an orientation vector within the molecule, and $\mathbf{r}(t)$ is the position of a specified atom or of the center of coordinates at time t . The number of MC moves takes here the place of time, and an approximate scaling, with an estimate of the time equivalent of a MC move, results in 1Mmove approximately equal to 2 ps. The τ functions are dimensionless numbers between 1 (complete correlation) and 0 (no correlation), and are averaged over all molecules in the box. They can be compared with experimentally determined correlation times, i.e. the time for the liquid to completely lose rotational memory (from $\tau = 1$ to $\tau = 0$). The D functions are averaged over the molecules within a radius of usually 30 Å from the overall center of the box.

8.3 The Mcfram module

The *Mcfram* module reads a *.dat* file and performs the following tasks:

- 1) check of the solute and solvent connectivity for bond distances, and of short intermolecular contacts
- 2) torsion angle monitoring
- 3) calculation of the center of mass radial distribution function for solute-solute, solvent-solvent and solute-solvent
- 4) calculation of the radial distribution function for any pair of atomic species, solute-solute, solvent-solvent and solute-solvent

8.3 The Mccorr module

The *Mccorr* module reads a trajectory *.dat* file (*.mcc* type) and performs the following tasks:

- calculate rotational correlation functions and self-diffusion coefficients;
- calculate distribution of rotation angles.

Equilibrium structure and dynamics in organic crystals by Monte Carlo simulation. Critical assessment of force fields and comparison with static packing analysis

Angelo Gavezzotti

Supporting Information

100 K runs, cell parameters, complete runs
For each crystal: a, b, c, α, β, γ
start: experimental crystal structure, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd	start	end	delt	aver	rmsd
#ABUMIT	3.949	3.588	-9.2	3.676	0.114	90.00	90.12	0.12	90.00	0.140
#ABUMIT	10.626	10.504	-1.2	10.450	0.065	97.00	101.10	4.10	100.73	1.272
#ABUMIT	15.270	15.110	-1.0	15.104	0.060	90.00	89.99	-0.01	90.16	0.336
#BENZEN07	7.398	7.439	0.6	7.324	0.059	90.00	89.92	-0.08	90.02	0.166
#BENZEN07	9.435	9.199	-2.5	9.237	0.061	90.00	89.92	-0.08	89.97	0.106
#BENZEN07	6.778	6.389	-5.7	6.524	0.107	90.00	89.68	-0.32	89.83	0.193
#BILNOZ01	10.018	9.782	-2.4	9.806	0.050	90.00	89.92	-0.08	90.00	0.178
#BILNOZ01	6.823	6.819	-0.1	6.817	0.007	90.04	90.82	0.78	90.51	0.218
#BILNOZ01	13.147	13.210	0.5	13.191	0.026	90.00	89.85	-0.15	90.02	0.127
#BNZQUI03	5.743	5.486	-4.5	5.544	0.074	90.00	92.79	2.79	90.51	0.702
#BNZQUI03	6.771	6.986	3.2	6.898	0.062	100.14	96.72	-3.42	97.99	0.912
#BNZQUI03	6.867	6.548	-4.7	6.678	0.078	90.00	87.11	-2.89	89.42	0.783
#BULVAL03	6.480	6.242	-3.7	6.266	0.055	90.00	90.11	0.11	89.98	0.088
#BULVAL03	20.584	20.907	1.6	20.856	0.101	90.17	92.93	2.76	92.71	0.642
#BULVAL03	10.370	10.385	0.1	10.367	0.014	90.00	89.96	-0.04	90.00	0.167
#CECGEX	4.717	4.608	-2.3	4.628	0.042	90.00	90.05	0.05	89.99	0.140
#CECGEX	7.461	7.143	-4.3	7.258	0.123	96.95	89.96	-6.99	90.56	1.476
#CECGEX	11.285	11.800	4.6	11.620	0.223	90.00	90.05	0.05	89.94	0.181
#CTCYDD	7.556	7.484	-1.0	7.465	0.026	90.00	89.96	-0.04	89.99	0.137
#CTCYDD	18.545	17.366	-6.4	17.648	0.332	113.73	115.62	1.89	115.26	0.352
#CTCYDD	8.496	8.673	2.1	8.584	0.076	90.00	89.74	-0.26	90.00	0.169
#DAZNAP	13.695	13.803	0.8	13.638	0.115	90.00	89.88	-0.12	90.03	0.127
#DAZNAP	10.557	10.171	-3.7	10.228	0.123	90.00	92.53	2.53	91.04	0.762
#DAZNAP	9.285	8.574	-7.7	8.778	0.192	90.00	89.87	-0.13	90.10	0.171
#DCBDOX10	5.983	5.931	-0.9	5.879	0.049	90.00	93.73	3.73	91.83	1.282
#DCBDOX10	7.114	6.470	-9.0	6.659	0.197	90.00	90.74	0.74	90.58	0.222
#DCBDOX10	24.637	24.774	0.6	24.721	0.088	90.00	90.00	-0.00	90.02	0.201
#DCLBEN01	14.762	14.633	-0.9	14.741	0.077	90.00	89.91	-0.09	89.99	0.201
#DCLBEN01	5.832	5.701	-2.3	5.677	0.056	112.78	109.60	-3.18	112.84	2.579
#DCLBEN01	4.039	3.508	-13.2	3.701	0.176	90.00	90.14	0.14	90.19	0.138
#DCLBEN02	7.320	7.398	1.1	7.392	0.038	93.17	84.76	-8.41	85.69	2.190
#DCLBEN02	5.950	5.522	-7.2	5.679	0.164	113.58	111.71	-1.87	115.41	3.633
#DCLBEN02	3.980	3.603	-9.5	3.709	0.112	93.50	97.70	4.20	96.15	1.346
#DEZDUH	14.963	14.761	-1.4	14.840	0.069	90.00	90.03	0.03	89.97	0.115
#DEZDUH	5.671	5.781	1.9	5.773	0.027	90.00	89.73	-0.27	89.98	0.130
#DEZDUH	9.559	9.898	3.5	9.846	0.082	90.00	90.29	0.29	89.97	0.151
#DEZXEL	11.881	11.914	0.3	11.902	0.025	90.00	89.93	-0.07	90.03	0.117
#DEZXEL	9.818	9.527	-3.0	9.553	0.080	90.00	89.96	-0.04	90.01	0.082
#DEZXEL	7.440	7.161	-3.7	7.201	0.076	90.00	89.84	-0.16	89.96	0.124
#DITBOX	7.733	6.934	-10.3	7.121	0.249	90.00	89.85	-0.15	89.88	0.138
#DITBOX	6.245	6.338	1.5	6.306	0.044	108.34	104.25	-4.09	104.94	1.379
#DITBOX	10.815	10.553	-2.4	10.562	0.081	90.00	90.11	0.11	90.14	0.146
#EZURUM	10.174	10.217	0.4	10.216	0.030	90.00	90.06	0.06	90.01	0.069
#EZURUM	6.582	6.473	-1.7	6.483	0.029	94.07	95.89	1.82	95.80	0.291
#EZURUM	12.466	12.520	0.4	12.511	0.015	90.00	90.00	-0.00	89.98	0.092
#FACGEV	5.809	5.810	0.0	5.759	0.033	90.00	90.17	0.17	89.89	0.371
#FACGEV	6.530	6.499	-0.5	6.475	0.040	101.89	96.00	-5.89	97.13	1.879
#FACGEV	7.190	6.567	-8.7	6.737	0.183	90.00	89.80	-0.20	90.04	0.170
#FACJAU	4.472	4.533	1.4	4.522	0.015	90.00	89.76	-0.24	89.94	0.237
#FACJAU	10.285	10.514	2.2	10.459	0.062	107.97	104.00	-3.97	103.95	0.822
#FACJAU	6.342	6.162	-2.8	6.197	0.067	90.00	90.10	0.10	90.02	0.187
#FMANUL01	9.111	9.152	0.4	9.039	0.091	90.00	89.99	-0.01	90.00	0.125
#FMANUL01	13.203	13.798	4.5	13.649	0.181	90.00	89.69	-0.31	89.96	0.189
#FMANUL01	6.981	6.225	-10.8	6.443	0.234	90.00	89.84	-0.16	89.98	0.143
#FOVNIN	7.721	7.658	-0.8	7.665	0.012	90.00	89.85	-0.15	90.01	0.126
#FOVNIN	11.379	11.239	-1.2	11.227	0.038	90.00	90.14	0.14	90.05	0.239
#FOVNIN	18.507	17.732	-4.2	17.831	0.164	90.00	90.09	0.09	89.89	0.234
#HAYYAH	7.918	7.665	-3.2	7.717	0.071	90.00	89.98	-0.02	89.99	0.160
#HAYYAH	14.109	13.752	-2.5	13.790	0.079	111.46	109.71	-1.75	110.38	0.862
#HAYYAH	8.193	8.047	-1.8	8.064	0.025	90.00	89.79	-0.21	90.11	0.232
#HCLBNZ11	8.048	7.931	-1.5	7.933	0.035	90.00	90.00	-0.00	89.92	0.181
#HCLBNZ11	3.836	3.549	-7.5	3.614	0.093	92.13	93.59	1.46	93.81	0.588
#HCLBNZ11	14.821	14.554	-1.8	14.549	0.076	90.00	89.83	-0.17	89.98	0.092

#HOWBAW	5.450	5.194	-4.7	5.236	0.061	93.27	94.17	0.90	93.91	0.305
#HOWBAW	5.449	5.607	2.9	5.588	0.041	94.10	95.46	1.36	95.41	0.350
#HOWBAW	7.678	7.674	-0.1	7.651	0.012	108.93	108.98	0.05	108.99	0.099
#NAPHTA10	8.213	7.426	-9.6	7.672	0.260	90.00	90.04	0.04	90.05	0.138
#NAPHTA10	5.973	5.933	-0.7	5.901	0.032	123.39	125.67	2.28	126.40	1.132
#NAPHTA10	8.675	8.687	0.1	8.713	0.040	90.00	89.97	-0.03	90.00	0.104
#NBORAN02	5.926	6.143	3.7	6.099	0.060	90.00	89.83	-0.17	89.99	0.145
#NBORAN02	9.489	9.593	1.1	9.599	0.027	90.00	89.94	-0.06	90.00	0.106
#NBORAN02	13.452	13.172	-2.1	13.254	0.111	90.00	90.05	0.05	90.00	0.094
#PUGDEB	7.424	7.256	-2.3	7.339	0.081	90.00	89.96	-0.04	90.29	0.342
#PUGDEB	11.590	12.082	4.2	11.986	0.156	112.78	108.82	-3.96	113.11	2.914
#PUGDEB	7.047	6.324	-10.3	6.562	0.216	90.00	89.91	-0.09	89.95	0.137
#TCHLBZ03	3.842	3.665	-4.6	3.680	0.057	90.00	89.95	-0.05	89.92	0.145
#TCHLBZ03	13.097	13.271	1.3	13.152	0.125	90.00	90.15	0.15	90.05	0.193
#TCHLBZ03	13.798	12.908	-6.5	13.163	0.253	90.00	90.21	0.21	89.92	0.201
#TEPNIT11	3.843	3.565	-7.2	3.619	0.085	114.50	115.41	0.91	115.21	0.521
#TEPNIT11	6.575	6.438	-2.1	6.414	0.055	93.53	83.30	-10.23	85.37	2.881
#TEPNIT11	7.313	7.004	-4.2	7.104	0.105	96.99	102.64	5.65	102.69	1.665
#VACCEH	7.070	7.078	0.1	7.037	0.050	90.00	89.87	-0.13	89.96	0.176
#VACCEH	7.169	6.862	-4.3	6.885	0.086	90.00	89.82	-0.18	89.99	0.111
#VACCEH	9.909	9.557	-3.6	9.628	0.082	90.00	90.01	0.01	90.01	0.098
#XAYMIT	3.761	3.430	-8.8	3.498	0.093	90.00	89.95	-0.05	90.00	0.092
#XAYMIT	8.271	8.532	3.2	8.442	0.107	90.00	90.14	0.14	89.97	0.165
#XAYMIT	26.110	25.391	-2.8	25.472	0.203	90.00	90.14	0.14	90.07	0.247
#YUYUPUD01	3.785	3.741	-1.2	3.718	0.028	90.00	89.93	-0.07	90.01	0.089
#YUYUPUD01	11.927	10.682	-10.4	11.082	0.388	91.62	93.28	1.66	94.78	1.560
#YUYUPUD01	14.597	14.380	-1.5	14.368	0.096	90.00	90.04	0.04	90.01	0.176
#ACANIL01	19.509	19.089	-2.2	19.059	0.104	90.00	90.12	0.12	90.03	0.156
#ACANIL01	9.364	9.381	0.2	9.439	0.044	90.00	90.01	0.01	89.97	0.131
#ACANIL01	7.778	7.747	-0.4	7.736	0.014	90.00	90.04	0.04	90.04	0.119
#ADIPAC07	7.187	7.361	2.4	7.276	0.047	90.00	89.66	-0.34	89.91	0.133
#ADIPAC07	5.163	5.009	-3.0	5.077	0.046	110.86	113.57	2.71	112.99	0.558
#ADIPAC07	10.015	10.241	2.3	10.175	0.064	90.00	89.98	-0.02	89.94	0.121
#ARCLAM01	8.206	8.151	-0.7	8.059	0.078	90.00	90.03	0.03	90.22	0.216
#ARCLAM01	5.748	5.051	-12.1	5.310	0.237	111.37	108.75	-2.62	108.02	0.882
#ARCLAM01	9.053	8.900	-1.7	8.859	0.064	90.00	89.85	-0.15	89.89	0.210
#AYOJED	5.901	5.557	-5.8	5.646	0.084	90.00	89.96	-0.04	90.04	0.113
#AYOJED	10.065	10.296	2.3	10.107	0.134	102.92	101.01	-1.91	102.54	1.024
#AYOJED	11.658	10.987	-5.8	11.174	0.190	90.00	89.97	-0.03	89.99	0.124
#BENZAC07	5.393	5.285	-2.0	5.312	0.035	90.00	90.08	0.08	89.98	0.074
#BENZAC07	5.003	4.902	-2.0	4.914	0.029	98.51	104.88	6.37	104.25	1.340
#BENZAC07	21.689	22.052	1.7	21.943	0.118	90.00	89.93	-0.07	89.99	0.090
#BIPHEN04	8.120	7.531	-7.3	7.688	0.179	90.00	90.26	0.26	90.16	0.223
#BIPHEN04	5.630	5.308	-5.7	5.352	0.105	95.10	86.94	-8.16	88.65	2.472
#BIPHEN04	9.510	9.307	-2.1	9.338	0.059	90.00	90.03	0.03	90.13	0.187
#BZAMID01	5.607	5.118	-8.7	5.270	0.153	90.00	90.14	0.14	89.92	0.198
#BZAMID01	5.046	5.150	2.1	5.095	0.056	90.66	81.40	-9.26	83.40	2.569
#BZAMID01	22.053	21.339	-3.2	21.373	0.264	90.00	89.91	-0.09	90.07	0.149
#DNBENZ14	14.069	14.817	5.3	14.566	0.201	90.00	104.07	14.07	96.22	5.166
#DNBENZ14	13.245	13.332	0.7	13.454	0.078	90.00	89.93	-0.07	89.93	0.213
#DNBENZ14	3.738	3.557	-4.8	3.576	0.073	90.00	90.05	0.05	90.10	0.144
#DNITBZ11	11.134	10.225	-8.2	10.524	0.309	90.00	90.03	0.03	89.92	0.145
#DNITBZ11	5.459	6.031	10.5	5.783	0.188	92.26	102.23	9.97	100.23	2.162
#DNITBZ11	5.681	5.597	-1.5	5.658	0.037	90.00	90.06	0.06	90.01	0.106
#EXODAW	5.604	5.422	-3.2	5.456	0.047	92.97	94.11	1.14	94.00	0.455
#EXODAW	6.117	6.098	-0.3	6.095	0.010	91.55	92.05	0.50	91.90	0.170
#EXODAW	7.840	7.704	-1.7	7.708	0.027	109.32	107.11	-2.21	107.35	0.612
#FAXTUU01	6.040	6.213	2.9	6.182	0.043	90.00	90.08	0.08	89.99	0.059
#FAXTUU01	10.157	9.861	-2.9	9.905	0.074	90.00	90.14	0.14	90.02	0.120
#FAXTUU01	15.549	15.590	0.3	15.575	0.019	90.00	90.01	0.01	89.98	0.101
#FOVQOX	9.524	9.179	-3.6	9.272	0.085	90.00	89.68	-0.32	90.02	0.164
#FOVQOX	11.006	10.990	-0.1	10.936	0.045	90.00	90.10	0.10	90.03	0.122
#FOVQOX	5.942	5.803	-2.3	5.797	0.033	90.00	89.95	-0.05	90.02	0.106
#GLURAC03	12.977	13.254	2.1	13.154	0.065	90.00	90.00	-0.00	90.02	0.105
#GLURAC03	4.748	4.579	-3.6	4.639	0.056	98.30	96.93	-1.37	97.27	0.340
#GLURAC03	9.696	9.813	1.2	9.821	0.032	90.00	89.92	-0.08	90.06	0.123
#HEPTAN02	4.116	4.178	1.5	4.169	0.015	78.11	78.36	0.25	78.15	0.332
#HEPTAN02	4.686	4.374	-6.7	4.424	0.078	81.79	83.77	1.98	83.50	0.506
#HEPTAN02	20.348	20.213	-0.7	20.218	0.036	74.25	77.38	3.13	76.69	1.173
#HEXANE01	4.131	4.171	1.0	4.167	0.013	83.40	82.32	-1.08	82.32	0.266
#HEXANE01	4.696	4.397	-6.4	4.450	0.083	87.26	89.02	1.76	88.79	0.365
#HEXANE01	8.539	8.563	0.3	8.554	0.020	75.17	77.72	2.55	76.92	1.116
#HITMUS	7.029	6.866	-2.3	6.865	0.036	90.00	89.97	-0.03	89.94	0.139
#HITMUS	8.586	8.446	-1.6	8.485	0.038	114.34	109.83	-4.51	110.78	1.347
#HITMUS	7.773	7.392	-4.9	7.478	0.120	90.00	89.99	-0.01	90.00	0.102
#JOHBUD	11.421	11.808	3.4	11.733	0.098	90.00	90.80	0.80	90.24	0.388
#JOHBUD	6.019	5.986	-0.5	6.002	0.021	104.62	109.10	4.48	107.82	1.744
#JOHBUD	10.177	10.730	5.4	10.656	0.158	90.00	89.58	-0.42	89.90	0.227
#MCINAM10	11.289	10.722	-5.0	10.833	0.162	90.00	89.75	-0.25	89.44	0.312
#MCINAM10	17.175	16.132	-6.1	16.321	0.316	90.00	90.02	0.02	89.75	0.404
#MCINAM10	9.528	9.758	2.4	9.714	0.083	90.00	90.06	0.06	90.00	0.128
#NITRBE01	3.801	3.582	-5.8	3.653	0.062	90.00	89.86	-0.14	90.05	0.148
#NITRBE01	11.615	11.063	-4.8	11.318	0.180	94.98	90.88	-4.10	88.89	1.642
#NITRBE01	12.984	13.918	7.2	13.452	0.289	90.00	89.92	-0.08	90.11	0.225
#OCTANE01	4.195	4.161	-0.8	4.170	0.007	85.11	84.17	-0.94	84.08	0.227
#OCTANE01	4.752	4.378	-7.9	4.434	0.102	83.77	85.37	1.60	85.08	0.392
#OCTANE01	10.998	10.980	-0.2	10.978	0.020	74.26	77.61	3.35	76.90	1.498
#PHBALD11	6.699	6.680	-0.3	6.679	0.008	90.00	90.12	0.12	89.98	0.142
#PHBALD11	13.555	13.697	1.0	13.600	0.063	112.87	119.04	6.17	119.39	1.608
#PHBALD11	7.144	6.733	-5.8	6.873	0.112	90.00	90.10	0.10	89.95	0.162

#QATTIO	5.014	4.945	-1.4	4.946	0.013	90.00	89.85	-0.15	90.09	0.154
#QATTIO	13.788	13.633	-1.1	13.660	0.028	107.27	107.46	0.19	107.40	0.160
#QATTIO	7.464	7.554	1.2	7.540	0.024	90.00	90.02	0.02	89.97	0.102
#QATTOU	5.323	5.323	-0.0	5.328	0.007	90.00	89.85	-0.15	89.90	0.150
#QATTOU	6.699	6.817	1.8	6.778	0.039	90.00	90.01	0.01	90.12	0.102
#QATTOU	17.040	16.696	-2.0	16.802	0.079	90.00	89.94	-0.06	90.05	0.128
#TEPHTH06	7.702	7.782	1.0	7.788	0.038	92.92	100.16	7.24	99.52	1.745
#TEPHTH06	6.346	6.514	2.7	6.425	0.063	107.91	107.01	-0.90	107.03	0.286
#TEPHTH06	3.668	3.445	-6.1	3.501	0.068	94.64	95.57	0.93	94.99	0.607
#XAYMEP	3.686	3.516	-4.6	3.536	0.047	102.43	99.03	-3.40	100.04	1.333
#XAYMEP	5.290	5.234	-1.1	5.227	0.024	92.78	101.17	8.39	99.86	2.170
#XAYMEP	9.470	9.098	-3.9	9.190	0.114	100.93	96.21	-4.72	96.11	1.206
#XOZBUK	9.037	9.356	3.5	9.316	0.069	90.00	90.08	0.08	89.99	0.078
#XOZBUK	5.201	5.281	1.5	5.255	0.021	97.58	91.71	-5.87	93.88	1.877
#XOZBUK	13.027	12.451	-4.4	12.642	0.165	90.00	90.01	0.01	89.94	0.127
#ZIVKOE '	6.547	6.845	4.6	6.747	0.093	107.48	110.15	2.67	107.55	1.474
#ZIVKOE '	7.057	6.149	-12.9	6.400	0.284	102.07	104.09	2.02	104.34	0.769
#ZIVKOE '	9.687	10.073	4.0	9.826	0.142	102.23	97.99	-4.24	98.58	0.984
#ZZZITY01	5.806	5.391	-7.2	5.545	0.132	90.00	90.04	0.04	90.03	0.102
#ZZZITY01	5.023	5.276	5.0	5.135	0.102	100.48	94.12	-6.36	96.00	1.947
#ZZZITY01	11.215	10.525	-6.2	10.688	0.201	90.00	90.04	0.04	90.11	0.099
#ZZZSPY01	10.516	9.900	-5.9	10.095	0.195	90.00	90.25	0.25	89.95	0.199
#ZZZSPY01	7.596	7.286	-4.1	7.315	0.100	90.00	90.16	0.16	90.04	0.113
#ZZZSPY01	16.868	16.809	-0.4	16.688	0.117	90.00	90.36	0.36	90.30	0.194

