Electronic Supplementary Material (ESI) for Chemical Communications

SUPPORTING INFORMATION FOR

1,2,4,5-Tetrakis(phenylsulfonyl)benzene: a novel quadruped host with D_2 symmetry having ordered sulfolane and *cyclo*heptanone guests

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Optimised structures of 1,2,4,5-tetrakis(phenylsulfonyl)benzene

B97-D3/def2-TZVP (Turbomole)

D2 (idealised symmetry) conformer (*abab*)

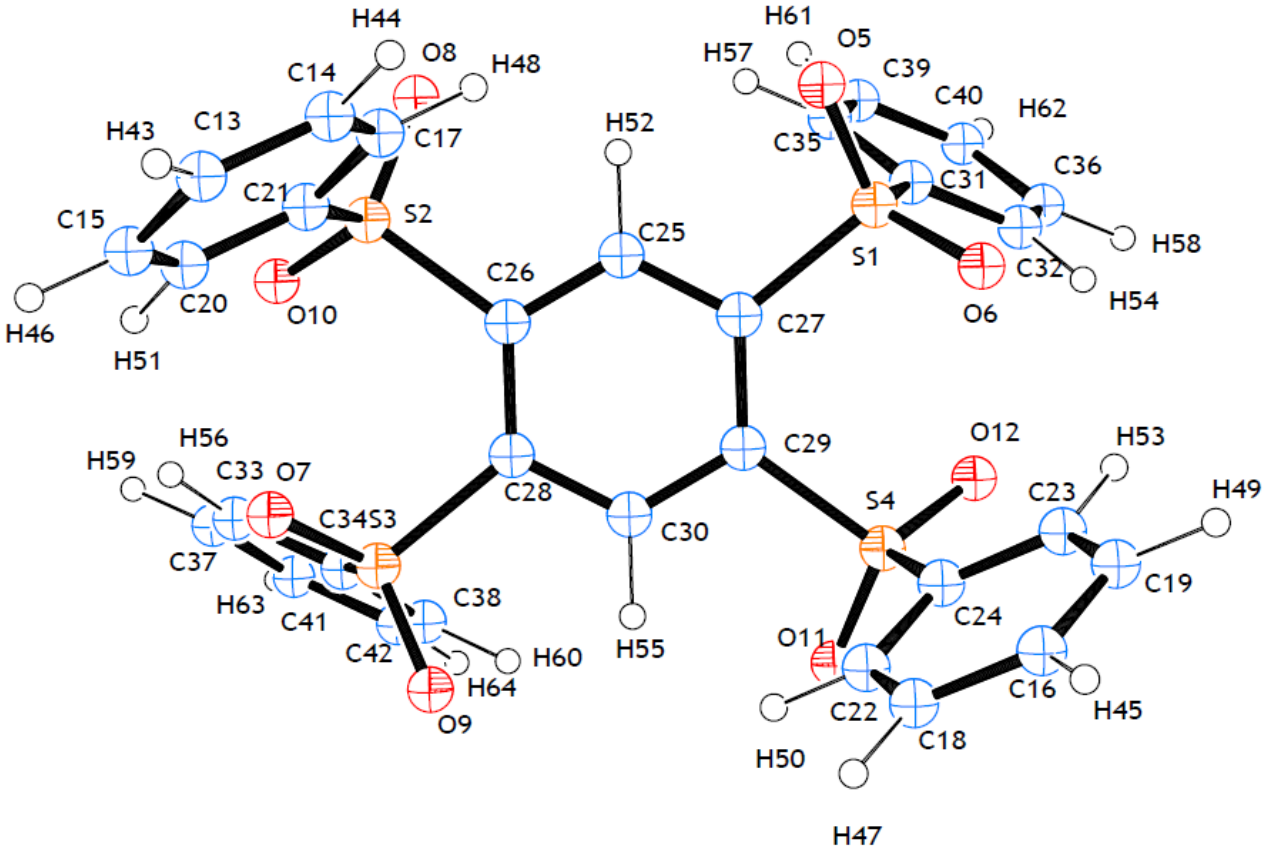

Fig. 1. Atomic labelling of optimised structure of D_2 conformer (*abab*)

