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The nature of the C-Br···Br-C intermolecular interactions found in molecular crystals: A general theoretical-database study

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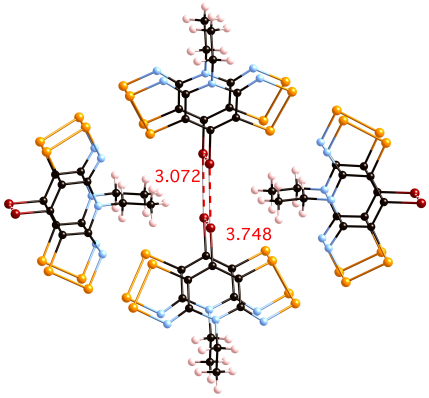

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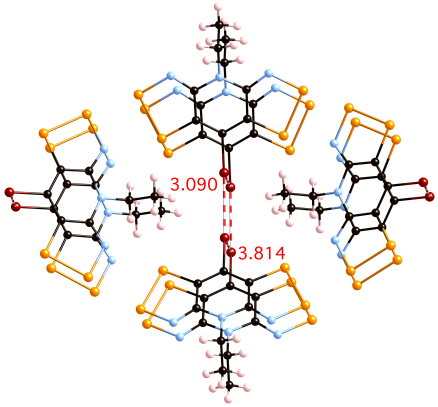

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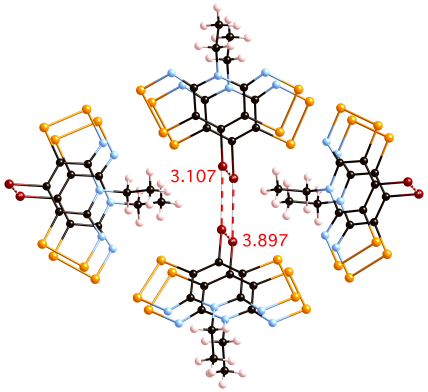

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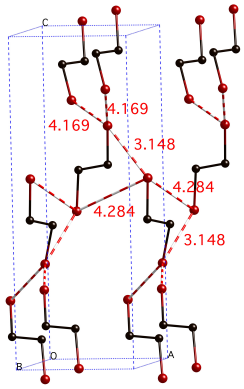

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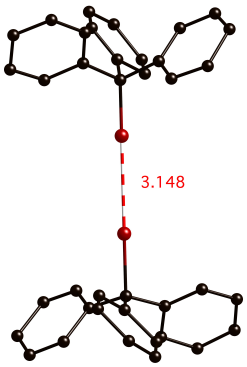

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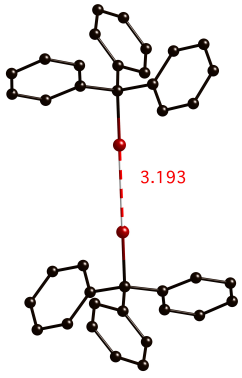

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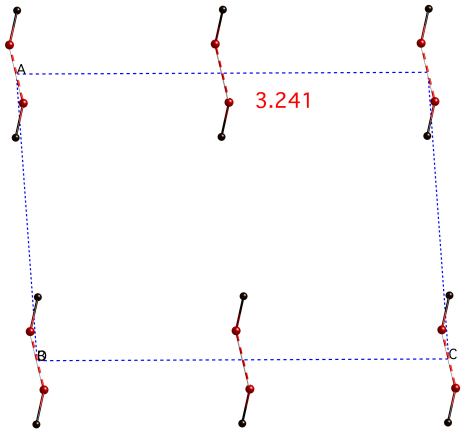

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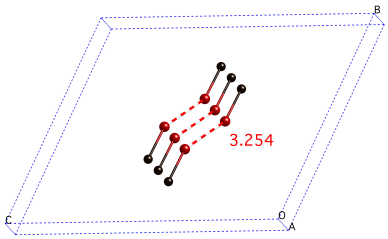

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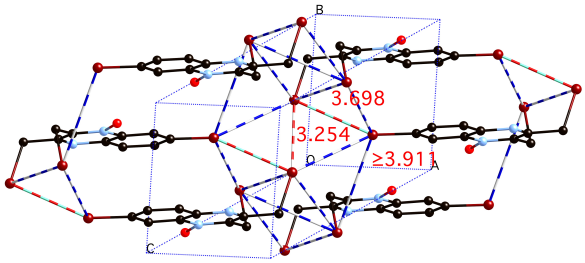

