Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Material for "A study of different approaches to the electrostatic interaction in force field methods for organic crystals" by S.Brodersen, S. Wilke, F.J.J. Leusen, and G. Engel

Containing the full results for Table 2 and Table 4

All force field minimizations start from the DMol-optimized structure and experimental lattice parameters.
ESP-charges and multipoles are fitted to the DMol3 optimized structures.

DMol3 settings:
Fine integration grid, nonlocal DFT (GGA -P91), hexadecapole expansion of density, DNP basis, ions and zwitterions spin unrestricted, ions with appropriate charges

Symbols:

DMol3-Exp.:	rms deviation in Ångstrøm between DMol3-optimized molecule (in vacuum) and experiment (crystal)
a,b,c:	Lattice constants in Ångstrøm
α, β, γ:	Lattice angles in degree
rms dev.:	rms-deviation between experimental structure and Force-Field optimized structure for a molecule in the crystal (for each molecule) in Ångstrøm
Δx:	Translation of the molecule in Ångstrøm
$\Delta\varphi$:	Rotation of the molecule in degree
F:	Structural drift factor = $(\Delta\varphi/2)^2 + (10\Delta x)^2 + (100\Delta a/a)^2 + (100\Delta b/b)^2 + (100\Delta c/c)^2 + \Delta\alpha^2 + \Delta\beta^2 + \Delta\gamma^2$

Results for Table 2: Full Optimization

Name	DMol3 - Exp. rms		Exp	esp-charges	% error	multi-1	% error	multi-2	% error	multi-3	% error	Gasteiger	% error
HACCIX	0.105848	a	11.295	11.339	0.38955	11.229	-0.5843	11.291	-0.0354	11.299	0.03541	11.352	0.50465
SpaceGroup	P21	b	6.08	6.292	3.48684	6.299	3.60197	6.322	3.98026	6.32	3.94737	6.283	3.33882
# Conform.	1	c	16.124	16.386	1.62491	16.418	1.82337	16.382	1.6001	16.373	1.54428	16.365	1.49467
# Molecules	1	α	90		-		-		-		-		-

		β	105.7	106.549	0.80322	105.543	-0.1485	106.526	0.78146	106.427	0.6878	106.015	0.29801
		γ	90		-		-		-		-		-
		Δx			0.063		0.025		0.049		0.051		0.033
		Δφ			3.717		1.758		4.856		3.716		1.687
		F			19.5219		17.5001		25.2216		22.2086		14.556
		rms dev.			0.12419		0.1267		0.13716		0.13886		0.11042
HACNUU	0.0986907	a	10.359	10.52	1.5542	10.513	1.48663	10.382	0.22203	10.468	1.05223	10.417	0.5599
SpaceGroup	P212121	b	11.657	11.762	0.90075	11.737	0.68628	11.997	2.9167	11.818	1.38114	11.986	2.82234
# Conform.	1	c	20.038	20.247	1.04302	20.242	1.01807	20.132	0.46911	20.274	1.17776	20.121	0.41421
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.048		0.021		0.052		0.067		0.04
		Δφ			0.833		1.19		1.79		0.767		2.123
		F			4.71865		4.11564		9.84794		4.99783		9.73744
		rms dev.			0.11197		0.11143		0.12751		0.11776		0.11145
LABHAX	0.0644755	a	8.654	8.805	1.74486	8.87	2.49596	8.772	1.36353	8.788	1.54842	8.79	1.57153
SpaceGroup	P21	b	6.428	6.547	1.85128	6.49	0.96453	6.557	2.00685	6.555	1.97573	6.597	2.62912
# Conform.	1	c	21.032	21.094	0.29479	21.148	0.55154	21.089	0.27102	21.077	0.21396	21.235	0.9652
# Molecules	1	α	90		-		-		-		-		-
		β	95.7	98.241	2.65517	97.373	1.74817	96.683	1.02717	96.607	0.94775	98.767	3.20481
		γ	90		-		-		-		-		-
		Δx			0.07		0.088		0.065		0.071		0.062
		Δφ			2.37		2.002		2.467		2.197		2.956
		F			14.9096		12.0396		8.87041		8.88034		22.289
		rms dev.			0.15232		0.13189		0.15876		0.15465		0.15353

LABHAX01	0.332749	a	10.83	10.064	-7.0729	10.093	-6.8052	10.92	0.83102	10.82	-0.0923	10.011	-7.5623
SpaceGroup	P212121	b	12.703	12.595	-0.8502	12.557	-1.1493	12.535	-1.3225	12.71	0.05511	12.873	1.33827
# Conform.	1	c	17.49	19.709	12.6872	19.674	12.4871	17.693	1.16066	17.647	0.89766	19.47	11.3208
# Molecules	1	α	90	-		-		-		-		-	
		β	90	-		-		-		-		-	
		γ	90	-		-		-		-		-	
		Δx		0.22		0.265		0.097		0.081		0.213	
		Δφ		7.909		8.028		3.523		3.454		5.522	
		F		232.194		226.695		7.83059		4.45598		199.299	
		rms dev.		0.32798		0.3214		0.12524		0.12576		0.30204	
VOXJEX	0.0765815	a	7.353	7.359	0.0816	7.399	0.62559	7.362	0.1224	7.351	-0.0272	7.35	-0.0408
SpaceGroup	P212121	b	10.153	10.366	2.0979	10.394	2.37368	10.419	2.61992	10.463	3.05328	10.364	2.0782
# Conform.	1	c	25.324	25.232	-0.3633	24.984	-1.3426	25.089	-0.928	25.049	-1.0859	25.409	0.33565
# Molecules	1	α	90	-		-		-		-		-	
		β	90	-		-		-		-		-	
		γ	90	-		-		-		-		-	
		Δx		0.035		0.049		0.063		0.063		0.058	
		Δφ		6.934		6.755		8.614		11.098		5.361	
		F		16.6824		19.4759		26.6872		41.6908		11.9547	
		rms dev.		0.09915		0.10397		0.12564		0.13301		0.08144	
WASROX	0.352915	a	6.4939	6.485	-0.1371	6.455	-0.599	6.502	0.12473	6.57	1.17187	6.425	-1.061
SpaceGroup	P212121	b	11.803	11.648	-1.3149	11.868	0.549	11.969	1.4047	11.817	0.11692	11.974	1.44707
# Conform.	1	c	35.021	35.932	2.60276	36.236	3.47082	36.412	3.97339	36.554	4.37886	36.376	3.87059
# Molecules	1	α	90	-		-		-		-		-	
		β	90	-		-		-		-		-	
		γ	90	-		-		-		-		-	
		Δx		0.219		0.258		0.088		0.432		0.249	
		Δφ		6.933		6.456		1.518		8.678		7.39	
		F		25.3348		29.7832		19.127		58.0507		38.0543	
		rms dev.		0.38525		0.37913		0.38967		0.47302		0.41969	

WERWUL	0.0694312	a	6.562	6.576	0.21335	6.508	-0.8229	6.572	0.15239	6.58	0.27431	6.523	-0.5943
SpaceGroup	P212121	b	13.583	13.633	0.36811	13.572	-0.081	13.684	0.74358	13.678	0.6994	13.596	0.09571
# Conform.	1	c	22.488	22.379	-0.4847	22.916	1.90324	22.286	-0.8983	22.274	-0.9516	22.083	-1.801
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.023		0.061		0.016		0.017		0.032
		Δφ			2.886		1.896		1.782		2.4		0.51
		F			2.55111		5.57687		2.20248		2.93889		3.77327
		rms dev.			0.10532		0.10357		0.10997		0.11271		0.09869
DETBAA03	0.0752807	a	12.585	12.266	-2.5348	12.345	-1.907	12.113	-3.7505	12.124	-3.6631	12.691	0.84227
	0.0843055	b	22.083	22.063	-0.0906	22.376	1.32681	22.37	1.29964	22.305	1.0053	22.051	-0.1449
	0.0697032	c	6.788	6.603	-2.7254	6.682	-1.5616	6.619	-2.4897	6.598	-2.7991	6.746	-0.6187
	0.0908798	α	90		-		-		-		-		-
SpaceGroup	P21	β	90.92	90.052	-0.9547	89.971	-1.0438	89.993	-1.0196	90.05	-0.9569	90	-1.0119
# Conform.	4	γ	90		-		-		-		-		-
# Molecules	1	Δx			0.705		0.709		0.724		0.712		0.826
		Δx			0.416		0.553		0.563		0.539		0.482
		Δx			0.75		0.72		0.72		0.721		0.874
		Δx			0.569		0.435		0.458		0.454		0.307
		Δφ			1.521		5.1		5.204		4.791		3.738
		Δφ			5.419		3.017		3.534		3.58		4.403
		Δφ			1.817		3.414		2.887		2.609		2.559
		Δφ			3.449		8.582		8.116		7.715		8.159
		F			25.074		20.0936		34.3991		34.1372		14.7029
		rms dev.			0.13498		0.07944		0.14089		0.14304		0.0907
		rms dev.			0.12767		0.06639		0.13644		0.13387		0.07917
		rms dev.			0.12892		0.06719		0.13239		0.13384		0.07914
		rms dev.			0.13145		0.0693		0.13087		0.13773		0.07584