100 K runs, cell parameters, convergence tests last 2 Msteps

For each crystal: a, b, c, α,β,γ

start: 3 Mstep frame, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd	start	end	delt	aver	rmsd
#ABUMIT	3.590	3.588	-0.1	3.588	0.003	89.81	90.12	0.31	90.03	0.118
#ABUMIT	10.475	10.504	0.3	10.480	0.013	101.05	101.10	0.05	100.96	0.218
#ABUMIT	15.114	15.110	-0.0	15.121	0.017	89.97	89.99	0.02	89.99	0.074
#BENZENO7	7.304	7.439	1.8	7.372	0.042	89.83	89.92	0.08	89.99	0.199
#BENZENO7	9.212	9.199	-0.1	9.215	0.012	89.92	89.92	0.01	89.96	0.091
#BENZENO7	6.481	6.389	-1.4	6.431	0.031	89.88	89.68	-0.20	89.90	0.187
#BILNOZ01	9.795	9.782	-0.1	9.782	0.013	90.22	89.92	-0.30	89.99	0.186
#BILNOZ01	6.820	6.819	-0.0	6.819	0.006	90.48	90.82	0.34	90.59	0.127
#BILNOZ01	13.205	13.210	0.0	13.210	0.011	90.00	89.85	-0.14	90.00	0.135
#BNZQUI03	5.496	5.486	-0.2	5.494	0.010	90.34	92.79	2.45	90.99	0.835
#BNZQUI03	6.910	6.986	1.1	6.958	0.029	97.56	96.72	-0.84	97.24	0.324
#BNZQUI03	6.671	6.548	-1.8	6.607	0.044	89.49	87.11	-2.37	88.78	0.829
#BULVAL03	6.257	6.242	-0.2	6.242	0.005	89.96	90.11	0.15	90.04	0.063
#BULVAL03	20.938	20.907	-0.1	20.908	0.019	93.03	92.93	-0.10	92.92	0.082
#BULVAL03	10.351	10.385	0.3	10.364	0.013	90.34	89.96	-0.38	89.91	0.150
#CECGEX	4.598	4.608	0.2	4.604	0.005	90.06	90.05	-0.02	89.99	0.126
#CECGEX	7.179	7.143	-0.5	7.147	0.012	90.04	89.96	-0.08	89.97	0.111
#CECGEX	11.792	11.800	0.1	11.816	0.018	90.01	90.05	0.04	90.03	0.099
#CTCYDD	7.479	7.484	0.1	7.479	0.008	89.94	89.96	0.01	89.92	0.086
#CTCYDD	17.458	17.366	-0.5	17.393	0.034	115.61	115.62	0.02	115.54	0.094
#CTCYDD	8.641	8.673	0.4	8.657	0.011	90.06	89.74	-0.32	90.05	0.129
#DAZNAP	13.670	13.803	1.0	13.747	0.036	90.08	89.88	-0.20	90.02	0.080
#DAZNAP	10.152	10.171	0.2	10.135	0.015	91.26	92.53	1.27	91.81	0.432
#DAZNAP	8.673	8.574	-1.1	8.639	0.032	90.12	89.87	-0.25	90.05	0.116
#DCBDOX10	5.877	5.931	0.9	5.916	0.015	92.53	93.73	1.20	93.18	0.330
#DCBDOX10	6.537	6.470	-1.0	6.496	0.018	90.58	90.74	0.15	90.70	0.125
#DCBDOX10	24.795	24.774	-0.1	24.782	0.014	90.02	90.00	-0.02	90.03	0.190
#DCLBEN01	14.771	14.633	-0.9	14.685	0.051	90.15	89.91	-0.24	90.01	0.139
#DCLBEN01	5.645	5.701	1.0	5.680	0.015	111.53	109.60	-1.94	110.21	0.624
#DCLBEN01	3.591	3.508	-2.3	3.536	0.021	90.10	90.14	0.03	90.12	0.123
#DCLBEN02	7.413	7.398	-0.2	7.403	0.008	84.99	84.76	-0.23	84.70	0.149
#DCLBEN02	5.559	5.522	-0.7	5.515	0.016	113.01	111.71	-1.30	111.95	0.312
#DCLBEN02	3.625	3.603	-0.6	3.614	0.007	96.87	97.70	0.83	97.56	0.218
#DEZDUH	14.813	14.761	-0.3	14.781	0.017	89.99	90.03	0.04	90.00	0.089
#DEZDUH	5.777	5.781	0.1	5.783	0.005	90.03	89.73	-0.31	89.95	0.128
#DEZDUH	9.878	9.898	0.2	9.896	0.011	90.02	90.29	0.27	90.01	0.145
#DEZXEL	11.919	11.914	-0.0	11.912	0.005	89.98	89.93	-0.05	90.00	0.057
#DEZXEL	9.523	9.527	0.0	9.518	0.007	90.00	89.96	-0.03	90.02	0.069
#DEZXEL	7.172	7.161	-0.2	7.166	0.008	89.98	89.84	-0.14	89.97	0.082
#DITBOX	6.945	6.934	-0.2	6.931	0.012	89.98	89.85	-0.13	89.94	0.121
#DITBOX	6.327	6.338	0.2	6.341	0.006	104.00	104.25	0.25	104.12	0.110
#DITBOX	10.521	10.553	0.3	10.548	0.018	90.09	90.11	0.01	90.07	0.098
#EZURUM	10.243	10.217	-0.3	10.226	0.012	90.13	90.06	-0.08	90.04	0.074
#EZURUM	6.479	6.473	-0.1	6.473	0.006	95.91	95.89	-0.02	95.87	0.115
#EZURUM	12.519	12.520	0.0	12.514	0.011	90.08	90.00	-0.08	90.03	0.084
#FACGEV	5.725	5.810	1.5	5.777	0.032	89.97	90.17	0.20	90.20	0.247
#FACGEV	6.494	6.499	0.1	6.506	0.007	95.67	96.00	0.33	96.03	0.195
#FACGEV	6.647	6.567	-1.2	6.591	0.031	89.82	89.80	-0.01	89.96	0.129
#FACJAU	4.531	4.533	0.1	4.535	0.005	89.62	89.76	0.14	89.93	0.171
#FACJAU	10.498	10.514	0.2	10.498	0.011	103.87	104.00	0.13	103.84	0.091
#FACJAU	6.168	6.162	-0.1	6.152	0.013	90.30	90.10	-0.20	90.06	0.128
#FMANUL01	9.101	9.152	0.6	9.120	0.018	89.99	89.99	0.00	90.02	0.109
#FMANUL01	13.765	13.798	0.2	13.796	0.015	90.02	89.69	-0.33	89.95	0.149
#FMANUL01	6.282	6.225	-0.9	6.253	0.018	89.91	89.84	-0.07	89.98	0.130
#FOVNIN	7.658	7.658	-0.0	7.664	0.005	90.03	89.85	-0.19	90.01	0.123
#FOVNIN	11.246	11.239	-0.1	11.228	0.018	89.81	90.14	0.32	89.98	0.164
#FOVNIN	17.746	17.732	-0.1	17.757	0.022	89.97	90.09	0.11	90.07	0.158
#HAYYAH	7.675	7.665	-0.1	7.673	0.007	90.19	89.98	-0.21	89.97	0.110

#HAYYAH	13.737	13.752	0.1	13.758	0.013	109.78	109.71	-0.06	109.83	0.193
#HAYYAH	8.059	8.047	-0.2	8.056	0.005	90.13	89.79	-0.34	90.07	0.163
#HCLBNZ11	7.933	7.931	-0.0	7.932	0.005	89.82	90.00	0.17	89.90	0.144
#HCLBNZ11	3.550	3.549	-0.0	3.547	0.004	93.48	93.59	0.10	93.52	0.081
#HCLBNZ11	14.530	14.554	0.2	14.541	0.012	89.92	89.83	-0.09	89.99	0.087
#HOWBAW	5.209	5.194	-0.3	5.212	0.010	93.96	94.17	0.21	94.02	0.104
#HOWBAW	5.599	5.607	0.2	5.605	0.008	95.58	95.46	-0.12	95.54	0.108
#HOWBAW	7.669	7.674	0.1	7.651	0.011	108.89	108.98	0.09	108.97	0.088
#NAPHTA10	7.504	7.426	-1.0	7.457	0.020	89.99	90.04	0.06	90.02	0.082
#NAPHTA10	5.903	5.933	0.5	5.923	0.009	125.96	125.67	-0.30	125.72	0.167
#NAPHTA10	8.713	8.687	-0.3	8.684	0.014	89.98	89.97	-0.01	90.00	0.087
#NBORAN02	6.138	6.143	0.1	6.144	0.004	90.09	89.83	-0.25	89.97	0.138
#NBORAN02	9.604	9.593	-0.1	9.596	0.008	89.88	89.94	0.06	89.99	0.088
#NBORAN02	13.182	13.172	-0.1	13.176	0.010	90.06	90.05	-0.01	90.01	0.064
#PUGDEB	7.302	7.256	-0.6	7.259	0.014	90.29	89.96	-0.33	90.11	0.269
#PUGDEB	12.084	12.082	-0.0	12.090	0.009	112.57	108.82	-3.76	110.20	1.240
#PUGDEB	6.439	6.324	-1.8	6.367	0.038	89.86	89.91	0.06	89.92	0.086
#TCHLBZ03	3.643	3.665	0.6	3.651	0.010	89.81	89.95	0.14	89.97	0.086
#TCHLBZ03	13.217	13.271	0.4	13.267	0.018	90.02	90.15	0.13	89.97	0.113
#TCHLBZ03	13.022	12.908	-0.9	12.964	0.044	89.97	90.21	0.24	89.92	0.187
#TEPNIT11	3.572	3.565	-0.2	3.565	0.005	114.92	115.41	0.49	115.12	0.167
#TEPNIT11	6.377	6.438	0.9	6.405	0.018	83.53	83.30	-0.22	83.36	0.149
#TEPNIT11	7.026	7.004	-0.3	7.017	0.008	103.45	102.64	-0.82	103.13	0.272
#VACCEH	7.094	7.078	-0.2	7.077	0.009	90.06	89.87	-0.19	90.06	0.132
#VACCEH	6.826	6.862	0.5	6.834	0.015	89.92	89.82	-0.10	89.98	0.133
#VACCEH	9.594	9.557	-0.4	9.582	0.014	89.97	90.01	0.05	90.00	0.101
#XAYMIT	3.444	3.430	-0.4	3.440	0.005	90.11	89.95	-0.15	89.99	0.080
#XAYMIT	8.509	8.532	0.3	8.511	0.010	90.03	90.14	0.12	90.01	0.111
#XAYMIT	25.415	25.391	-0.1	25.400	0.021	89.89	90.14	0.25	90.24	0.201
#YUYUPUD01	3.705	3.741	1.0	3.733	0.014	89.87	89.93	0.06	89.99	0.079
#YUYUPUD01	10.919	10.682	-2.2	10.732	0.078	94.81	93.28	-1.53	93.49	0.505
#YUYUPUD01	14.257	14.380	0.9	14.355	0.045	90.06	90.04	-0.01	89.99	0.094
#ACANIL01	19.028	19.089	0.3	19.069	0.022	89.80	90.12	0.32	90.02	0.119
#ACANIL01	9.409	9.381	-0.3	9.404	0.020	90.06	90.01	-0.05	89.92	0.117
#ACANIL01	7.742	7.747	0.1	7.736	0.009	90.01	90.04	0.03	90.04	0.103
#ADIPAC07	7.314	7.361	0.6	7.319	0.019	89.95	89.66	-0.30	89.84	0.107
#ADIPAC07	5.063	5.009	-1.1	5.035	0.016	113.46	113.57	0.11	113.40	0.095
#ADIPAC07	10.230	10.241	0.1	10.226	0.010	90.05	89.98	-0.07	89.89	0.104
#ARCLAM01	8.006	8.151	1.8	8.088	0.047	90.01	90.03	0.02	90.05	0.089
#ARCLAM01	5.175	5.051	-2.4	5.087	0.035	107.64	108.75	1.11	108.35	0.358
#ARCLAM01	8.817	8.900	0.9	8.873	0.026	90.06	89.85	-0.21	89.93	0.140
#AYOJED	5.606	5.557	-0.9	5.579	0.015	89.92	89.96	0.04	90.04	0.091
#AYOJED	10.164	10.296	1.3	10.244	0.034	102.30	101.01	-1.29	101.56	0.310
#AYOJED	11.102	10.987	-1.0	11.017	0.027	89.99	89.97	-0.02	90.01	0.088
#BENZAC07	5.287	5.285	-0.0	5.285	0.006	89.98	90.08	0.10	89.99	0.068
#BENZAC07	4.898	4.902	0.1	4.905	0.007	104.68	104.88	0.20	104.75	0.119
#BENZAC07	21.985	22.052	0.3	22.028	0.022	90.04	89.93	-0.11	89.98	0.084
#BIPHEN04	7.571	7.531	-0.5	7.558	0.015	90.04	90.26	0.22	90.07	0.137
#BIPHEN04	5.271	5.308	0.7	5.289	0.012	87.54	86.94	-0.60	87.14	0.190
#BIPHEN04	9.311	9.307	-0.0	9.307	0.008	89.96	90.03	0.06	90.03	0.104
#BZAMID01	5.175	5.118	-1.1	5.142	0.019	89.83	90.14	0.31	89.99	0.123
#BZAMID01	5.135	5.150	0.3	5.144	0.004	81.61	81.40	-0.21	81.54	0.073
#BZAMID01	21.132	21.339	1.0	21.263	0.075	90.02	89.91	-0.11	89.96	0.092
#DNBENZ14	14.664	14.817	1.0	14.747	0.043	98.12	104.07	5.95	101.74	1.764
#DNBENZ14	13.522	13.332	-1.4	13.432	0.062	89.81	89.93	0.11	90.05	0.162
#DNBENZ14	3.501	3.557	1.6	3.532	0.019	90.11	90.05	-0.05	90.05	0.146
#DNITBZ11	10.327	10.225	-1.0	10.248	0.032	89.90	90.03	0.14	89.96	0.140
#DNITBZ11	5.869	6.031	2.8	5.966	0.048	100.81	102.23	1.42	101.63	0.415
#DNITBZ11	5.661	5.597	-1.1	5.620	0.023	90.04	90.06	0.02	89.99	0.086
#EXODAW	5.443	5.422	-0.4	5.429	0.007	94.18	94.11	-0.07	94.13	0.076
#EXODAW	6.094	6.098	0.1	6.096	0.007	92.06	92.05	-0.01	91.99	0.109
#EXODAW	7.705	7.704	-0.0	7.704	0.006	107.10	107.11	0.01	107.08	0.100
#FAXTUU01	6.210	6.213	0.0	6.206	0.005	89.98	90.08	0.10	89.99	0.055
#FAXTUU01	9.879	9.861	-0.2	9.868	0.008	90.12	90.14	0.02	90.00	0.097
#FAXTUU01	15.578	15.590	0.1	15.576	0.013	89.84	90.01	0.17	89.99	0.084
#FOVQOX	9.224	9.179	-0.5	9.199	0.022	89.94	89.68	-0.26	89.97	0.177
#FOVQOX	10.941	10.990	0.4	10.974	0.012	89.96	90.10	0.15	89.99	0.094
#FOVQOX	5.782	5.803	0.4	5.789	0.006	90.02	89.95	-0.07	90.01	0.068
#GLURAC03	13.189	13.254	0.5	13.214	0.024	89.86	90.00	0.14	90.04	0.095
#GLURAC03	4.601	4.579	-0.5	4.587	0.009	97.15	96.93	-0.21	96.98	0.100
#GLURAC03	9.837	9.813	-0.2	9.839	0.011	90.13	89.92	-0.21	90.09	0.118
#HEPTAN02	4.180	4.178	-0.0	4.178	0.005	78.22	78.36	0.14	78.29	0.135
#HEPTAN02	4.389	4.374	-0.4	4.384	0.006	83.70	83.77	0.07	83.75	0.133
#HEPTAN02	20.192	20.213	0.1	20.223	0.029	77.04	77.38	0.34	77.34	0.143
#HEXANE01	4.176	4.171	-0.1	4.172	0.005	81.94	82.32	0.39	82.25	0.139
#HEXANE01	4.402	4.397	-0.1	4.402	0.006	89.08	89.02	-0.06	88.99	0.099
#HEXANE01	8.557	8.563	0.1	8.561	0.006	77.57	77.72	0.15	77.67	0.114
#HITMUS	6.857	6.866	0.1	6.855	0.008	89.92	89.97	0.05	89.96	0.116
#HITMUS	8.465	8.446	-0.2	8.461	0.009	109.95	109.83	-0.12	109.97	0.102
#HITMUS	7.407	7.392	-0.2	7.397	0.007	89.82	89.99	0.17	89.98	0.115
#JOHBUD	11.814	11.808	-0.1	11.799	0.012	90.12	90.80	0.69	90.53	0.368
#JOHBUD	5.981	5.986	0.1	5.988	0.003	109.00	109.10	0.10	109.03	0.157
#JOHBUD	10.746	10.730	-0.2	10.746	0.010	90.25	89.58	-0.68	89.83	0.257
#MCINAM10	10.722	10.722	0.0	10.719	0.009	89.37	89.75	0.37	89.60	0.167
#MCINAM10	16.125	16.132	0.0	16.120	0.016	89.81	90.02	0.21	89.93	0.166
#MCINAM10	9.774	9.758	-0.2	9.773	0.007	89.91	90.06	0.15	90.04	0.092
#NITRBE01	3.620	3.582	-1.0	3.604	0.013	90.18	89.86	-0.32	90.11	0.142
#NITRBE01	11.218	11.063	-1.4	11.140	0.067	87.95	90.88	2.93	89.20	0.956
#NITRBE01	13.606	13.918	2.3	13.744	0.108	90.24	89.92	-0.32	90.19	0.268
#OCTANE01	4.176	4.161	-0.4	4.168	0.006	83.93	84.17	0.24	84.01	0.116

#OCTANE01	4.381	4.378	-0.1	4.378	0.003	85.28	85.37	0.09	85.28	0.122
#OCTANE01	11.000	10.980	-0.2	10.992	0.009	77.91	77.61	-0.30	77.80	0.130
#PHBALD11	6.687	6.680	-0.1	6.679	0.006	90.11	90.12	0.01	90.03	0.135
#PHBALD11	13.603	13.697	0.7	13.665	0.030	119.92	119.04	-0.88	119.51	0.237
#PHBALD11	6.816	6.733	-1.2	6.772	0.022	90.06	90.10	0.04	89.99	0.082
#QATTIO	4.937	4.945	0.2	4.941	0.003	90.05	89.85	-0.19	90.02	0.162
#QATTIO	13.652	13.633	-0.1	13.652	0.012	107.36	107.46	0.09	107.50	0.126
#QATTIO	7.546	7.554	0.1	7.554	0.007	89.97	90.02	0.05	89.97	0.062
#QATTOU	5.323	5.323	0.0	5.324	0.007	89.90	89.85	-0.04	89.77	0.118
#QATTOU	6.801	6.817	0.2	6.815	0.011	90.08	90.01	-0.07	90.11	0.123
#QATTOU	16.788	16.696	-0.5	16.731	0.034	89.87	89.94	0.06	90.06	0.093
#TEPHTH06	7.828	7.782	-0.6	7.796	0.024	99.89	100.16	0.27	100.03	0.279
#TEPHTH06	6.447	6.514	1.0	6.489	0.023	107.31	107.01	-0.30	107.22	0.133
#TEPHTH06	3.452	3.445	-0.2	3.453	0.006	95.49	95.57	0.07	95.49	0.082
#XAYMEP	3.521	3.516	-0.1	3.516	0.006	99.14	99.03	-0.11	99.26	0.125
#XAYMEP	5.203	5.234	0.6	5.228	0.011	100.94	101.17	0.22	101.14	0.133
#XAYMEP	9.128	9.098	-0.3	9.117	0.012	95.63	96.21	0.58	95.88	0.263
#XOZBUK	9.365	9.356	-0.1	9.360	0.005	89.93	90.08	0.15	89.98	0.079
#XOZBUK	5.258	5.281	0.4	5.271	0.007	92.58	91.71	-0.87	92.13	0.291
#XOZBUK	12.572	12.451	-1.0	12.510	0.043	90.02	90.01	-0.00	89.99	0.125
#ZIVKOE '	6.813	6.845	0.5	6.835	0.009	107.96	110.15	2.18	109.07	0.700
#ZIVKOE '	6.223	6.149	-1.2	6.160	0.028	104.50	104.09	-0.42	104.22	0.167
#ZIVKOE '	9.847	10.073	2.3	9.972	0.081	97.98	97.99	0.01	98.15	0.178
#ZZZITY01	5.457	5.391	-1.2	5.425	0.025	89.97	90.04	0.06	90.04	0.079
#ZZZITY01	5.194	5.276	1.6	5.239	0.030	94.71	94.12	-0.59	94.40	0.258
#ZZZITY01	10.545	10.525	-0.2	10.533	0.012	90.19	90.04	-0.15	90.12	0.080
#ZZZSPY01	9.966	9.900	-0.7	9.916	0.019	90.14	90.25	0.11	90.01	0.170
#ZZZSPY01	7.247	7.286	0.5	7.274	0.010	90.21	90.16	-0.06	90.09	0.103
#ZZZSPY01	16.682	16.809	0.8	16.779	0.037	90.50	90.36	-0.14	90.33	0.140

100 K runs, density, complete runs
start: experimental crystal structure, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd
#ABUMIT	1.535	1.748	13.83	1.715	0.0603
#BENZEN07	1.097	1.187	8.21	1.176	0.0237
#BILNOZ01	1.262	1.287	1.98	1.286	0.0049
#BNZQUI03	1.366	1.444	5.70	1.421	0.0200
#BULVAL03	1.250	1.278	2.20	1.278	0.0068
#CECGEX	1.349	1.370	1.50	1.364	0.0084
#CTCYDD	1.645	1.765	7.24	1.754	0.0259
#DAZNAP	1.288	1.438	11.63	1.414	0.0417
#DCBDOX10	1.603	1.772	10.55	1.740	0.0454
#DCLBEN01	1.523	1.771	16.31	1.716	0.0656
#DCLBEN02	1.545	1.803	16.70	1.756	0.0694
#DEZDUH	1.770	1.700	-3.95	1.702	0.0161
#DEZXEL	1.669	1.782	6.76	1.769	0.0295
#DITBOX	1.208	1.332	10.28	1.308	0.0350
#EZURUM	1.385	1.401	1.12	1.399	0.0029
#FACGEV	1.420	1.537	8.24	1.522	0.0321
#FACJAU	1.796	1.749	-2.64	1.753	0.0092
#FMANUL01	1.409	1.506	6.84	1.490	0.0240
#FOVNIN	1.815	1.934	6.55	1.923	0.0246
#HAYYAH	1.218	1.300	6.68	1.290	0.0160
#HCLBNZ11	2.069	2.314	11.85	2.275	0.0708
#HOWBAW	1.303	1.336	2.51	1.333	0.0073
#NAPHTA10	1.198	1.369	14.25	1.342	0.0413
#NBORAN02	1.442	1.405	-2.56	1.406	0.0072
#PUGDEB	1.569	1.672	6.53	1.657	0.0303
#TCHLBZ03	1.736	1.920	10.61	1.893	0.0508
#TEPNIT11	1.285	1.503	16.95	1.466	0.0643
#VACCEH	1.060	1.147	8.19	1.141	0.0202
#XAYMIT	1.490	1.628	9.29	1.610	0.0344
#YUYPUD01	1.292	1.484	14.82	1.445	0.0566
#ACANIL01	1.264	1.294	2.42	1.290	0.0064
#ADIPAC07	1.398	1.402	0.32	1.403	0.0023
#ARCLAM01	1.187	1.361	14.59	1.313	0.0616
#AYOJED	1.143	1.250	9.36	1.241	0.0256
#BENZAC07	1.402	1.469	4.81	1.462	0.0171
#BIPHEN04	1.183	1.379	16.57	1.337	0.0623
#BZAMID01	1.290	1.447	12.17	1.415	0.0471
#DNBENZ14	1.603	1.638	2.20	1.610	0.0211
#DNITBZ11	1.618	1.655	2.30	1.650	0.0129
#EXODAW	1.530	1.597	4.37	1.589	0.0149
#FAXTUU01	1.800	1.798	-0.13	1.801	0.0031
#FOVQOX	1.324	1.409	6.40	1.403	0.0192
#GLURAC03	1.484	1.484	-0.01	1.476	0.0072
#HEPTAN02	0.904	0.945	4.50	0.940	0.0079
#HEXANE01	0.900	0.941	4.59	0.935	0.0092
#HITMUS	1.353	1.435	6.01	1.421	0.0214
#JOHBUD	1.551	1.466	-5.54	1.471	0.0196
#MCINAM10	1.159	1.269	9.45	1.248	0.0311
#NITRBE01	1.432	1.483	3.56	1.472	0.0177
#OCTANE01	0.906	0.978	7.95	0.967	0.0152
#PHBALD11	1.357	1.506	10.98	1.493	0.0364
#QATTIO	1.215	1.232	1.43	1.231	0.0029
#QATTOU	1.138	1.142	0.30	1.140	0.0016
#TEPHTH06	1.628	1.700	4.41	1.690	0.0233
#XAYMEP	1.490	1.636	9.80	1.612	0.0425

#XOZBUK	1.522	1.503	-1.30	1.497	0.0050
#ZIVKOE '	1.450	1.545	6.58	1.524	0.0364
###ZZZITY01	1.096	1.181	7.73	1.167	0.0244
###ZZZSPY01	1.047	1.163	11.13	1.145	0.0336