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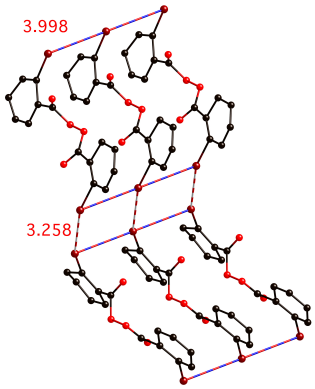

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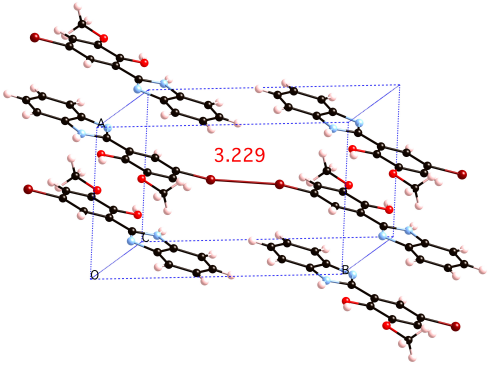

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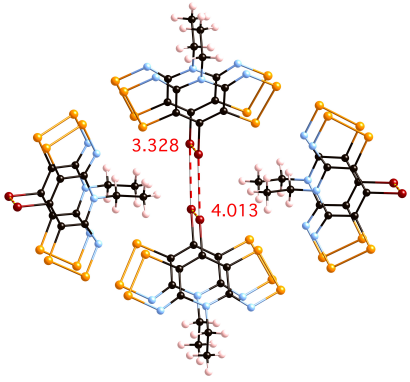

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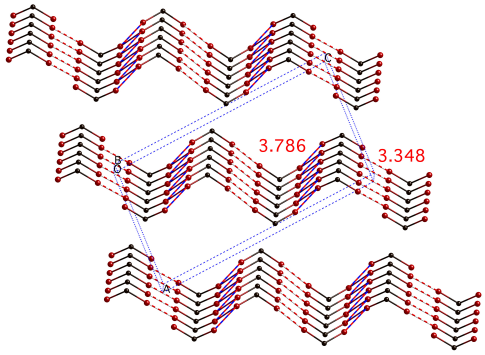

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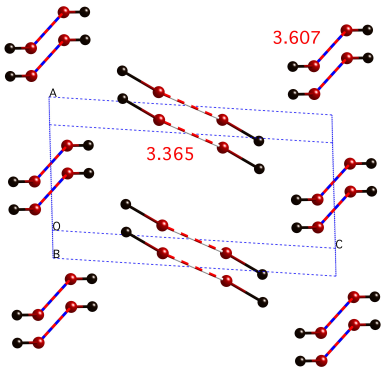

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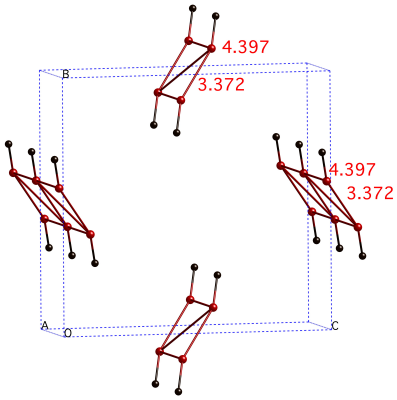

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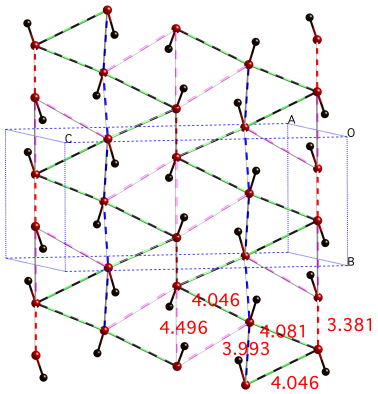

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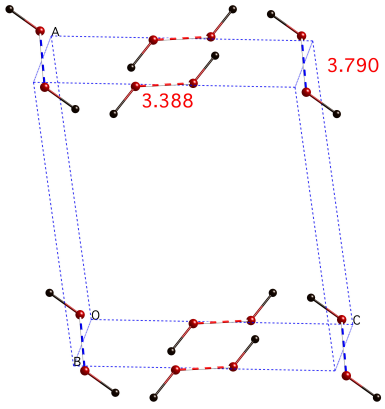