DIWWEL	0.115189	a	8.373	8.547	2.07811	8.53	1.87507	8.587	2.55583	8.547	2.07811	8.514	1.68398
SpaceGroup	P21/C	b	7.268	7.05	-2.9994	7.14	-1.7611	7.285	0.2339	7.044	-3.082	7.014	-3.4948
# Conform.	1	c	17.311	17.995	3.95124	17.828	2.98654	17.539	1.31708	18.012	4.04945	18.099	4.55202
# Molecules	1	α	90		-		-		-		-		-
		β	96.75	99.371	2.70904	99.112	2.44134	99.968	3.3261	99.156	2.48682	99.213	2.54574
		γ	90		-		-		-		-		-
		Δx			0.162		0.191		0.237		0.133		0.114
		Δφ			5.118		3.889		3.603		6.12		6.745
		F			44.9701		28.5452		27.5395		47.1366		54.5098
		rms dev.			0.21544		0.22102		0.22101		0.22877		0.19752
DIWWEL01	0.207507	a	33.15	31.673	-4.4555	32.529	-1.8733	34.845	5.11312	31.247	-5.7406	34.051	2.71795
	0.0803654	b	8.272	8.432	1.93424	8.372	1.2089	8.378	1.28143	8.448	2.12766	8.335	0.76161
	0.0707215	c	26.09	26.752	2.53737	26.417	1.25335	25.367	-2.7712	26.854	2.92833	25.721	-1.4143
SpaceGroup	C2/C	α	90		-		-		-		-		-
# Conform.	3	β	115.22	113.411	-1.57	114.823	-0.3446	117.568	2.03784	112.821	-2.0821	115.404	0.15969
# Molecules	1	γ	90		-		-		-		-		-
		Δx			0.141		0.156		0.174		0.163		0.378
		Δx			0.329		0.347		0.393		0.281		0.074
		Δx			0.177		0.206		0.117		0.219		0.155
		Δφ			4.875		3.509		8.693		5.478		9.67
		Δφ			7.175		9.958		13.377		5.573		14.92
		Δφ			8.992		11.956		16.88		7.88		8.061
		F			39.4114		15.8462		58.1678		56.938		22.5028
		rms dev.			0.24437		0.23482		0.19337		0.29215		0.19892
		rms dev.			0.26398		0.24895		0.28558		0.28773		0.26247
		rms dev.			0.24297		0.18694		0.17358		0.29638		0.14557
DIWWEL02	0.0973831	a	8.429	8.441	0.14237	8.4	-0.3441	8.496	0.79487	8.949	6.16918	8.378	-0.6051

	0.0924936	b	21.053	22.897	8.75885	22.82	8.3931	22.939	8.95834	20.224	-3.9377	20.404	-3.0827
	0.0771921	c	10.199	10.752	5.4221	10.801	5.90254	9.561	-6.2555	11.583	13.57	11.628	14.0112
SpaceGroup	Pc	α	90		-		-		-		-		-
# Conform.	3	β	111.86	120.621	7.83211	120.031	7.30467	111.289	-0.5105	121.834	8.9165	118.935	6.32487
# Molecules	1	γ	90		-		-		-		-		-
		Δx			0.348		0.379		0.442		0.185		0.301
		Δx			1.122		1.276		3.761		1.069		2.281
		Δx			0.791		0.791		0.655		3.445		3.525
		Δφ			34.368		32.638		18.081		11.811		37.009
		Δφ			25.764		25.458		13.489		37.262		35.906
		Δφ			5.236		5.921		5.523		9.582		5.719
		F			257.187		247.373		299.43		527.127		527.885
		rms dev.			0.50317		0.49644		0.23646		0.38883		0.44494
		rms dev.			0.456		0.2678		0.19097		0.51791		0.34122
		rms dev.			0.3676		0.33773		0.28145		0.37403		0.41541
ACSALA	0.0574557	a	11.446	11.243	-1.7735	14.211	24.1569	10.841	-5.2857	10.901	-4.7615	11.12	-2.8482
SpaceGroup	P21/C	b	6.596	6.734	2.09218	5.222	-20.831	6.922	4.94239	6.844	3.75985	6.934	5.12432
# Conform.	1	c	11.388	11.063	-2.8539	11.251	-1.203	11.313	-0.6586	11.223	-1.4489	11.163	-1.9758
# Molecules	1	α	90		-		-		-		-		-
		β	95.55	94.922	-0.6572	82.289	-13.879	97.419	1.95604	95.74	0.19885	96.136	0.61329
		γ	90		-		-		-		-		-
		Δx			0.12		0.154		0.054		0.1		0.173
		Δφ			3.159		13.325		5.589		3.722		3.322
		F			19.9965		1241.54		64.3935		43.407		44.3695
		rms dev.			0.1047		0.56389		0.23264		0.14869		0.19151
AMSALA01	0.0403029	a	7.209	6.671	-7.4629	6.669	-7.4906	6.717	-6.8248	6.679	-7.3519	6.888	-4.4528
SpaceGroup	P21/C	b	3.786	4.343	14.7121	3.862	2.0074	3.821	0.92446	3.843	1.50555	3.854	1.79609
# Conform.	1	c	25.109	25.539	1.71253	25.045	-0.2549	25.263	0.61333	25.26	0.60138	25.585	1.89573
# Molecules	1	α	90		-		-		-		-		-
		β	103.22	117.712	14.0399	102.256	-0.9339	103.255	0.03391	102.966	-0.2461	104.249	0.9969

		γ	90		-		-		-		-		-
		Δx			0.831		0.16		0.173		0.153		0.374
		Δφ			21.023		4.455		5.699		5.522		8.049
		F			664.639		68.6553		58.9225		66.7076		57.8899
		rms dev.			0.07299		0.05152		0.08873		0.06978		0.07468
IBPRAC	0.273649	a	14.667	14.612	-0.375	14.956	1.97041	15.192	3.57946	14.834	1.13861	14.945	1.89541
SpaceGroup	P21/C	b	7.886	7.71	-2.2318	7.754	-1.6739	7.609	-3.5126	7.717	-2.143	7.576	-3.931
# Conform.	1	c	10.73	10.682	-0.4473	10.521	-1.9478	10.694	-0.3355	10.605	-1.165	10.717	-0.1212
# Molecules	1	α	90		-		-		-		-		-
		β	99.362	96.174	-3.2085	97.271	-2.1044	97.389	-1.9857	96.652	-2.7274	94.639	-4.7533
		γ	90		-		-		-		-		-
		Δx			0.092		0.115		0.13		0.108		0.124
		Δφ			7.947		4.506		6.01		6.33		5.632
		F			32.1201		21.249		39.8759		25.7739		50.8343
		rms dev.			0.16107		0.18266		0.23607		0.17531		0.18809
JEKNOC	0.224119	a	12.462	12.453	-0.0722	12.419	-0.345	12.453	-0.0722	12.455	-0.0562	12.507	0.3611
	0.0982151	b	8.035	8.016	-0.2365	7.976	-0.7343	8.12	1.05787	8.06	0.31114	7.862	-2.1531
SpaceGroup	P21	c	13.539	13.223	-2.334	13.241	-2.201	13.22	-2.3562	13.203	-2.4817	13.476	-0.4653
# Conform.	2	α	90		-		-		-		-		-
# Molecules	1	β	112.89	112.893	0.00266	110.547	-2.0755	112.771	-0.1054	112.599	-0.2578	110.959	-1.7105
		γ	90		-		-		-		-		-
		Δx			0.078		0.025		0.097		0.067		0.066
		Δx			0.161		0.116		0.187		0.167		0.15
		Δφ			9.582		6.246		6.482		7.891		15.455
		Δφ			10.616		2.836		7.127		5.989		16.178
		F			11.9898		12.6516		10.3775		9.87903		23.288
		rms dev.			0.18357		0.15607		0.25118		0.20867		0.1773
		rms dev.			0.19527		0.13188		0.20127		0.1619		0.26674

ACMDOB	0.229617	a	8.444	8.6409	2.33183	8.6416	2.34012	8.5777	1.58337	8.5878	1.70298	8.7024	3.06016
SpaceGroup	P21/c	b	19.083	18.5914	-2.5761	18.575	-2.6621	18.7453	-1.7696	18.7034	-1.9892	18.3639	-3.7683
# Conform.	1	c	9.177	9.3753	2.16084	9.3115	1.46562	9.3978	2.40602	9.3578	1.97014	9.5816	4.40885
# Molecules	1	α	90		-		-		-		-		-
		β	109	110.8104	1.66092	109.9636	0.88404	107.987	-0.9294	110.2886	1.1822	111.3661	2.17073
		γ	90		-		-		-		-		-
		Δx			0.157		0.102		0.221		0.143		0.223
		Δφ			3.356		2.617		7.422		3.692		2.819
		F			25.3012		18.3919		31.1094		17.8517		55.5604
		rms dev.			0.16561		0.12309		0.26721		0.16538		0.17322
ACNPHB	0.0634363	a	5.046	5.398	6.97582	5.319	5.41023	4.575	-9.3341	failure		5.155	2.16013
SpaceGroup	P21/c	b	17.84	17.555	-1.5975	17.427	-2.315	19.197	7.6065			17.875	0.19619
# Conform.	1	c	15.689	15.599	-0.5737	16.066	2.40296	16.277	3.74785			16.172	3.07859
# Molecules	1	α	90		-		-		-				-
		β	96.16	113.071	17.5863	113.284	17.8078	97.611	1.50894			110.782	15.2059
		γ	90		-		-		-				-
		Δx			1.491		1.493		0.466				1.448
		Δφ			6.46		4.408		3.346				4.662
		F			570.266		561.398		185.651				443.089
		rms dev.			0.10799		0.07616		0.21871				0.08453
BANGOM01	0.0768037	a	12.738	12.912	1.36599	failure		12.911	1.35814	12.96	1.74282	12.945	1.62506
SpaceGroup	P2	b	7.263	7.965	9.66543			8.178	12.5981	8.329	14.6771	8.184	12.6807
# Conform.	1	c	6.039	6	-2.5832			5.874	-2.7322	5.652	-6.4083	5.788	-4.1563
# Molecules	1	α	90		-				-		-		-
		β	98.15	104.56	6.53082			105.837	7.83189	103.024	4.96587	107.004	9.02089
		γ	90		-				-		-		-
		Δx			0.272				0.328		0.258		0.291
		Δφ			38.57				40.758		40.461		39.878