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Schoenflies symbol = D2       CSM =  0.0007     Molecular RMS =  0.0026
 CSM,see: Zabrodsky et al. (1993) JACS, 115, 8278-8298
 Symmetry element its CSM and Max.Diff.  Symmetry element its CSM and Max.Diff.
  1) [E  ]  x,y,z       0.0000  0.0000    2) [C2 ]  -x,-y,z     0.0001  0.0017
  3) [C2 ]  -x,y,-z     0.0006  0.0040    4) [C2 ]  x,-y,-z     0.0007  0.0054
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Table 1. Atomic Angstrom coordinates of optimised structure of D_2 conformer (*abab*)

Energy = -3350.484819022

S	1	-2.68084892	-0.11758566	-1.82634806
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S	3	2.67839884	-0.11112128	1.82625408
S	4	-2.68129756	0.11800527	1.82528733
O	5	-2.14236181	-0.56360668	-3.09887454
O	6	-3.72928247	-0.87376500	-1.17787625
O	7	3.72606819	-0.87118609	1.18101948
O	8	2.14097990	0.55091872	-3.10068112
O	9	2.13996907	-0.55070129	3.10106869
O	10	3.72654860	0.87057804	-1.17996850
O	11	-2.14328961	0.56512773	3.09762486
O	12	-3.73005174	0.87314449	1.17616910
C	13	3.95159428	-4.22862104	-2.38230795
C	14	2.73814012	-3.78006665	-2.91686305
C	15	4.77703696	-3.35404320	-1.67001014
C	16	-3.94873174	-4.22001228	2.40523018
C	17	2.34648360	-2.45380229	-2.74067277
C	18	-2.73687538	-3.76654389	2.93926298
C	19	-4.77413409	-3.35088443	1.68626221
C	20	4.39214259	-2.02592909	-1.47552093
C	21	3.17924782	-1.59343420	-2.01409315
C	22	-2.34676159	-2.44080852	2.75585698
C	23	-4.39080067	-2.02337526	1.48456451
C	24	-3.17948028	-1.58594592	2.02275220
C	25	-0.00105480	-0.00214370	-1.37486235
C	26	1.22453939	0.01452778	-0.70290754
C	27	-1.22688520	-0.01675683	-0.70318832
C	28	1.22434445	-0.01450391	0.70297490
C	29	-1.22706978	0.01713632	0.70254865
C	30	-0.00143267	0.00248767	1.37457812
C	31	-3.17997624	1.58620439	-2.02288909
C	32	-4.39206898	2.02247117	-1.48551868
C	33	4.39257625	2.02497303	1.47659574
C	34	3.17902950	1.59319953	2.01429439
C	35	-2.34712409	2.44212609	-2.75460807
C	36	-4.77608255	3.34986589	-1.68665995
C	37	4.77781910	3.35303391	1.67076748
C	38	2.34594823	2.45423735	2.73970035
C	39	-2.73790279	3.76774796	-2.93742191
C	40	-3.95056054	4.22004831	-2.40421833
C	41	3.95208536	4.22826548	2.38192327
C	42	2.73796262	3.78044101	2.91557556
H	43	4.25362488	-5.26406616	-2.52327598
H	44	2.10073729	-4.46022575	-3.47661774
H	45	-4.24953988	-5.25502453	2.55185471
H	46	5.71908133	-3.70581264	-1.25657428
H	47	-2.09950538	-4.44242908	3.50420757
H	48	1.41737028	-2.08664444	-3.16742418
H	49	-5.71501054	-3.70639902	1.27338355
H	50	-1.41902593	-2.06975509	3.18219662
H	51	5.00370131	-1.33449942	-0.90850870
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H	53	-5.00236941	-1.33618620	0.91242020
H	54	-5.00371087	1.33449750	-0.91439782
H	55	-0.00153075	0.00456536	2.45855773
H	56	5.00434111	1.33303225	0.91042007
H	57	-1.41874187	2.07196438	-3.18032610
H	58	-5.71758862	3.70447721	-1.27443907
H	59	5.72034629	3.70425264	1.25796513
H	60	1.41630814	2.08768196	3.16582088
H	61	-2.10043730	4.44445383	-3.50127640
H	62	-4.25190811	5.25496655	-2.55039986
H	63	4.25439367	5.26365731	2.52268684
H	64	2.10030054	4.46113640	3.47438303

Table 2. Interatomic distances (Å) of optimised structure of D_2 conformer (*abab*)