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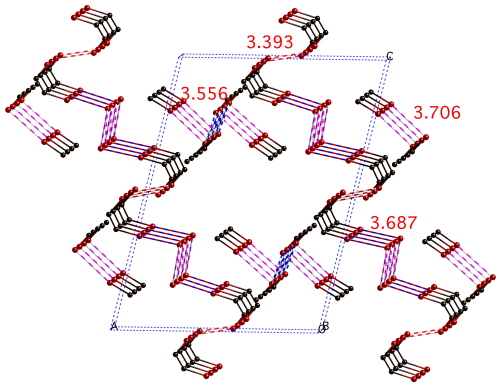

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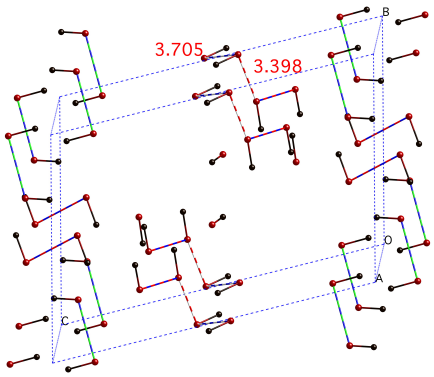

LOGNIF

Figure S1. Intermolecular C-Br···Br-C interactions found in the ten crystals presenting the shortest Br···Br interactions (see Table S1), as well as in structure number 20, 30, 40, 50 60 70 80, 90 and 100 of Table S1. Each crystal is identified by its refcode. In some crystals (for instance, DBRDOX, DANZIC, and ZILNIT), in order to better visualize the position and superstructure of the C-Br functional groups and the C-Br···Br-C interactions shorter than 5 Å among them, only the C-Br groups are plotted.