		F		522.357			653.174		699.208		665.141		
		rms dev.		0.66104			0.71596		0.71901		0.66284		
BANGOM02	0.0752221	a	12.101	12.832	6.04082	11.7	-3.3138	11.45	-5.3797	12.393	2.41302	12.903	6.62755
SpaceGroup	P21/c	b	7.373	7.637	3.58063	7.6	3.0788	7.859	6.59162	8.553	16.0043	7.611	3.22799
# Conform.	1	c	12.89	12.422	-3.6307	14.167	9.9069	13.66	5.97362	11.274	-12.537	12.339	-4.2746
# Molecules	1	α	90	-		-		-		-		-	
		β	95.89	108.808	13.4717	91.016	-5.0829	94.899	-1.0335	98.877	3.11503	101.995	6.36667
		γ	90	-		-		-		-		-	
		Δx		0.244		0.376		0.536		0.57		0.746	
		Δφ		29.477		34.312		42.248		42.383		25.931	
		F		452.546		450.829		584.01		909.626		333.644	
		rms dev.		0.61432		0.73556		0.75972		0.71007		0.6163	
BETPIZ	0.321246	a	17.929	17.005	-5.1537	16.587	-7.4851	16.673	-7.0054	16.785	-6.3807	17.16	-4.2891
SpaceGroup	C2/c	b	5.232	5.33	1.87309	5.424	3.66972	5.503	5.17966	5.402	3.24924	5.666	8.29511
# Conform.	1	c	24.804	24.687	-0.4717	24.835	0.12498	24.631	-0.6975	24.609	-0.7862	25.265	1.85857
# Molecules	1	α	90	-		-		-		-		-	
		β	103.59	104.94	1.30321	105.218	1.57158	106.518	2.82653	105.654	1.99247	117.032	12.9762
		γ	90	-		-		-		-		-	
		Δx		0.083		0.092		0.12		0.066		0.553	
		Δφ		2.634		2.238		4.392		3.289		17.057	
		F		34.5371		74.2579		91.2267		59.2893		374.663	
		rms dev.		0.18552		0.15557		0.2248		0.19608		0.19779	
CICVOZ	0.0580315	a	5.547	5.81	4.7413	5.46	-1.5684	5.845	5.37227	5.778	4.16441	5.968	7.58969
SpaceGroup	P-1	b	10.382	9.594	-7.5901	10.304	-0.7513	9.503	-8.4666	9.666	-6.8966	9.244	-10.961
# Conform.	1	c	10.696	11.008	2.91698	10.677	-0.1776	11.106	3.83321	10.901	1.9166	11.754	9.89155
# Molecules	1	α	87.01	83.419	-4.1271	90.423	3.92254	82.686	-4.9695	83.856	-3.6249	85.404	-1.8458
		β	89.63	90.627	1.11235	89.85	0.24545	90.936	1.4571	89.023	-0.6772	100.806	12.469

		γ	79.9	75.562	-5.4293	78.792	-1.3867	75.347	-5.6984	75.79	-5.1439	74.696	-6.5131
		Δx			0.189		0.087		0.24		0.195		0.407
		Δφ			16.959		3.066		19.202		13.872		35.195
		F			196.779		19.0876		254.309		147.697		756.396
		rms dev.			0.22155		0.15117		0.24851		0.17546		0.3529
JECYIZ	0.346044	a	5.488	5.455	-0.6013	5.477	-0.2004	7.02	27.9155	5.494	0.10933	5.535	0.85641
SpaceGroup	P1	b	8.14	8.241	1.24079	8.233	1.14251	9.004	10.6143	8.28	1.7199	7.952	-2.3096
# Conform.	1	c	8.664	8.764	1.1542	8.742	0.90028	7.454	-13.966	8.676	0.1385	8.557	-1.235
# Molecules	1	α	85.68	87.788	2.46032	87.751	2.41713	84.271	-1.6445	86.958	1.4916	93.53	9.162
		β	74.52	75.687	1.56602	75.265	0.99973	63.209	-15.178	75.444	1.23994	86.372	15.9045
		γ	72.5	72.301	-0.2745	72.342	-0.2179	64.825	-10.586	71.818	-0.9407	82.458	13.7352
		Δx			0		0		0		0		0
		Δφ			16.329		13.263		63.033		18.992		20.259
		F			75.7375		51.0018		2269.1		96.1154		411.454
		rms dev.			0.20284		0.19542		1.09345		0.21733		0.42992
CENRIW	0.112452	a	21.1	20.81	-1.3744	20.515	-2.7725	20.34	-3.6019	17.933	-15.009	20.982	-0.5592
SpaceGroup	C2/c	b	7.45	8.127	9.08725	7.79	4.56376	7.917	6.26846	9.074	21.7987	7.662	2.84564
# Conform.	1	c	17.7	17.021	-3.8362	17.567	-0.7514	17.5	-1.1299	17.681	-0.1073	17.572	-0.7232
# Molecules	1	α	90		-		-		-		-		-
		β	108.3	105.101	-2.9538	101.922	-5.8892	105.958	-2.1625	98.089	-9.4284	108.265	-0.0323
		γ	90		-		-		-		-		-
		Δx			0.088		0.299		0.337		0.35		0.268
		Δφ			8.955		2.902		4.726		13.69		3.302
		F			130.239		80.8037		75.9696		863.846		18.8428
		rms dev.			0.15732		0.25765		0.24839		0.37302		0.15451

DUPTOX	0.145694	a	8.14	8.047	-1.1425	8.039	-1.2408	8.035	-1.2899	8.057	-1.0197	8.053	-1.0688
SpaceGroup	P-1	b	9.504	9.638	1.40993	9.627	1.29419	9.624	1.26263	9.651	1.54672	9.665	1.69402
# Conform.	1	c	10.699	10.684	-0.1402	10.656	-0.4019	10.684	-0.1402	10.555	-1.3459	10.764	0.60753
# Molecules	1	α	76.55	75.896	-0.8543	76.191	-0.469	76.042	-0.6636	76.474	-0.0993	75.571	-1.2789
		β	81.16	80.17	-1.2198	80.44	-0.8871	80.122	-1.279	81.078	-0.101	79.605	-1.916
		γ	74.02	75.763	2.35477	75.936	2.58849	75.981	2.64928	76.807	3.7652	75.27	1.68873
		Δx			0.057		0.063		0.058		0.095		0.071
		Δφ			4.118		4.762		4.47		6.74		3.968
		F			12.3231		13.7604		13.7904		25.2828		13.7605
		rms dev.			0.16545		0.17237		0.1682		0.19306		0.18249
DUPTOX01	0.12554	a	9.269	9.339	0.75521	9.382	1.21912	9.309	0.43155	9.347	0.84151	9.493	2.41666
SpaceGroup	Pbca	b	22.072	22.127	0.24918	20.872	-5.4368	22.284	0.96049	21.017	-4.7798	22.398	1.47698
# Conform.	1	c	14.779	14.992	1.44123	15.691	6.17092	14.873	0.63604	15.64	5.82583	14.749	-0.203
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.454		1.107		0.368		1.07		0.219
		Δφ			10.071		13.737		8.905		13.502		6.564
		F			48.6774		238.846		34.8805		217.561		23.6305
		rms dev.			0.34295		0.38076		0.31463		0.38406		0.30443
EABMEZ	0.174176	a	18.222	18.858	3.49029	18.521	1.64087	18.057	-0.9055	19.084	4.73055	18.634	2.261
SpaceGroup	C2/c	b	11.254	10.647	-5.3936	10.828	-3.7853	11.353	0.87969	10.482	-6.8598	11.157	-0.8619
# Conform.	1	c	18.99	19.577	3.0911	19.126	0.71617	19.495	2.65929	19.493	2.64876	19.248	1.35861
# Molecules	1	α	90		-		-		-		-		-
		β	127.88	127.715	-0.129	126.556	-1.0353	128.867	0.77182	127.454	-0.3331	128.032	0.11886
		γ	90		-		-		-		-		-
		Δx			0.192		0.211		0.038		0.146		0.317
		Δφ			4.702		2.707		4.598		4.357		3.786
		F			60.0692		25.5711		15.0696		83.5096		21.3563