S	1	-	O	5	1.45197340
S	1	-	O	6	1.44621430
S	1	-	C	27	1.84001760
S	1	-	C	31	1.78624102
S	2	-	O	8	1.45198505
S	2	-	O	10	1.44626702
S	2	-	C	21	1.78624389
S	2	-	C	26	1.83995202
S	3	-	O	7	1.44624938
S	3	-	O	9	1.45199500
S	3	-	C	28	1.83993620
S	3	-	C	34	1.78625296
S	4	-	O	11	1.45196895
S	4	-	O	12	1.44619330
S	4	-	C	24	1.78623292
S	4	-	C	29	1.83997150
C	13	-	C	14	1.39979327
C	13	-	C	15	1.39771606
C	13	-	H	43	1.08776885
C	14	-	C	17	1.39406420
C	14	-	H	44	1.08730128
C	15	-	C	20	1.39637273
C	15	-	H	46	1.08725275
C	16	-	C	18	1.39979301
C	16	-	C	19	1.39770784
C	16	-	H	45	1.08776590
C	17	-	C	21	1.40058825
C	17	-	H	48	1.08635778
C	18	-	C	22	1.39405911
C	18	-	H	47	1.08730111
C	19	-	C	23	1.39639073
C	19	-	H	49	1.08724786
C	20	-	C	21	1.39578852
C	20	-	H	51	1.08331987
C	22	-	C	24	1.40059027
C	22	-	H	50	1.08634230
C	23	-	C	24	1.39581070
C	23	-	H	53	1.08332555
C	25	-	C	26	1.39781341
C	25	-	C	27	1.39786255
C	25	-	H	52	1.08398709
C	26	-	C	28	1.40618217
C	27	-	C	29	1.40614552
C	28	-	C	30	1.39780870
C	29	-	C	30	1.39786427
C	30	-	H	55	1.08398161
C	31	-	C	32	1.39580245
C	31	-	C	35	1.40059178
C	32	-	C	36	1.39638854
C	32	-	H	54	1.08332479
C	33	-	C	34	1.39579508
C	33	-	C	37	1.39637403
C	33	-	H	56	1.08332506
C	34	-	C	38	1.40058001
C	35	-	C	39	1.39405962
C	35	-	H	57	1.08634667
C	36	-	C	40	1.39771029
C	36	-	H	58	1.08724832
C	37	-	C	41	1.39771566
c	37	-	h	59	1.08725244
c	38	-	c	42	1.39406726
c	38	-	h	60	1.08635733
c	39	-	c	40	1.39979301
c	39	-	h	61	1.08730168
c	40	-	h	62	1.08776613
c	41	-	c	42	1.39979483
c	41	-	h	63	1.08776879
c	42	-	h	64	1.08730167

C_i (idealised symmetry) conformer (*abba*)