100 K runs, density, convergence test last 2 Mstep
start: 3 Mstep frame, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd
#ABUMIT	1.750	1.748	-0.16	1.749	0.0020
#BENZEN07	1.190	1.187	-0.27	1.188	0.0020
#BILNOZ01	1.285	1.287	0.11	1.287	0.0018
#BNZQUI03	1.430	1.444	0.99	1.434	0.0054
#BULVAL03	1.277	1.278	0.04	1.280	0.0019
#CECGEX	1.367	1.370	0.22	1.368	0.0020
#CTCYDD	1.763	1.765	0.11	1.765	0.0023
#DAZNAP	1.437	1.438	0.06	1.437	0.0016
#DCBDOX10	1.767	1.772	0.32	1.768	0.0021
#DCLBEN01	1.753	1.771	1.04	1.764	0.0051
#DCLBEN02	1.790	1.803	0.73	1.801	0.0035
#DEZDUH	1.698	1.700	0.10	1.697	0.0024
#DEZZEL	1.779	1.782	0.15	1.783	0.0022
#DITBOX	1.335	1.332	-0.22	1.331	0.0018
#EZURUM	1.396	1.401	0.34	1.400	0.0018
#FACGEV	1.541	1.537	-0.27	1.538	0.0033
#FACJAU	1.750	1.749	-0.06	1.753	0.0030
#FMANUL01	1.504	1.506	0.13	1.504	0.0017
#FOVNIN	1.931	1.934	0.15	1.931	0.0027
#HAYYAH	1.298	1.300	0.13	1.297	0.0019
#HCLBNZ11	2.315	2.314	-0.08	2.316	0.0022
#HOWBAW	1.334	1.336	0.15	1.336	0.0016
#NAPHTA10	1.363	1.369	0.45	1.367	0.0022
#NBOBAN02	1.403	1.405	0.10	1.404	0.0017
#PUGDEB	1.672	1.672	-0.03	1.674	0.0037
#TCHLBZ03	1.922	1.920	-0.12	1.920	0.0024
#TEPNIT11	1.508	1.503	-0.34	1.506	0.0019
#VACCEH	1.146	1.147	0.09	1.149	0.0019
#XAYMIT	1.625	1.628	0.21	1.627	0.0018
#YUYPU01	1.481	1.484	0.18	1.483	0.0018
#ACANIL01	1.296	1.294	-0.09	1.294	0.0018
#ADIPAC07	1.397	1.402	0.41	1.403	0.0025
#ARCLAM01	1.356	1.361	0.32	1.363	0.0024
#AYOJED	1.249	1.250	0.14	1.251	0.0016
#BENZAC07	1.473	1.469	-0.26	1.469	0.0018
#BIPHEN04	1.380	1.379	-0.07	1.378	0.0011
#BZAMID01	1.448	1.447	-0.13	1.446	0.0013
#DNBENZ14	1.625	1.638	0.83	1.631	0.0048
#DNITBZ11	1.657	1.655	-0.08	1.659	0.0030
#EXODAW	1.592	1.597	0.33	1.595	0.0026
#FAXTUU01	1.797	1.798	0.05	1.800	0.0019
#FOVQOX	1.413	1.409	-0.31	1.411	0.0028
#GLURAC03	1.482	1.484	0.17	1.482	0.0016
#HEPTAN02	0.944	0.945	0.12	0.943	0.0016
#HEXANE01	0.941	0.941	0.01	0.940	0.0013
#HITMUS	1.431	1.435	0.23	1.434	0.0023
#JOHBUD	1.463	1.466	0.19	1.464	0.0019
#MCINAM10	1.267	1.269	0.11	1.268	0.0016
#NITRBE01	1.481	1.483	0.10	1.483	0.0032
#OCTANE01	0.971	0.978	0.67	0.975	0.0016
#PHBALD11	1.510	1.506	-0.23	1.508	0.0020
#QATTIO	1.233	1.232	-0.09	1.232	0.0011
#QATTOU	1.138	1.142	0.32	1.140	0.0015
#TEPPTH06	1.705	1.700	-0.29	1.700	0.0021
#XAYMEP	1.635	1.636	0.07	1.634	0.0027
#XOZBUK	1.494	1.503	0.56	1.498	0.0030
#ZIVKOE '	1.547	1.545	-0.15	1.550	0.0026
###ZZZITY01	1.184	1.181	-0.22	1.181	0.0017
###ZZZSPY01	1.171	1.163	-0.63	1.165	0.0021

100 K runs, energies, complete runs
for each crystal: intramolecular, LP, Coulombic, total lattice energy
start: experimental crystal structure, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd	
#ABUMIT	0.00	0.00	0.00	0.00	0.0000	intram
#ABUMIT	-61.46	-68.90	-7.44	-67.78	2.1015	LP
#ABUMIT	-2.72	-3.32	-0.60	-3.31	0.1454	Coulombic
#ABUMIT	-64.18	-72.21	-8.03	-71.09	2.2167	Total
#BENZEN07	0.00	0.00	0.00	0.00	0.0000	
#BENZEN07	-43.51	-43.56	-0.06	-43.35	0.4552	
#BENZEN07	-7.29	-8.45	-1.16	-8.32	0.2643	
#BENZEN07	-50.80	-52.01	-1.21	-51.67	0.6827	
#BILNOZ01	0.00	0.00	0.00	0.00	0.0000	
#BILNOZ01	-68.73	-67.94	0.78	-67.84	0.2048	
#BILNOZ01	-3.20	-3.19	0.01	-3.19	0.0111	
#BILNOZ01	-71.92	-71.13	0.79	-71.03	0.2008	
#BNZQUI03	0.00	0.00	0.00	0.00	0.0000	

#BNZQUI03	-33.83	-49.01	-15.18	-47.30	2.0480
#BNZQUI03	-31.68	-28.22	3.46	-29.25	0.5720
#BNZQUI03	-65.51	-77.23	-11.72	-76.55	1.6903
#BULVAL03	0.00	0.00	0.00	0.00	0.0000
#BULVAL03	-64.53	-63.46	1.07	-63.55	0.2213
#BULVAL03	-6.03	-8.06	-2.03	-7.87	0.5122
#BULVAL03	-70.56	-71.52	-0.96	-71.43	0.5765
#CECGEX	0.00	0.00	0.00	0.00	0.0000
#CECGEX	-61.42	-65.74	-4.32	-65.20	0.8095
#CECGEX	-34.14	-34.18	-0.03	-34.08	0.4128
#CECGEX	-95.56	-99.91	-4.35	-99.28	1.0873
#CTCYDD	0.00	0.00	0.00	0.00	0.0000
#CTCYDD	-85.75	-89.65	-3.90	-89.07	1.0941
#CTCYDD	-2.52	-2.14	0.38	-2.26	0.1567
#CTCYDD	-88.26	-91.79	-3.53	-91.33	0.9682
#DAZNAP	0.00	0.00	0.00	0.00	0.0000
#DAZNAP	-63.65	-71.55	-7.90	-70.70	1.5868
#DAZNAP	-21.58	-22.25	-0.67	-21.99	0.6465
#DAZNAP	-85.23	-93.80	-8.58	-92.69	2.1440
#DCBDOX10	0.00	0.00	0.00	0.00	0.0000
#DCBDOX10	-110.93	-119.15	-8.21	-117.77	2.3928
#DCBDOX10	0.12	-2.01	-2.13	-1.31	0.6986
#DCBDOX10	-110.82	-121.16	-10.34	-119.07	3.0386
#DCLBEN01	0.00	0.00	0.00	0.00	0.0000
#DCLBEN01	-62.14	-71.30	-9.16	-68.87	2.9080
#DCLBEN01	-2.69	-2.79	-0.10	-2.90	0.0973
#DCLBEN01	-64.83	-74.09	-9.26	-71.77	2.8853
#DCLBEN02	0.00	0.00	0.00	0.00	0.0000
#DCLBEN02	-62.61	-73.62	-11.00	-71.39	3.1785
#DCLBEN02	-3.09	-3.59	-0.49	-3.62	0.1654
#DCLBEN02	-65.71	-77.20	-11.50	-75.00	3.2847
#DEZDUH	0.00	0.00	0.00	0.00	0.0000
#DEZDUH	-49.59	-49.33	0.26	-49.17	0.2807
#DEZDUH	-16.96	-16.68	0.28	-16.73	0.0787
#DEZDUH	-66.55	-66.01	0.54	-65.91	0.2467
#DEZXEL	0.00	0.00	0.00	0.00	0.0000
#DEZXEL	-77.90	-87.94	-10.05	-87.49	1.4400
#DEZXEL	-17.44	-17.42	0.02	-17.19	0.5307
#DEZXEL	-95.34	-105.36	-10.03	-104.68	1.6670
#DITBOX	0.00	0.00	0.00	0.00	0.0000
#DITBOX	-83.25	-90.97	-7.71	-89.35	2.5682
#DITBOX	-8.00	-8.60	-0.60	-8.60	0.1144
#DITBOX	-91.25	-99.57	-8.32	-97.95	2.6225
#EZURUM	0.00	0.00	0.00	0.00	0.0000
#EZURUM	-68.39	-71.78	-3.40	-71.72	0.4806
#EZURUM	-23.20	-21.09	2.10	-21.09	0.3078
#EZURUM	-91.59	-92.88	-1.29	-92.81	0.1930
#FACGEV	0.00	0.00	0.00	0.00	0.0000
#FACGEV	-41.44	-46.15	-4.71	-45.69	0.8851
#FACGEV	-6.41	-6.12	0.29	-5.89	0.3523
#FACGEV	-47.85	-52.26	-4.41	-51.58	1.1113
#FACJAU	0.00	0.00	0.00	0.00	0.0000
#FACJAU	-40.53	-42.52	-1.99	-42.52	0.4043
#FACJAU	-11.22	-11.19	0.03	-11.15	0.1387
#FACJAU	-51.75	-53.72	-1.96	-53.67	0.3531
#FMANUL01	0.00	0.00	0.00	0.00	0.0000
#FMANUL01	-67.36	-73.24	-5.88	-72.15	1.3585
#FMANUL01	-10.52	-10.43	0.09	-10.37	0.1942
#FMANUL01	-77.88	-83.66	-5.79	-82.52	1.5135
#FOVNIN	0.00	0.00	0.00	0.00	0.0000
#FOVNIN	-98.56	-102.14	-3.58	-101.85	0.8887
#FOVNIN	-3.20	-3.84	-0.64	-3.74	0.1465
#FOVNIN	-101.76	-105.97	-4.21	-105.59	1.0233
#HAYYAH	0.00	0.00	0.00	0.00	0.0000
#HAYYAH	-75.39	-76.20	-0.81	-76.10	0.3388
#HAYYAH	-7.00	-8.58	-1.58	-8.40	0.3031
#HAYYAH	-82.39	-84.78	-2.39	-84.49	0.5944
#HCLBNZ11	0.00	0.00	0.00	0.00	0.0000
#HCLBNZ11	-100.01	-110.12	-10.11	-108.27	3.0313
#HCLBNZ11	7.31	9.16	1.85	8.48	0.9188
#HCLBNZ11	-92.70	-100.96	-8.26	-99.79	2.2155
#HOWBAW	0.00	0.00	0.00	0.00	0.0000
#HOWBAW	-81.31	-81.44	-0.13	-81.08	0.3160
#HOWBAW	-10.78	-11.22	-0.44	-11.23	0.1459
#HOWBAW	-92.08	-92.66	-0.57	-92.31	0.4036
#NAPHTA10	0.00	0.00	0.00	0.00	0.0000
#NAPHTA10	-68.97	-77.56	-8.59	-76.01	2.2930
#NAPHTA10	-7.63	-8.61	-0.98	-8.68	0.3170
#NAPHTA10	-76.60	-86.17	-9.57	-84.70	2.5274
#NBORAN02	0.00	0.00	0.00	0.00	0.0000
#NBORAN02	-63.64	-62.43	1.20	-62.78	0.2057
#NBORAN02	-33.76	-34.24	-0.48	-33.77	0.3066
#NBORAN02	-97.39	-96.68	0.72	-96.55	0.2301
#PUGDEB	0.00	0.00	0.00	0.00	0.0000
#PUGDEB	-42.93	-48.59	-5.66	-47.66	1.4669
#PUGDEB	-6.70	-7.79	-1.10	-7.57	0.2448
#PUGDEB	-49.63	-56.38	-6.75	-55.23	1.6806
#TCHLBZ03	0.00	0.00	0.00	0.00	0.0000
#TCHLBZ03	-76.88	-82.05	-5.17	-81.48	1.4727
#TCHLBZ03	1.00	0.55	-0.45	0.76	0.1894

#TCHLBZ03	-75.89	-81.51	-5.62	-80.72	1.5928
#TEPNIT11	0.00	0.00	0.00	0.00	0.0000
#TEPNIT11	-62.73	-74.90	-12.16	-73.37	3.0798
#TEPNIT11	-30.42	-31.99	-1.57	-31.29	0.9090
#TEPNIT11	-93.15	-106.89	-13.74	-104.66	3.8703
#VACCEH	0.00	0.00	0.00	0.00	0.0000
#VACCEH	-47.31	-47.94	-0.63	-47.91	0.3973
#VACCEH	-4.84	-6.83	-1.98	-6.69	0.3312
#VACCEH	-52.15	-54.77	-2.62	-54.60	0.6779
#XAYMIT	0.00	0.00	0.00	0.00	0.0000
#XAYMIT	-93.28	-105.28	-12.01	-104.00	2.2680
#XAYMIT	-16.76	-15.59	1.17	-15.85	0.3461
#XAYMIT	-110.03	-120.87	-10.83	-119.85	2.1586
#YUYPUD01	0.00	0.00	0.00	0.00	0.0000
#YUYPUD01	-63.68	-71.65	-7.97	-70.48	1.9207
#YUYPUD01	-26.76	-31.03	-4.27	-30.14	0.9694
#YUYPUD01	-90.45	-102.69	-12.24	-100.62	2.8141
#ACANIL01	14.71	3.05	-11.66	3.76	1.8311
#ACANIL01	-69.73	-72.54	-2.81	-72.48	0.4123
#ACANIL01	-37.88	-36.19	1.70	-36.39	0.3678
#ACANIL01	-92.91	-105.68	-12.77	-105.11	1.9129
#ADIPAC07	1.12	3.13	2.01	3.01	0.2851
#ADIPAC07	-78.80	-89.45	-10.66	-88.83	1.4246
#ADIPAC07	-47.32	-46.65	0.67	-46.86	0.2247
#ADIPAC07	-124.99	-132.97	-7.97	-132.68	1.0902
#ARCLAM01	0.72	2.07	1.34	1.90	0.2276
#ARCLAM01	-33.55	-51.72	-18.18	-49.63	2.9703
#ARCLAM01	-39.43	-33.87	5.56	-33.84	0.8834
#ARCLAM01	-72.26	-83.53	-11.27	-81.58	2.4788
#AYOJED	0.14	0.12	-0.02	0.13	0.0041
#AYOJED	-63.01	-67.16	-4.15	-66.67	0.8778
#AYOJED	-5.40	-5.89	-0.49	-5.85	0.2596
#AYOJED	-68.26	-72.93	-4.67	-72.38	1.1198
#BENZAC07	4.31	1.29	-3.02	1.36	0.4347
#BENZAC07	-53.82	-66.29	-12.47	-65.88	1.7764
#BENZAC07	-28.90	-23.64	5.25	-23.75	0.7304
#BENZAC07	-78.40	-88.64	-10.24	-88.26	1.5106
#BIPHEN04	5.99	5.88	-0.11	5.68	0.3330
#BIPHEN04	-77.14	-89.43	-12.29	-86.73	4.1693
#BIPHEN04	-10.75	-12.77	-2.02	-12.32	0.7496
#BIPHEN04	-81.91	-96.32	-14.41	-93.38	4.6241
#BZAMID01	4.58	2.16	-2.42	2.28	0.3553
#BZAMID01	-63.19	-73.09	-9.90	-71.68	2.2259
#BZAMID01	-33.45	-33.40	0.06	-32.92	0.4985
#BZAMID01	-92.07	-104.32	-12.25	-102.33	2.8248
#DNBENZ14	0.38	0.38	-0.00	0.50	0.1196
#DNBENZ14	-64.94	-72.26	-7.33	-70.20	2.1805
#DNBENZ14	-17.60	-13.64	3.96	-14.37	1.1166
#DNBENZ14	-82.15	-85.52	-3.37	-84.07	1.2180
#DNITBZ11	0.22	0.15	-0.07	0.17	0.0509
#DNITBZ11	-64.35	-72.77	-8.41	-71.82	1.5987
#DNITBZ11	-22.25	-20.44	1.80	-20.28	0.4136
#DNITBZ11	-86.38	-93.06	-6.68	-91.93	1.6098
#EXODAW	19.45	0.84	-18.61	1.35	2.6548
#EXODAW	-83.96	-87.24	-3.28	-86.77	0.5741
#EXODAW	-29.58	-29.05	0.53	-29.12	0.1804
#EXODAW	-94.09	-115.45	-21.36	-114.54	3.0380
#FAXTUU01	0.00	0.34	0.34	0.34	0.0620
#FAXTUU01	-84.09	-86.38	-2.29	-86.44	0.3568
#FAXTUU01	-28.55	-28.03	0.52	-27.95	0.2026
#FAXTUU01	-112.63	-114.06	-1.43	-114.05	0.3577
#FOVQOX	5.59	6.16	0.56	6.20	0.1261
#FOVQOX	-73.90	-73.47	0.43	-73.18	0.2322
#FOVQOX	-60.18	-62.84	-2.66	-62.85	0.5809
#FOVQOX	-128.48	-130.15	-1.67	-129.83	0.5323
#GLURAC03	14.77	6.36	-8.41	6.64	1.2518
#GLURAC03	-74.90	-82.33	-7.42	-81.78	1.0036
#GLURAC03	-62.68	-55.00	7.68	-55.20	1.0713
#GLURAC03	-122.82	-130.97	-8.16	-130.35	1.1728
#HEPTAN02	0.10	1.54	1.43	1.59	0.2347
#HEPTAN02	-64.53	-64.89	-0.36	-64.54	0.5016
#HEPTAN02	0.70	0.41	-0.29	0.38	0.0598
#HEPTAN02	-63.73	-62.95	0.78	-62.57	0.4511
#HEXANE01	0.08	1.46	1.38	1.40	0.2246
#HEXANE01	-57.94	-57.88	0.06	-57.58	0.4660
#HEXANE01	0.70	0.21	-0.49	0.21	0.0783
#HEXANE01	-57.16	-56.21	0.95	-55.97	0.4268
#HITMUS	0.51	1.52	1.01	1.39	0.1925
#HITMUS	-67.72	-75.78	-8.06	-74.95	1.4225
#HITMUS	-34.32	-31.88	2.44	-32.08	0.3495
#HITMUS	-101.53	-106.14	-4.61	-105.63	0.9599
#JOHBUD	1.26	1.13	-0.13	1.17	0.0461
#JOHBUD	-47.76	-54.67	-6.91	-53.79	1.4854
#JOHBUD	-29.79	-24.46	5.33	-25.15	1.0589
#JOHBUD	-76.29	-78.01	-1.71	-77.77	0.4997
#MCINAM10	18.03	5.05	-12.98	5.43	1.8903
#MCINAM10	-62.89	-81.50	-18.61	-79.18	3.6766
#MCINAM10	-26.08	-22.19	3.89	-22.97	0.9330
#MCINAM10	-70.93	-98.64	-27.70	-96.72	4.4404
#NITRBE01	0.00	0.10	0.09	0.08	0.0200

#NITRBE01	-57.21	-60.62	-3.40	-59.55	1.0221
#NITRBE01	-11.86	-12.50	-0.64	-12.73	0.2534
#NITRBE01	-69.07	-73.02	-3.95	-72.20	1.0336
#OCTANE01	0.13	1.81	1.68	1.79	0.2598
#OCTANE01	-72.58	-75.15	-2.57	-74.47	1.0164
#OCTANE01	0.97	0.58	-0.39	0.49	0.1058
#OCTANE01	-71.48	-72.76	-1.28	-72.18	0.8712
#PHBALD11	2.08	1.22	-0.86	1.23	0.1337
#PHBALD11	-61.81	-71.10	-9.29	-70.26	1.6065
#PHBALD11	-43.60	-42.67	0.93	-43.05	0.3439
#PHBALD11	-103.32	-112.55	-9.23	-112.08	1.8023
#QATTIO	4.45	3.37	-1.07	3.41	0.1660
#QATTIO	-62.60	-57.68	4.92	-58.01	0.7476
#QATTIO	-58.55	-64.61	-6.06	-64.28	1.0048
#QATTIO	-116.71	-118.92	-2.21	-118.87	0.3735
#QATTOU	8.95	9.08	0.13	9.17	0.1001
#QATTOU	-61.96	-59.12	2.85	-59.11	0.4456
#QATTOU	-60.51	-62.31	-1.80	-62.18	0.2988
#QATTOU	-113.52	-112.35	1.18	-112.12	0.2572
#TEPHTH06	11.27	2.25	-9.03	2.52	1.2759
#TEPHTH06	-78.89	-97.92	-19.03	-96.66	2.9737
#TEPHTH06	-62.02	-52.41	9.61	-52.61	1.3439
#TEPHTH06	-129.64	-148.08	-18.44	-146.75	2.9842
#XAYMEP	0.00	0.09	0.09	0.10	0.0287
#XAYMEP	-84.82	-95.20	-10.38	-93.87	2.4081
#XAYMEP	-10.35	-11.53	-1.17	-11.55	0.3702
#XAYMEP	-95.17	-106.63	-11.46	-105.32	2.7260
#XOZBUK	-0.13	0.66	0.79	0.60	0.1228
#XOZBUK	-59.73	-63.88	-4.15	-63.26	0.7409
#XOZBUK	-27.54	-27.92	-0.38	-28.03	0.1868
#XOZBUK	-87.39	-91.14	-3.75	-90.69	0.6511
#ZIVKOE '	1.73	1.56	-0.17	1.47	0.1704
#ZIVKOE '	-71.73	-86.25	-14.52	-84.34	2.9269
#ZIVKOE '	-35.83	-35.13	0.70	-34.55	0.8214
#ZIVKOE '	-105.83	-119.82	-13.99	-117.42	3.3759
#ZZZITY01	0.00	0.09	0.09	0.10	0.0230
#ZZZITY01	-56.72	-62.64	-5.92	-61.97	1.5007
#ZZZITY01	-3.84	-7.28	-3.43	-6.63	0.8858
#ZZZITY01	-60.56	-69.82	-9.27	-68.51	2.3611
#ZZZSPY01	0.00	0.16	0.16	0.15	0.0281
#ZZZSPY01	-58.03	-61.95	-3.93	-61.29	1.3197
#ZZZSPY01	-3.61	-6.12	-2.52	-5.66	0.5433
#ZZZSPY01	-61.63	-67.92	-6.28	-66.79	1.8245

100 K runs, energies, convergence test last 2 Mstep
for each crystal: intramolecular, LP, Coulombic, total lattice energy
start: 3 Mstep frame, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd
#ABUMIT	0.00	0.00	0.00	0.00	0.0000
#ABUMIT	-68.92	-68.90	0.02	-68.95	0.0660
#ABUMIT	-3.32	-3.32	0.00	-3.31	0.0166
#ABUMIT	-72.24	-72.21	0.03	-72.26	0.0593
#BENZEN07	0.00	0.00	0.00	0.00	0.0000
#BENZEN07	-43.50	-43.56	-0.06	-43.57	0.0364
#BENZEN07	-8.50	-8.45	0.05	-8.42	0.0296
#BENZEN07	-52.00	-52.01	-0.01	-51.99	0.0318
#BILNOZ01	0.00	0.00	0.00	0.00	0.0000
#BILNOZ01	-67.80	-67.94	-0.14	-67.85	0.0668
#BILNOZ01	-3.19	-3.19	0.00	-3.19	0.0076
#BILNOZ01	-70.99	-71.13	-0.14	-71.03	0.0684
#BNZQUI03	0.00	0.00	0.00	0.00	0.0000
#BNZQUI03	-47.57	-49.01	-1.45	-48.20	0.4548
#BNZQUI03	-29.40	-28.22	1.18	-28.84	0.3954
#BNZQUI03	-76.96	-77.23	-0.27	-77.04	0.0879
#BULVAL03	0.00	0.00	0.00	0.00	0.0000
#BULVAL03	-63.46	-63.46	-0.01	-63.51	0.0737
#BULVAL03	-8.14	-8.06	0.08	-8.11	0.0388
#BULVAL03	-71.60	-71.52	0.08	-71.62	0.0677
#CECGEX	0.00	0.00	0.00	0.00	0.0000
#CECGEX	-65.49	-65.74	-0.25	-65.58	0.0759
#CECGEX	-34.36	-34.18	0.19	-34.24	0.0876
#CECGEX	-99.85	-99.91	-0.06	-99.82	0.1002
#CTCYDD	0.00	0.00	0.00	0.00	0.0000
#CTCYDD	-89.50	-89.65	-0.15	-89.65	0.1103
#CTCYDD	-2.11	-2.14	-0.03	-2.13	0.0298
#CTCYDD	-91.61	-91.79	-0.18	-91.78	0.1065
#DAZNAP	0.00	0.00	0.00	0.00	0.0000
#DAZNAP	-71.43	-71.55	-0.12	-71.49	0.0857
#DAZNAP	-22.44	-22.25	0.19	-22.34	0.0611
#DAZNAP	-93.88	-93.80	0.08	-93.83	0.0761
#DCBDOX10	0.00	0.00	0.00	0.00	0.0000
#DCBDOX10	-119.01	-119.15	-0.14	-119.12	0.0984
#DCBDOX10	-1.76	-2.01	-0.25	-1.89	0.0688
#DCBDOX10	-120.77	-121.16	-0.39	-121.01	0.0946
#DCLBEN01	0.00	0.00	0.00	0.00	0.0000
#DCLBEN01	-70.82	-71.30	-0.48	-71.13	0.1357
#DCLBEN01	-2.87	-2.79	0.08	-2.82	0.0262
#DCLBEN01	-73.69	-74.09	-0.40	-73.95	0.1184
#DCLBEN02	0.00	0.00	0.00	0.00	0.0000