		rms dev.		0.17285		0.12093		0.15971		0.17216	0.1403
EABSIJ	0.130504	a	5.933	5.765	-2.8316	5.691	-4.0789	6.496	9.4893	5.717 -3.6407	5.821 -1.8877
SpaceGroup	P212121	b	13.326	13.934	4.56251	14.475	8.62224	17.693	32.7705	14.47 8.58472	13.542 1.62089
# Conform.	1	c	17.546	17.659	0.64402	17.295	-1.4305	12.585	-28.274	17.089 -2.6046	18.026 2.73567
# Molecules	1	α	90		-		-		-	-	-
		β	90		-		-		-	-	-
		γ	90		-		-		-	-	-
		Δx			0.502		0.174		1.298	0.414	1.313
		Δφ			5.448		5.403		51.51	4.314	14.709
		F			61.8699		103.352		2795.19	115.528	240.16
		rms dev.			0.27539		0.18571		0.89829	0.34057	0.27664
EACBOZ	0.341182	a	5.751	6.093	5.94679	5.833	1.42584	5.717	-0.5912	5.87 2.06921	5.745 -0.1043
SpaceGroup	P21	b	10.647	10.394	-2.3763	10.895	2.32929	11.18	5.00611	10.872 2.11327	11.055 3.83207
# Conform.	1	c	12.085	11.671	-3.4257	11.518	-4.6918	11.427	-5.4448	11.524 -4.6421	11.308 -6.4295
# Molecules	1	α	90		-		-		-	-	-
		β	91.95	90.588	-1.4812	89.83	-2.3056	88.584	-3.6607	89.747 -2.3959	88.729 -3.503
		γ	90		-		-		-	-	-
		Δx			0.032		0.04		0.013	0.014	0.067
		Δφ			9.65		5.66		6.92	7.525	12.164
		F			77.9847		42.1346		78.3745	49.326	103.848
		rms dev.			0.2964		0.25028		0.26334	0.29179	0.27232
HAXBUD	0.149316	a	12.642	12.585	-0.4509	12.403	-1.8905	12.63	-0.0949	12.726 0.66445	12.865 1.76396
	0.00922617	b	9.857	8.984	-8.8567	8.77	-11.028	8.811	-10.612	10.157 3.04352	8.125 -17.571
SpaceGroup	Pbca	c	17.383	18.67	7.40379	19.14	10.1076	19.103	9.89472	17.048 -1.9272	12.987 -25.289
# Conform.	1	α	90		-		-		-	-	-
# Molecules	2	β	90		-		-		-	-	-
		γ	90		-		-		-	-	-
		Δx			0.313		0.361		0.427	0.15	0.346

		Δx		0.558		0.351		0.603		0.476	0.172
		Δφ		9.251		9.992		9.524		3.871	13.411
		Δφ		51.926		65.946		74.938		16.218	70.65
		F		317.561		511.73		580.823		37.0209	1278.34
		rms dev.		0.12581		0.16229		0.13319		0.17343	0.14289
HECNAE	0.13227	a	8.771	8.589	-2.075	8.799	0.31923	8.809	0.43325	8.734 -0.4218	8.735 -0.4104
	0.0613704	b	22.553	22.857	1.34794	22.214	-1.5031	22.167	-1.7115	22.41 -0.6341	22.74 0.82916
SpaceGroup	P21/c	c	7.257	7.155	-1.4055	7.102	-2.1359	7.123	-1.8465	7.112 -1.9981	7.224 -0.4547
# Conform.	1	α	90	-		-		-		-	-
# Molecules	2	β	99.33	100.787	1.46683	100.249	0.9252	99.402	0.07249	99.238 -0.0926	102.295 2.985
		γ	90	-		-		-		-	-
		Δx		0.283		0.138		0.129		0.127	0.672
		Δx		0.136		0.407		0.409		0.297	0.185
		Δφ		2.128		1.42		1.857		0.683	2.678
		Δφ		5.776		23.785		20.97		14.308	16.144
		F		15.0538		47.869		38.8291		20.0133	38.7367
		rms dev.		0.08792		0.09346		0.09055		0.09582	0.06373
JAWJIA	0.255955	a	6.9811	6.768	-3.0525	6.855	-1.8063	6.92	-0.8752	6.9926 0.16473	6.701 -4.0123
	0.0315456	b	9.808	9.696	-1.1419	9.775	-0.3365	9.658	-1.5294	9.4997 -3.1434	10.105 3.02814
SpaceGroup	P212121	c	20.61	21.119	2.46967	20.097	-2.4891	20.077	-2.5861	20.4151 -0.9457	21.052 2.14459
# Conform.	1	α	90	-		-		-		-	-
# Molecules	2	β	90	-		-		-		-	-
		γ	90	-		-		-		-	-
		Δx		0.556		0.193		0.075		0.215	0.234
		Δx		0.379		0.213		0.098		0.12	0.336
		Δφ		10.598		12.256		10.716		11.501	11.907
		Δφ		34.928		9.487		11.342		12.952	20.909
		F		111.308		26.6502		25.3908		31.0694	70.2436
		rms dev.		0.14304		0.08226		0.11425		0.32736	0.13223

JIGFUA	0.140091	a	11.77	11.902	1.1215	11.945	1.48683	11.44	-2.8037	11.69	-0.6797	12.37	5.09771
	0.0317166	b	14.276	14.125	-1.0577	13.795	-3.3693	13.894	-2.6758	13.899	-2.6408	14.426	1.05071
SpaceGroup	P212121	c	9.488	9.621	1.40177	9.782	3.09865	10.081	6.25	9.858	3.89966	9.263	-2.3714
# Conform.	1	α	90		-		-		-		-		-
# Molecules	2	β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.101		0.115		0.073		0.138		0.063
		Δx			0.471		0.556		0.687		0.61		0.266
		Δφ			3.486		3.338		6.335		3.888		2.449
		Δφ			13.114		10.118		6.771		6.976		27.419
		F			21.6506		38.3182		71.3896		36.4081		81.9448
		rms dev.			0.32622		0.35267		0.49366		0.36976		0.30358
KUHPAE	0.243098	a	14.348	13.694	-4.5581	13.745	-4.2027	13.782	-3.9448	13.892	-3.1781	13.398	-6.6211
	0.0328502	b	13.086	13.538	3.45407	13.318	1.77289	14.486	10.6985	13.477	2.98793	13.913	6.31973
SpaceGroup	P212121	c	11.851	11.874	0.19408	11.947	0.81006	11.75	-0.8522	11.681	-1.4345	12.199	2.93646
# Conform.	1	α	90		-		-		-		-		-
# Molecules	2	β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.101		0.068		0.1		0.142		0.185
		Δx			0.171		0.385		0.39		0.291		0.247
		Δφ			17.617		12.736		18.072		18.755		13.987
		Δφ			13.639		18.422		15.02		12.604		14.037
		F			64.7547		56.6315		169.31		55.6203		119.324
		rms dev.			0.15067		0.10763		0.14363		0.17787		0.15135
CHAPEP01	0.396506	a	5.892	5.704	-3.1908	5.696	-3.3265	5.64	-4.277	5.643	-4.2261	5.76	-2.2403

	0.0484289	b	12.22	11.138	-8.8543	11.519	-5.7365	11.163	-8.6498	11.146	-8.7889	11.159	-8.6825
SpaceGroup	P212121	c	18.12	19.388	6.99779	18.864	4.10596	19.332	6.68874	19.554	7.91391	19.311	6.57285
# Conform.	1	α	90		-		-		-		-		-
# Molecules	2	β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.247		0.197		0.259		0.221		0.291
		Δx			0.068		0.084		0.156		0.087		0.101
		Δφ			25.653		21.54		20.246		24.582		20.956
		Δφ			8.288		5.537		6.489		8.975		6.256
		F			184.613		92.8932		168.386		201.946		155.872
		rms dev.			0.17235		0.16051		0.17472		0.17971		0.15262
		rms dev.			0.07467		0.05536		0.08286		0.08622		0.12334
CHAPEP02	0.0435696	a	13.48	13.494	0.10386	13.84	2.67062	13.574	0.69733	13.458	-0.1632	13.821	2.52967
	0.0971247	b	8.104	7.665	-5.4171	7.824	-3.4551	7.21	-11.032	7.741	-4.4793	7.264	-10.365
SpaceGroup	P21/c	c	12.98	12.379	-4.6302	11.924	-8.1356	13.006	0.20031	12.353	-4.8305	12.711	-2.0724
# Conform.	1	α	90		-		-		-		-		-
# Molecules	2	β	112.81	114.572	1.56192	113.154	0.30494	116.076	2.89513	114.716	1.68957	115.669	2.53435
		γ	90		-		-		-		-		-
		Δx			0.552		0.624		0.508		0.588		0.52
		Δx			0.221		0.364		0.155		0.24		0.263
		Δφ			19.302		22.224		13.923		20.677		19.049
		Δφ			12.499		13.829		21.633		9.122		22.054
		F			95.7871		141.245		181.306		89.0626		187.873
		rms dev.			0.06762		0.0577		0.06881		0.07898		0.07216
		rms dev.			0.64032		0.6645		0.71762		0.65262		0.65486
GEBMEF	0.174188	a	18.799	18.863	0.34044	19.107	1.63839	19.521	3.84063	19.085	1.52136	18.661	-0.7341
	0.0538661	b	7.726	7.615	-1.4367	7.723	-0.0388	8.59	11.183	7.896	2.20036	10.24	32.5395
SpaceGroup	Pbca	c	22.878	23.964	4.74692	23.195	1.38561	21.027	-8.0907	22.558	-1.3987	20.388	-10.884