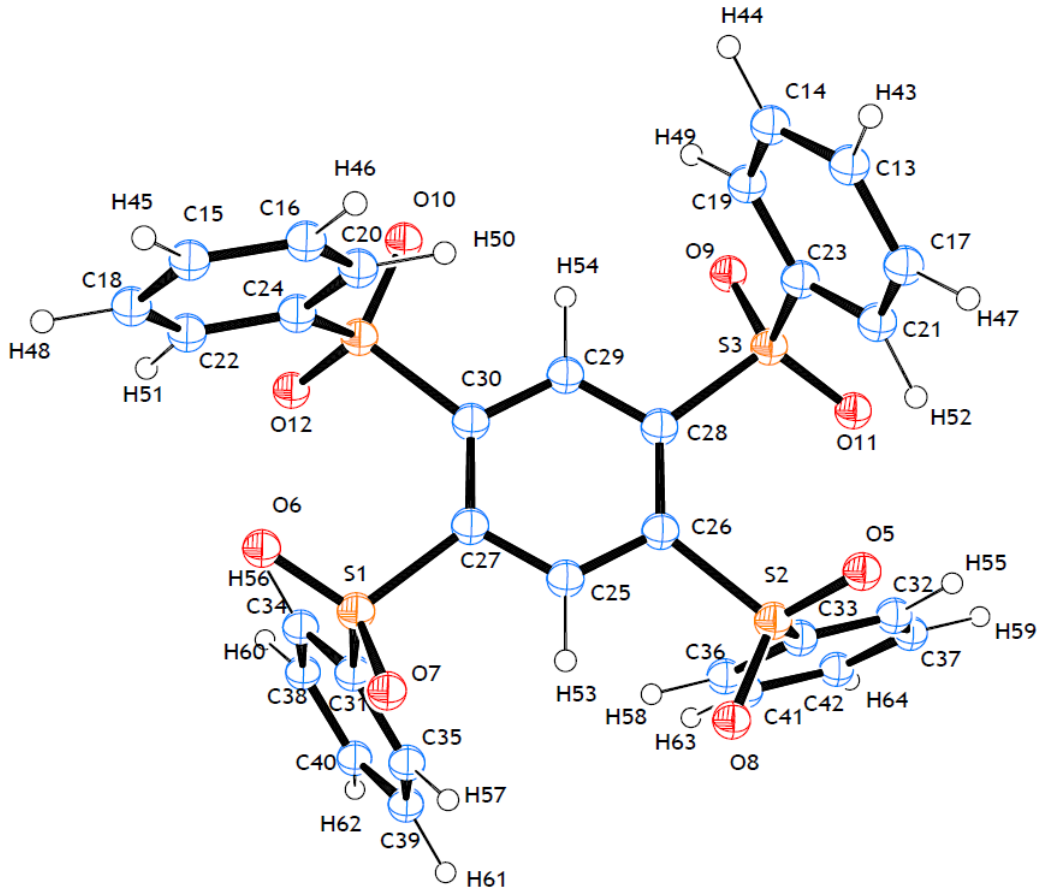

Fig. 2. Atomic labelling of optimised structure of C_i conformer (*abba*)

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 CSM,see: Zabrodsky et al. (1993) JACS, 115, 8278-8298
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  1) [E  ]  x,y,z        0.0000  0.0000    2) [Ci ]  -x,-y,-z    4.5685  0.4061
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Table3. Atomic Angstrom coordinates of optimised structure of C_i conformer (*abba*)

Energy = -3350.482656032

S	1	2.65567472	-1.19594684	-1.30574568
S	2	-2.67950785	-1.08328578	-1.45388398
S	3	-2.69246380	1.32368529	1.32728031
S	4	2.66065537	1.16229883	1.50957089
O	5	-3.65995572	-0.06377790	-1.75785314
O	6	3.87341302	-0.50679773	-0.94712418
O	7	2.29280940	-1.39168783	-2.69587471
O	8	-2.10631890	-1.87191533	-2.53079370
O	9	-2.27355430	1.61490755	2.68473013
O	10	2.09645246	2.04509497	2.51562020
O	11	-3.87368595	0.53203430	1.07242112
O	12	3.49793115	0.05372646	1.91833692
C	13	-2.93277844	5.28123586	-0.92440786
C	14	-2.12829461	5.17374299	0.21603919
C	15	4.87234117	3.91710298	-1.36293625
C	16	3.50368133	4.09969294	-1.13637383
C	17	-3.67349598	4.18366313	-1.37396672
C	18	5.55992589	2.87491649	-0.73431773
C	19	-2.05753243	3.96535511	0.90937146
C	20	2.82032026	3.24395096	-0.27277172
C	21	-3.61246188	2.96635522	-0.69209414
C	22	4.88387955	2.00017533	0.11734818
C	23	-2.80217202	2.87482645	0.44326256
C	24	3.52154072	2.19991137	0.33841577
C	25	-0.00318920	-0.76469071	-1.08262729
C	26	-1.23380449	-0.33348449	-0.58298540
C	27	1.21560862	-0.37202643	-0.52177037
C	28	-1.23983717	0.54982546	0.51193271
C	29	-0.01999248	0.95636788	1.06190836
C	30	1.21035890	0.50830928	0.57365803
C	31	2.59874727	-2.78764286	-0.48875699
C	32	-4.64494692	-2.13506447	0.17386315
C	33	-3.31827396	-2.23353983	-0.24417355
C	34	3.26727223	-2.96143807	0.72661629
C	35	1.85142844	-3.81643464	-1.07431348
C	36	-2.47198867	-3.24689779	0.21988965
C	37	-5.13489702	-3.07912341	1.07801724
C	38	3.17812741	-4.19885134	1.36786885
C	39	1.77249114	-5.04676516	-0.42114298
C	40	2.43174950	-5.23583193	0.79892538
C	41	-2.96916282	-4.17299209	1.13553289
C	42	-4.29965563	-4.08989706	1.56182947
H	43	-2.98493852	6.22599214	-1.46114171
H	44	-1.56202227	6.03217613	0.56993045
H	45	5.40304686	4.58799133	-2.03465822
H	46	2.97048057	4.91051777	-1.62678273
H	47	-4.30093910	4.27231279	-2.25751741
H	48	6.62209356	2.73191332	-0.91764615
H	49	-1.45441466	3.86552015	1.80711402
H	50	1.76084436	3.38531963	-0.07338487
H	51	5.38617886	1.16297083	0.58918880
H	52	-4.16880187	2.09846529	-1.02831068
H	53	0.00348616	-1.43295320	-1.93661795
H	54	-0.02600791	1.62837642	1.91333451
H	55	-5.26276745	-1.32135384	-0.18964714
H	56	3.82952217	-2.13899615	1.15553950
H	57	1.35950101	-3.65321575	-2.02902419
H	58	-1.44469433	-3.30958566	-0.13032543
H	59	-6.16644055	-3.01432997	1.41543886
H	60	3.69241037	-4.35064999	2.31384249
H	61	1.20194056	-5.85798092	-0.86748289
H	62	2.36627792	-6.19637608	1.30553137
H	63	-2.32026943	-4.95978258	1.51316455
H	64	-4.68394460	-4.81401874	2.27683986