#DCLBEN02	-73.30	-73.62	-0.31	-73.59	0.0907
#DCLBEN02	-3.60	-3.59	0.02	-3.60	0.0179
#DCLBEN02	-76.91	-77.20	-0.30	-77.18	0.0963
#DEZDUH	0.00	0.00	0.00	0.00	0.0000
#DEZDUH	-49.06	-49.33	-0.27	-49.29	0.1048
#DEZDUH	-16.75	-16.68	0.07	-16.69	0.0400
#DEZDUH	-65.80	-66.01	-0.21	-65.98	0.1104
#DEZXEL	0.00	0.00	0.00	0.00	0.0000
#DEZXEL	-87.88	-87.94	-0.06	-87.87	0.0871
#DEZXEL	-17.36	-17.42	-0.06	-17.41	0.0534
#DEZXEL	-105.24	-105.36	-0.12	-105.28	0.0919
#DITBOX	0.00	0.00	0.00	0.00	0.0000
#DITBOX	-91.06	-90.97	0.09	-90.93	0.0989
#DITBOX	-8.72	-8.60	0.13	-8.66	0.0437
#DITBOX	-99.78	-99.57	0.21	-99.59	0.0973
#EZURUM	0.00	0.00	0.00	0.00	0.0000
#EZURUM	-71.91	-71.78	0.12	-71.80	0.0902
#EZURUM	-20.91	-21.09	-0.18	-21.05	0.0795
#EZURUM	-92.81	-92.88	-0.06	-92.85	0.0655
#FACGEV	0.00	0.00	0.00	0.00	0.0000
#FACGEV	-46.12	-46.15	-0.03	-46.09	0.0549
#FACGEV	-6.10	-6.12	-0.02	-6.12	0.0429
#FACGEV	-52.21	-52.26	-0.05	-52.21	0.0714
#FACJAU	0.00	0.00	0.00	0.00	0.0000
#FACJAU	-42.56	-42.52	0.03	-42.57	0.0924
#FACJAU	-11.15	-11.19	-0.04	-11.21	0.0536
#FACJAU	-53.71	-53.72	-0.00	-53.78	0.0909
#FMANUL01	0.00	0.00	0.00	0.00	0.0000
#FMANUL01	-73.00	-73.24	-0.23	-73.02	0.1068
#FMANUL01	-10.44	-10.43	0.02	-10.45	0.0280
#FMANUL01	-83.44	-83.66	-0.22	-83.47	0.1135
#FOVNIN	0.00	0.00	0.00	0.00	0.0000
#FOVNIN	-102.08	-102.14	-0.06	-102.12	0.1163
#FOVNIN	-3.85	-3.84	0.01	-3.82	0.0313
#FOVNIN	-105.93	-105.97	-0.04	-105.94	0.1089
#HAYYAH	0.00	0.00	0.00	0.00	0.0000
#HAYYAH	-76.20	-76.20	-0.00	-76.18	0.0831
#HAYYAH	-8.59	-8.58	0.01	-8.56	0.0498
#HAYYAH	-84.79	-84.78	0.00	-84.73	0.0830
#HCLBNZ11	0.00	0.00	0.00	0.00	0.0000
#HCLBNZ11	-110.21	-110.12	0.09	-110.14	0.0853
#HCLBNZ11	9.16	9.16	0.01	9.19	0.0533
#HCLBNZ11	-101.05	-100.96	0.09	-100.95	0.0621
#HOWBAW	0.00	0.00	0.00	0.00	0.0000
#HOWBAW	-81.16	-81.44	-0.28	-81.19	0.1341
#HOWBAW	-11.31	-11.22	0.09	-11.27	0.0637
#HOWBAW	-92.47	-92.66	-0.18	-92.46	0.0990
#NAPHTA10	0.00	0.00	0.00	0.00	0.0000
#NAPHTA10	-77.32	-77.56	-0.24	-77.46	0.0926
#NAPHTA10	-8.71	-8.61	0.10	-8.66	0.0379
#NAPHTA10	-86.03	-86.17	-0.14	-86.11	0.0893
#NBORAN02	0.00	0.00	0.00	0.00	0.0000
#NBORAN02	-62.53	-62.43	0.09	-62.68	0.1475
#NBORAN02	-34.05	-34.24	-0.19	-33.98	0.1206
#NBORAN02	-96.58	-96.68	-0.10	-96.67	0.1067
#PUGDEB	0.00	0.00	0.00	0.00	0.0000
#PUGDEB	-48.40	-48.59	-0.18	-48.50	0.0908
#PUGDEB	-7.63	-7.79	-0.17	-7.75	0.0437
#PUGDEB	-56.03	-56.38	-0.35	-56.25	0.1210
#TCHLBZ03	0.00	0.00	0.00	0.00	0.0000
#TCHLBZ03	-82.30	-82.05	0.25	-82.12	0.0928
#TCHLBZ03	0.66	0.55	-0.11	0.58	0.0468
#TCHLBZ03	-81.64	-81.51	0.14	-81.54	0.0598
#TEPNIT11	0.00	0.00	0.00	0.00	0.0000
#TEPNIT11	-74.78	-74.90	-0.11	-74.90	0.0901
#TEPNIT11	-31.96	-31.99	-0.03	-31.94	0.0740
#TEPNIT11	-106.74	-106.89	-0.14	-106.84	0.0870
#VACCEH	0.00	0.00	0.00	0.00	0.0000
#VACCEH	-48.04	-47.94	0.10	-48.04	0.0777
#VACCEH	-6.82	-6.83	-0.00	-6.82	0.0391
#VACCEH	-54.87	-54.77	0.09	-54.85	0.0716
#XAYMIT	0.00	0.00	0.00	0.00	0.0000
#XAYMIT	-105.07	-105.28	-0.21	-105.16	0.0964
#XAYMIT	-15.54	-15.59	-0.04	-15.66	0.0965
#XAYMIT	-120.61	-120.87	-0.26	-120.81	0.0908
#YUYPUD01	0.00	0.00	0.00	0.00	0.0000
#YUYPUD01	-71.29	-71.65	-0.37	-71.59	0.1379
#YUYPUD01	-30.60	-31.03	-0.43	-30.93	0.1599
#YUYPUD01	-101.88	-102.69	-0.80	-102.52	0.2364
#ACANIL01	3.19	3.05	-0.14	3.12	0.0878
#ACANIL01	-72.47	-72.54	-0.07	-72.65	0.0894
#ACANIL01	-36.34	-36.19	0.15	-36.16	0.0926
#ACANIL01	-105.62	-105.68	-0.06	-105.69	0.1334
#ADIPAC07	3.06	3.13	0.07	3.03	0.1128
#ADIPAC07	-88.86	-89.45	-0.59	-89.22	0.1798
#ADIPAC07	-46.83	-46.65	0.17	-46.68	0.1246
#ADIPAC07	-132.63	-132.97	-0.34	-132.87	0.1451
#ARCLAM01	2.08	2.07	-0.02	2.02	0.0378
#ARCLAM01	-50.89	-51.72	-0.84	-51.43	0.1954
#ARCLAM01	-34.21	-33.87	0.34	-34.09	0.0980

#ARCLAM01	-83.02	-83.53	-0.51	-83.49	0.1552
#AYOJED	0.12	0.12	-0.00	0.12	0.0023
#AYOJED	-66.92	-67.16	-0.25	-67.09	0.1139
#AYOJED	-5.88	-5.89	-0.00	-5.94	0.0446
#AYOJED	-72.68	-72.93	-0.25	-72.90	0.1160
#BENZAC07	1.28	1.29	0.01	1.29	0.0448
#BENZAC07	-66.25	-66.29	-0.04	-66.34	0.0993
#BENZAC07	-23.79	-23.64	0.15	-23.60	0.1069
#BENZAC07	-88.76	-88.64	0.12	-88.65	0.0957
#BIPHEN04	5.89	5.88	-0.01	5.87	0.0124
#BIPHEN04	-89.42	-89.43	-0.01	-89.25	0.1303
#BIPHEN04	-12.85	-12.77	0.08	-12.83	0.0555
#BIPHEN04	-96.39	-96.32	0.07	-96.21	0.0996
#BZAMID01	2.23	2.16	-0.07	2.20	0.0451
#BZAMID01	-73.03	-73.09	-0.06	-73.05	0.0660
#BZAMID01	-33.29	-33.40	-0.11	-33.28	0.0977
#BZAMID01	-104.09	-104.32	-0.23	-104.13	0.1017
#DNBENZ14	0.43	0.38	-0.05	0.40	0.0335
#DNBENZ14	-71.68	-72.26	-0.58	-72.17	0.2000
#DNBENZ14	-13.54	-13.64	-0.10	-13.51	0.1273
#DNBENZ14	-84.79	-85.52	-0.74	-85.29	0.2611
#DNITBZ11	0.15	0.15	-0.00	0.15	0.0104
#DNITBZ11	-72.61	-72.77	-0.16	-72.66	0.1153
#DNITBZ11	-20.32	-20.44	-0.12	-20.50	0.0882
#DNITBZ11	-92.78	-93.06	-0.28	-93.00	0.1201
#EXODAW	0.95	0.84	-0.11	0.84	0.0489
#EXODAW	-87.12	-87.24	-0.12	-87.02	0.1250
#EXODAW	-29.02	-29.05	-0.03	-29.06	0.1060
#EXODAW	-115.20	-115.45	-0.26	-115.24	0.1213
#FAXTUU01	0.33	0.34	0.01	0.34	0.0219
#FAXTUU01	-86.44	-86.38	0.07	-86.51	0.0995
#FAXTUU01	-28.03	-28.03	0.00	-28.00	0.0587
#FAXTUU01	-114.15	-114.06	0.09	-114.17	0.0799
#FOVQOX	6.25	6.16	-0.09	6.23	0.0545
#FOVQOX	-72.97	-73.47	-0.50	-73.24	0.1767
#FOVQOX	-63.29	-62.84	0.45	-63.03	0.1827
#FOVQOX	-130.01	-130.15	-0.14	-130.04	0.1087
#GLURAC03	6.50	6.36	-0.14	6.44	0.0747
#GLURAC03	-82.02	-82.33	-0.31	-82.14	0.1438
#GLURAC03	-55.07	-55.00	0.07	-55.07	0.1192
#GLURAC03	-130.59	-130.97	-0.39	-130.77	0.1316
#HEPTAN02	1.70	1.54	-0.17	1.61	0.0716
#HEPTAN02	-64.68	-64.89	-0.20	-64.77	0.1179
#HEPTAN02	0.38	0.41	0.03	0.38	0.0152
#HEPTAN02	-62.60	-62.95	-0.34	-62.77	0.1455
#HEXANE01	1.46	1.46	-0.01	1.43	0.0533
#HEXANE01	-57.75	-57.88	-0.12	-57.84	0.0886
#HEXANE01	0.21	0.21	-0.01	0.20	0.0218
#HEXANE01	-56.08	-56.21	-0.13	-56.21	0.1170
#HITMUS	1.54	1.52	-0.02	1.51	0.0324
#HITMUS	-75.69	-75.78	-0.10	-75.73	0.1172
#HITMUS	-32.02	-31.88	0.13	-31.94	0.1013
#HITMUS	-106.17	-106.14	0.02	-106.15	0.1219
#JOHBUD	1.13	1.13	-0.00	1.13	0.0091
#JOHBUD	-54.64	-54.67	-0.03	-54.59	0.0792
#JOHBUD	-24.42	-24.46	-0.04	-24.54	0.0749
#JOHBUD	-77.93	-78.01	-0.07	-77.99	0.0727
#MCINAM10	5.24	5.05	-0.19	5.04	0.1408
#MCINAM10	-81.56	-81.50	0.06	-81.48	0.1634
#MCINAM10	-22.52	-22.19	0.33	-22.33	0.1482
#MCINAM10	-98.84	-98.64	0.20	-98.77	0.1757
#NITRBE01	0.07	0.10	0.02	0.08	0.0127
#NITRBE01	-60.17	-60.62	-0.45	-60.37	0.1775
#NITRBE01	-12.68	-12.50	0.18	-12.54	0.0765
#NITRBE01	-72.78	-73.02	-0.24	-72.83	0.1154
#OCTANE01	1.82	1.81	-0.01	1.86	0.0557
#OCTANE01	-74.95	-75.15	-0.20	-74.99	0.1083
#OCTANE01	0.54	0.58	0.04	0.53	0.0312
#OCTANE01	-72.59	-72.76	-0.17	-72.60	0.1201
#PHBALD11	1.20	1.22	0.02	1.23	0.0470
#PHBALD11	-70.82	-71.10	-0.28	-71.00	0.1040
#PHBALD11	-43.18	-42.67	0.51	-42.95	0.1571
#PHBALD11	-112.79	-112.55	0.24	-112.71	0.0936
#QATTIO	3.48	3.37	-0.11	3.37	0.0587
#QATTIO	-57.73	-57.68	0.05	-57.80	0.1132
#QATTIO	-64.69	-64.61	0.08	-64.57	0.1182
#QATTIO	-118.95	-118.92	0.03	-118.99	0.1272
#QATTOU	9.10	9.08	-0.02	9.15	0.0761
#QATTOU	-59.18	-59.12	0.06	-59.02	0.0903
#QATTOU	-61.99	-62.31	-0.32	-62.29	0.1402
#QATTOU	-112.07	-112.35	-0.27	-112.16	0.1081
#TEPPTH06	2.27	2.25	-0.02	2.26	0.0503
#TEPPTH06	-97.69	-97.92	-0.23	-97.78	0.1362
#TEPPTH06	-52.45	-52.41	0.04	-52.33	0.1270
#TEPPTH06	-147.87	-148.08	-0.21	-147.85	0.1453
#XAYMEP	0.09	0.09	-0.00	0.09	0.0054
#XAYMEP	-94.84	-95.20	-0.36	-95.06	0.1146
#XAYMEP	-11.68	-11.53	0.16	-11.61	0.0922
#XAYMEP	-106.43	-106.63	-0.21	-106.58	0.1036
#XOZBUK	0.58	0.66	0.08	0.64	0.0359

#XOZBUK	-63.68	-63.88	-0.21	-63.77	0.1124
#XOZBUK	-27.96	-27.92	0.05	-27.93	0.0561
#XOZBUK	-91.06	-91.14	-0.08	-91.05	0.1038
#ZIVKOE '	1.53	1.56	0.03	1.59	0.0560
#ZIVKOE '	-86.12	-86.25	-0.13	-86.25	0.1415
#ZIVKOE '	-34.85	-35.13	-0.28	-35.17	0.1318
#ZIVKOE '	-119.44	-119.82	-0.39	-119.83	0.2004
#ZZZITY01	0.09	0.09	0.00	0.09	0.0030
#ZZZITY01	-62.87	-62.64	0.23	-62.72	0.0868
#ZZZITY01	-7.21	-7.28	-0.06	-7.28	0.0354
#ZZZITY01	-69.99	-69.82	0.17	-69.91	0.0744
#ZZZSPY01	0.16	0.16	-0.00	0.16	0.0026
#ZZZSPY01	-62.03	-61.95	0.08	-62.06	0.0801
#ZZZSPY01	-5.95	-6.12	-0.18	-6.04	0.0594
#ZZZSPY01	-67.82	-67.92	-0.10	-67.95	0.1020

300 K runs, cell parameters, complete runs
For each crystal: a, b, c, α , β , γ
start: experimental crystal structure, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd	start	end	delt	aver	rmsd	
#ABUMIT	3.588	3.689	2.8	3.672	0.021	90.12	89.9	-0.22	90.01	0.226	
#ABUMIT	10.504	10.779	2.6	10.711	0.06	101.1	101.01	-0.09	100.2	0.399	
#ABUMIT	15.11	15.197	0.6	15.232	0.035	89.99	89.53	-0.45	90.02	0.249	
#BENZENO	7.439	7.806	4.9	7.713	0.09	89.92	89.14	-0.78	89.89	0.378	
#BENZENO	9.199	9.426	2.5	9.44	0.069	89.92	89.7	-0.22	89.9	0.291	
#BENZENO	6.389	6.536	2.3	6.499	0.042	89.68	88.14	-1.55	90.05	0.98	
#BILNOZO	9.782	9.88	1	9.931	0.058	89.92	89.19	-0.73	89.71	0.369	
#BILNOZO	6.819	7.039	3.2	6.962	0.047	90.82	90.88	0.06	91	0.238	
#BILNOZO	13.21	13.822	4.6	13.643	0.169	89.85	89.8	-0.05	90.07	0.3	
#BNZQUIO	5.486	5.51	0.4	5.517	0.015	92.79	90.91	-1.88	91.92	1.133	
#BNZQUIO	6.986	7.111	1.8	7.093	0.025	96.72	97.09	0.37	97.23	0.284	
#BNZQUIO	6.548	6.638	1.4	6.655	0.035	87.11	89.22	2.11	88.29	1.003	
#BULVALO	6.242	6.35	1.7	6.332	0.02	90.11	89.97	-0.14	90.03	0.23	
#BULVALO	20.907	21.403	2.4	21.303	0.124	92.93	92.9	-0.02	92.97	0.185	
#BULVALO	10.385	10.492	1	10.523	0.035	89.96	89.55	-0.41	90.02	0.394	
#CECGEX	4.608	4.622	0.3	4.63	0.014	90.05	90.15	0.1	90.03	0.23	
#CECGEX	7.143	7.263	1.7	7.257	0.062	89.96	90.07	0.11	90.15	0.207	
#CECGEX	11.8	12.043	2.1	11.978	0.078	90.05	90.02	-0.02	90.02	0.221	
#CTCYDD	7.484	7.553	0.9	7.532	0.015	89.96	90.11	0.15	89.97	0.217	
#CTCYDD	17.366	17.574	1.2	17.635	0.073	115.62	115.9	0.28	115.73	0.169	
#CTCYDD	8.673	8.794	1.4	8.752	0.025	89.74	90.03	0.29	90.08	0.326	
#DAZNAP	13.803	14.043	1.7	13.939	0.056	89.88	90.12	0.24	89.99	0.167	
#DAZNAP	10.171	10.231	0.6	10.289	0.032	92.53	88.96	-3.57	90.58	1.15	
#DAZNAP	8.574	8.636	0.7	8.634	0.025	89.87	90.1	0.23	89.91	0.202	
#DCBDOX1	5.931	6.027	1.6	6.017	0.022	93.73	93.84	0.12	93.56	0.498	
#DCBDOX1	6.47	6.529	0.9	6.526	0.014	90.74	90.72	-0.02	90.65	0.273	
#DCBDOX1	24.774	24.994	0.9	24.954	0.045	90	90.25	0.25	90	0.208	
#DCLBEN0	14.633	14.811	1.2	14.793	0.04	89.91	89.95	0.04	89.88	0.243	
#DCLBEN0	5.701	5.875	3.1	5.838	0.035	109.6	110.55	0.96	110.13	0.474	
#DCLBEN0	3.508	3.6	2.6	3.596	0.019	90.14	90.27	0.13	90.13	0.315	
#DCLBEN0	7.398	7.475	1	7.484	0.025	84.76	85.63	0.87	85.45	0.25	
#DCLBEN0	5.522	5.638	2.1	5.627	0.027	111.71	111.53	-0.18	112.38	0.518	
#DCLBEN0	3.603	3.667	1.8	3.674	0.021	97.7	96.48	-1.22	96.55	0.297	
#DEZDUH	14.761	15.009	1.7	15.04	0.083	90.03	90.27	0.24	90.09	0.286	
#DEZDUH	5.781	5.921	2.4	5.888	0.033	89.73	90.56	0.83	89.9	0.458	
#DEZDUH	9.898	10.213	3.2	10.157	0.075	90.29	89.69	-0.6	90.09	0.393	
#DEZXEL	11.914	11.97	0.5	11.962	0.021	89.93	89.68	-0.25	90	0.152	
#DEZXEL	9.527	9.633	1.1	9.595	0.024	89.96	89.71	-0.25	89.96	0.188	
#DEZXEL	7.161	7.24	1.1	7.261	0.022	89.84	90.44	0.6	90.01	0.184	
#DITBOX	6.934	7.052	1.7	7.015	0.025	89.85	89.47	-0.37	90.07	0.278	
#DITBOX	6.338	6.384	0.7	6.4	0.016	104.25	104.64	0.39	104.37	0.276	
#DITBOX	10.553	10.679	1.2	10.675	0.046	90.11	90.13	0.02	90.01	0.282	
#EZURUM	10.217	10.29	0.7	10.332	0.036	90.06	89.86	-0.2	90.05	0.136	
#EZURUM	6.473	6.557	1.3	6.539	0.022	95.89	95.66	-0.24	95.44	0.192	
#EZURUM	12.52	12.612	0.7	12.633	0.033	90	90.27	0.27	90.05	0.209	
#FACGEV	5.81	5.834	0.4	5.866	0.021	90.17	89.12	-1.05	89.99	0.599	
#FACGEV	6.499	6.925	6.6	6.836	0.112	96	97.8	1.81	97.96	0.698	
#FACGEV	6.567	6.865	4.5	6.8	0.068	89.8	89.37	-0.43	89.75	0.455	
#FACJAU	4.533	4.609	1.7	4.581	0.019	89.76	91.08	1.32	89.95	0.543	
#FACJAU	10.514	11.239	6.9	11.024	0.205	104	109.47	5.47	107.25	1.953	
#FACJAU	6.162	6.517	5.8	6.45	0.091	90.1	89.46	-0.65	90.07	0.406	
#FMANUL0	9.152	9.319	1.8	9.333	0.049	89.99	89.7	-0.29	90.03	0.301	
#FMANUL0	13.798	13.932	1	13.925	0.035	89.69	89.66	-0.03	89.89	0.239	
#FMANUL0	6.225	6.278	0.9	6.289	0.015	89.84	89.74	-0.1	89.94	0.331	
#FOVNIN	7.658	7.737	1	7.725	0.016	89.85	90.47	0.62	90.06	0.206	
#FOVNIN	11.239	11.388	1.3	11.37	0.034	90.14	89.89	-0.24	89.91	0.235	
#FOVNIN	17.732	17.838	0.6	17.849	0.04	90.09	90.3	0.22	90	0.205	
#HAYYAH	7.665	7.837	2.2	7.813	0.036	89.98	89.99	0	89.96	0.261	
#HAYYAH	13.752	13.895	1	13.888	0.033	109.71	109.9	0.19	109.73	0.357	
#HAYYAH	8.047	8.114	0.8	8.114	0.017	89.79	90.43	0.64	90.15	0.398	
#HCLBNZ1	7.931	8.029	1.2	8.033	0.029	90	89.84	-0.16	90.08	0.37	
#HCLBNZ1	3.549	3.636	2.5	3.609	0.018	93.59	94.16	0.57	93.85	0.228	
#HCLBNZ1	14.554	14.627	0.5	14.624	0.034	89.83	89.58	-0.25	89.91	0.227	
#HOWBAW	5.194	5.283	1.7	5.279	0.021	94.17	94.7	0.53	94.26	0.197	
#HOWBAW	5.607	5.673	1.2	5.663	0.02	95.46	94.8	-0.67	94.98	0.213	
#HOWBAW	7.674	7.727	0.7	7.704	0.018	108.98	109.04	0.06	109.17	0.249	
#NAPHTA1	7.426	7.614	2.5	7.559	0.041	90.04	90.02	-0.02	90.01	0.225	
#NAPHTA1	5.933	5.918	-0.2	5.949	0.015	125.67	125.02	-0.65	124.61	0.351	
#NAPHTA1	8.687	8.792	1.2	8.76	0.023	89.97	90.16	0.19	89.97	0.223	
#NBORAN0	6.143	6.144	0	6.148	0.015	89.83	89.82	-0.01	89.96	0.198	
#NBORAN0	9.593	9.753	1.7	9.707	0.038	89.94	89.89	-0.05	89.99	0.149	
#NBORAN0	13.172	13.456	2.2	13.446	0.082	90.05	89.99	-0.05	90.02	0.164	
#PUGDEB	7.256	7.457	2.8	7.459	0.069	89.96	90.18	0.21	90.45	0.483	
#PUGDEB	12.082	12.511	3.5	12.402	0.097	108.82	104.63	-4.18	106.83	0.985	
#PUGDEB	6.324	6.485	2.5	6.468	0.047	89.91	89.94	0.03	89.89	0.213	
#TCHLBZ0	3.665	3.768	2.8	3.735	0.022	89.95	89.66	-0.29	90.02	0.21	
#TCHLBZ0	13.271	13.846	4.3	13.729	0.163	90.15	89.81	-0.34	90.03	0.186	
#TCHLBZ0	12.908	12.694	-1.7	12.822	0.114	90.21	89.56	-0.65	89.94	0.381	
#TEPNIT1	3.565	3.607	1.2	3.621	0.022	115.41	115.63	0.21	115.41	0.216	
#TEPNIT1	6.438	6.564	2	6.503	0.026	83.3	83.56	0.25	83.33	0.219	
#TEPNIT1	7.004	7.049	0.6	7.038	0.014	102.64	101.72	-0.92	102.41	0.325	
#VACCEH	7.078	7.395	4.5	7.303	0.074	89.87	90.22	0.35	89.99	0.38	
#VACCEH	6.862	6.933	1	6.957	0.033	89.82	90.34	0.52	90.02	0.293	
#VACCEH	9.557	9.793	2.5	9.791	0.072	90.01	90.22	0.21	90.01	0.249	

