

Supplementary Material for:

**The *Hybrid* Big Bang-Big Crunch method for solving crystal structure
from powder diffraction data**

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Table S1 For each test structure: code, compound name, molecular formula and reference.

Code	Name	Molecular Formula	Reference
1	Silver(I)-pyrazolate	[Ag(C ₃ H ₃ N ₂)] _n	Masciocchi <i>et al.</i> (1994)
2	<i>N,N'</i> -Bis[1-pyridin-4-yl-meth-(<i>E</i>)-ylidene]hydrazine	C ₁₂ H ₁₀ N ₄	Florence <i>et al.</i> (2005)
3	Hydrochlorothiazide	C ₇ H ₈ ClN ₃ O ₄ S ₂	Florence <i>et al.</i> (2005)
4	2-Mercaptobenzoic acid	C ₇ H ₆ O ₂ S	Florence <i>et al.</i> (2005)
5	Paracetamol (form I polymorph)	C ₈ H ₉ NO ₂	Florence <i>et al.</i> (2005)
6	Phenylacetic acid	C ₈ H ₈ O ₂	Florence <i>et al.</i> (2005)
7	Aspirin	C ₉ H ₈ O ₄	http://en.wikipedia.org/wiki/Aspirin
8	Hydroflumethiazide	C ₈ H ₈ F ₃ N ₃ O ₄ S ₂	Florence <i>et al.</i> (2005)
9	Triphenylphosphine	P(C ₆ H ₅) ₃	http://en.wikipedia.org/wiki/Triphenylphosphine
10	Ethyl 1',2',3',4',4a',5',6',7'-octahydrodispiro[cyclohexane-1,2'-quinazoline-4',1"-cyclohexane]-8'-carbodithioate	C ₂₁ H ₃₄ N ₂ S ₂	Avila <i>et al.</i> (2009)
11	2,6-diamino-5-hydroxy-3-nitro-4 <i>H</i> -pyrazolo[1,5-a]pyrimidin-7-one monohydrate	C ₆ H ₆ N ₆ O ₄ ·H ₂ O	Chernyshev <i>et al.</i> (1999)
12	<i>Fluorescein diacetate</i>	C ₂₄ H ₁₆ O ₇	Knudsen <i>et al.</i> (1998)
13	Ibuprofen	C ₁₃ H ₁₈ O ₂	Shankland <i>et al.</i> (1998)
14	Tetracycline hydrochloride	C ₂₂ H ₂₄ N ₂ O ₈ ·HCl	www.cristal.org/SDPDRR/samples.html (Sample2) (1998)
15	2-(4-Hydroxy-2-oxo-2,3-dihydro-1,3-benzothiazol-7-yl)ethylammonium chloride	C ₉ H ₁₁ N ₂ O ₂ S·Cl	Florence <i>et al.</i> (2005)
16	Citric acid	C ₆ H ₈ O ₇	http://en.wikipedia.org/wiki/Citric_acid
17	Citric acid	C ₆ H ₈ O ₇	http://en.wikipedia.org/wiki/Citric_acid