# Conform.	1	α	90		-		-		-		-		-
# Molecules	2	β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.384		0.21		0.21		0.206		0.409
		Δx			0.399		0.224		0.375		0.066		0.478
		Δφ			5.079		5.897		15.164		9.122		34.495
		Δφ			2.851		1.483		8.427		2.751		46.246
		F			34.5		9.2735		228.699		15.956		1395.75
		rms dev.			0.17326		0.15347		0.17831		0.16567		0.2139
		rms dev.			0.14041		0.1026		0.3498		0.10473		0.18655
LEKRIC	0.23735	a	9.997	9.966	-0.3101	10.29	2.93088	9.973	-0.2401	10.003	0.06002	9.882	-1.1503
	0.0567607	b	10.347	10.562	2.0779	10.351	0.03866	10.474	1.22741	10.472	1.20808	10.647	2.89939
SpaceGroup	P212121	c	12.68	12.557	-0.97	12.464	-1.7035	12.597	-0.6546	12.58	-0.7886	12.629	-0.4022
# Conform.	1	α	90		-		-		-		-		-
# Molecules	2	β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.113		0.141		0.24		0.175		0.456
		Δx			0.184		0.223		0.293		0.21		0.323
		Δφ			6.194		5.404		6.315		5.956		10.378
		Δφ			4.896		5.154		9.556		7.944		11.836
		F			10.4164		16.719		13.7786		10.1145		33.1853
		rms dev.			0.12348		0.08857		0.15637		0.11382		0.09733
		rms dev.			0.08242		0.07405		0.1084		0.09194		0.09253
LEKROI	0.288239	a	6.228	6.164	-1.0276	6.42	3.08285	6.041	-3.0026	6.167	-0.9794	6.152	-1.2203
	0.0856834	b	6.819	7.634	11.9519	7.489	9.82549	7.78	14.093	7.582	11.1893	6.97	2.2144
SpaceGroup	P1	c	7.494	7.177	-4.2301	6.975	-6.9255	7.202	-3.8965	7.074	-5.6045	7.567	0.97411
# Conform.	1	α	95.42	96.338	0.96206	96.013	0.62146	98.591	3.3232	97.227	1.89373	97.508	2.18822
# Molecules	2	β	99.48	100.358	0.88259	100.288	0.81222	98.216	-1.2706	99.377	-0.1035	103.263	3.80277

		γ	108.99	110.831	1.68915	111.964	2.72869	111.046	1.88641	110.411	1.30379	105.051	-3.6141
		Δx			0		0		0		0		0
		Δx			0.106		0.11		0.169		0.112		0.105
		Δφ			8.538		4.913		12.689		7.774		4.459
		Δφ			6.886		1.672		10.035		5.752		5.012
		F			174.601		165.842		255.761		169.024		44.6164
		rms dev.			0.17673		0.18702		0.32025		0.19733		0.14596
		rms dev.			0.13388		0.11306		0.14366		0.11572		0.89192
PEAMAN01	0.113005	a	8.322	8.581	3.11223	8.978	7.88272	failure		8.457	1.62221	8.482	1.92261
	0.116525	b	6.801	6.668	-1.9556	6.735	-0.9704			6.695	-1.5586	6.683	-1.735
SpaceGroup	P21	c	12.885	12.822	-0.4889	12.687	-1.5367			12.925	0.31044	13.126	1.87039
# Conform.	1	α	90		-		-				-		-
# Molecules	2	β	91.74	86.926	-5.2474	80.608	-12.134			86.098	-6.15	95.85	4.48005
		γ	90		-		-				-		-
		Δx			0.166		0.378				0.05		0.428
		Δx			0.161		0.221				0.232		0.374
		Δφ			18.809		4.007				3.421		17.144
		Δφ			2.362		13.361				19.742		7.354
		F			60.7208		206.316				63.488		56.9237
		rms dev.			0.20981		0.17479				0.141		0.20981
		rms dev.			0.18663		0.29281				0.20043		0.12242
XIMBZB	0.0581995	a	25.47	24.293	-4.6211	25.099	-1.4566	23.583	-7.4087	25.347	-0.4829	26.897	5.60267
	0.12483	b	7.01	7.299	4.12268	7.137	1.8117	7.103	1.32668	7.124	1.62625	6.495	-7.3466
SpaceGroup	C2/c	c	16.29	15.78	-3.1308	15.798	-3.0203	15.989	-1.8478	16.016	-1.682	15.555	-4.512
# Conform.	1	α	90		-		-		-		-		-
# Molecules	2	β	109.1	107.027	-1.9001	110.536	1.31622	112.891	3.47479	112.557	3.16865	81.117	-25.649
		γ	90		-		-		-		-		-

		Δx			0.277		0.13		0.082		0.127		0.925
		Δx			0.106		0.112		0.088		0.054		1.139
		Δφ			2.001		6.251		7.687		6.819		7.875
		Δφ			4.581		2.892		3.099		3.051		14.748
		F			56.2112		20.289		79.0901		21.622		960.063
		rms dev.			0.07901		0.08525		0.09291		0.09214		0.05534
		rms dev.			0.11422		0.11431		0.11265		0.11477		0.28459
XIMBZB01	0.0612426	a	11.55	11.869	2.7619	11.874	2.80519	12.001	3.90476	11.989	3.80087	12.281	6.329
	0.10036	b	27.4	26.761	-2.3321	26.528	-3.1825	26.444	-3.4891	26.565	-3.0474	27.253	-0.5365
SpaceGroup	Pbca	c	8.57	8.396	-2.0303	8.443	-1.4819	8.402	-1.9603	8.385	-2.1587	7.915	-7.6429
# Conform.	1	α	90		-		-		-		-		-
# Molecules	2	β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.085		0.076		0.073		0.056		0.343
		Δx			0.177		0.186		0.203		0.155		0.21
		Δφ			7.451		4.857		6.051		6.587		21.124
		Δφ			5.24		4.25		6.688		5.586		7.579
		F			23.3389		23.806		37.511		33.7345		134.281
		rms dev.			0.06893		0.06134		0.07439		0.07667		0.06197
		rms dev.			0.07344		0.07458		0.06913		0.07004		0.10987
HECFIE	0.433575	a	9.218	9	-2.3649	9.084	-1.4537	9.613	4.28509	8.928	-3.146	8.001	-13.202
	0.0248209	b	7.279	7.377	1.34634	7.297	0.24729	7.312	0.45336	7.313	0.4671	7.683	5.55021
	0.0609003	c	10.957	10.693	-2.4094	10.439	-4.7276	9.82	-10.377	10.623	-3.0483	11.197	2.19038
	0.0711885	α	90		-		-		-		-		-
SpaceGroup	P21	β	110.43	110.702	0.24631	111.653	1.10749	107.499	-2.6542	111.223	0.7181	98.402	-10.892
# Conform.	1	γ	90		-		-		-		-		-
# Molecules	4	Δx			0.067		0.145		0.283		0.089		0.222
		Δx			0.131		0.207		0.517		0.199		1.561
		Δx			0.203		0.317		0.996		0.338		0.596

		Δx			0.328		0.312		1.05		0.352		1.155
		Δφ			3.102		5.505		26.448		2.944		34.354
		Δφ			3.652		2.626		10.207		3.486		29.098
		Δφ			17.391		9.661		64.315		20.426		61.845
		Δφ			17.256		31.389		34.114		26.983		14.341
		F			24.0872		45.0901		245.474		40.0426		475.321
		rms dev.			0.12394		0.15293		0.51315		0.11723		0.14496
		rms dev.			0.0313		0.03022		0.03639		0.03261		0.03097
JILTUT	0.120527	a	17.968	17.77	-1.102	17.765	-1.1298	17.778	-1.0574	17.806	-0.9016	17.367	-3.3448
	0.408685	b	5.7859	5.794	0.14	5.695	-1.5711	5.654	-2.2797	5.642	-2.4871	5.214	-9.8844
	0.0365284	c	14.844	14.349	-3.3347	14.528	-2.1288	14.636	-1.4012	14.618	-1.5225	16.289	9.73457
SpaceGroup	P21/c	α	90		-		-		-		-		-
# Conform.	1	β	103.61	102.483	-1.0916	103.575	-0.0376	102.866	-0.7219	103.497	-0.1129	95.92	-7.4256
# Molecules	3	γ	90		-		-		-		-		-
		Δx			0.111		0.144		0.186		0.197		0.175
		Δx			0.105		0.068		0.057		0.062		0.401
		Δx			0.246		0.161		0.167		0.293		0.208
		Δφ			7.637		1.477		2.804		9.236		10.123
		Δφ			18.867		17.04		14.944		17.027		24.893
		Δφ			9.864		10.184		12.139		13.477		14.909
		F			28.7757		19.8549		20.0835		26.2261		291.69
		rms dev.			0.11483		0.11255		0.13897		0.14506		0.14624
		rms dev.			0.11967		0.06342		0.08837		0.08094		0.32178
BEYZIO	0.0366202	a	7.893	7.9855	1.17192	8.0867	2.45407	7.9583	0.82732	7.979	1.08957	8.216	4.09223
SpaceGroup	P-1	b	8.028	7.8727	-1.9345	7.8681	-1.9918	7.8532	-2.1774	7.8545	-2.1612	8.1911	2.03164
# Conform.	1	c	10.228	10.1661	-0.6052	10.2613	0.32558	10.2255	-0.0244	10.1753	-0.5153	10.2241	-0.0381
# Molecules	1	α	92.61	90.676	-2.0883	90.3824	-2.4054	91.8584	-0.8116	90.4892	-2.29	89.1518	-3.7342
		β	131.84	132.6625	0.62386	133.8457	1.52131	132.3301	0.37174	132.2516	0.3122	134.267	1.84087
		γ	107.68	108.9578	1.18666	108.3946	0.66363	108.1802	0.46452	109.324	1.52675	109.7977	1.96666
		Δx			0.043		0.035		0.045		0.047		0.151
		Δφ			4.852		2.586		4.175		6.347		2.666