Table4. Interatomic distances (Å) of optimised structure of C_i conformer (*abba*)

S	1	O	6	1.44444538
S	1	O	7	1.44998086
S	1	C	27	1.83500749
S	1	C	31	1.79003002
S	2	O	5	1.44674517
S	2	O	8	1.45265849
S	2	C	26	1.84681470
S	2	C	33	1.78731806
S	3	O	9	1.45016054
S	3	O	11	1.44462807
S	3	C	23	1.78873200
S	3	C	28	1.83678384
S	4	O	10	1.45251133
S	4	O	12	1.44812054
S	4	C	24	1.78588008
S	4	C	30	1.84580472
C	13	C	14	1.39977442
C	13	C	17	1.39836746
C	13	H	43	1.08782734
C	14	C	19	1.39496171
C	14	H	44	1.08757107
C	15	C	16	1.39924957
C	15	C	18	1.39788651
C	15	H	45	1.08763509
C	16	C	20	1.39466315
C	16	H	46	1.08730899
C	17	C	21	1.39660800
C	17	H	47	1.08729272
C	18	C	22	1.39554490
C	18	H	48	1.08731751
C	19	C	23	1.40035652
C	19	H	49	1.08612142
C	20	C	24	1.39831289
C	20	H	50	1.08730373
C	21	C	23	1.39784907
C	21	H	52	1.08433790
C	22	C	24	1.39453665
C	22	H	51	1.08436596
C	25	C	26	1.39642214
C	25	C	27	1.39793199
C	25	H	53	1.08439816
C	26	C	28	1.40681148
C	27	C	30	1.40534049
C	28	C	29	1.39848884
C	29	C	30	1.39746535
C	29	H	54	1.08469265
C	31	C	34	1.39794942
C	31	C	35	1.39991942
C	32	C	33	1.39445804
C	32	C	37	1.39599176
C	32	H	55	1.08442008
C	33	C	36	1.39944553
C	34	C	38	1.39654690
C	34	H	56	1.08467084
C	35	C	39	1.39519748
C	35	H	57	1.08632663
C	36	C	41	1.39399976
C	36	H	58	1.08715870
C	37	C	42	1.39762865
C	37	H	59	1.08725967
C	38	C	40	1.39860838
C	38	H	60	1.08738030
C	39	C	40	1.39961946
C	39	H	61	1.08757450
C	40	H	62	1.08792519
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C	41	H	63	1.08752359
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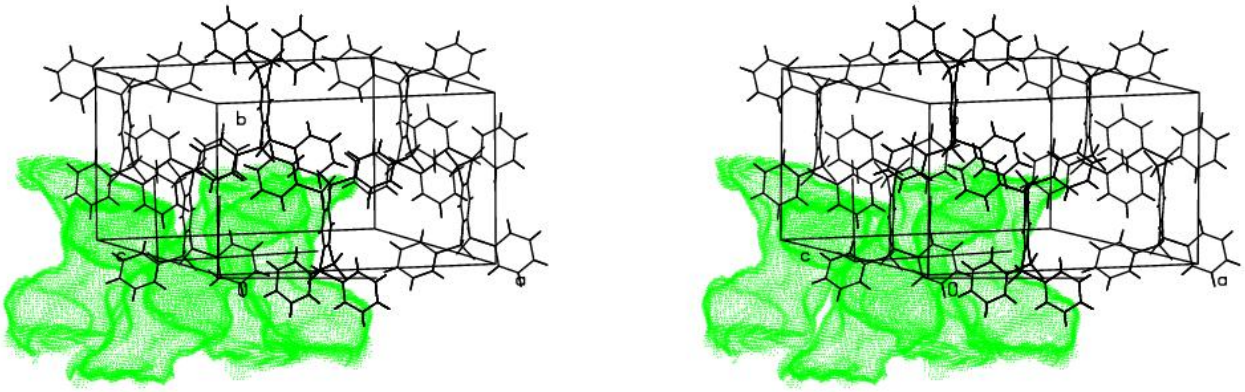