18	Salbutamol	C ₁₃ H ₂₁ NO ₃	Florence <i>et al.</i> (2005)
19	Tetracycline hydrochloride	C ₂₂ H ₂₄ N ₂ O ₈ ·HCl	www.cristal.org/SDPDRR/samples.html (Sample2) (1998)
20	2-[1-(2-aminoethyl)-2-imidazolidinylidene]-2-nitroacetonitrile	C ₇ H ₁₁ N ₅ O ₂	Chernyshev <i>et al.</i> (1999)
21	2,5-dioxopyrrolidin-1-yl 2-(benzoylsulfanyl)acetate	C ₁₃ H ₁₁ NO ₅ S	Rukiah & Al-Ktaifani (2011)
22	Creatine monohydrate	C ₄ H ₉ N ₃ O ₂ ·H ₂ O	Florence <i>et al.</i> (2005)
23	<i>m</i> -Toluidine	C ₇ H ₉ N	Rukiah <i>et al.</i> (2004)
24	Promazine hydrochloride	C ₁₇ H ₂₁ N ₂ S·Cl	Florence <i>et al.</i> (2005)
25	Clomipramine hydrochloride	C ₁₉ H ₂₄ ClN ₂ ·Cl	Florence <i>et al.</i> (2005)
26	α-Lactose monohydrate	C ₁₂ H ₂₂ O ₁₁ ·H ₂ O	Florence <i>et al.</i> (2005)
27	Tolbutamide	C ₁₂ H ₁₈ N ₂ O ₃ S	Florence <i>et al.</i> (2005)
28	Benzene-Hexafluorobenzene	C ₆ H ₆ :C ₆ F ₆	Williams <i>et al.</i> (1992)
29	Capecitabine	C ₁₅ H ₂₂ FN ₃ O ₆	Rohlicek <i>et al.</i> (2009);
30	Carbamazepine dihydrate	C ₁₅ H ₁₂ N ₂ O·2H ₂ O	Florence <i>et al.</i> (2005)
31	<i>catena</i> -Poly[[dipyridinenickel(II)]-trans-di-μ-chlorido]	[NiCl ₂ (C ₅ H ₅ N) ₂] _n	Alig <i>et al.</i> (2010)
32	Pigment Orange 36 (β phase)	C ₁₇ H ₁₃ ClN ₆ O ₅	van de Streek <i>et al.</i> (2009)
33	Pigment Orange 62	C ₁₇ H ₁₄ N ₆ O ₅	van de Streek <i>et al.</i> (2009)
34	Pigment Yellow 151	C ₁₈ H ₁₅ N ₅ O ₅	van de Streek <i>et al.</i> (2009)
35	Pigment Yellow 154 (α phase)	C ₁₈ H ₁₄ F ₃ N ₅ O ₃	van de Streek <i>et al.</i> (2009)
36	Barium sulfate	BaSO ₄	Lee <i>et al.</i> (2005)
37	Bromotrifluoromethane	CBrF ₃	Jouanneaux <i>et al.</i> (1992)
38	Cimetidine	C ₁₀ H ₁₆ N ₆ S	Diffraction data courtesy of Dr. A. Himeda, Rigaku, Japan
39	Famotidine	C ₈ H ₁₅ N ₇ O ₂ S ₃	Florence <i>et al.</i> (2005)
40	Famotidine	C ₈ H ₁₅ N ₇ O ₂ S ₃	Shankland <i>et al.</i> (2002)
41	[D ₃]Methylsodium	NaCD ₃	Weiss <i>et al.</i> (1990)