		F		17.6019		21.3857		11.0415		23.7853		47.2665	
		rms dev.		0.08109		0.08201		0.07441		0.10202		0.11428	
BEYZIO01	0.0466016	a	7.147	6.877	-3.7778	6.875	-3.8058	6.94	-2.8963	7.003	-2.0148	6.967	-2.5185
SpaceGroup	P21/c	b	16.258	16.711	2.78632	16.743	2.98315	16.586	2.01747	16.493	1.44544	16.62	2.2266
# Conform.	1	c	8.068	8.255	2.3178	8.184	1.43778	8.204	1.68567	8.286	2.70203	8.426	4.43728
# Molecules	1	α	90	-		-		-		-		-	
		β	115.38	117.372	1.72647	116.345	0.83637	116.916	1.33125	117.644	1.96221	116.828	1.25498
		γ	90	-		-		-		-		-	
		Δx		0.152		0.093		0.048		0.061		0.136	
		Δφ		8.544		4.773		5.002		10.558		8.693	
		F		51.9361		32.9419		24.145		46.8155		53.8286	
		rms dev.		0.08492		0.10336		0.08546		0.10471		0.12365	
CAXMOD	0.0519055	a	12.799	14.021	9.54762	12.623	-1.3751	12.034	-5.977	13.688	6.94586	13.38	4.53942
SpaceGroup	Pna21	b	4.846	4.692	-3.1779	4.767	-1.6302	4.857	0.22699	4.739	-2.208	4.654	-3.962
# Conform.	1	c	8.285	7.261	-12.36	8.57	3.43995	8.811	6.34882	7.339	-11.418	7.265	-12.311
# Molecules	1	α	90	-		-		-		-		-	
		β	90	-		-		-		-		-	
		γ	90	-		-		-		-		-	
		Δx		0.188		0.09		0.161		0.246		0.245	
		Δφ		12.782		6.032		6.898		11.803		9.408	
		F		298.397		26.288		90.5717		224.375		216.005	
		rms dev.		0.22696		0.12355		0.10977		0.2067		0.27141	
CAXMOD01	0.154979	a	7.589	7.728	1.8316	7.641	0.6852	7.892	3.99262	7.736	1.93701	6.836	-9.9223
SpaceGroup	P21/a	b	8.13	8.928	9.8155	8.671	6.65437	8.76	7.74908	8.928	9.8155	8.044	-1.0578
# Conform.	1	c	7.812	7.277	-6.8484	7.441	-4.7491	7.361	-5.7732	7.237	-7.3605	8.347	6.84844
# Molecules	1	α	90	-		-		-		-		-	
		β	95.76	90.4575	-5.5373	91.532	-4.4152	91.354	-4.6011	90.884	-5.0919	86.733	-9.4267

		γ	90		-		-		-		-		-
		Δx			0.235		0.599		0.298		0.245		0.801
		Δφ			40.176		50.044		34.446		39.704		36.184
		F			583.767		747.161		434.244		578.152		619.439
		rms dev.			0.27961		0.17046		0.28372		0.27983		0.58916
DIPTOX10	0.0615612	a	5.103	4.935	-3.2922	5.023	-1.5677	5.2562	3.00216	5.018	-1.6657	5.252	2.91985
SpaceGroup	P212121	b	15.209	14.116	-7.1865	14.103	-7.272	12.8464	-15.534	13.745	-9.6259	13.088	-13.946
# Conform.	1	c	8.114	8.243	1.58984	8.098	-0.1972	8.1229	0.10969	8.242	1.57752	7.994	-1.4789
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.255		0.201		0.304		0.313		0.336
		Δφ			19.349		7.963		34.69		17.173		22.748
		F			165.111		75.2712		560.428		181.446		345.852
		rms dev.			0.16544		0.13314		0.46316		0.17427		0.228

Results for Table 4: Rigid Body Optimization

Name	DMol3 - Exp. rms		Exp	esp-charges	% error	multi-1	% error	multi-2	% error	multi-3	% error	Gasteiger	% error
HACCIX	0.105848	a	11.295	11.3358	0.36122	11.3198	0.21957	11.3104	0.13634	11.3215	0.23462	11.3837	0.7853
SpaceGroup	P21	b	6.08	6.3269	4.06086	6.3313	4.13322	6.3297	4.10691	6.3306	4.12171	6.3303	4.11678
# Conform.	1	c	16.124	16.4332	1.91764	16.4461	1.99764	16.4542	2.04788	16.4399	1.95919	16.4248	1.86554

# Molecules	1	α	90		-		-		-		-		-
		β	105.7	106.3782	0.64163	106.4043	0.66632	106.3064	0.5737	106.3744	0.63803	106.4693	0.72781
		γ	90		-		-		-		-		-
		Δx			0.027		0.021		0.023		0.022		0.025
		Δφ			3.652		4.122		3.997		4.016		3.329
		F			24.1655		25.9102		25.4937		25.4173		24.4697
HACNUU	0.0986907	a	10.359	10.5971	2.29848	10.5806	2.1392	10.5807	2.14017	10.5835	2.1672	10.5844	2.17589
SpaceGroup	P212121	b	11.657	11.9121	2.18838	11.9	2.08458	11.8977	2.06485	11.8933	2.02711	11.971	2.69366
# Conform.	1	c	20.038	20.2272	0.94421	20.2562	1.08893	20.2544	1.07995	20.2451	1.03354	20.2337	0.97664
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.029		0.02		0.02		0.02		0.042
		Δφ			0.927		1.013		1.024		0.962		0.973
		F			11.2625		10.404		10.3124		10.1455		13.3572
LABHAX	0.0644755	a	8.654	8.7147	0.70141	8.7286	0.86203	8.7273	0.84701	8.7246	0.81581	8.715	0.70488
SpaceGroup	P21	b	6.428	6.5727	2.25109	6.5715	2.23242	6.5683	2.18264	6.5691	2.19508	6.6163	2.92937
# Conform.	1	c	21.032	21.2425	1.00086	21.1681	0.64711	21.1851	0.72794	21.1975	0.7869	21.2251	0.91812
# Molecules	1	α	90		-		-		-		-		-
		β	95.7	95.4403	-0.2714	95.8159	0.12111	95.5754	-0.1302	95.5646	-0.1415	95.6909	-0.0095
		γ	90		-		-		-		-		-
		Δx			0.034		0.036		0.039		0.039		0.044
		Δφ			1.071		0.899		0.872		0.919		1.262
		F			7.03089		6.49063		6.36895		6.48472		10.5129
LABHAX01	0.332749	a	10.83	11.8168	9.11173	10.0401	-7.2936	10.0662	-7.0526	10.0575	-7.133	10.1766	-6.0332
SpaceGroup	P212121	b	12.703	13.2366	4.20058	12.8114	0.85334	12.7682	0.51326	12.86	1.23593	13.2797	4.53987
# Conform.	1	c	17.49	17.3115	-1.0206	20.4278	16.797	20.5031	17.2276	20.4456	16.8988	19.3709	10.7541
# Molecules	1	α	90		-		-		-		-		-

		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.387		0.2		0.199		0.203		0.235
		Δφ			14.685		8.136		8.464		8.831		4.717
		F			170.599		356.614		368.662		361.594		183.747
VOXJEX	0.0765815	a	7.353	7.4284	1.02543	7.4625	1.48919	7.4602	1.45791	7.4745	1.65239	7.3744	0.29104
SpaceGroup	P212121	b	10.153	10.2781	1.23215	10.2819	1.26958	10.2786	1.23707	10.2774	1.22525	10.3303	1.74628
# Conform.	1	c	25.324	25.4194	0.37672	25.3341	0.03988	25.3395	0.06121	25.3113	-0.0502	25.6238	1.18386
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.011		0.048		0.044		0.051		0.017
		Δφ			0.878		1.429		1.243		1.54		2.057
		F			2.91644		4.572		4.23945		5.08714		5.62243
WASROX	0.352915	a	6.4939	6.7166	3.42937	6.7157	3.41551	6.7188	3.46325	6.7239	3.54179	6.6309	2.10967
SpaceGroup	P212121	b	11.803	11.8159	0.1076	11.8249	0.18385	11.8275	0.20588	11.8105	0.06185	11.9885	1.56991
# Conform.	1	c	35.021	35.5931	1.63504	35.5377	1.47685	35.5042	1.38119	35.539	1.48056	35.5834	1.60734
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.23		0.234		0.234		0.226		0.235
		Δφ			11.362		10.803		10.637		10.794		11.126
		F			52.0093		48.5324		47.7062		48.9753		45.9684
WERWUL	0.0694312	a	6.562	6.5342	-0.4237	6.5266	-0.5395	6.5321	-0.4557	6.5351	-0.4099	6.535	-0.4115
SpaceGroup	P212121	b	13.583	13.5845	0.01104	13.5811	-0.014	13.5892	0.04565	13.5924	0.0692	13.5977	0.10822
# Conform.	1	c	22.488	22.8272	1.50836	22.8747	1.71958	22.841	1.56973	22.8311	1.5257	22.8277	1.51058
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-

		γ	90	-		-		-		-	
		Δx		0.018		0.024		0.022		0.023	
		Δφ		0.737		0.816		0.621		0.601	
		F		2.62294		3.47226		2.81855		2.64381	
DIWWEL	0.115189	a	8.373	8.6414	3.20554	8.6411	3.20196	8.6404	3.1936	8.6471	3.27362
SpaceGroup	P21/C	b	7.268	7.2867	0.25729	7.3018	0.46505	7.2994	0.43203	7.2965	0.39213
# Conform.	1	c	17.311	17.7516	2.5452	17.6827	2.14719	17.6878	2.17665	17.7165	2.34244
# Molecules	1	α	90	-		-		-		-	
		β	96.75	97.9196	1.20889	97.7146	0.997	97.8005	1.08579	98.0083	1.30057
		γ	90	-		-		-		-	
		Δx		0.218		0.18		0.184		0.192	
		Δφ		2.676		2.749		2.805		2.614	
		F		24.7304		21.1389		21.5797		23.3353	
ACSALA	0.0574557	a	11.446	11.6441	1.73074	11.4206	-0.2219	11.4561	0.08824	11.4544	0.07339
SpaceGroup	P21/C	b	6.596	6.5274	-1.04	6.5298	-1.0036	6.5241	-1.0901	6.5404	-0.8429
# Conform.	1	c	11.388	11.3161	-0.6314	11.5102	1.07306	11.4715	0.73323	11.4629	0.65771
# Molecules	1	α	90	-		-		-		-	
		β	95.55	95.9336	0.40147	96.6297	1.12998	96.3585	0.84615	96.6007	1.09963
		γ	90	-		-		-		-	
		Δx		0.09		0.078		0.073		0.086	
		Δφ		2.214		1.503		1.485		1.649	
		F		6.65832		4.5469		3.47151		3.67188	
AMSALA01	0.0403029	a	7.209	6.8288	-5.274	6.85	-4.9799	6.8464	-5.0298	6.8264	-5.3073
SpaceGroup	P21/C	b	3.786	4.2617	12.5647	3.8555	1.83571	3.8472	1.61648	3.8701	2.22134
# Conform.	1	c	25.109	26.0976	3.93723	25.336	0.90406	25.4612	1.40268	25.5897	1.91445
# Molecules	1	α	90	-		-		-		-	