#XAYMIT	3.43	3.496	1.9	3.49	0.014	89.95	90.16	0.2	90.03	0.165
#XAYMIT	8.532	8.596	0.7	8.593	0.018	90.14	90.06	-0.08	89.94	0.181
#XAYMIT	25.391	25.476	0.3	25.474	0.058	90.14	89.9	-0.24	90.24	0.324
#YUYUPUD0	3.741	3.819	2.1	3.799	0.016	89.93	90.16	0.23	89.97	0.247
#YUYUPUD0	10.682	10.938	2.4	10.919	0.068	93.28	94.71	1.43	94.34	0.41
#YUYUPUD0	14.38	14.442	0.4	14.435	0.022	90.04	90.1	0.06	89.96	0.258
#ACANIL0	19.089	19.17	0.4	19.156	0.04	90.12	89.82	-0.3	90.05	0.298
#ACANIL0	9.381	9.543	1.7	9.558	0.063	90.01	90.19	0.18	90	0.286
#ACANIL0	7.747	7.949	2.6	7.91	0.041	90.04	90.57	0.53	90.01	0.25
#ADIPAC0	7.361	7.53	2.3	7.514	0.042	89.66	90.05	0.4	89.88	0.22
#ADIPAC0	5.009	5.135	2.5	5.113	0.034	113.57	114.23	0.66	114.28	0.281
#ADIPAC0	10.241	10.297	0.5	10.308	0.033	89.98	90.21	0.24	89.91	0.236
#ARCLAM0	8.151	7.913	-2.9	8.104	0.11	90.03	90.31	0.29	90.21	0.29
#ARCLAM0	5.051	5.287	4.7	5.205	0.057	108.75	111.41	2.66	110.75	0.677
#ARCLAM0	8.9	9.591	7.8	9.357	0.197	89.85	89.95	0.1	90.11	0.273
#AYOJED	5.557	5.657	1.8	5.646	0.021	89.96	89.83	-0.14	89.99	0.237
#AYOJED	10.296	10.521	2.2	10.457	0.052	101.01	100.52	-0.49	100.36	0.326
#AYOJED	10.987	11.161	1.6	11.143	0.047	89.97	90.31	0.34	90.04	0.226
#BENZAC0	5.285	5.358	1.4	5.368	0.021	90.08	90.04	-0.03	90	0.193
#BENZAC0	4.902	4.95	1	4.966	0.017	104.88	103.84	-1.04	103.92	0.257
#BENZAC0	22.052	22.481	1.9	22.338	0.129	89.93	89.68	-0.25	89.98	0.189
#BIPHEN0	7.531	7.75	2.9	7.688	0.048	90.26	89.93	-0.33	89.87	0.381
#BIPHEN0	5.308	5.376	1.3	5.4	0.023	86.94	87.08	0.13	86.91	0.411
#BIPHEN0	9.307	9.33	0.2	9.347	0.027	90.03	89.76	-0.26	89.96	0.243
#BZAMID0	5.118	5.156	0.7	5.172	0.019	90.14	90.03	-0.11	89.99	0.238
#BZAMID0	5.15	5.163	0.3	5.162	0.01	81.4	83.25	1.85	83.21	0.45
#BZAMID0	21.339	21.875	2.5	21.796	0.128	89.91	89.9	0	90.01	0.218
#DNBENZ1	14.817	15.177	2.4	15.081	0.067	104.07	103.84	-0.23	103.54	0.315
#DNBENZ1	13.332	13.488	1.2	13.506	0.049	89.93	90.07	0.15	90.07	0.263
#DNBENZ1	3.557	3.673	3.3	3.656	0.03	90.05	90	-0.05	90	0.234
#DNITBZ1	10.225	10.571	3.4	10.511	0.067	90.03	89.79	-0.25	90.03	0.3
#DNITBZ1	6.031	6.177	2.4	6.146	0.047	102.23	101.9	-0.33	101.79	0.321
#DNITBZ1	5.597	5.55	-0.8	5.587	0.032	90.06	89.99	-0.07	89.98	0.215
#EXODAW	5.422	5.512	1.7	5.495	0.022	94.11	93.74	-0.37	93.76	0.257
#EXODAW	6.098	6.192	1.5	6.174	0.02	92.05	92.01	-0.04	92.17	0.265
#EXODAW	7.704	7.773	0.9	7.77	0.015	107.11	107.99	0.88	107.64	0.286
#FAXTUU0	6.213	6.296	1.3	6.289	0.02	90.08	89.85	-0.23	89.98	0.119
#FAXTUU0	9.861	9.99	1.3	9.954	0.028	90.14	89.87	-0.27	89.98	0.187
#FAXTUU0	15.59	15.645	0.3	15.694	0.032	90.01	89.96	-0.05	90.01	0.17
#FOVQOX	9.179	9.315	1.5	9.283	0.036	89.68	90.04	0.37	89.99	0.301
#FOVQOX	10.99	10.983	-0.1	10.995	0.021	90.1	89.98	-0.12	90	0.156
#FOVQOX	5.803	5.825	0.4	5.842	0.013	89.95	89.9	-0.05	90	0.172
#GLURAC0	13.254	13.093	-1.2	13.268	0.089	90	90.08	0.08	90.05	0.204
#GLURAC0	4.579	4.729	3.3	4.678	0.037	96.93	96.91	-0.03	96.15	0.39
#GLURAC0	9.813	10.028	2.2	9.955	0.048	89.92	90.08	0.16	90.15	0.215
#HEPTAN0	4.178	4.451	6.5	4.386	0.069	78.36	78.33	-0.04	78.73	0.262
#HEPTAN0	4.374	4.585	4.8	4.546	0.053	83.77	85.08	1.3	85.13	0.406
#HEPTAN0	20.213	20.521	1.5	20.472	0.066	77.38	73.85	-3.53	75.01	1.29
#HEXANE0	4.171	4.49	7.7	4.415	0.083	82.32	82.97	0.65	82.44	0.334
#HEXANE0	4.397	4.595	4.5	4.566	0.052	89.02	88.73	-0.29	89.47	0.391
#HEXANE0	8.563	8.618	0.6	8.664	0.037	77.72	74.24	-3.48	75.24	1.102
#HITMUS	6.866	6.974	1.6	6.97	0.027	89.97	89.97	0	90.08	0.257
#HITMUS	8.446	8.706	3.1	8.67	0.057	109.83	111.07	1.24	110.81	0.614
#HITMUS	7.392	7.662	3.7	7.611	0.088	89.99	90.34	0.35	89.96	0.28
#JOHBUD	11.808	11.911	0.9	11.903	0.036	90.8	89.89	-0.91	90.2	0.673
#JOHBUD	5.986	6.169	3.1	6.147	0.054	109.1	105.7	-3.4	106.48	0.812
#JOHBUD	10.73	10.947	2	10.923	0.049	89.58	89.99	0.42	89.97	0.49
#MCINAM1	10.722	10.978	2.4	10.945	0.076	89.75	89.72	-0.03	89.85	0.344
#MCINAM1	16.132	16.543	2.6	16.465	0.11	90.02	90.09	0.07	89.79	0.341
#MCINAM1	9.758	9.84	0.8	9.825	0.022	90.06	89.84	-0.22	90.01	0.201
#NITRBE0	3.582	3.68	2.7	3.681	0.033	89.86	90.48	0.62	89.95	0.265
#NITRBE0	11.063	11.137	0.7	11.172	0.044	90.88	92.34	1.45	91.5	0.53
#NITRBE0	13.918	14.312	2.8	14.276	0.108	89.92	89.78	-0.14	90.07	0.299
#OCTANE0	4.161	4.387	5.4	4.363	0.065	84.17	83.89	-0.28	84.03	0.253
#OCTANE0	4.378	4.524	3.3	4.513	0.035	85.37	85.68	0.31	85.73	0.241
#OCTANE0	10.98	11.097	1.1	11.061	0.03	77.61	75.65	-1.96	75.73	0.895
#PHBALD1	6.68	6.723	0.6	6.73	0.015	90.12	90.52	0.4	89.96	0.391
#PHBALD1	13.697	14.074	2.8	13.963	0.097	119.04	117.38	-1.66	117.83	0.298
#PHBALD1	6.733	6.64	-1.4	6.675	0.034	90.1	90.18	0.08	90.01	0.158
#QATTIO	4.945	4.975	0.6	4.973	0.008	89.85	90.15	0.3	89.79	0.263
#QATTIO	13.633	13.698	0.5	13.702	0.022	107.46	106.47	-0.98	106.29	0.352
#QATTIO	7.554	7.674	1.6	7.668	0.037	90.02	90.01	-0.01	90.02	0.113
#QATTOU	5.323	5.411	1.6	5.392	0.021	89.85	89.57	-0.28	90.1	0.214
#QATTOU	6.817	7.011	2.8	6.953	0.045	90.01	90.42	0.41	90.13	0.241
#QATTOU	16.696	16.539	-0.9	16.619	0.067	89.94	90.02	0.09	89.93	0.205
#TEPHTH0	7.782	7.85	0.9	7.892	0.037	100.16	98.21	-1.95	98.21	0.465
#TEPHTH0	6.514	6.644	2	6.58	0.041	107.01	108.44	1.43	108.24	0.627
#TEPHTH0	3.445	3.471	0.8	3.477	0.01	95.57	96.83	1.27	96.72	0.347
#XAYMEP	3.516	3.613	2.8	3.583	0.021	99.03	98.98	-0.05	99.39	0.319
#XAYMEP	5.234	5.243	0.2	5.274	0.016	101.17	100.79	-0.37	100.65	0.306
#XAYMEP	9.098	9.128	0.3	9.165	0.026	96.21	96.06	-0.15	96.11	0.232
#XOZBUK	9.356	9.413	0.6	9.425	0.015	90.08	89.82	-0.26	89.88	0.289
#XOZBUK	5.281	5.323	0.8	5.323	0.017	91.71	90.96	-0.75	91.05	0.438
#XOZBUK	12.451	13.033	4.7	12.873	0.148	90.01	89.98	-0.04	89.98	0.189
#ZIVKOE	6.845	6.894	0.7	6.896	0.016	110.15	110.04	-0.1	110.3	0.284
#ZIVKOE	6.149	6.257	1.8	6.242	0.025	104.09	104.5	0.42	104.36	0.208
#ZIVKOE	10.073	10.158	0.8	10.169	0.024	97.99	98.05	0.07	98.1	0.276
#ZZZITY0	5.391	5.432	0.8	5.463	0.035	90.04	89.97	-0.06	90	0.218
#ZZZITY0	5.276	5.758	9.1	5.574	0.124	94.12	89.72	-4.4	91.48	1.12
#ZZZITY0	10.525	10.344	-1.7	10.484	0.07	90.04	89.68	-0.36	90.03	0.231

#ZZZSPY0	9.9	10.163	2.7	10.117	0.078	90.25	89.75	-0.5	89.97	0.399
#ZZZSPY0	7.286	7.529	3.3	7.5	0.065	90.16	90.07	-0.08	90.06	0.248
#ZZZSPY0	16.809	16.952	0.8	16.908	0.059	90.36	90.26	-0.1	90.08	0.304

300 K runs, cell parameters, convergence tests last 2 Msteps
For each crystal: a, b, c, α, β, γ
start: 3 Mstep frame, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd	start	end	delt	aver	rmsd
#ABUMIT	3.667	3.689	0.6	3.685	0.006	90.23	89.90	-0.33	90.08	0.202
#ABUMIT	10.745	10.779	0.3	10.760	0.011	99.69	101.01	1.32	100.29	0.363
#ABUMIT	15.279	15.197	-0.5	15.230	0.023	90.13	89.53	-0.60	90.05	0.274
#BENZEN07	7.745	7.806	0.8	7.780	0.035	90.40	89.14	-1.27	89.79	0.413
#BENZEN07	9.446	9.426	-0.2	9.424	0.020	90.04	89.70	-0.34	89.80	0.327
#BENZEN07	6.533	6.536	0.1	6.535	0.009	91.00	88.14	-2.87	89.34	0.754
#BILNOZ01	9.926	9.880	-0.5	9.897	0.026	89.42	89.19	-0.22	89.52	0.333
#BILNOZ01	6.960	7.039	1.1	7.001	0.019	90.97	90.88	-0.09	91.04	0.193
#BILNOZ01	13.681	13.822	1.0	13.799	0.044	90.04	89.80	-0.23	90.08	0.380
#BNZQUI03	5.517	5.510	-0.1	5.520	0.015	91.07	90.91	-0.16	90.81	0.252
#BNZQUI03	7.091	7.111	0.3	7.108	0.008	97.08	97.09	0.01	97.23	0.285
#BNZQUI03	6.662	6.638	-0.4	6.647	0.009	88.91	89.22	0.32	89.30	0.196
#BULVAL03	6.340	6.350	0.2	6.333	0.010	89.88	89.97	0.09	89.97	0.187
#BULVAL03	21.337	21.403	0.3	21.390	0.053	93.51	92.90	-0.61	92.97	0.182
#BULVAL03	10.550	10.492	-0.6	10.531	0.020	90.08	89.55	-0.53	89.83	0.361
#CECGEX	4.625	4.622	-0.1	4.624	0.016	89.75	90.15	0.40	90.11	0.185
#CECGEX	7.324	7.263	-0.8	7.307	0.036	90.17	90.07	-0.10	90.12	0.168
#CECGEX	11.877	12.043	1.4	11.933	0.049	89.59	90.02	0.43	90.01	0.209
#CTCYDD	7.517	7.553	0.5	7.530	0.014	90.06	90.11	0.05	89.96	0.189
#CTCYDD	17.607	17.574	-0.2	17.599	0.038	115.94	115.90	-0.04	115.79	0.135
#CTCYDD	8.772	8.794	0.3	8.770	0.018	89.94	90.03	0.09	90.20	0.218
#DAZNAP	13.933	14.043	0.8	13.997	0.028	90.19	90.12	-0.07	90.00	0.176
#DAZNAP	10.308	10.231	-0.7	10.281	0.028	90.19	88.96	-1.23	89.33	0.363
#DAZNAP	8.638	8.636	-0.0	8.617	0.021	89.78	90.10	0.32	89.93	0.180
#DCBDOX10	6.031	6.027	-0.1	6.029	0.011	93.13	93.84	0.72	93.89	0.381
#DCBDOX10	6.521	6.529	0.1	6.531	0.013	90.91	90.72	-0.18	90.72	0.233
#DCBDOX10	24.978	24.994	0.1	24.969	0.017	89.89	90.25	0.35	89.98	0.256
#DCLBEN01	14.833	14.811	-0.1	14.798	0.023	89.52	89.95	0.43	89.85	0.228
#DCLBEN01	5.852	5.875	0.4	5.846	0.013	110.52	110.55	0.03	110.28	0.342
#DCLBEN01	3.602	3.600	-0.1	3.604	0.006	90.23	90.27	0.03	90.14	0.333
#DCLBEN02	7.486	7.475	-0.1	7.494	0.016	85.77	85.63	-0.14	85.51	0.260
#DCLBEN02	5.626	5.638	0.2	5.638	0.018	112.62	111.53	-1.09	112.55	0.386
#DCLBEN02	3.696	3.667	-0.8	3.683	0.011	96.48	96.48	-0.00	96.49	0.204
#DEZDUH	15.061	15.009	-0.3	15.080	0.042	90.30	90.27	-0.03	90.07	0.291
#DEZDUH	5.897	5.921	0.4	5.902	0.011	89.38	90.56	1.18	89.85	0.425
#DEZDUH	10.213	10.213	0.0	10.207	0.022	90.42	89.69	-0.73	90.06	0.370
#DEZXEL	11.971	11.970	-0.0	11.955	0.014	89.98	89.68	-0.30	89.97	0.164
#DEZXEL	9.612	9.633	0.2	9.609	0.020	90.20	89.71	-0.49	89.97	0.233
#DEZXEL	7.269	7.240	-0.4	7.269	0.014	89.87	90.44	0.57	90.05	0.223
#DITBOX	7.022	7.052	0.4	7.030	0.017	89.95	89.47	-0.48	90.05	0.317
#DITBOX	6.393	6.384	-0.1	6.397	0.011	104.73	104.64	-0.10	104.48	0.230
#DITBOX	10.723	10.679	-0.4	10.685	0.030	90.01	90.13	0.11	89.98	0.286
#EZURUM	10.329	10.290	-0.4	10.324	0.023	90.14	89.86	-0.28	90.04	0.141
#EZURUM	6.518	6.557	0.6	6.553	0.018	95.40	95.66	0.25	95.46	0.177
#EZURUM	12.578	12.612	0.3	12.620	0.016	90.16	90.27	0.12	90.07	0.201
#FACGEV	5.887	5.834	-0.9	5.858	0.024	89.14	89.12	-0.02	90.27	0.703
#FACGEV	6.881	6.925	0.6	6.903	0.033	98.46	97.80	-0.66	98.39	0.527
#FACGEV	6.850	6.865	0.2	6.855	0.016	90.32	89.37	-0.95	89.42	0.351
#FACJAU	4.586	4.609	0.5	4.590	0.013	89.15	91.08	1.94	90.11	0.699
#FACJAU	11.170	11.239	0.6	11.200	0.022	108.58	109.47	0.90	108.99	0.383
#FACJAU	6.494	6.517	0.4	6.512	0.011	90.68	89.46	-1.23	89.97	0.521
#FMANUL01	9.367	9.319	-0.5	9.351	0.016	90.09	89.70	-0.39	90.07	0.273
#FMANUL01	13.941	13.932	-0.1	13.918	0.021	89.95	89.66	-0.29	89.84	0.211
#FMANUL01	6.295	6.278	-0.3	6.290	0.011	89.61	89.74	0.13	90.00	0.324
#FOVNIN	7.740	7.737	-0.0	7.727	0.011	90.19	90.47	0.28	90.10	0.229
#FOVNIN	11.392	11.388	-0.0	11.385	0.014	90.16	89.89	-0.27	89.84	0.235
#FOVNIN	17.883	17.838	-0.3	17.848	0.026	90.04	90.30	0.27	90.00	0.183
#HAYYAH	7.795	7.837	0.5	7.822	0.021	89.93	89.99	0.05	89.90	0.232
#HAYYAH	13.902	13.895	-0.0	13.894	0.010	109.98	109.90	-0.07	109.78	0.309
#HAYYAH	8.133	8.114	-0.2	8.115	0.012	89.77	90.43	0.66	90.24	0.340
#HCLBNZ11	8.045	8.029	-0.2	8.030	0.009	89.66	89.84	0.18	90.15	0.306
#HCLBNZ11	3.609	3.636	0.8	3.618	0.013	93.88	94.16	0.28	93.93	0.220
#HCLBNZ11	14.664	14.627	-0.3	14.629	0.019	90.01	89.58	-0.43	89.84	0.200
#HOWBAW	5.273	5.283	0.2	5.279	0.008	94.13	94.70	0.58	94.31	0.220
#HOWBAW	5.667	5.673	0.1	5.661	0.010	95.12	94.80	-0.33	94.92	0.176
#HOWBAW	7.700	7.727	0.4	7.710	0.016	109.23	109.04	-0.20	109.12	0.191
#NAPHTA10	7.584	7.614	0.4	7.579	0.021	90.33	90.02	-0.30	89.96	0.187
#NAPHTA10	5.933	5.918	-0.3	5.950	0.016	123.89	125.02	1.12	124.75	0.270
#NAPHTA10	8.747	8.792	0.5	8.773	0.017	89.83	90.16	0.33	90.02	0.153
#NBORAN02	6.154	6.144	-0.2	6.141	0.011	89.74	89.82	0.08	89.95	0.187
#NBORAN02	9.703	9.753	0.5	9.740	0.017	90.01	89.89	-0.13	89.96	0.128
#NBORAN02	13.491	13.456	-0.3	13.489	0.026	89.72	89.99	0.28	89.99	0.164
#PUGDEB	7.503	7.457	-0.6	7.507	0.024	90.52	90.18	-0.35	90.24	0.457
#PUGDEB	12.403	12.511	0.9	12.468	0.029	107.29	104.63	-2.66	106.52	1.226
#PUGDEB	6.481	6.485	0.1	6.497	0.023	89.82	89.94	0.12	89.95	0.186
#TCHLBZ03	3.753	3.768	0.4	3.748	0.011	90.11	89.66	-0.45	89.94	0.183
#TCHLBZ03	13.785	13.846	0.4	13.871	0.040	89.88	89.81	-0.07	90.02	0.202
#TCHLBZ03	12.741	12.694	-0.4	12.707	0.027	89.43	89.56	0.13	89.82	0.377
#TEPNIT11	3.658	3.607	-1.4	3.629	0.012	115.21	115.63	0.42	115.43	0.211
#TEPNIT11	6.480	6.564	1.3	6.510	0.023	83.51	83.56	0.05	83.29	0.210