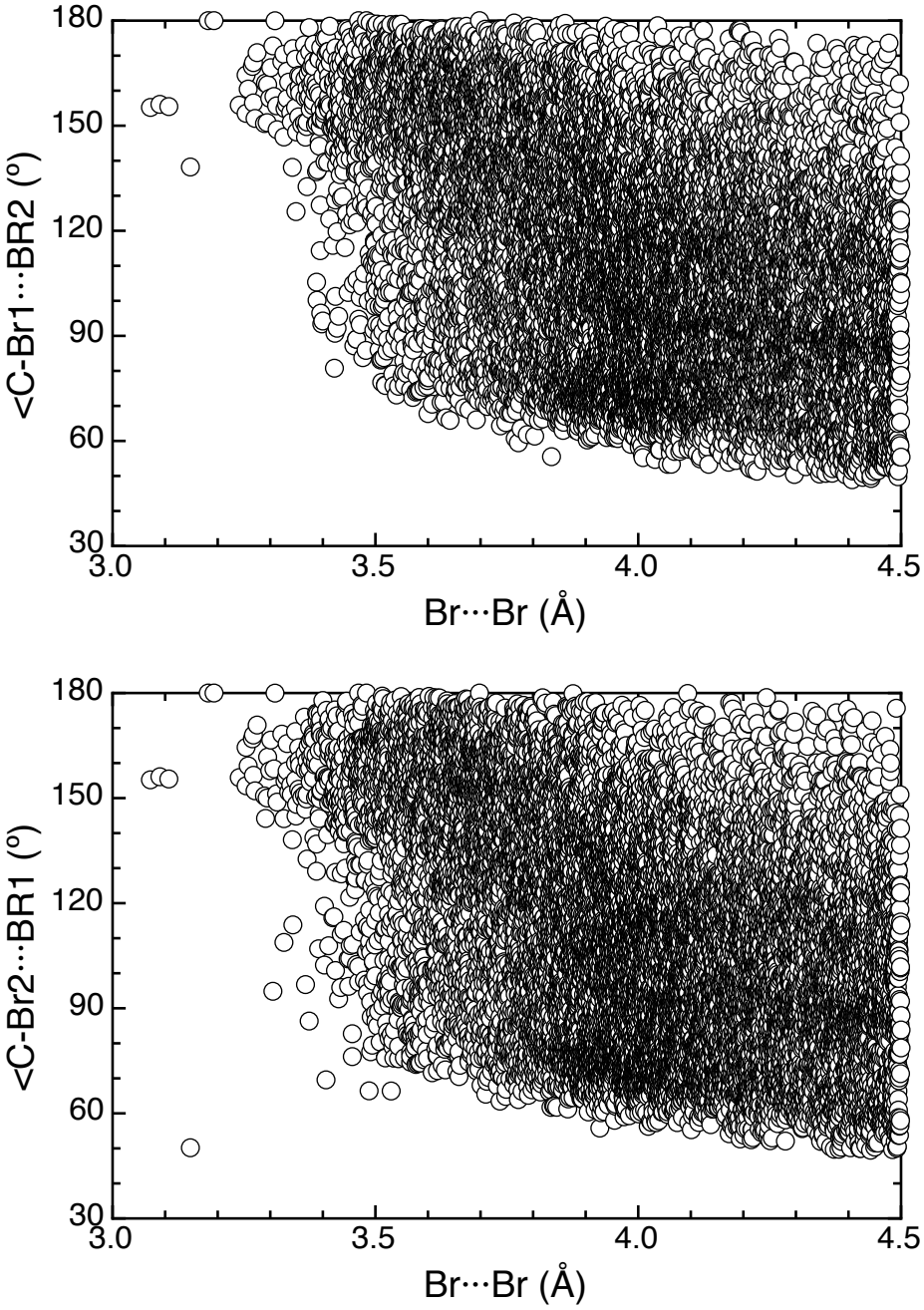

Figure S2. Distribution of the <C-Br1··Br2 (top) and <C-Br2···Br1 (bottom) angles as a function of the Br···Br distance.

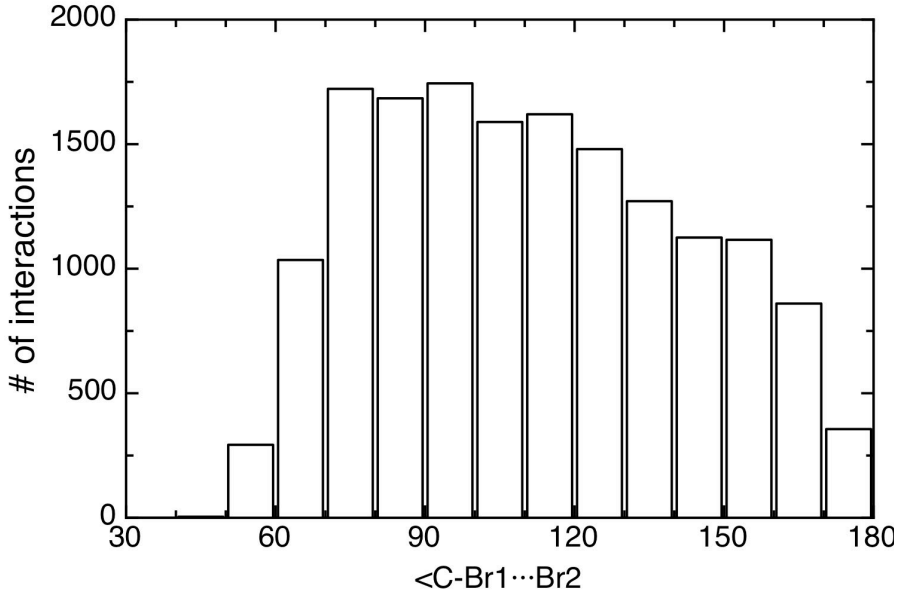

Figure S3. Probability distribution for the < C-Br···Br angles, computed for the set of C-Br···Br-C contacts found in the CSD that have a Br···Br distance smaller than 4.5 Å.