		β	103.22	115.8464	12.2325	103.5685	0.33763	103.4762	0.24821	104.0002	0.75586	104.8863	1.61432
		γ	90		-		-		-		-		-
		Δx			0.654		0.124		0.124		0.106		0.217
		Δφ			18.133		4.996		5.655		6.194		9.239
		F			485.587		36.8855		39.4777		48.0902		103.526
IBPRAC	0.273649	a	14.667	15.7961	7.69823	15.911	8.48163	15.902	8.42026	15.9116	8.48572	15.8449	8.03095
SpaceGroup	P21/C	b	7.886	7.5086	-4.7857	7.4687	-5.2917	7.4707	-5.2663	7.4796	-5.1534	7.4747	-5.2156
# Conform.	1	c	10.73	10.9648	2.18826	10.8319	0.94967	10.8481	1.10065	10.8569	1.18267	11.0018	2.53308
# Molecules	1	α	90		-		-		-		-		-
		β	99.362	95.2212	-4.1674	96.1294	-3.2534	96.0736	-3.3095	95.8987	-3.4855	94.909	-4.4816
		γ	90		-		-		-		-		-
		Δx			0.23		0.196		0.2		0.21		0.336
		Δφ			10.209		9.602		9.688		9.652		6.854
		F			135.446		138.182		138.124		139.659		140.978
ACMDOB	0.229617	a	8.444	8.5483	1.2352	8.5616	1.3927	8.5516	1.27428	8.5279	0.9936	8.4528	0.10422
SpaceGroup	P21/c	b	19.083	19.3932	1.62553	19.3312	1.30063	19.3624	1.46413	19.4683	2.01907	19.1388	0.29241
# Conform.	1	c	9.177	9.5436	3.99477	9.542	3.97733	9.534	3.89016	9.5057	3.58178	9.9415	8.33061
# Molecules	1	α	90		-		-		-		-		-
		β	109	111.4062	2.20752	111.6607	2.44101	111.585	2.37156	111.1132	1.93872	113.6465	4.26284
		γ	90		-		-		-		-		-
		Δx			0.038		0.056		0.063		0.053		0.092
		Δφ			2.438		2.386		2.23		2.269		1.797
		F			27.5464		28.2666		27.2232		23.9267		92.7391
ACNPHB	0.0634363	a	5.046	5.3632	6.28617	5.1652	2.36227	5.095	0.97107	4.6403	-8.04	5.011	-0.6936
SpaceGroup	P21/c	b	17.84	17.9111	0.39854	18.3764	3.00673	18.4171	3.23487	18.9795	6.38733	18.742	5.05605
# Conform.	1	c	15.689	15.0601	-4.0085	15.5001	-1.204	15.6609	-0.1791	16.5052	5.20237	15.3784	-1.9797
# Molecules	1	α	90		-		-		-		-		-
		β	96.16	96.3906	0.23981	92.2218	-4.0955	92.3952	-3.9151	94.291	-1.9436	94.4861	-1.7407
		γ	90		-		-		-		-		-

		Δx			1.773		1.614		1.595		1.656		1.77
		Δφ			10.348		10.26		9.858		13.023		12.82
		F			396.919		318.396		304.311		452.631		387.144
BANGOM01	0.0768037	a	12.738	12.9776	1.88099	12.9572	1.72084	12.9564	1.71455	12.9708	1.8276	13.0511	2.458
SpaceGroup	P2	b	7.263	7.2626	-0.0055	7.2652	0.03029	7.2631	0.00138	7.2753	0.16935	7.2735	0.14457
# Conform.	1	c	6.039	6	5.73108	6.3708	5.49429	6.3697	5.47607	6.3713	5.50257	6.4254	6.39841
# Molecules	1	α	90		-		-		-		-		-
		β	98.15	100.5166	2.41121	100.0649	1.95099	100.0535	1.93938	100.2918	2.18217	102.6504	4.58523
		γ	90		-		-		-		-		-
		Δx			0.166		0.125		0.149		0.162		0.658
		Δφ			1.246		1.213		1.26		1.174		1.47
		F			45.128		38.7466		39.1674		41.2033		111.093
BANGOM02	0.0752221	a	12.101	12.2954	1.60648	12.288	1.54533	12.2902	1.56351	12.3108	1.73374	12.2613	1.32468
SpaceGroup	P21/c	b	7.373	7.3247	-0.6551	7.342	-0.4205	7.3416	-0.4259	7.346	-0.3662	7.3398	-0.4503
# Conform.	1	c	12.89	13.103	1.65244	13.07	1.39643	13.0646	1.35454	13.0552	1.28161	13.041	1.17145
# Molecules	1	α	90		-		-		-		-		-
		β	95.89	97.1056	1.2677	97.1428	1.3065	97.1427	1.30639	97.3499	1.52247	96.7117	0.85692
		γ	90		-		-		-		-		-
		Δx			0.211		0.201		0.198		0.24		0.171
		Δφ			1.333		1.129		1.098		1.113		1.549
		F			12.1145		10.4431		10.2518		12.9835		7.52899
BETPIZ	0.321246	a	17.929	16.4616	-8.1845	16.5913	-7.4611	16.5664	-7.6	16.5435	-7.7277	17.7124	-1.2081
SpaceGroup	C2/c	b	5.232	6.099	16.5711	6.1778	18.0772	6.1538	17.6185	6.1121	16.8215	6.1257	17.0814
# Conform.	1	c	24.804	24.9072	0.41606	24.7669	-0.1496	24.792	-0.0484	24.8338	0.12014	25.055	1.01193
# Molecules	1	α	90		-		-		-		-		-
		β	103.59	109.9271	6.11748	110.879	7.03639	110.5042	6.67458	110.3427	6.51868	119.0255	14.9006
		γ	90		-		-		-		-		-
		Δx			0.193		0.211		0.202		0.19		0.595
		Δφ			8.791		8.87		8.598		8.932		19.522

		F			404.965		459.727		438.542		411.848		663.193
CICVOZ	0.0580315	a	5.547	5.6708	2.23184	5.5576	0.19109	5.5586	0.20912	5.6513	1.8803	5.9574	7.39859
SpaceGroup	P-1	b	10.382	10.0925	-2.7885	10.3763	-0.0549	10.3426	-0.3795	10.1421	-2.3107	9.6704	-6.8542
# Conform.	1	c	10.696	10.7813	0.79749	10.6512	-0.4188	10.6912	-0.0449	10.7768	0.75542	11.3199	5.83302
# Molecules	1	α	87.01	87.6484	0.73371	91.0728	4.66935	90.6964	4.23675	87.6021	0.6805	90.0839	3.53281
		β	89.63	87.4507	-2.4314	87.7425	-2.1059	87.5869	-2.2795	86.98	-2.9566	95.7306	6.80643
		γ	79.9	77.7894	-2.6416	80.1606	0.32616	79.8579	-0.0527	78.2077	-2.118	74.1943	-7.1411
		Δx			0.099		0.068		0.085		0.081		0.344
		Δφ			4.541		2.787		2.209		3.711		18.76
		F			29.1395		22.7561		19.8978		23.7816		314.782
JECYIZ	0.346044	a	5.488	5.8209	6.06596	5.7818	5.3535	5.7902	5.50656	5.7497	4.76859	5.7708	5.15306
SpaceGroup	P1	b	8.14	8.6294	6.01229	8.5762	5.35872	8.5939	5.57617	8.9156	9.52826	8.4476	3.77887
# Conform.	1	c	8.664	9.1575	5.69598	9.1278	5.35319	9.1186	5.247	9.7225	12.2172	8.7106	0.53786
# Molecules	1	α	85.68	90.5434	5.67624	91.1851	6.42519	91.191	6.43207	89.8895	4.91305	92.9341	8.4665
		β	74.52	74.667	0.19726	75.3832	1.15835	75.4753	1.28194	74.9468	0.57273	77.7414	4.32287
		γ	72.5	71.4111	-1.5019	72.2069	-0.4043	72.0579	-0.6098	62.3104	-14.055	76.0473	4.89283
		Δx			0		0		0		0		0
		Δφ			7.094		7.224		7.269		25.829		8.597
		F			142.829		130.216		133.636		551.302		135.183
CENRIW	0.112452	a	21.1	20.8179	-1.337	20.4977	-2.8545	20.5486	-2.6133	20.4266	-3.1915	21.4318	1.57251
SpaceGroup	C2/c	b	7.45	8.3737	12.3987	8.5399	14.6295	8.5264	14.4483	8.6072	15.5329	7.5733	1.65503
# Conform.	1	c	17.7	17.0814	-3.4949	17.2306	-2.652	17.1901	-2.8808	17.2413	-2.5915	18.058	2.0226
# Molecules	1	α	90		-		-		-		-		-
		β	108.3	103.0993	-4.8021	102.2835	-5.5554	102.3491	-5.4948	102.2982	-5.5418	108.1543	-0.1345
		γ	90		-		-		-		-		-
		Δx			0.088		0.102		0.106		0.114		0.059
		Δφ			10.476		10.927		10.986		10.088		0.722
		F			222.987		296.293		290.592		320.935		9.80249