#TEPNIT11	7.025	7.049	0.4	7.032	0.008	102.67	101.72	-0.96	102.36	0.357
#VACCCH	7.318	7.395	1.1	7.361	0.021	89.81	90.22	0.40	89.88	0.355
#VACCCH	6.947	6.933	-0.2	6.947	0.016	89.68	90.34	0.67	90.02	0.319
#VACCCH	9.829	9.793	-0.4	9.845	0.022	90.11	90.22	0.12	90.04	0.226
#XAYMIT	3.491	3.496	0.1	3.489	0.008	90.02	90.16	0.14	90.04	0.176
#XAYMIT	8.590	8.596	0.1	8.593	0.014	89.74	90.06	0.32	89.88	0.143
#XAYMIT	25.545	25.476	-0.3	25.503	0.044	90.74	89.90	-0.84	90.16	0.387
#YUYUPUD01	3.806	3.819	0.4	3.807	0.014	90.36	90.16	-0.20	90.01	0.254
#YUYUPUD01	10.942	10.938	-0.0	10.944	0.031	94.65	94.71	0.06	94.49	0.337
#YUYUPUD01	14.389	14.442	0.4	14.429	0.022	90.01	90.10	0.09	89.94	0.215
#ACANIL01	19.103	19.170	0.3	19.127	0.025	90.09	89.82	-0.27	90.05	0.226
#ACANIL01	9.634	9.543	-0.9	9.587	0.024	90.41	90.19	-0.22	89.96	0.259
#ACANIL01	7.919	7.949	0.4	7.925	0.020	89.74	90.57	0.83	90.06	0.231
#ADIPAC07	7.535	7.530	-0.1	7.538	0.010	89.81	90.05	0.24	89.97	0.221
#ADIPAC07	5.141	5.135	-0.1	5.134	0.008	114.12	114.23	0.11	114.30	0.110
#ADIPAC07	10.279	10.297	0.2	10.294	0.014	89.72	90.21	0.49	89.91	0.233
#ARCLAM01	8.093	7.913	-2.2	7.992	0.055	90.52	90.31	-0.21	90.14	0.311
#ARCLAM01	5.234	5.287	1.0	5.255	0.021	110.83	111.41	0.58	111.27	0.188
#ARCLAM01	9.447	9.591	1.5	9.540	0.043	90.10	89.95	-0.15	89.99	0.175
#AYOJED	5.644	5.657	0.2	5.651	0.014	89.85	89.83	-0.02	89.89	0.186
#AYOJED	10.492	10.521	0.3	10.480	0.023	99.61	100.52	0.92	100.26	0.264
#AYOJED	11.156	11.161	0.0	11.129	0.024	90.03	90.31	0.29	89.98	0.190
#BENZAC07	5.369	5.358	-0.2	5.360	0.008	90.25	90.04	-0.21	89.96	0.177
#BENZAC07	4.976	4.950	-0.5	4.961	0.010	103.84	103.84	-0.01	103.81	0.166
#BENZAC07	22.378	22.481	0.5	22.454	0.052	89.69	89.68	-0.01	89.93	0.174
#BIPHEN04	7.701	7.750	0.6	7.721	0.022	89.41	89.93	0.53	89.58	0.343
#BIPHEN04	5.439	5.376	-1.2	5.403	0.019	86.09	87.08	0.99	86.70	0.323
#BIPHEN04	9.318	9.330	0.1	9.334	0.016	90.11	89.76	-0.35	89.85	0.245
#BZAMID01	5.176	5.156	-0.4	5.172	0.016	90.03	90.03	0.00	89.99	0.213
#BZAMID01	5.155	5.163	0.2	5.166	0.008	83.67	83.25	-0.42	83.38	0.180
#BZAMID01	21.934	21.875	-0.3	21.860	0.046	90.04	89.90	-0.14	89.94	0.173
#DNBENZ14	15.066	15.177	0.7	15.103	0.050	103.61	103.84	0.24	103.70	0.171
#DNBENZ14	13.467	13.488	0.2	13.512	0.022	90.13	90.07	-0.06	90.06	0.238
#DNBENZ14	3.691	3.673	-0.5	3.677	0.010	90.08	90.00	-0.08	89.98	0.263
#DNITBZ11	10.483	10.571	0.8	10.535	0.032	90.01	89.79	-0.23	90.01	0.293
#DNITBZ11	6.161	6.177	0.3	6.187	0.011	101.84	101.90	0.07	102.02	0.205
#DNITBZ11	5.564	5.550	-0.3	5.558	0.015	89.87	89.99	0.12	90.03	0.208
#EXODAW	5.498	5.512	0.3	5.509	0.008	93.53	93.74	0.21	93.78	0.261
#EXODAW	6.171	6.192	0.3	6.177	0.011	92.22	92.01	-0.21	92.15	0.247
#EXODAW	7.762	7.773	0.1	7.773	0.012	107.65	107.99	0.34	107.74	0.208
#FAXTUU01	6.282	6.296	0.2	6.300	0.007	90.06	89.85	-0.20	89.94	0.115
#FAXTUU01	9.961	9.990	0.3	9.971	0.014	90.01	89.87	-0.14	90.00	0.195
#FAXTUU01	15.709	15.645	-0.4	15.688	0.024	89.96	89.96	-0.00	90.00	0.141
#FOVQOX	9.324	9.315	-0.1	9.313	0.011	90.17	90.04	-0.13	90.07	0.340
#FOVQOX	10.991	10.983	-0.1	10.991	0.012	89.83	89.98	0.15	89.99	0.142
#FOVQOX	5.849	5.825	-0.4	5.833	0.007	90.07	89.90	-0.17	89.90	0.152
#GLURAC03	13.243	13.093	-1.1	13.179	0.049	90.18	90.08	-0.10	89.98	0.178
#GLURAC03	4.692	4.729	0.8	4.714	0.013	96.39	96.91	0.51	96.49	0.197
#GLURAC03	9.965	10.028	0.6	9.994	0.024	90.40	90.08	-0.32	90.18	0.245
#HEPTAN02	4.416	4.451	0.8	4.433	0.018	78.39	78.33	-0.06	78.67	0.262
#HEPTAN02	4.575	4.585	0.2	4.578	0.013	84.97	85.08	0.11	85.16	0.375
#HEPTAN02	20.516	20.521	0.0	20.496	0.038	74.53	73.85	-0.69	74.13	0.566
#HEXANE01	4.458	4.490	0.7	4.480	0.008	82.59	82.97	0.38	82.65	0.335
#HEXANE01	4.593	4.595	0.1	4.601	0.006	89.72	88.73	-0.99	89.40	0.452
#HEXANE01	8.686	8.618	-0.8	8.653	0.029	74.39	74.24	-0.15	74.44	0.259
#HITMUS	6.977	6.974	-0.0	6.972	0.013	89.82	89.97	0.15	89.97	0.265
#HITMUS	8.697	8.706	0.1	8.686	0.018	110.92	111.07	0.15	111.27	0.233
#HITMUS	7.687	7.662	-0.3	7.690	0.016	90.13	90.34	0.21	90.14	0.249
#JOHBUD	11.911	11.911	-0.0	11.902	0.021	88.97	89.89	0.93	89.82	0.370
#JOHBUD	6.202	6.169	-0.5	6.185	0.014	106.39	105.70	-0.69	105.83	0.320
#JOHBUD	10.968	10.947	-0.2	10.944	0.020	90.81	89.99	-0.81	90.20	0.317
#MCINAM10	10.991	10.978	-0.1	10.984	0.029	89.99	89.72	-0.27	89.98	0.243
#MCINAM10	16.592	16.543	-0.3	16.530	0.036	89.02	90.09	1.07	89.82	0.438
#MCINAM10	9.818	9.840	0.2	9.830	0.017	89.80	89.84	0.05	89.92	0.196
#NITRBE01	3.713	3.680	-0.9	3.702	0.011	90.01	90.48	0.47	89.92	0.276
#NITRBE01	11.203	11.137	-0.6	11.144	0.020	91.22	92.34	1.12	91.76	0.378
#NITRBE01	14.357	14.312	-0.3	14.355	0.026	90.01	89.78	-0.23	90.04	0.272
#OCTANE01	4.394	4.387	-0.2	4.405	0.012	83.79	83.89	0.10	84.05	0.227
#OCTANE01	4.526	4.524	-0.0	4.524	0.006	85.86	85.68	-0.18	85.80	0.202
#OCTANE01	11.078	11.097	0.2	11.081	0.014	75.19	75.65	0.45	75.13	0.337
#PHBALD11	6.729	6.723	-0.1	6.734	0.009	89.34	90.52	1.18	89.93	0.410
#PHBALD11	14.009	14.074	0.5	14.038	0.024	117.46	117.38	-0.08	117.77	0.246
#PHBALD11	6.647	6.640	-0.1	6.650	0.010	90.16	90.18	0.02	90.05	0.164
#QATTTO	4.958	4.975	0.3	4.972	0.006	89.83	90.15	0.32	89.91	0.268
#QATTTO	13.753	13.698	-0.4	13.712	0.013	106.14	106.47	0.33	106.31	0.253
#QATTTO	7.697	7.674	-0.3	7.689	0.008	90.12	90.01	-0.12	90.04	0.106
#QATTOU	5.382	5.411	0.5	5.407	0.012	90.12	89.57	-0.55	90.05	0.230
#QATTOU	6.992	7.011	0.3	6.988	0.010	89.79	90.42	0.62	90.15	0.283
#QATTOU	16.618	16.539	-0.5	16.560	0.027	90.31	90.02	-0.29	89.88	0.187
#TEPHTH06	7.948	7.850	-1.2	7.886	0.025	97.55	98.21	0.66	98.12	0.253
#TEPHTH06	6.575	6.644	1.1	6.618	0.032	108.91	108.44	-0.47	108.59	0.400
#TEPHTH06	3.487	3.471	-0.4	3.477	0.008	97.10	96.83	-0.27	96.90	0.160
#XAYMEP	3.585	3.613	0.8	3.600	0.011	99.42	98.98	-0.44	99.17	0.218
#XAYMEP	5.263	5.243	-0.4	5.267	0.013	100.42	100.79	0.37	100.86	0.253
#XAYMEP	9.188	9.128	-0.7	9.148	0.019	95.89	96.06	0.17	96.09	0.219
#XOZBUK	9.421	9.413	-0.1	9.423	0.011	89.46	89.82	0.36	89.87	0.244
#XOZBUK	5.324	5.323	-0.0	5.311	0.011	91.41	90.96	-0.45	90.93	0.273
#XOZBUK	12.872	13.033	1.3	12.987	0.052	90.06	89.98	-0.08	90.05	0.201
#ZIVKOE	6.918	6.894	-0.3	6.892	0.013	110.26	110.04	-0.22	110.40	0.286
#ZIVKOE	6.258	6.257	-0.0	6.258	0.014	104.23	104.50	0.27	104.40	0.189

#ZIVKOE '	10.158	10.158	-0.0	10.179	0.016	98.24	98.05	-0.18	97.96	0.257
###ZZZITY01	5.447	5.432	-0.3	5.434	0.017	90.04	89.97	-0.07	90.04	0.247
###ZZZITY01	5.630	5.758	2.3	5.686	0.038	90.74	89.72	-1.02	90.48	0.460
###ZZZITY01	10.479	10.344	-1.3	10.416	0.041	89.96	89.68	-0.28	90.04	0.296
###ZZZSPY01	10.166	10.163	-0.0	10.148	0.022	89.68	89.75	0.07	90.23	0.373
###ZZZSPY01	7.548	7.529	-0.3	7.522	0.011	90.01	90.07	0.06	90.04	0.223
###ZZZSPY01	16.877	16.952	0.4	16.901	0.052	90.20	90.26	0.06	90.05	0.325

300 K runs, density, complete runs
start: experimental crystal structure, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd
#ABUMIT	1.748	1.646	-5.78	1.657	0.0211
#BENZEN07	1.187	1.080	-9.03	1.097	0.0241
#BILNOZ01	1.287	1.180	-8.31	1.202	0.0227
#BNZQUI03	1.444	1.391	-3.62	1.391	0.0109
#BULVAL03	1.278	1.215	-4.95	1.220	0.0132
#CECGEX	1.370	1.316	-3.93	1.322	0.0098
#CTCYDD	1.765	1.708	-3.22	1.713	0.0101
#DAZNAP	1.438	1.394	-3.06	1.397	0.0077
#DCBDOX10	1.772	1.713	-3.33	1.719	0.0108
#DCLBEN01	1.771	1.665	-6.01	1.675	0.0192
#DCLBEN02	1.803	1.710	-5.18	1.719	0.0178
#DEZDUH	1.700	1.582	-6.94	1.597	0.0291
#DEZXEL	1.782	1.735	-2.62	1.738	0.0090
#DITBOX	1.332	1.287	-3.36	1.290	0.0088
#EZURUM	1.401	1.362	-2.75	1.358	0.0097
#FACGEV	1.537	1.379	-10.24	1.404	0.0355
#FACJAU	1.749	1.566	-10.44	1.604	0.0439
#FMANUL01	1.506	1.452	-3.58	1.448	0.0126
#FOVNIN	1.934	1.877	-2.90	1.882	0.0110
#HAYYAH	1.300	1.249	-3.89	1.252	0.0091
#HCLBNZ11	2.314	2.221	-4.01	2.236	0.0169
#HOWBAW	1.336	1.289	-3.50	1.297	0.0080
#NAPHTA10	1.369	1.312	-4.16	1.313	0.0099
#NBORAN02	1.405	1.352	-3.72	1.359	0.0113
#PUGDEB	1.672	1.499	-10.34	1.533	0.0377
#TCHLBZ03	1.920	1.820	-5.21	1.834	0.0207
#TEPNT11	1.503	1.445	-3.85	1.456	0.0092
#VACCEH	1.147	1.060	-7.54	1.070	0.0207
#XAYMIT	1.628	1.581	-2.92	1.584	0.0084
#YUYUPD01	1.484	1.415	-4.59	1.426	0.0141
#ACANIL01	1.294	1.235	-4.59	1.240	0.0133
#ADIPAC07	1.402	1.337	-4.66	1.345	0.0158
#ARCLAM01	1.361	1.264	-7.11	1.280	0.0223
#AYOJED	1.250	1.181	-5.51	1.192	0.0121
#BENZAC07	1.469	1.401	-4.62	1.404	0.0141
#BIPHEN04	1.379	1.319	-4.31	1.322	0.0117
#BZAMID01	1.447	1.391	-3.83	1.393	0.0129
#DNBENZ14	1.638	1.529	-6.65	1.543	0.0227
#DNITBZ11	1.655	1.574	-4.89	1.581	0.0160
#EXODAW	1.597	1.540	-3.57	1.547	0.0105
#FAXTUU01	1.798	1.745	-2.93	1.748	0.0111
#FOVQOX	1.409	1.384	-1.77	1.383	0.0052
#GLURAC03	1.484	1.424	-4.08	1.429	0.0118
#HEPTAN02	0.945	0.845	-10.55	0.862	0.0220
#HEXANE01	0.941	0.843	-10.46	0.856	0.0241
#HITMUS	1.435	1.332	-7.12	1.346	0.0223
#JOHBUD	1.466	1.356	-7.46	1.371	0.0254
#MCINAM10	1.269	1.198	-5.55	1.210	0.0167
#NITRBE01	1.483	1.395	-5.89	1.394	0.0229
#OCTANE01	0.978	0.895	-8.43	0.905	0.0188
#PHBALD11	1.506	1.454	-3.45	1.462	0.0088
#QATTIO	1.232	1.194	-3.12	1.194	0.0079
#QATTOU	1.142	1.103	-3.42	1.110	0.0076
#TEPHTH06	1.700	1.648	-3.02	1.650	0.0104
#XAYMEP	1.636	1.581	-3.38	1.580	0.0106
#XOZBUK	1.503	1.415	-5.83	1.431	0.0173
#ZIVKOE '	1.545	1.498	-3.05	1.502	0.0091
###ZZZITY01	1.181	1.090	-7.73	1.106	0.0185
###ZZZSPY01	1.163	1.087	-6.52	1.100	0.0171

300 K runs, density, convergence test last 2 Mstep
start: 3 Mstep frame, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd
#ABUMIT	1.645	1.646	0.06	1.643	0.0028
#BENZEN07	1.086	1.080	-0.58	1.083	0.0043
#BILNOZ01	1.200	1.180	-1.67	1.186	0.0057
#BNZQUI03	1.389	1.391	0.21	1.388	0.0032
#BULVAL03	1.214	1.215	0.03	1.214	0.0030
#CECGEX	1.322	1.316	-0.49	1.319	0.0038
#CTCYDD	1.718	1.708	-0.58	1.714	0.0041
#DAZNAP	1.394	1.394	-0.00	1.394	0.0029
#DCBDOX10	1.714	1.713	-0.05	1.714	0.0023
#DCLBEN01	1.667	1.665	-0.16	1.669	0.0037
#DCLBEN02	1.711	1.710	-0.03	1.711	0.0048
#DEZDUH	1.583	1.582	-0.07	1.581	0.0072

#DEZXEL	1.732	1.735	0.19	1.735	0.0024
#DITBOX	1.286	1.287	0.09	1.287	0.0023
#EZURUM	1.368	1.362	-0.44	1.357	0.0055
#FACGEV	1.381	1.379	-0.09	1.382	0.0040
#FACJAU	1.581	1.566	-0.91	1.575	0.0049
#FMANUL01	1.440	1.452	0.85	1.446	0.0037
#FOVNIN	1.871	1.877	0.33	1.879	0.0045
#HAYYAH	1.253	1.249	-0.30	1.250	0.0038
#HCLBNZ11	2.227	2.221	-0.27	2.231	0.0057
#HOWBAW	1.299	1.289	-0.72	1.296	0.0045
#NAPHTA10	1.303	1.312	0.70	1.309	0.0029
#NBORAN02	1.354	1.352	-0.08	1.351	0.0021
#PUGDEB	1.524	1.499	-1.61	1.506	0.0070
#TCHLBZ03	1.828	1.820	-0.46	1.825	0.0056
#TEPNIT11	1.448	1.445	-0.22	1.453	0.0043
#VACCEH	1.065	1.060	-0.48	1.057	0.0038
#XAYMIT	1.580	1.581	0.07	1.583	0.0022
#YUYPU01	1.425	1.415	-0.69	1.420	0.0077
#ACANIL01	1.232	1.235	0.22	1.236	0.0025
#ADIPAC07	1.336	1.337	0.09	1.337	0.0029
#ARCLAM01	1.263	1.264	0.11	1.265	0.0024
#AYOJED	1.185	1.181	-0.26	1.190	0.0052
#BENZAC07	1.398	1.401	0.26	1.399	0.0042
#BIPHEN04	1.315	1.319	0.29	1.318	0.0038
#BZAMID01	1.383	1.391	0.57	1.387	0.0034
#DNBENZ14	1.534	1.529	-0.30	1.532	0.0053
#DNITBZ11	1.588	1.574	-0.82	1.576	0.0043
#EXODAW	1.548	1.540	-0.54	1.543	0.0033
#FAXTUU01	1.747	1.745	-0.11	1.742	0.0036
#FOVQOX	1.376	1.384	0.58	1.381	0.0031
#GLURAC03	1.426	1.424	-0.16	1.423	0.0036
#HEPTAN02	0.851	0.845	-0.68	0.849	0.0045
#HEXANE01	0.843	0.843	-0.05	0.840	0.0027
#HITMUS	1.328	1.332	0.37	1.333	0.0037
#JOHBUD	1.351	1.356	0.36	1.355	0.0042
#MCINAM10	1.196	1.198	0.18	1.200	0.0035
#NITRBE01	1.370	1.395	1.87	1.382	0.0067
#OCTANE01	0.897	0.895	-0.16	0.895	0.0022
#PHBALD11	1.459	1.454	-0.34	1.458	0.0038
#QATTIO	1.187	1.194	0.53	1.190	0.0026
#QATT0U	1.106	1.103	-0.33	1.106	0.0019
#TEPHTH06	1.641	1.648	0.46	1.646	0.0039
#XAYMEP	1.577	1.581	0.26	1.577	0.0028
#XOZBUK	1.432	1.415	-1.16	1.422	0.0042
#ZIVKOE '	1.494	1.498	0.25	1.498	0.0042
#ZZZTTY01	1.097	1.090	-0.69	1.096	0.0045
#ZZZSPY01	1.089	1.087	-0.16	1.093	0.0039

300 K runs, energies, complete runs
for each crystal: intramolecular, LP, Coulombic, total lattice energy
start: experimental crystal structure, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd	
#ABUMIT	0.00	0.00	0.00	0.00	0.0000	intram
#ABUMIT	-68.90	-62.14	6.76	-62.80	1.0285	LP
#ABUMIT	-3.32	-2.94	0.37	-2.96	0.0820	Coulombic
#ABUMIT	-72.21	-65.08	7.13	-65.76	1.1007	total
#BENZEN07	0.00	0.00	0.00	0.00	0.0000	
#BENZEN07	-43.56	-37.18	6.38	-37.69	1.0569	
#BENZEN07	-8.45	-6.73	1.72	-6.90	0.3560	
#BENZEN07	-52.01	-43.91	8.10	-44.59	1.3970	
#BILNOZ01	0.00	0.00	0.00	0.00	0.0000	
#BILNOZ01	-67.94	-57.78	10.16	-59.44	1.7836	
#BILNOZ01	-3.19	-2.88	0.31	-2.98	0.0596	
#BILNOZ01	-71.13	-60.65	10.48	-62.42	1.8377	
#BNZQUI03	0.00	0.00	0.00	0.00	0.0000	
#BNZQUI03	-49.01	-45.95	3.06	-46.26	0.4357	
#BNZQUI03	-28.22	-25.18	3.04	-25.13	0.5897	
#BNZQUI03	-77.23	-71.14	6.10	-71.40	0.8884	
#BULVAL03	0.00	0.00	0.00	0.00	0.0000	
#BULVAL03	-63.46	-57.73	5.74	-58.08	0.8730	
#BULVAL03	-8.06	-7.32	0.74	-7.27	0.1591	
#BULVAL03	-71.52	-65.05	6.47	-65.35	0.9926	
#CECGEX	0.00	0.00	0.00	0.00	0.0000	
#CECGEX	-65.74	-61.67	4.07	-61.92	0.5881	
#CECGEX	-34.18	-31.89	2.28	-31.96	0.4184	
#CECGEX	-99.91	-93.56	6.35	-93.88	0.9132	
#CTCYDD	0.00	0.00	0.00	0.00	0.0000	
#CTCYDD	-89.65	-84.05	5.60	-84.27	0.8268	
#CTCYDD	-2.14	-2.09	0.05	-2.11	0.0497	
#CTCYDD	-91.79	-86.14	5.65	-86.39	0.8304	
#DAZNAP	0.00	0.00	0.00	0.00	0.0000	
#DAZNAP	-71.55	-66.96	4.59	-67.30	0.6415	
#DAZNAP	-22.25	-21.07	1.18	-21.16	0.1867	
#DAZNAP	-93.80	-88.03	5.78	-88.46	0.8031	
#DCBDOX10	0.00	0.00	0.00	0.00	0.0000	
#DCBDOX10	-119.15	-113.12	6.03	-113.49	0.8764	
#DCBDOX10	-2.01	-1.77	0.25	-1.84	0.0782	