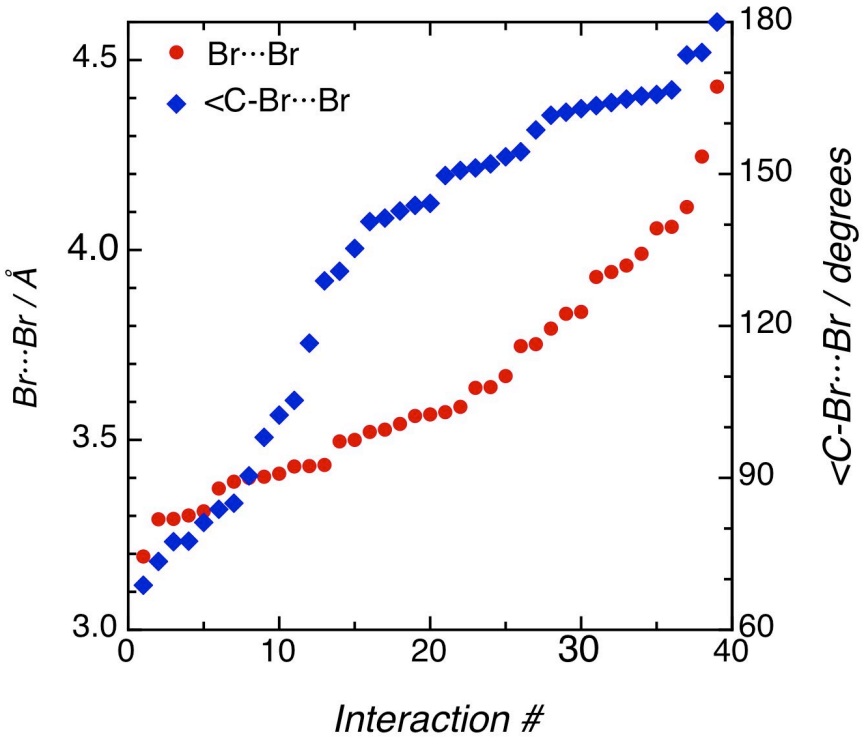

Figure S4. Distribution of the Br···Br distance and <C-Br···Br angle for Table 4 dimers.

Table S1. Value of the Br···Br distance (Br···Br_1, in Å), the <C-Br1···Br2 (ANG1), and <C-Br2···Br1 (ANG2) angles (both in degrees) for the shortest 100 C-Br···Br-C contacts found in the Cambridge Crystallographic Database (all Br···Br values are within the 3.07 and 3.40 Å range). Also given is the difference between the ANG1 and ANG2 angles, which allows to determine if the contact is of the Type I class, and the values of the Br···Br distance (Br···Br_2, in Å) and <C-Br1···Br2 angle (ANG3, in degrees) for the second shortest C-Br···Br-C contact (see Figure S1 to determine the relative disposition of the shortest and the next C-Br···Br-C contacts within the crystal).

#	REFCODE	Br···Br_1	ANG1	ANG2	ANG1-ANG2	Br···Br_2	ANG3	
1	IZOXOL04	3.072	155.2	155.2	0.0	3.748	114.7	a
2	IZOXOL03	3.090	156.1	156.1	0.0	3.814	113.9	a
3	IZOXOL02	3.107	155.5	155.5	0.0	3.897	114.5	a
4	DBRDOX	3.148	138.2	50.2	88.0	4.169	141.0	
5	TPHMBR01	3.182	180.0	180.0	0.0	> 5 Å		b
6	TPHMBR02	3.193	180.0	180.0	0.0	> 5 Å		b
7	DANZIC	3.241	155.9	155.9	0.0	> 5 Å		b
8	ZILNIT	3.254	153.5	153.5	0.0	> 5 Å		b
9	NIGXIL	3.254	164.5	164.5	0.0	3.698	96.4	
10	DBBZPO	3.258	160.5	159.2	1.3	3.998	69.3	
11	ESIWUY01	3.266	166.9	166.9	0.0			
12	APATOB	3.268	168.0	168.0	0.0			
13	EHINEP	3.268	156.5	156.5	0.0			
14	POXZOR	3.271	152.1	152.1	0.0			
15	DISWIN	3.275	170.9	170.9	0.0			
16	GUJSIN	3.289	150.6	150.6	0.0			
17	QAQLUQ	3.291	162.2	144.2	18.0			
18	QECGEM	3.294	150.9	150.0	0.8			
19	YOZLII	3.295	161.7	161.7	0.0			
20	SACJAJ	3.299	157.8	157.8	0.0	> 5 Å		b
21	YIHDEY	3.301	166.6	166.6	0.0			
22	OHIKUL	3.305	172.8	94.9	77.9			
23	SACJAJ01	3.307	158.3	158.3	0.0			
24	ZERJIP	3.309	180.0	180.0	0.0			
25	BAWJAL	3.312	155.7	151.2	4.5			
26	IPEXAD	3.313	148.9	148.9	0.0			
27	QETVER	3.322	168.3	168.3	0.0			
28	VOBCIZ	3.326	146.8	144.1	2.6			
29	XEFGEW	3.326	170.4	108.8	61.6			
30	IZOXOL01	3.328	154.9	154.9	0.0	4.013	115.1	a
31	ROFLOO01	3.331	156.1	156.1	0.0			
32	DUFWIL	3.332	157.7	157.7	0.0			
33	GESTII	3.332	165.6	165.6	0.0			
34	ERITOP	3.335	162.4	151.7	10.7			
35	AFACIU	3.339	153.7	153.7	0.0			
36	KEJDEI	3.340	151.0	151.0	0.0			
37	SOSTUQ	3.342	138.1	138.1	0.0			
38	HUDDAM	3.343	172.0	113.8	58.2			
39	EQIFIU	3.348	160.0	160.0	0.0			
40	PUJRAO	3.348	155.2	155.2	0.0	3.786	153.8	
41	VOQWAA	3.348	169.0	169.0	0.0			
42	XACXEE	3.349	125.5	144.9	-19.4			
43	UDURAN	3.350	148.2	148.2	0.0			
44	AXUKIO	3.354	164.4	164.4	0.0			
45	YICDUK	3.354	152.5	152.5	0.0			
46	XAZMES	3.355	160.9	160.9	0.0			
47	DABPYR	3.356	159.3	159.3	0.0			