DUPTOX	0.145694	a	8.14	8.6139	5.82187	9.241	13.5258	8.6121	5.79975	9.2373	13.4803	8.6496	6.26044
SpaceGroup	P-1	b	9.504	9.6931	1.98969	10.1475	6.77083	9.6919	1.97706	10.1383	6.67403	9.6576	1.61616
# Conform.	1	c	10.699	10.5134	-1.7347	9.8462	-7.9708	10.5404	-1.4824	9.853	-7.9073	10.5621	-1.2796
# Molecules	1	α	76.55	74.336	-2.8922	75.1764	-1.7944	74.2111	-3.0554	75.2057	-1.7561	74.1613	-3.1204
		β	81.16	83.1303	2.42767	86.3231	6.36163	82.9493	2.20466	86.2834	6.31272	83.6198	3.0308
		γ	74.02	73.1109	-1.2282	65.0303	-12.145	73.0168	-1.3553	65.0938	-12.059	73.494	-0.7106
		Δx			0.098		0.204		0.088		0.203		0.129
		Δφ			0.329		12.966		0.675		12.795		1.621
		F			51.4601		447.876		50.3101		441.57		57.7966
DUPTOX01	0.12554	a	9.269	9.514	2.64322	9.4923	2.40911	9.4849	2.32927	9.4874	2.35624	9.5073	2.57094
SpaceGroup	Pbca	b	22.072	22.4688	1.79775	22.6474	2.60692	22.6263	2.51133	22.6236	2.49909	22.641	2.57793
# Conform.	1	c	14.779	14.5477	-1.5651	14.4726	-2.0732	14.4875	-1.9724	14.4839	-1.9968	14.5488	-1.5576
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.123		0.153		0.143		0.142		0.145
		Δφ			1.255		1.542		1.379		1.398		1.792
		F			14.5746		19.8334		18.1429		18.2894		18.5869
EABMEZ	0.174176	a	18.222	18.7838	3.08309	18.8157	3.25815	18.8298	3.33553	18.7905	3.11986	18.6374	2.27966
SpaceGroup	C2/c	b	11.254	11.2459	-0.072	11.1805	-0.6531	11.1788	-0.6682	11.1947	-0.5269	11.8021	4.87027
# Conform.	1	c	18.99	18.9517	-0.2017	18.857	-0.7004	18.8935	-0.5082	18.8885	-0.5345	19.0563	0.34913
# Molecules	1	α	90		-		-		-		-		-
		β	127.88	124.1682	-2.9026	123.5032	-3.4226	123.7744	-3.2105	123.737	-3.2398	126.909	-0.7593
		γ	90		-		-		-		-		-
		Δx			0.222		0.244		0.253		0.249		0.381
		Δφ			3.799		4.838		4.461		4.459		2.785
		F			31.8652		42.4941		40.0625		38.632		46.4363

EABSIJ	0.130504	a	5.933	6.0134	1.35513	5.9941	1.02983	6.0295	1.6265	6.0199	1.46469	6.1892	4.31822
SpaceGroup	P212121	b	13.326	13.7987	3.5472	13.8129	3.65376	13.7488	3.17275	14	3.05268	13.6586	2.49587
# Conform.	1	c	17.546	17.5551	0.05186	17.607	0.34766	17.6098	0.36362	17.6088	0.35792	17.8588	1.78274
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.109		0.093		0.122		0.113		2.307
		Δφ			2.698		1.998		1.843		2.055		0.939
		F			17.4296		16.3943		15.1816		13.9249		560.5
EACBOZ	0.341182	a	5.751	6.242	8.53765	6.2337	8.39332	6.2315	8.35507	6.2087	7.95862	6.3231	9.94784
SpaceGroup	P21	b	10.647	9.9529	-6.5192	9.9847	-6.2205	9.9776	-6.2872	9.9788	-6.2759	9.783	-8.115
# Conform.	1	c	12.085	12.168	0.6868	12.1779	0.76872	12.191	0.87712	12.2269	1.17418	12.2325	1.22052
# Molecules	1	α	90		-		-		-		-		-
		β	91.95	91.0402	-0.9895	90.9476	-1.0902	90.8749	-1.1692	90.6113	-1.4559	87.9689	-4.3296
		γ	90		-		-		-		-		-
		Δx			0.044		0.039		0.04		0.039		0.124
		Δφ			9.008		9.007		8.961		8.611		11.107
		F			137.171		131.172		131.496		124.587		214.53
BEYZIO		a	7.893	7.9993	1.34676	8.0331	1.77499	8.0243	1.6635	8.0498	1.98657	8.0744	2.29824
SpaceGroup	P-1	b	8.028	7.9417	-1.075	7.9049	-1.5334	7.9081	-1.4935	7.9073	-1.5035	8.1522	1.54709
# Conform.	1	c	10.228	10.1398	-0.8623	10.1871	-0.3999	10.1854	-0.4165	10.1771	-0.4977	10.0677	-1.5673
# Molecules	1	α	92.61	91.5463	-1.1486	91.2985	-1.4162	91.2629	-1.4546	91.2551	-1.463	92.4272	-0.1974
		β	131.84	132.6832	0.63956	132.9536	0.84466	132.8696	0.78095	133.0126	0.88941	132.1799	0.25781
		γ	107.68	108.1584	0.44428	108.0082	0.30479	108.0618	0.35457	108.1034	0.3932	107.2196	-0.4276
		Δx			0.05		0.054		0.05		0.054		0.068
		Δφ			3.409		3.566		3.481		3.557		3.684
		F			8.93963		12.2003		11.4712		13.2993		14.348
BEYZIO01	0.0466016	a	7.147	7.3191	2.408	7.0542	-1.2984	7.0474	-1.3936	6.995	-2.1268	7.31	2.28068
SpaceGroup	P21/c	b	16.258	15.8894	-2.2672	16.516	1.58691	16.5238	1.63489	16.6534	2.43203	16.0254	-1.4307

# Conform.	1	c	8.068	8.4669	4.94422	8.1611	1.15394	8.1567	1.09941	8.1725	1.29524	8.5619	6.12172
# Molecules	1	α	90		-		-		-		-		-
		β	115.38	119.7095	3.75238	116.2928	0.79112	116.22	0.72803	116.3807	0.86731	118.0544	2.31791
		γ	90		-		-		-		-		-
		Δx			0.208		0.042		0.038		0.044		0.255
		Δφ			15.811		6.053		5.753		6.292		15.774
		F			120.952		15.7051		14.9479		23.2079		120.583
CAXMOD	0.0519055	a	12.799	12.3773	-3.2948	12.4711	-2.5619	13.1211	2.5166	12.2084	-4.6144	11.4606	-10.457
SpaceGroup	Pna21	b	4.846	4.9502	2.15023	4.9091	1.3021	4.8463	0.00619	4.9664	2.48452	5.114	5.53033
# Conform.	1	c	8.285	8.9983	8.60954	8.9162	7.61859	8.2343	-0.6119	8.9821	8.414	8.8211	6.47073
# Molecules	1	α	90		-		-		-		-		-
		β	90		-		-		-		-		-
		γ	90		-		-		-		-		-
		Δx			0.147		0.119		0.227		0.153		0.241
		Δφ			3.205		3.693		3.523		4.034		8.948
		F			94.3321		71.1274		14.9636		104.67		207.63
CAXMOD01	0.154979	a	7.589	7.806	2.8594	7.899	4.08486	7.962	4.91501	7.849	3.42601	7.495	-1.2386
SpaceGroup	P21/a	b	8.13	8.604	5.83026	8.685	6.82657	8.73	7.38007	8.683	6.80197	8.571	5.42435
# Conform.	1	c	7.812	8.182	4.7363	7.979	2.13774	7.95	1.76651	8.094	3.60983	7.851	0.49923
# Molecules	1	α	90		-		-		-		-		-
		β	95.76	89.144	-6.9089	90.959	-5.0136	91.842	-4.0915	90.843	-5.1347	93.423	-2.4405
		γ	90		-		-		-		-		-
		Δx			0.467		0.32		0.39		0.36		0.353
		Δφ			16.232		17.649		18.75		16.236		15.051
		F			196.05		179.019		200.195		174.074		105.763
DIPTOX10	0.0615612	a	5.103	5.1387	0.69959	5.1233	0.39781	5.1415	0.75446	5.1726	1.3639	5.0291	-1.4482
SpaceGroup	P212121	b	15.209	15.1128	-0.6325	15.2372	0.18542	15.1451	-0.4201	14.9733	-1.5497	14.6049	-3.972
# Conform.	1	c	8.114	8.1092	-0.0592	8.0581	-0.6889	8.0832	-0.3796	8.1025	-0.1417	8.1759	0.76288
# Molecules	1	α	90										
		β	90		-		-		-		-		-

γ	90	-	-	-	-	-
Δx		0.051	0.073	0.077	0.072	0.352
Δφ		2.936	2.725	1.008	1.253	10.957
F		3.30813	3.05656	1.73673	5.19292	60.8602