(a)

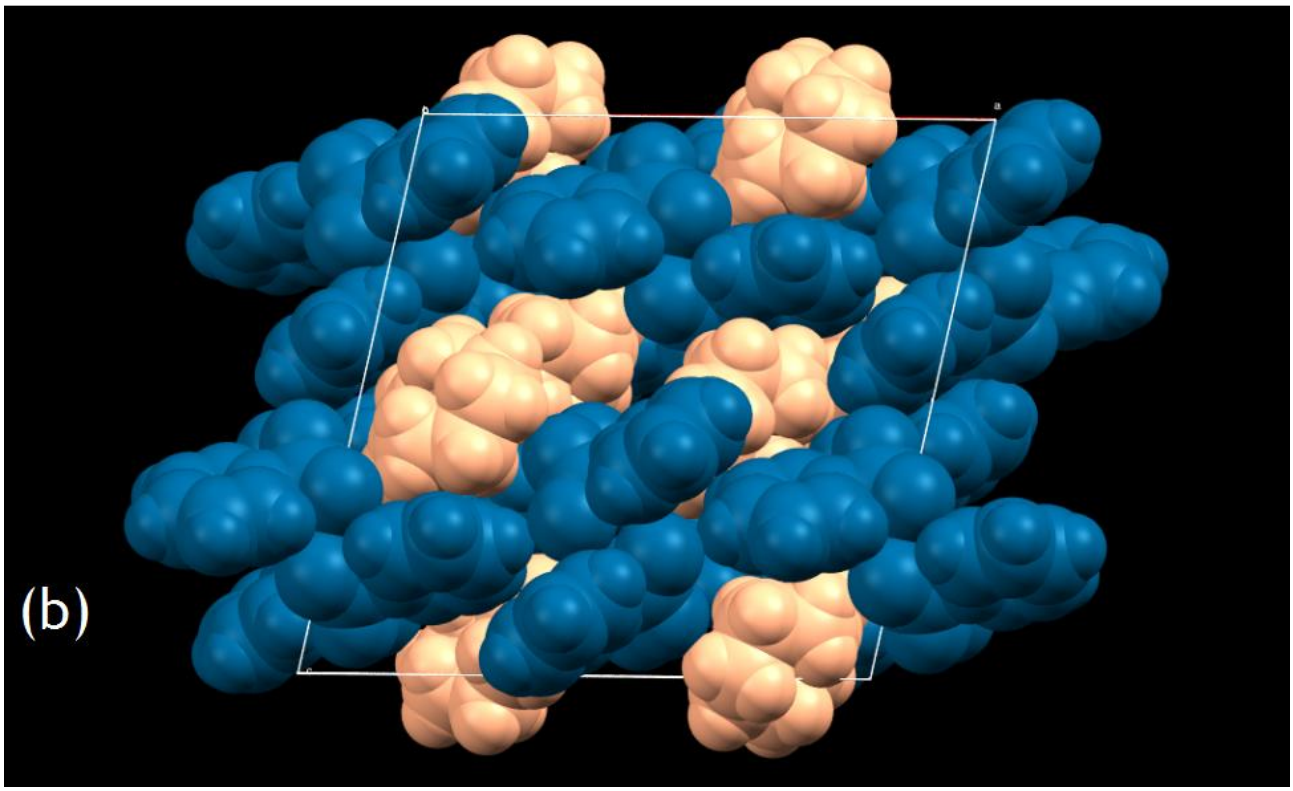

Fig. 2 (a) Stereo plot showing the voids in the packing of the host molecule in **1b**, (b) Spacefill view of packing in **1b** along the b axis with host molecules **1** in blue and guest *cyclo*heptanone molecules in pink.