48	OWECEZ	3.357	164.2	151.5	12.7			
49	EGIDEE	3.360	150.2	150.2	0.0			
50	CEPVID	3.365	173.1	173.1	0.0	3.607	158.1	
51	LADVOB	3.365	150.9	150.9	0.0			
52	TUVFEW	3.366	158.0	158.0	0.0			
53	YUBLUD	3.366	163.3	162.7	0.7			
54	CIBRAI	3.367	146.7	146.8	-0.1			
55	OHIKOF	3.367	169.5	96.8	72.8			
56	ARIZUX	3.369	149.7	149.7	0.0			
57	DBCYOC	3.370	160.7	160.7	0.0			
58	NUQLAN	3.370	132.6	132.6	0.0			
59	XAZMES	3.370	151.0	151.0	0.0			
60	BAPRER	3.372	157.9	157.9	0.0	4.372	117.1	
61	IFOKOD	3.372	164.8	164.8	0.0			
62	BRGUOS01	3.374	178.0	86.4	91.7			
63	BAGVIO	3.375	171.0	170.1	0.9			
64	ROFFIC	3.375	158.5	158.5	0.0			
65	GUCRUR	3.376	166.1	166.1	0.0			
66	RIQHIJ	3.376	154.6	154.6	0.0			
67	KIKPUQ	3.377	161.8	161.8	0.0			
68	GURLIP	3.379	167.1	167.1	0.0			
69	NUWKIA	3.380	160.9	160.9	0.0			
70	RUPSAW	3.381	162.8	162.8	0.0	3.993	98.5	
71	JAWXAG	3.382	168.5	168.5	0.0			
72	RANZIQ	3.382	155.7	155.7	0.0			
73	XACXEE	3.382	157.0	167.7	-10.7			
74	ESAWUQ	3.383	166.8	166.8	0.0			
75	WEWWIE	3.383	173.3	138.7	34.6			
76	IJUSAI	3.385	159.5	159.5	0.0			
77	LEBRAN	3.386	150.5	160.2	-9.7			
78	SAGKOC	3.386	150.1	150.1	0.0			
79	BZMOCO	3.387	162.2	162.2	0.0			
80	BPPHOX	3.388	136.9	136.9	0.0	3.790	109.9	
81	LALCEI	3.388	161.0	129.1	31.9			
82	QESBEW	3.388	105.3	174.3	-69.0			
83	SEPXES	3.389	100.2	172.0	-71.8			
84	LILBAJ	3.389	150.8	150.8	0.0			
85	LIKFIU	3.390	137.4	174.0	-36.7			
86	ZIXNAX	3.391	159.5	159.5	0.0			
87	BHXPAM10	3.392	169.1	107.0	62.2			
88	EBMZDC	3.393	168.9	163.6	5.3			
89	IBUCEN	3.393	145.6	145.6	0.0			
90	YUNWUA	3.393	144.2	144.2	0.0	3.556	95.7	
91	NAWXIU	3.394	158.6	171.3	-12.7			
92	JEHYAX	3.395	149.7	149.7	0.0			
93	KUCBEQ	3.395	154.6	174.1	-19.5			
94	MUTRAU	3.395	127.3	168.2	-40.8			
95	SEDRIE	3.395	114.3	170.0	-55.6			
96	AZOZOF	3.396	172.4	172.4	0.0			
97	OHIKOF	3.396	96.5	169.3	-72.8			
98	XUQYUE	3.396	151.8	151.8	0.0			
99	EWUBAZ	3.397	152.1	152.1	0.0			
100	LOGNIF	3.398	93.4	167.7	-74.2	3.705	88.4	

[a] Crystal structure determined under pressure

[b] No C-Br···Br-C short contact below 5 Å other than reported in this table below 3.4 Å

Table S2. Proportion of symmetric C-Br···Br-C interactions (i.e., those that have their <C-Br1···Br2 angle equal to the <C-Br2···Br1 angle) for contacts whose Br···Br distance is smaller than the indicated cutoff.