#DCBDOX10	-121.16	-114.88	6.28	-115.33	0.8948
#DCLBEN01	0.00	0.00	0.00	0.00	0.0000
#DCLBEN01	-71.30	-64.73	6.58	-65.09	0.9959
#DCLBEN01	-2.79	-2.49	0.30	-2.52	0.0493
#DCLBEN01	-74.09	-67.21	6.88	-67.61	1.0358
#DCLBEN02	0.00	0.00	0.00	0.00	0.0000
#DCLBEN02	-73.62	-67.67	5.94	-67.97	0.8890
#DCLBEN02	-3.59	-3.12	0.47	-3.25	0.0693
#DCLBEN02	-77.20	-70.79	6.41	-71.22	0.9390
#DEZDUH	0.00	0.00	0.00	0.00	0.0000
#DEZDUH	-49.33	-43.43	5.90	-43.87	0.9523
#DEZDUH	-16.68	-15.33	1.35	-15.52	0.2732
#DEZDUH	-66.01	-58.75	7.26	-59.39	1.2073
#DEZZXEL	0.00	0.00	0.00	0.00	0.0000
#DEZZXEL	-87.94	-83.62	4.33	-83.47	0.6701
#DEZZXEL	-17.42	-16.07	1.35	-16.24	0.2184
#DEZZXEL	-105.36	-99.68	5.68	-99.70	0.8486
#DITBOX	0.00	0.00	0.00	0.00	0.0000
#DITBOX	-90.97	-85.64	5.33	-85.65	0.8276
#DITBOX	-8.60	-8.13	0.46	-8.16	0.0901
#DITBOX	-99.57	-93.77	5.80	-93.82	0.8911
#EZURUM	0.00	0.00	0.00	0.00	0.0000
#EZURUM	-71.78	-67.38	4.41	-67.30	0.6971
#EZURUM	-21.09	-20.06	1.03	-19.88	0.2441
#EZURUM	-92.88	-87.44	5.44	-87.18	0.8984
#FACGEV	0.00	0.00	0.00	0.00	0.0000
#FACGEV	-46.15	-38.48	7.66	-39.48	1.3005
#FACGEV	-6.12	-4.56	1.56	-4.88	0.3063
#FACGEV	-52.26	-43.04	9.22	-44.35	1.5950
#FACJAU	0.00	0.00	0.00	0.00	0.0000
#FACJAU	-42.52	-36.01	6.51	-37.00	1.0943
#FACJAU	-11.19	-9.35	1.85	-9.58	0.3874
#FACJAU	-53.72	-45.35	8.36	-46.58	1.4567
#FMANUL01	0.00	0.00	0.00	0.00	0.0000
#FMANUL01	-73.24	-68.00	5.24	-67.85	0.8538
#FMANUL01	-10.43	-9.91	0.51	-9.81	0.1361
#FMANUL01	-83.66	-77.91	5.75	-77.67	0.9692
#FOVNIN	0.00	0.00	0.00	0.00	0.0000
#FOVNIN	-102.14	-96.60	5.54	-96.59	0.8918
#FOVNIN	-3.84	-3.74	0.10	-3.70	0.0458
#FOVNIN	-105.97	-100.33	5.64	-100.28	0.9133
#HAYYAH	0.00	0.00	0.00	0.00	0.0000
#HAYYAH	-76.20	-71.38	4.82	-71.31	0.7351
#HAYYAH	-8.58	-7.85	0.73	-7.94	0.1520
#HAYYAH	-84.78	-79.23	5.55	-79.24	0.8411
#HCLBNZ11	0.00	0.00	0.00	0.00	0.0000
#HCLBNZ11	-110.12	-102.86	7.26	-103.73	1.0384
#HCLBNZ11	9.16	8.32	-0.84	8.60	0.1974
#HCLBNZ11	-100.96	-94.54	6.42	-95.13	0.8962
#HOWBAW	0.00	0.00	0.00	0.00	0.0000
#HOWBAW	-81.44	-76.26	5.18	-76.62	0.7314
#HOWBAW	-11.22	-10.13	1.09	-10.33	0.2126
#HOWBAW	-92.66	-86.39	6.27	-86.95	0.8741
#NAPHTA10	0.00	0.00	0.00	0.00	0.0000
#NAPHTA10	-77.56	-72.17	5.39	-72.08	0.8455
#NAPHTA10	-8.61	-8.20	0.41	-8.13	0.0957
#NAPHTA10	-86.17	-80.37	5.80	-80.21	0.9103
#NBORAN02	0.00	0.00	0.00	0.00	0.0000
#NBORAN02	-62.43	-58.16	4.28	-58.61	0.6053
#NBORAN02	-34.24	-32.73	1.51	-32.44	0.3217
#NBORAN02	-96.68	-90.89	5.79	-91.05	0.8639
#PUGDEB	0.00	0.00	0.00	0.00	0.0000
#PUGDEB	-48.59	-41.65	6.94	-42.69	1.2228
#PUGDEB	-7.79	-5.46	2.33	-6.13	0.5663
#PUGDEB	-56.38	-47.11	9.27	-48.82	1.7635
#TCHLBZ03	0.00	0.00	0.00	0.00	0.0000
#TCHLBZ03	-82.05	-75.09	6.96	-75.71	1.0492
#TCHLBZ03	0.55	-0.01	-0.56	0.12	0.1695
#TCHLBZ03	-81.51	-75.10	6.41	-75.59	0.9366
#TEPNIT11	0.00	0.00	0.00	0.00	0.0000
#TEPNIT11	-74.90	-70.94	3.96	-70.83	0.6161
#TEPNIT11	-31.99	-30.14	1.85	-30.38	0.2765
#TEPNIT11	-106.89	-101.08	5.81	-101.21	0.8660
#VACCEH	0.00	0.00	0.00	0.00	0.0000
#VACCEH	-47.94	-41.72	6.22	-42.43	0.9934
#VACCEH	-6.83	-5.55	1.28	-5.64	0.2777
#VACCEH	-54.77	-47.27	7.50	-48.07	1.2550
#XAYMIT	0.00	0.00	0.00	0.00	0.0000
#XAYMIT	-105.28	-100.20	5.08	-100.61	0.7139
#XAYMIT	-15.59	-14.57	1.01	-14.64	0.1978
#XAYMIT	-120.87	-114.77	6.10	-115.25	0.8400
#YUYPUD01	0.00	0.00	0.00	0.00	0.0000
#YUYPUD01	-71.65	-67.39	4.27	-67.27	0.6773
#YUYPUD01	-31.03	-28.93	2.10	-29.15	0.3718
#YUYPUD01	-102.68	-96.32	6.37	-96.42	1.0084
#ACANIL01	3.05	4.44	1.39	4.65	0.2984
#ACANIL01	-72.54	-66.71	5.83	-67.15	0.9128
#ACANIL01	-36.19	-33.42	2.77	-33.63	0.4685
#ACANIL01	-105.68	-95.68	9.99	-96.13	1.5233
#ADIPAC07	3.13	8.87	5.74	8.27	0.9187

#ADIPAC07	-89.45	-82.20	7.25	-82.57	1.2668
#ADIPAC07	-46.65	-42.22	4.43	-42.88	0.6629
#ADIPAC07	-132.97	-115.55	17.41	-117.18	2.7342
#ARCLAM01	2.07	5.25	3.19	5.54	0.5650
#ARCLAM01	-51.72	-46.07	5.66	-46.91	0.9267
#ARCLAM01	-33.87	-30.50	3.37	-30.77	0.6382
#ARCLAM01	-83.53	-71.32	12.21	-72.15	2.0281
#AYOJED	0.12	0.10	-0.02	0.10	0.0054
#AYOJED	-67.16	-61.28	5.88	-61.76	0.8365
#AYOJED	-5.89	-4.71	1.18	-4.87	0.2091
#AYOJED	-72.93	-65.90	7.03	-66.53	1.0115
#BENZAC07	1.29	3.28	1.99	3.15	0.3000
#BENZAC07	-66.29	-61.16	5.13	-61.20	0.8019
#BENZAC07	-23.64	-21.09	2.55	-21.19	0.4355
#BENZAC07	-88.64	-78.98	9.66	-79.23	1.4714
#BIPHEN04	5.88	5.59	-0.29	5.57	0.0627
#BIPHEN04	-89.43	-82.85	6.58	-83.02	0.9857
#BIPHEN04	-12.77	-11.85	0.92	-11.93	0.1802
#BIPHEN04	-96.32	-89.11	7.21	-89.37	1.0829
#BZAMID01	2.16	5.78	3.62	5.75	0.5508
#BZAMID01	-73.09	-68.32	4.77	-68.31	0.7683
#BZAMID01	-33.40	-30.42	2.97	-30.68	0.5032
#BZAMID01	-104.32	-92.96	11.36	-93.23	1.7461
#DNBENZ14	0.38	0.70	0.32	0.62	0.0579
#DNBENZ14	-72.26	-65.06	7.21	-65.77	1.1213
#DNBENZ14	-13.64	-11.97	1.67	-11.97	0.3322
#DNBENZ14	-85.52	-76.32	9.20	-77.12	1.4235
#DNITBZ11	0.15	0.53	0.38	0.51	0.0664
#DNITBZ11	-72.77	-65.99	6.78	-66.45	0.9765
#DNITBZ11	-20.44	-19.56	0.88	-19.60	0.2057
#DNITBZ11	-93.06	-85.02	8.05	-85.53	1.1940
#EXODAW	0.84	2.71	1.87	2.59	0.3092
#EXODAW	-87.24	-81.93	5.31	-82.48	0.7406
#EXODAW	-29.05	-27.61	1.43	-27.74	0.2719
#EXODAW	-115.45	-106.84	8.61	-107.63	1.2028
#FAXTUU01	0.34	0.92	0.58	0.90	0.0885
#FAXTUU01	-86.38	-81.71	4.66	-81.69	0.7200
#FAXTUU01	-28.03	-26.72	1.31	-26.92	0.2182
#FAXTUU01	-114.06	-107.51	6.55	-107.71	0.9650
#FOVQOX	6.16	8.30	2.14	8.19	0.3166
#FOVQOX	-73.47	-69.63	3.84	-69.93	0.5750
#FOVQOX	-62.84	-58.41	4.42	-58.44	0.6819
#FOVQOX	-130.15	-119.74	10.41	-120.18	1.4763
#GLURAC03	6.36	10.60	4.25	10.33	0.6688
#GLURAC03	-82.33	-76.04	6.28	-76.81	0.9582
#GLURAC03	-55.00	-49.99	5.01	-50.28	0.8232
#GLURAC03	-130.97	-115.43	15.54	-116.76	2.3804
#HEPTAN02	1.54	5.87	4.34	5.45	0.8154
#HEPTAN02	-64.89	-53.13	11.76	-54.95	2.0180
#HEPTAN02	0.41	0.03	-0.37	0.10	0.0831
#HEPTAN02	-62.95	-47.22	15.73	-49.40	2.7374
#HEXANE01	1.46	1.17	-0.29	3.57	1.6779
#HEXANE01	-57.88	-47.57	10.30	-48.87	1.8748
#HEXANE01	0.21	0.05	-0.16	0.10	0.0655
#HEXANE01	-56.21	-46.35	9.85	-45.20	2.4090
#HITMUS	1.52	3.17	1.65	3.03	0.2976
#HITMUS	-75.78	-65.86	9.93	-67.00	1.5639
#HITMUS	-31.88	-29.20	2.68	-29.24	0.4814
#HITMUS	-106.14	-91.89	14.25	-93.21	2.2685
#JOHBUD	1.13	0.92	-0.21	0.92	0.0500
#JOHBUD	-54.67	-47.86	6.81	-48.33	1.1686
#JOHBUD	-24.46	-21.17	3.29	-21.58	0.6480
#JOHBUD	-78.01	-68.11	9.89	-69.00	1.7492
#MCINAM10	5.05	8.11	3.06	8.46	0.5658
#MCINAM10	-81.50	-73.51	7.99	-74.27	1.4822
#MCINAM10	-22.19	-20.60	1.59	-20.62	0.3355
#MCINAM10	-98.64	-85.99	12.64	-86.43	2.0777
#NITRBE01	0.10	0.22	0.13	0.23	0.0282
#NITRBE01	-60.62	-54.71	5.90	-54.56	1.0147
#NITRBE01	-12.50	-11.34	1.15	-11.37	0.2234
#NITRBE01	-73.02	-65.83	7.19	-65.71	1.2349
#OCTANE01	1.81	-3.09	-4.90	2.39	2.9614
#OCTANE01	-75.15	-64.59	10.56	-65.49	1.8378
#OCTANE01	0.58	0.29	-0.29	0.27	0.0809
#OCTANE01	-72.76	-67.39	5.38	-62.82	2.9805
#PHBALD11	1.22	2.93	1.71	2.77	0.2571
#PHBALD11	-71.10	-67.80	3.30	-67.71	0.5590
#PHBALD11	-42.67	-38.66	4.01	-39.57	0.6431
#PHBALD11	-112.55	-103.52	9.03	-104.51	1.2883
#QATTIO	3.37	7.44	4.07	7.25	0.6221
#QATTIO	-57.68	-54.29	3.39	-54.65	0.5051
#QATTIO	-64.61	-60.37	4.24	-60.24	0.7129
#QATTIO	-118.92	-107.21	11.70	-107.63	1.7147
#QATTOU	9.08	13.75	4.67	13.32	0.7617
#QATTOU	-59.12	-56.01	3.10	-56.29	0.4655
#QATTOU	-62.31	-56.71	5.60	-56.88	0.8680
#QATTOU	-112.35	-98.97	13.38	-99.85	1.9409
#TEPPTH06	2.25	5.93	3.69	5.97	0.6158
#TEPPTH06	-97.92	-93.03	4.89	-93.29	0.7494
#TEPPTH06	-52.41	-48.38	4.02	-48.23	0.7240

#TEPHTH06	-148.08	-135.48	12.60	-135.55	1.9620
#XAYMEP	0.09	0.27	0.18	0.29	0.0401
#XAYMEP	-95.20	-89.90	5.30	-89.74	0.8388
#XAYMEP	-11.52	-10.72	0.81	-10.66	0.1761
#XAYMEP	-106.63	-100.34	6.29	-100.11	0.9819
#XOZBUK	0.66	1.87	1.21	1.80	0.2057
#XOZBUK	-63.88	-57.05	6.83	-57.68	1.0378
#XOZBUK	-27.92	-26.54	1.38	-26.54	0.2400
#XOZBUK	-91.14	-81.72	9.42	-82.42	1.4091
#ZIVKOE '	1.56	1.44	-0.11	1.51	0.0614
#ZIVKOE '	-86.25	-81.49	4.76	-81.99	0.6677
#ZIVKOE '	-35.13	-33.01	2.12	-33.13	0.3864
#ZIVKOE '	-119.82	-113.05	6.77	-113.61	0.9656
#ZZZITY01	0.09	0.15	0.06	0.15	0.0115
#ZZZITY01	-62.64	-54.62	8.01	-55.65	1.3092
#ZZZITY01	-7.28	-6.06	1.21	-6.08	0.2484
#ZZZITY01	-69.82	-60.53	9.29	-61.58	1.5438
#ZZZSPY01	0.16	0.16	0.00	0.16	0.0047
#ZZZSPY01	-61.95	-55.41	6.55	-55.75	1.0897
#ZZZSPY01	-6.12	-5.13	1.00	-5.26	0.2217
#ZZZSPY01	-67.92	-60.37	7.55	-60.85	1.2846

300 K runs, energies, convergence test last 2 Mstep
for each crystal: intramolecular, LP, Coulombic, total lattice energy
start: 3 Mstep frame, end: end of the 5Mstep MC run

	start	end	%delt	aver	rmsd
#ABUMIT	0.00	0.00	0.00	0.00	0.0000
#ABUMIT	-62.24	-62.14	0.10	-62.21	0.1748
#ABUMIT	-2.90	-2.94	-0.04	-2.91	0.0272
#ABUMIT	-65.14	-65.08	0.06	-65.13	0.1856
#BENZEN07	0.00	0.00	0.00	0.00	0.0000
#BENZEN07	-37.27	-37.18	0.09	-37.14	0.2140
#BENZEN07	-6.85	-6.73	0.12	-6.73	0.0828
#BENZEN07	-44.12	-43.91	0.21	-43.86	0.2791
#BILNOZ01	0.00	0.00	0.00	0.00	0.0000
#BILNOZ01	-58.94	-57.78	1.16	-58.15	0.4314
#BILNOZ01	-2.95	-2.88	0.07	-2.94	0.0324
#BILNOZ01	-61.89	-60.65	1.23	-61.09	0.4480
#BNZQUI03	0.00	0.00	0.00	0.00	0.0000
#BNZQUI03	-46.24	-45.95	0.29	-46.24	0.2020
#BNZQUI03	-24.89	-25.18	-0.30	-24.93	0.1414
#BNZQUI03	-71.13	-71.14	-0.01	-71.17	0.2043
#BULVAL03	0.00	0.00	0.00	0.00	0.0000
#BULVAL03	-57.90	-57.73	0.17	-57.72	0.1810
#BULVAL03	-7.17	-7.32	-0.15	-7.28	0.0796
#BULVAL03	-65.07	-65.05	0.02	-64.99	0.1933
#CECGEX	0.00	0.00	0.00	0.00	0.0000
#CECGEX	-62.29	-61.67	0.62	-61.81	0.2841
#CECGEX	-31.98	-31.89	0.09	-31.93	0.1703
#CECGEX	-94.27	-93.56	0.71	-93.74	0.2761
#CTCYDD	0.00	0.00	0.00	0.00	0.0000
#CTCYDD	-84.54	-84.05	0.49	-84.17	0.2976
#CTCYDD	-2.12	-2.09	0.03	-2.11	0.0514
#CTCYDD	-86.66	-86.14	0.52	-86.28	0.3178
#DAZNAP	0.00	0.00	0.00	0.00	0.0000
#DAZNAP	-66.98	-66.96	0.03	-67.13	0.1645
#DAZNAP	-21.24	-21.07	0.17	-21.09	0.0926
#DAZNAP	-88.22	-88.03	0.20	-88.22	0.1573
#DCBDOX10	0.00	0.00	0.00	0.00	0.0000
#DCBDOX10	-113.07	-113.12	-0.04	-113.16	0.2244
#DCBDOX10	-1.83	-1.77	0.06	-1.87	0.0691
#DCBDOX10	-114.90	-114.88	0.02	-115.03	0.2466
#DCLBEN01	0.00	0.00	0.00	0.00	0.0000
#DCLBEN01	-64.93	-64.73	0.20	-64.80	0.1803
#DCLBEN01	-2.52	-2.49	0.03	-2.51	0.0311
#DCLBEN01	-67.45	-67.21	0.24	-67.31	0.1882
#DCLBEN02	0.00	0.00	0.00	0.00	0.0000
#DCLBEN02	-67.73	-67.67	0.06	-67.63	0.2362
#DCLBEN02	-3.26	-3.12	0.14	-3.23	0.0521
#DCLBEN02	-70.99	-70.79	0.20	-70.87	0.2481
#DEZDUH	0.00	0.00	0.00	0.00	0.0000
#DEZDUH	-43.44	-43.43	0.01	-43.38	0.2650
#DEZDUH	-15.40	-15.33	0.08	-15.38	0.0681
#DEZDUH	-58.85	-58.75	0.09	-58.76	0.3039
#DEZXEL	0.00	0.00	0.00	0.00	0.0000
#DEZXEL	-83.44	-83.62	-0.17	-83.32	0.1977
#DEZXEL	-16.10	-16.07	0.03	-16.14	0.0769
#DEZXEL	-99.54	-99.68	-0.14	-99.47	0.1889
#DITBOX	0.00	0.00	0.00	0.00	0.0000
#DITBOX	-85.72	-85.64	0.08	-85.50	0.2458
#DITBOX	-8.16	-8.13	0.03	-8.14	0.0561
#DITBOX	-93.88	-93.77	0.11	-93.64	0.2653
#EZURUM	0.00	0.00	0.00	0.00	0.0000
#EZURUM	-67.83	-67.38	0.45	-67.23	0.3305
#EZURUM	-20.05	-20.06	-0.01	-19.86	0.1558
#EZURUM	-87.88	-87.44	0.44	-87.09	0.3963
#FACGEV	0.00	0.00	0.00	0.00	0.0000
#FACGEV	-38.74	-38.48	0.26	-38.73	0.1828

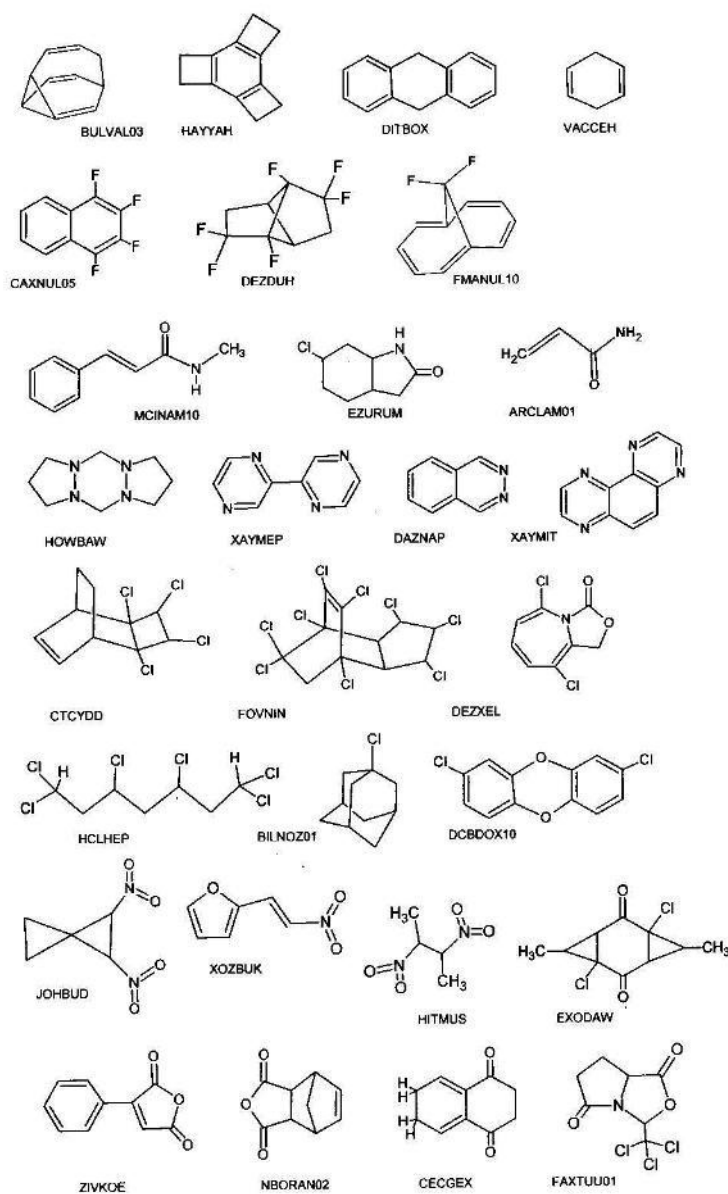
#FACGEV	-4.68	-4.56	0.12	-4.67	0.0787
#FACGEV	-43.42	-43.04	0.38	-43.41	0.2219
#FACJAU	0.00	0.00	0.00	0.00	0.0000
#FACJAU	-36.73	-36.01	0.72	-36.34	0.2744
#FACJAU	-9.50	-9.35	0.15	-9.35	0.0607
#FACJAU	-46.23	-45.35	0.87	-45.69	0.2926
#FMANUL01	0.00	0.00	0.00	0.00	0.0000
#FMANUL01	-67.22	-68.00	-0.78	-67.71	0.2049
#FMANUL01	-9.74	-9.91	-0.17	-9.81	0.0674
#FMANUL01	-76.97	-77.91	-0.94	-77.52	0.2330
#FOVNIN	0.00	0.00	0.00	0.00	0.0000
#FOVNIN	-96.19	-96.60	-0.41	-96.55	0.3677
#FOVNIN	-3.70	-3.74	-0.03	-3.70	0.0402
#FOVNIN	-99.90	-100.33	-0.44	-100.25	0.3731
#HAYYAH	0.00	0.00	0.00	0.00	0.0000
#HAYYAH	-71.54	-71.38	0.16	-71.18	0.2466
#HAYYAH	-7.97	-7.85	0.12	-7.90	0.0754
#HAYYAH	-79.51	-79.23	0.28	-79.09	0.2641
#HCLBNZ11	0.00	0.00	0.00	0.00	0.0000
#HCLBNZ11	-103.47	-102.86	0.61	-103.44	0.3799
#HCLBNZ11	8.58	8.32	-0.26	8.51	0.1550
#HCLBNZ11	-94.89	-94.54	0.35	-94.94	0.2578
#HOWBAW	0.00	0.00	0.00	0.00	0.0000
#HOWBAW	-76.84	-76.26	0.59	-76.59	0.2744
#HOWBAW	-10.39	-10.13	0.26	-10.33	0.1421
#HOWBAW	-87.24	-86.39	0.85	-86.91	0.3525
#NAPHTA10	0.00	0.00	0.00	0.00	0.0000
#NAPHTA10	-71.70	-72.17	-0.47	-71.87	0.2441
#NAPHTA10	-8.09	-8.20	-0.11	-8.13	0.0802
#NAPHTA10	-79.79	-80.37	-0.58	-80.00	0.2596
#NBOAN02	0.00	0.00	0.00	0.00	0.0000
#NBOAN02	-58.13	-58.16	-0.02	-58.37	0.1584
#NBOAN02	-32.32	-32.73	-0.41	-32.37	0.1576
#NBOAN02	-90.45	-90.89	-0.44	-90.74	0.1901
#PUGDEB	0.00	0.00	0.00	0.00	0.0000
#PUGDEB	-42.41	-41.65	0.76	-41.80	0.2172
#PUGDEB	-5.98	-5.46	0.52	-5.64	0.1390
#PUGDEB	-48.39	-47.11	1.28	-47.44	0.3169
#TCHLBZ03	0.00	0.00	0.00	0.00	0.0000
#TCHLBZ03	-75.37	-75.09	0.29	-75.28	0.2490
#TCHLBZ03	0.03	-0.01	-0.05	-0.03	0.0334
#TCHLBZ03	-75.34	-75.10	0.24	-75.31	0.2505
#TEPNIT11	0.00	0.00	0.00	0.00	0.0000
#TEPNIT11	-70.85	-70.94	-0.09	-70.71	0.2050
#TEPNIT11	-30.39	-30.14	0.25	-30.31	0.0935
#TEPNIT11	-101.24	-101.08	0.16	-101.03	0.2303
#VACCEH	0.00	0.00	0.00	0.00	0.0000
#VACCEH	-42.06	-41.72	0.34	-41.83	0.2218
#VACCEH	-5.53	-5.55	-0.02	-5.45	0.0530
#VACCEH	-47.59	-47.27	0.32	-47.28	0.2323
#XAYMIT	0.00	0.00	0.00	0.00	0.0000
#XAYMIT	-100.38	-100.20	0.18	-100.57	0.2800
#XAYMIT	-14.45	-14.57	-0.12	-14.57	0.1434
#XAYMIT	-114.82	-114.77	0.06	-115.14	0.2462
#YUYPUD01	0.00	0.00	0.00	0.00	0.0000
#YUYPUD01	-67.43	-67.39	0.05	-67.17	0.2763
#YUYPUD01	-28.98	-28.93	0.05	-29.04	0.1639
#YUYPUD01	-96.41	-96.32	0.10	-96.21	0.3905
#ACANIL01	4.62	4.44	-0.18	4.66	0.1390
#ACANIL01	-66.88	-66.71	0.17	-66.87	0.2328
#ACANIL01	-33.40	-33.42	-0.01	-33.49	0.1473
#ACANIL01	-95.66	-95.68	-0.03	-95.71	0.3258
#ADIPAC07	8.70	8.87	0.17	8.58	0.2355
#ADIPAC07	-81.70	-82.20	-0.50	-82.06	0.3211
#ADIPAC07	-42.71	-42.22	0.49	-42.65	0.3457
#ADIPAC07	-115.71	-115.55	0.16	-116.13	0.4433
#ARCLAM01	5.78	5.25	-0.53	5.61	0.1795
#ARCLAM01	-46.48	-46.07	0.41	-46.30	0.1697
#ARCLAM01	-30.29	-30.50	-0.21	-30.46	0.1342
#ARCLAM01	-70.99	-71.32	-0.33	-71.15	0.2228
#AYOJED	0.10	0.10	-0.00	0.10	0.0021
#AYOJED	-61.38	-61.28	0.09	-61.62	0.2523
#AYOJED	-4.76	-4.71	0.05	-4.78	0.0801
#AYOJED	-66.03	-65.90	0.14	-66.31	0.2918
#BENZAC07	3.30	3.28	-0.02	3.24	0.1177
#BENZAC07	-61.17	-61.16	0.00	-60.99	0.1703
#BENZAC07	-21.12	-21.09	0.03	-21.01	0.1898
#BENZAC07	-78.99	-78.98	0.01	-78.76	0.2275
#BIPHEN04	5.57	5.59	0.02	5.56	0.0382
#BIPHEN04	-82.46	-82.85	-0.39	-82.72	0.2560
#BIPHEN04	-11.80	-11.85	-0.05	-11.88	0.0874
#BIPHEN04	-88.69	-89.11	-0.42	-89.04	0.3018
#BZAMID01	5.57	5.78	0.21	5.86	0.1550
#BZAMID01	-67.79	-68.32	-0.53	-68.03	0.2466
#BZAMID01	-30.30	-30.42	-0.12	-30.51	0.1929
#BZAMID01	-92.52	-92.96	-0.44	-92.68	0.3375
#DNBENZ14	0.64	0.70	0.06	0.62	0.0508
#DNBENZ14	-65.46	-65.06	0.40	-65.20	0.2057
#DNBENZ14	-12.00	-11.97	0.04	-11.97	0.1377
#DNBENZ14	-76.82	-76.32	0.50	-76.56	0.2300