42	<i>trans</i> -Dichlorobis(triphenylphosphine)nickel(II)	C ₃₆ H ₃₀ Cl ₂ NiP ₂	Florence <i>et al.</i> (2005)
43	Diltiazem hydrochloride	C ₂₂ H ₂₇ N ₂ O ₄ S·Cl	Florence <i>et al.</i> (2005)
44	Poly[(μ_2 -2,2-dimethylpropane-1,3-diyl diisocyanide)- μ_2 -iodido-silver(I)]	[AgI(C ₇ H ₁₀ N ₂)] _n	Rukiah & Al-Ktaifani (2009)
45	Zopiclone dihydrate	C ₁₇ H ₁₇ ClN ₆ O ₃ ·2H ₂ O	Florence <i>et al.</i> (2005)
46	Capsaicin	C ₁₈ H ₂₇ NO ₃	Florence <i>et al.</i> (2005)
47	Lithium benzilate hemihydrate	C ₂₈ H ₂₂ O ₆ Li ₂ ·H ₂ O	Mora <i>et al.</i> (2003)
48	S-Bupivacaine Hydrochloride (Form A)	C ₁₈ H ₂₈ N ₂ O·HCl	Niederwanger <i>et al.</i> (2009)
49	Tetracaine hydrochloride	C ₁₅ H ₂₅ N ₂ O ₂ ⁺ Cl ⁻	Nowell <i>et al.</i> (2002)
50	2-{[3-(2-Phenylethoxy)propyl]sulfonyl}ethyl benzoate	C ₂₀ H ₂₄ O ₅ S	Florence <i>et al.</i> (2005)
51	N-formylurea	C ₂ H ₄ N ₂ O ₂	Harris <i>et al.</i> (1998)
52	Lanthanum disilicate	La ₂ Si ₂ O ₇	Christensen (1994)
53	Nimustine hydrochloride	C ₉ H ₁₄ ClN ₆ O ₂ ⁺ ·Cl ⁻	Beko <i>et al.</i> (2012)
54	7-oxanorbornane	C ₆ H ₁₀ O	Palin <i>et al.</i> (2007)
55	Sodium 4-[(<i>E</i>)-(4-hydroxyphenyl)diazenyl]benzene sulfonate dihydrate	C ₁₂ H ₉ N ₂ O ₄ S·Na·2H ₂ O	Florence <i>et al.</i> (2005)
56	Ampicillin trihydrate	C ₁₆ H ₁₉ N ₃ O ₄ S·3H ₂ O	Burley <i>et al.</i> (2006)
57	L-arabinitol	C ₅ H ₁₂ O ₅	Derollez <i>et al.</i> (2012)
58	S-Ibuprofen	C ₁₃ H ₁₈ O ₂	Florence <i>et al.</i> (2005)
59	Dapsone	C ₁₂ H ₁₂ N ₂ O ₂ S	Florence <i>et al.</i> (2005)
60	Verapamil hydrochloride	C ₂₇ H ₃₉ N ₂ O ₄ ·Cl	Florence <i>et al.</i> (2005)
61	Amodiaquinium dichloride dihydrate	C ₂₀ H ₂₄ ClN ₃ O ²⁺ ·2Cl ⁻ ·2H ₂ O	Llinàs <i>et al.</i> (2006)
62	Deuterated potassium uranyl phosphate trihydrate	KUO ₂ PO ₄ ·3D ₂ O	Fitch & Cole (1991)

63	barbituric acid:calcium iodide pentahydrate <i>co-crystal</i>	C ₄ H ₄ N ₂ O ₃ ·CaI ₂ ·5H ₂ O	Braga <i>et al.</i> (2012)
64	Nifedipine (C polymorph)	C ₁₇ H ₁₈ N ₂ O ₆	Bortolotti <i>et al.</i> (2011)
65	Antimony phosphate	Sb ₂ (PO ₄) ₃	Jouanneaux <i>et al.</i> (1991b)
66	Calcium tartrate tetrahydrate	CaC ₄ H ₄ O ₆ ·4H ₂ O	Le Bail <i>et al.</i> (2009)
67	Nickel zirconium phosphate	Ni _{0.5} Zr ₂ (PO ₄) ₃	Jouanneaux <i>et al.</i> (1991a)
68	Potassium titanium silicate monohydrate	K ₂ TiSi ₃ O ₉ H ₂ O	Dadachov & Le Bail (1997)
69	<i>l</i> -Glutamic acid	C ₅ H ₉ NO ₄	Kariuki <i>et al.</i> (1998)

Table S2 For each test structure: code, type of radiation (X for conventional X-ray, S for synchrotron data, N for neutron data); space group; the number of atoms (non-H) to be correctly located in the asymmetric unit (NAT_{asym}); the experimental resolution (RES) and the number of reflections (NREF) used in SA and *HBB-BC* runs; the total (internal and external) number of degrees of freedom: DOFs.