Cutoff	3.1	3.2	3.3	3.4	3.5	3.6	3.7	3.8
# contacts	2	8	20	100	431	1179	2320	3705
% symmetric	1.00	0.88	0.90	0.77	0.67	0.51	0.44	0.40

Table S3. Cartesian coordinates of all optimized dimers computed in this paper:

$(CH_3Br)_2$ (180,180)

C	-3.95880700	0.00014100	-0.00086500
H	-4.31603800	0.18841800	1.00987200
H	-4.33013200	0.78095800	-0.66199400
H	-4.32136700	-0.97104100	-0.33253800
Br	-2.02861100	-0.00004100	-0.00039900
Br	2.02906800	0.00011900	0.00012200
C	3.95926400	0.00045200	0.00015200
H	4.31619000	0.97958800	0.31407700
H	4.31621000	-0.76338100	0.68848200
H	4.31640600	-0.22084900	-1.00390300

$(CH_3Br)_2$ (180,90)

C	2.27164600	1.50319700	0.00137500
H	1.79119100	1.91068200	-0.88630100
H	1.79904400	1.92232300	0.88784600
H	3.32864200	1.76280200	-0.01327700
Br	2.08075400	-0.41760500	0.00015900
Br	-1.70501600	-0.04136900	-0.00005000
C	-3.62578700	0.14983500	-0.00003500
H	-3.87959700	1.20833900	0.00074300
H	-4.03258700	-0.32846100	-0.88919000
H	-4.03270500	-0.32979500	0.88834700

$(CH_3Br)_2$ (90,90)

C	-2.51892100	1.40821600	-0.00112700
H	-2.11178900	1.86568400	0.89865200
H	-2.08205800	1.88930200	-0.87425000
H	-3.59996700	1.53447800	-0.00702600
Br	-2.09400700	-0.47319000	-0.00037300
Br	2.09395000	0.47265700	-0.00010800
C	2.51886500	-1.40874900	0.00064600
H	2.09793700	-1.86932900	-0.89116200
H	3.60054300	-1.52960900	0.00084900
H	2.09766000	-1.86867700	0.89266000

$(H_2CCHBr)_2$ (180,180)

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.345300
H	0.906600	0.000000	1.954000
H	-0.925000	0.000000	-0.579500
H	0.956400	0.000000	-0.529200
Br	-1.589800	0.000000	2.374500
Br	-4.579000	-0.000600	4.309700

C	-6.168700	-0.000600	5.338900
C	-6.168700	-0.001200	6.684200
H	-5.243700	-0.001800	7.263600
H	-7.125200	-0.001200	7.213300
H	-7.075300	-0.000100	4.730100

$(H_2CCHBr)_2$ (180,90)

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.345300
H	0.910700	0.000000	1.947900
H	-0.925500	0.000000	-0.578800
H	0.955300	0.000000	-0.531400
Br	-1.585800	0.000000	2.381200
Br	-4.556200	-0.000600	4.321500
C	-4.556400	1.893600	4.321700
C	-3.937900	2.621700	5.268800
H	-3.397600	2.157200	6.095800
H	-3.977600	3.712500	5.208500
H	-5.105300	2.324300	3.481600

$(H_2CCHBr)_2$ (90,90)

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.345600
H	0.907800	0.000000	1.952300
H	-0.925600	0.000000	-0.578600
H	0.955900	0.000000	-0.530100
Br	-1.587300	0.000000	2.374500
Br	-1.587300	-3.895200	2.374500
C	-3.174600	-3.895200	3.403500
C	-3.174600	-3.895200	4.749000
H	-2.249000	-3.895200	5.327600
H	-4.130600	-3.895200	5.279100
H	-4.082400	-3.895200	2.796700

$(HCCBr)_2$ (180,180)

C	0.00058000	5.26044300	0.00000000
C	0.00015500	4.04085300	0.00000000
H	0.00113800	6.32630700	0.00000000
Br	-0.00015900	2.24676800	0.00000000
Br	-0.00015900	-2.24676800	0.00000000
C	0.00015500	-4.04085300	0.00000000
C	0.00058000	-5.26044300	0.00000000
H	0.00113800	-6.32630700	0.00000000

$(HCCBr)_2$ (180,90)