#DNITBZ11	0.50	0.53	0.03	0.54	0.0296
#DNITBZ11	-66.63	-65.99	0.64	-66.17	0.2810
#DNITBZ11	-19.67	-19.56	0.11	-19.60	0.0910
#DNITBZ11	-85.80	-85.02	0.78	-85.24	0.3253
#EXODAW	2.56	2.71	0.15	2.66	0.1039
#EXODAW	-82.11	-81.93	0.18	-82.28	0.2824
#EXODAW	-27.82	-27.61	0.21	-27.69	0.1302
#EXODAW	-107.38	-106.84	0.53	-107.31	0.3280
#FAXTUU01	0.89	0.92	0.03	0.91	0.0380
#FAXTUU01	-81.20	-81.71	-0.51	-81.43	0.1785
#FAXTUU01	-27.00	-26.72	0.27	-26.85	0.1156
#FAXTUU01	-107.31	-107.51	-0.21	-107.37	0.1630
#FOVQOX	8.20	8.30	0.11	8.27	0.1160
#FOVQOX	-69.53	-69.63	-0.09	-69.76	0.2203
#FOVQOX	-58.14	-58.41	-0.27	-58.25	0.2259
#FOVQOX	-119.48	-119.74	-0.26	-119.75	0.2636
#GLURAC03	10.81	10.60	-0.21	10.65	0.1505
#GLURAC03	-76.82	-76.04	0.77	-76.43	0.2612
#GLURAC03	-50.26	-49.99	0.27	-49.96	0.2618
#GLURAC03	-116.27	-115.43	0.83	-115.74	0.3816
#HEPTAN02	5.96	5.87	-0.08	5.94	0.1104
#HEPTAN02	-53.80	-53.13	0.67	-53.74	0.4628
#HEPTAN02	0.10	0.03	-0.07	0.04	0.0390
#HEPTAN02	-47.74	-47.22	0.52	-47.77	0.4819
#HEXANE01	5.44	1.17	-4.27	2.23	1.5853
#HEXANE01	-47.47	-47.57	-0.10	-47.64	0.1849
#HEXANE01	0.01	0.05	0.03	0.05	0.0269
#HEXANE01	-42.02	-46.35	-4.34	-45.37	1.6296
#HITMUS	3.44	3.17	-0.27	3.07	0.1578
#HITMUS	-65.91	-65.86	0.05	-66.21	0.2842
#HITMUS	-28.85	-29.20	-0.35	-29.11	0.1603
#HITMUS	-91.32	-91.89	-0.58	-92.25	0.4517
#JOHBUD	0.89	0.92	0.02	0.89	0.0178
#JOHBUD	-47.61	-47.86	-0.26	-47.63	0.1990
#JOHBUD	-21.20	-21.17	0.03	-21.23	0.1122
#JOHBUD	-67.92	-68.11	-0.20	-67.97	0.2507
#MCINAM10	8.72	8.11	-0.61	8.52	0.2836
#MCINAM10	-72.82	-73.51	-0.68	-73.43	0.3296
#MCINAM10	-20.57	-20.60	-0.04	-20.60	0.2645
#MCINAM10	-84.67	-85.99	-1.33	-85.50	0.5419
#NITRBE01	0.22	0.22	0.00	0.24	0.0210
#NITRBE01	-53.73	-54.71	-0.98	-54.12	0.3202
#NITRBE01	-11.22	-11.34	-0.13	-11.28	0.0650
#NITRBE01	-64.73	-65.83	-1.10	-65.16	0.3484
#OCTANE01	1.75	-3.09	-4.84	-0.13	2.2358
#OCTANE01	-64.67	-64.59	0.08	-64.54	0.2476
#OCTANE01	0.21	0.29	0.08	0.23	0.0361
#OCTANE01	-62.70	-67.39	-4.68	-64.44	2.2054
#PHBALD11	2.76	2.93	0.17	2.86	0.1053
#PHBALD11	-67.49	-67.80	-0.31	-67.59	0.3132
#PHBALD11	-39.57	-38.66	0.92	-39.22	0.3040
#PHBALD11	-104.30	-103.52	0.78	-103.95	0.3755
#QATTIO	7.32	7.44	0.12	7.41	0.1579
#QATTIO	-54.70	-54.29	0.41	-54.53	0.1827
#QATTIO	-59.45	-60.37	-0.92	-60.07	0.3374
#QATTIO	-106.83	-107.21	-0.39	-107.19	0.3474
#QATTOU	13.26	13.75	0.49	13.68	0.1969
#QATTOU	-56.12	-56.01	0.11	-56.10	0.2361
#QATTOU	-56.58	-56.71	-0.12	-56.75	0.2305
#QATTOU	-99.45	-98.97	0.48	-99.17	0.2907
#TEPHTH06	5.84	5.93	0.09	6.11	0.2678
#TEPHTH06	-92.89	-93.03	-0.13	-93.07	0.2935
#TEPHTH06	-47.60	-48.38	-0.78	-47.97	0.3011
#TEPHTH06	-134.66	-135.48	-0.82	-134.93	0.3936
#XAYMEP	0.28	0.27	-0.01	0.29	0.0151
#XAYMEP	-89.78	-89.90	-0.12	-89.58	0.2722
#XAYMEP	-10.45	-10.72	-0.27	-10.69	0.1397
#XAYMEP	-99.95	-100.34	-0.39	-99.98	0.2895
#XOZBUK	1.82	1.87	0.05	1.87	0.1057
#XOZBUK	-57.68	-57.05	0.63	-57.29	0.2074
#XOZBUK	-26.56	-26.54	0.02	-26.56	0.0962
#XOZBUK	-82.42	-81.72	0.70	-81.98	0.2713
#ZIVKOE '	1.54	1.44	-0.09	1.49	0.0588
#ZIVKOE '	-81.89	-81.49	0.40	-81.82	0.2537
#ZIVKOE '	-32.89	-33.01	-0.13	-32.97	0.1901
#ZIVKOE '	-113.23	-113.05	0.18	-113.30	0.2907
#ZZZZITY01	0.15	0.15	-0.00	0.16	0.0031
#ZZZZITY01	-55.22	-54.62	0.60	-54.93	0.3290
#ZZZZITY01	-5.99	-6.06	-0.07	-6.03	0.0802
#ZZZZITY01	-61.06	-60.53	0.53	-60.81	0.3440
#ZZZZSPY01	0.16	0.16	0.01	0.16	0.0049
#ZZZZSPY01	-55.42	-55.41	0.01	-55.45	0.3051
#ZZZZSPY01	-5.17	-5.13	0.05	-5.16	0.0576
#ZZZZSPY01	-60.43	-60.37	0.06	-60.45	0.3267

Equilibrium structure and dynamics in organic crystals by Monte Carlo simulation. Critical assessment of force fields and comparison with static packing analysis

Angelo Gavezzotti

Electronic Supplementary Information: Supplementary Figures 1-16.



Scheme. Compounds considered with their Cambridge Structural Database refcodes.

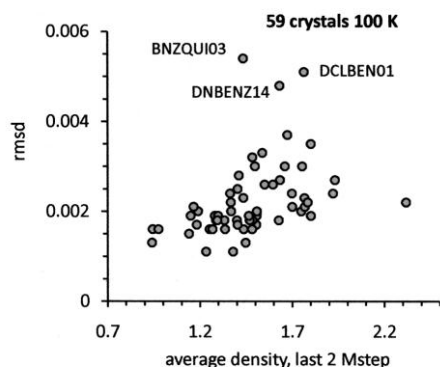
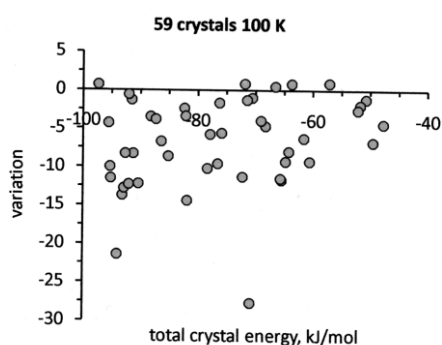
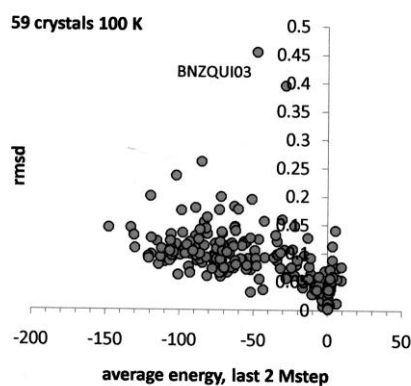


Fig. S1. Convergence of density in the last 2 million steps of the simulations: average values with their root-mean-square deviations (rmsd). Deviating crystals are labeled with their CSD refcode (see Scheme)

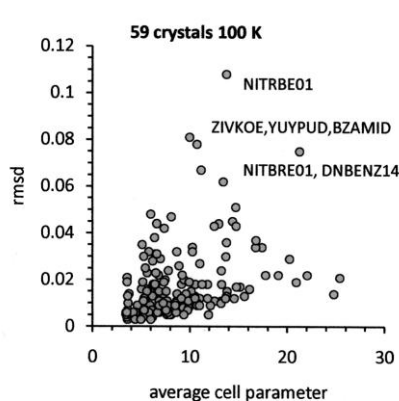


(a)

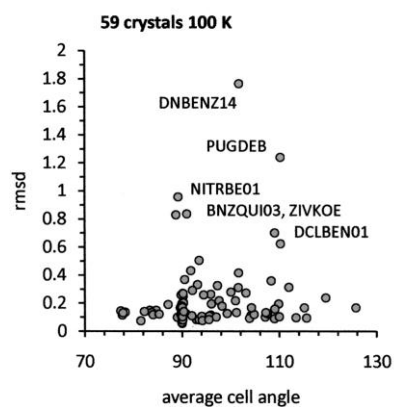


(b)

Fig. S2. (a) Variation in total crystal energy from the experimental crystal structure to the end of the 100 K simulation. (b) Convergence of LP, Coulombic and total energies: average values with their rmsd's.



(a)



(b)

Figure S3. Convergence of cell parameters: (a) average cell edges with their rmsd in the last 2 Msteps of the simulation. (b) The same for cell angles. Deviating crystals are labeled with their CSD refcodes (see Scheme)

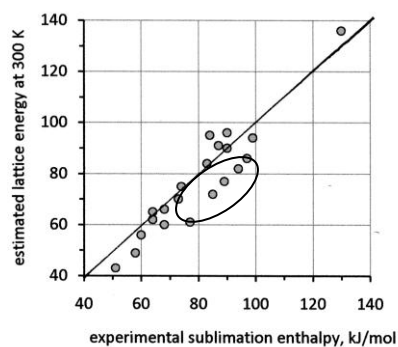


Fig. S4. Comparison between experimental sublimation enthalpies and lattice energies estimated as $E = -U_{\text{lattice}} - 2RT$ at 300 K. For the low-melting compounds (n-alkanes, bullvalene, encircled) this is a rough approximation and results in an underestimation of the sublimation enthalpy.

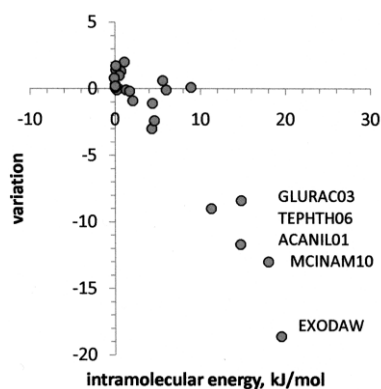


Fig. S5. Variation in intramolecular energies from the experimental crystal structure to the end of the 100 K simulations at 100 K.

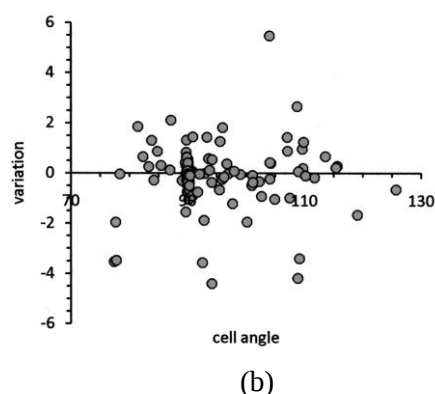
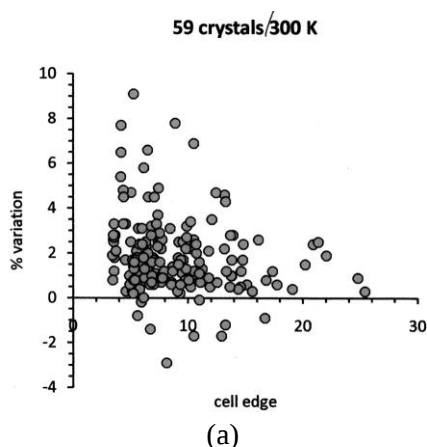


Fig. S6. Percent variation in cell edges (a), and absolute values of variation in cell angles (b), on going from 100 to 300 K.

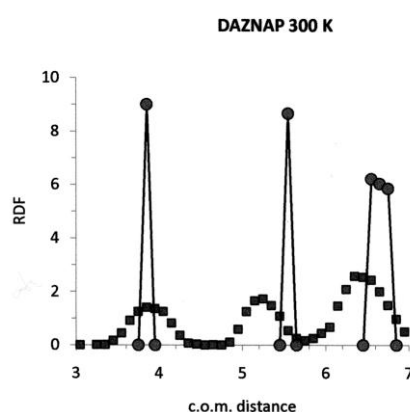
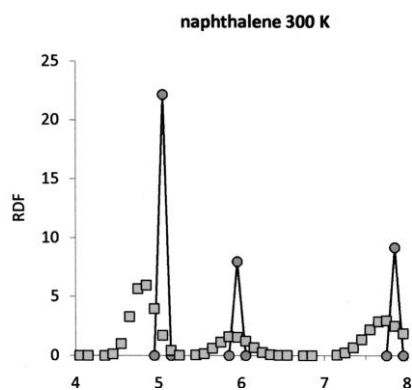


Fig. S7. Shifts in the center-of-mass radial distribution functions from static experimental crystal structure (peaks) to end of simulation (squares).

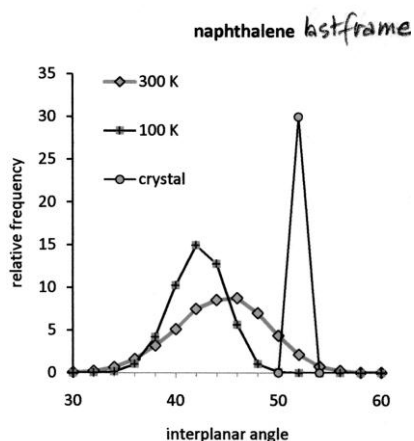


Fig. S8. Spread in the values of angles between molecular planes in the last frame of the simulation of the naphthalene crystal. The single peak at 52° is the value in the static experimental crystal structure.

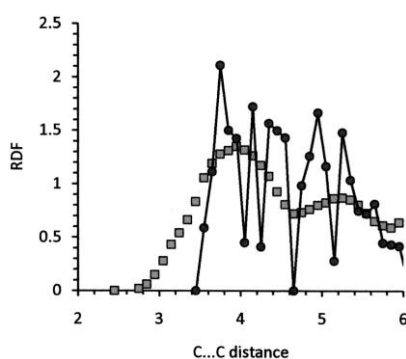
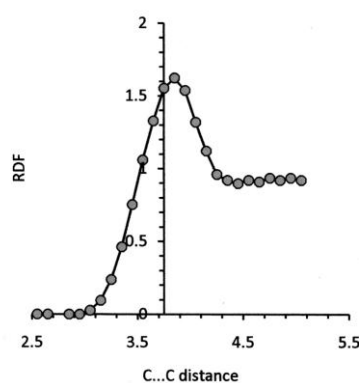


Fig. S9. (a) Radial distribution function of intermolecular C...C distances in the last frame of the naphthalene crystal simulation at 300 K. The vertical axis marks the sum of accepted average intermolecular radii. (b) Similar picture for the 2,3-diazanaphthalene crystal (DAZNAP): squares, last frame of the simulation; circles joined by lines, the single values in the static experimental crystal structure.

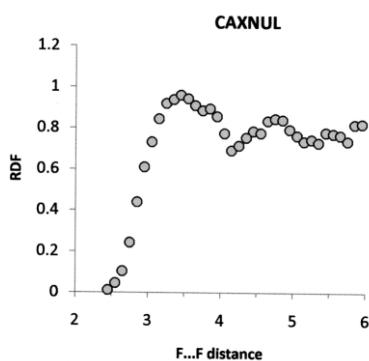


Fig. S10. The inexplicable radial distribution function of F...F contacts in the final frame of the simulation of 1,2,3,4-tetrafluoronaphthalene (CAXNUL).

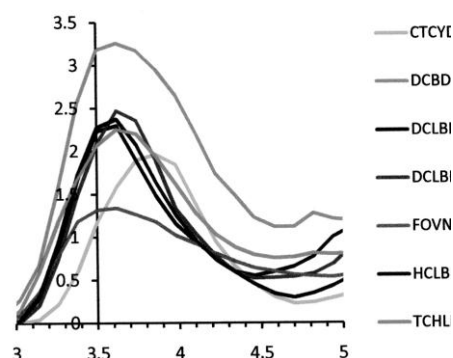


Fig. S11. The Cl...Cl radial distribution functions from the simulation of crystals of chlorinated compounds at 300 K (the picture from the average of the last 10 frames is quite similar with slightly sharper peaks). The areas on the left of the vertical axis are for contacts below the sum of accepted average intermolecular radii.

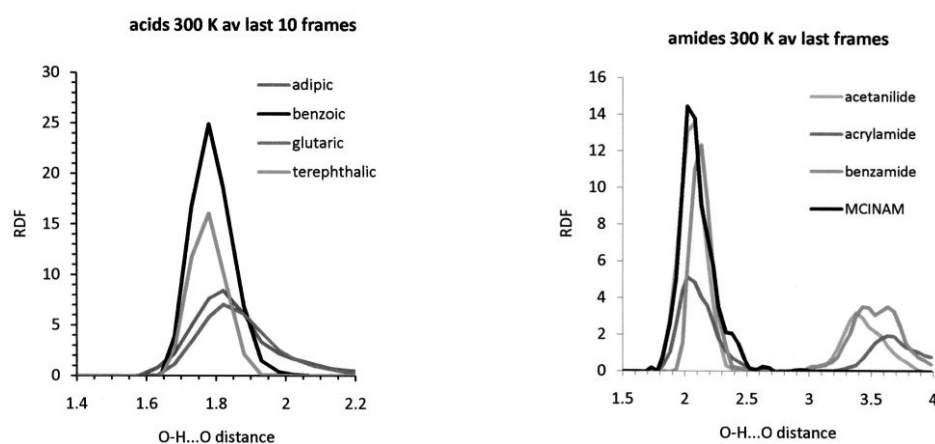


Fig. S12. The radial distribution functions of hydrogen-bonding (a) OH...O distances in acids, and (b) NH...O distances in amides, from the average of the last 10 frames of the crystal simulations at 300 K.

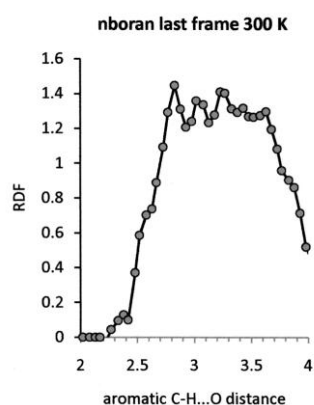


Fig. S13. The dome-shaped radial distribution function of C-H...O distances in the final frame of the simulation at 300 K of the norbornene anhydride crystal (NBORAN02).

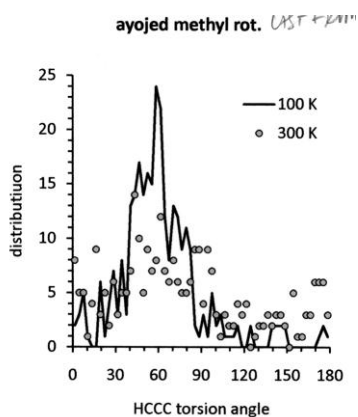


Fig. S14. Spread of methyl torsion angles in the snapshot last frame of the simulation of the methyl ethynylbenzene crystal (AYOJED). Free rotation at 300 K is evident.

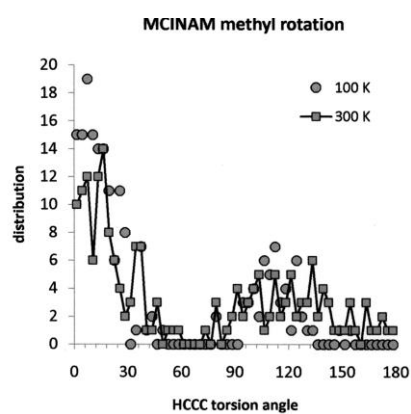
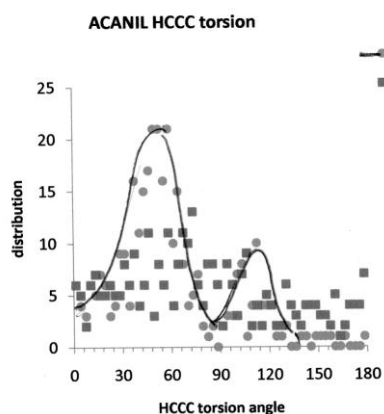


Fig. S15. (a) Methyl rotation in the acetanilide crystal simulation: partial localization (hindered rotation) at 100 K, almost free rotation at 300 K. (b) The same for the methyl group in the MCINAM crystal: hindered rotation at both temperatures. Snapshot (last) frames in both cases.

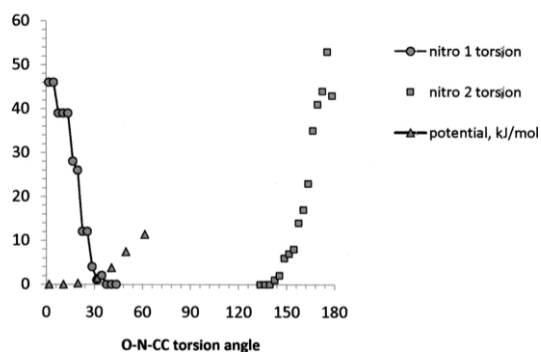


Fig. S16. The spread around planarity ($0-30^\circ$) of nitro group rotations in 1,4-dinitrobenzene: circles, squares, number of molecules in the computational box for each value of the torsion angle. The distribution drops to zero even before the rise of the intramolecular potential (triangles, kJ/mol) above $3RT$.