Code	Type of radiation	Space Group	NAT_{asym}	RES	NREF	DOFs
1	X	<i>P b c a</i>	6	2.0	55	6
2	X	<i>P 2₁/c</i>	8	2.0	67	7
3	X	<i>P 2₁</i>	17	2.0	90	7
4	X	<i>P 2₁/c</i>	10	2.0	85	7
5	X	<i>P 2₁/n</i>	11	2.0	103	8
6	X	<i>P 2₁/a</i>	10	2.0	98	8
7	S	<i>P 2₁/c</i>	13	2.0	114	9
8	X	<i>P 2₁</i>	20	2.0	92	9
9	X	<i>P 2₁/c</i>	19	2.0	192	9
10	S	<i>P 2₁/n</i>	25	2.0	262	9
11	S	<i>P 2₁/n</i>	17	2.0	116	10
12	S	<i>P -1</i>	31	2.0	242	10
13	S	<i>P 2₁/c</i>	15	2.0	160	10
14	X	<i>P 2₁ 2₁ 2₁</i>	33	2.0	191	11
15	X	<i>P 2₁/a</i>	15	2.0	138	11
16	X	<i>P 2₁/c</i>	13	2.0	100	11
17	S	<i>P 2₁/c</i>	13	2.0	100	11
18	X	<i>P b c a</i>	17	2.0	184	11
19	S	<i>P 2₁ 2₁ 2₁</i>	33	2.0	191	11
20	N	<i>P 2₁/n</i>	25	2.0	118	12
21	X	<i>P -1</i>	20	2.0	175	12
22	X	<i>P 2₁/c</i>	10	2.0	96	12

23	X	$P 2_1/c$	16	2.0	162	12
24	X	$P 2_1/c$	21	2.0	221	13
25	X	$P 2_1/c$	23	2.0	241	13
26	X	$P 2_1$	25	2.0	106	13
27	X	$P n a 2_1$	18	2.0	106	13
28	S	$P 2_1/a$	9	1.78	98	14
29	S	$P 2_1 2_1 2_1$	25	2.0	164	14
30	X	$C m c a$	12	2.0	101	14
31	X	$P 2/c$	16	2.0	142	14
32	X	$P -1$	29	2.0	227	14
33	X	$P -1$	28	2.64	95	14
34	X	$P -1$	28	2.0	218	14
35	X	$P 2_1/c$	29	2.0	226	14
36	N	$P n a m$	5	1.26	105	15
37	N	$P 2_1/a$	5	1.52	105	15
38	X	$P 2_1/n$	17	2.0	167	15
39	X	$P 2_1/c$	20	2.0	187	15
40	S	$P 2_1/c$	20	2.0	187	15
41	S	$I \bar{2} \bar{2} 2$	5	1.44	105	15
42	X	$P 2/c$	21	2.0	208	15
43	X	$P 2_1 2_1 2_1$	30	2.16	164	16
44	X	$P b c a$	11	2.0	136	16
45	X	$P 2_1/c$	29	2.0	257	16
46	X	$P 2_1/c$	22	2.0	232	17
47	S	$P 2_1/a$	34	2.0	314	18
48	S	$P 2_1$	22	2.0	141	18
49	S	$P -1$	20	2.0	213	18
50	X	$P 2_1/n$	26	2.0	251	18
51	S	$P n 2_1 a$	6	1.20	126	18

52	N	$P\ 2_1/c$	11	1.71	126	18
53	X	$P\ 2_1/c$	19	2.0	188	18
54	S	$C\ 2/c$	21	2.0	216	18
55	X	$P\ b\ c\ n$	22	2.0	180	19
56	S	$P\ 2_1\ 2_1\ 2_1$	27	2.0	176	20
57	X	$P\ 1$	20	1.71	140	20
58	X	$P\ 2_1$	30	2.0	193	20
59	X	$P\ 2_1\ 2_1\ 2_1$	17	1.82	147	21
60	X	$P\ -1$	34	2.0	363	23
61	X	$P\ 2_1/c$	29	2.0	300	24
62	S	$P\ 4/n\ c\ c$	7	1.12	168	24
63	X	$P\ 2_1/c$	22	2.0	185	24
64	S	$P\ -1$	50	2.39	258	24
65	S	$P\ 2_1/n$	17	1.76	168	24
66	X	$P\ -1$	15	1.84	168	24
67	S	$P\ 2_1/n$	18	1.75	189	27
68	X	$P\ 2_1\ 2_1\ 2_1$	16	1.44	210	30
69	S	$P\ 2_1\ 2_1\ 2_1$	10	1.35	183	30

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