

Electron Diffraction Data (Known)

(with D. Dorset and M. McCourt)

Structure	Atoms	Space Group	Success Rate	3-D
Copper Chloride	5	$P2_1/m$	21%	52%
Poly-Butene-1	8	$P2_12_12_1$	28%	37%
Poly- ϵ -Caprolactone	8	$P2_12_12_1$	41%	15%
Copper Perchloro-phthalocyanine	16	$Cmm2$	Yes	0%
<i>n</i> -Paraffin	36	$Pca2_1$	Yes	50%

Cost-Effectiveness

Structure	Atoms	S.G.	T.R.	P.S.
Nordihydroquaiaretic Acid	22	$P2_1/c$	213.48	123.15
Prostaglandin E_2	25	$P1$	194.60	80.70
9 α -Methoxycortisol	28	$P2_12_12_1$	101.44	37.43
3 β -hydroxy-16-methyl-5,16-pregnadien-20-one	48	$P1$	405.3	209.3
Tetrahymanol	63	$P2_1$	3.01	2.91
Emerimycin	74	$P1$	65.51	46.41
Isoleucinomycin	84	$P2_12_12_1$	4.10	1.88
Meso-valinomycin	84	$P\bar{1}$	1.03	0.67
Synthetic Pyrrole	96	$P1$	12.09	9.27
Ternatin	105	$P2_12_12_1$	0.03	0.06
Hexadeca Isoleucinomycin	127	$P2_12_12_1$	0.05	0.06
Cholesterol Butanoate	132	$P2_1$	0.43	0.30
Gramicidin A	317	$P2_12_12_1$	No	Yes
Crambin	400	$P2_1$	0.02	0.02

Fragment Recycling

CBT: 132 atoms, $P2_1$, 20-atom fragment

Base: 20-atom random trials yield 2.5% success

	Tangent Formula (RANTAN)	Shake-and-Bake (<i>SnB</i>)		
	Deformed RMS Model	Deformed RMS Model	Angular RMS Model	Positional RMS Model
RMS Å	Soln. (%)	Soln. (%)	Soln. (%)	Soln. (%)
0.0	19.80			
0.1	7.20			
0.15	2.20			
0.2	0.15			100
0.3		100	100	96
0.4		86	96	72
0.5		50	72	22
0.6		12	66	0
0.7		2	57	
0.8		0	40	
1.0			32	
1.2			6	
1.4			0	