C	0.65659100	4.51989500	0.00000000
C	0.39081300	3.32944700	0.00000000
H	0.88902300	5.56012500	0.00000000
Br	0.00000000	1.57751600	0.00000000
Br	-0.81925000	-2.09802200	0.00000000
C	0.93275000	-2.48852900	0.00000000
C	2.12333700	-2.75368400	0.00000000
H	3.16376900	-2.98520700	0.00000000

$(HCCBr)_2$ (90,90)

C	-1.20902600	3.42381600	0.00000000
C	-0.23008600	2.69568400	0.00000000
H	-2.06434500	4.05976600	0.00000000
Br	1.20902600	1.62488900	0.00000000

Br	-1.20902600	-1.62488900	0.00000000
C	0.23008600	-2.69568400	0.00000000
C	1.20902600	-3.42381600	0.00000000
H	2.06434500	-4.05976600	0.00000000

$(C_6H_5Br)_2$ (180,180)

C	5.93540200	-0.40826700	1.14135600
C	4.53577100	-0.40824000	1.14127800
C	3.83622200	0.00005800	-0.00016300
C	4.53649600	0.40821500	-1.14121000
C	5.93612600	0.40796100	-1.14050000
C	6.63509400	0.00000300	-0.00000800
H	6.47911500	-0.72525800	2.02753900
H	3.98876600	-0.72458800	2.02566300
H	3.99005200	0.72467300	-2.02590300
H	6.47995100	0.72493100	-2.02662300
H	7.72203000	-0.00001900	0.00005200
Br	1.94204900	0.00009600	-0.00026800
Br	-1.94213900	-0.00005500	0.00015500
C	-3.83637600	-0.00001800	0.00005000
C	-4.53599800	-1.14148900	-0.40804300
C	-4.53599800	1.14148100	0.40806500
C	-5.93562800	-1.14146100	-0.40812000
C	-6.63524900	0.00003800	-0.00010500
C	-5.93562800	1.14150800	0.40798700
H	-3.98904700	-2.02597900	-0.72419300
H	-3.98904700	2.02594900	0.72427600
H	-6.47894500	-2.02791300	-0.72504000
H	-6.47894500	2.02798200	0.72484700
H	-7.72218500	0.00005900	-0.00016500

$(C_6H_5Br)_2$ (180,90)

C	-4.95721300	0.68520000	1.21221100
C	-3.62820200	0.24607100	1.21213500
C	-2.96398300	0.02653400	-0.00018600
C	-3.62898000	0.24619500	-1.21205800
C	-4.95799000	0.68532500	-1.21123600
C	-5.62159600	0.90465800	-0.00003400
H	-5.47350800	0.85584500	2.15338500
H	-3.10842600	0.07437900	2.15120000
H	-3.10980700	0.07460000	-2.15147500
H	-5.47441300	0.85590900	-2.15235200
H	-6.65367900	1.24567800	0.00002500
Br	-1.16513600	-0.56783800	-0.00028900
Br	2.31583700	-1.71801500	0.00015100
C	2.91009700	0.08049400	0.00005300
C	3.12947600	0.74490000	1.21230000
C	3.12971300	0.74468900	-1.21226600
C	3.56860500	2.07391100	1.21222700
C	3.78822100	2.73810700	-0.00009200
C	3.56884300	2.07370000	-1.21233900
H	2.95766200	0.22527000	2.15142400
H	2.95808300	0.22489600	-2.15133300
H	3.73897000	2.58987600	2.15363300
H	3.73939200	2.58950100	-2.15380100
H	4.12924000	3.77019000	-0.00014900

$(C_6H_5Br)_2$ (90,90)

C	4.40305300	-0.61018900	1.21218600
C	3.24273900	0.17273100	1.21219400

C	2.66270700	0.56406500	-0.00012300
C	3.24314000	0.17237700	-1.21213500
C	4.40345300	-0.61054400	-1.21151400
C	4.98303400	-1.00157300	-0.00014000
H	4.85382200	-0.91431300	2.15335600
H	2.78884000	0.47903200	2.15115100
H	2.78955100	0.47840300	-2.15133100
H	4.85418300	-0.91470600	-2.15269000
H	5.88406500	-1.60954300	-0.00014600
Br	1.09452500	1.62219400	-0.00011200
Br	-1.09459200	-1.62214900	0.00000000
C	-2.66283000	-0.56398200	0.00001100
C	-3.24286200	-0.17264800	-1.21230700
C	-3.24281100	-0.17259900	1.21233600
C	-4.40317500	0.61027200	-1.21229800
C	-4.98315600	1.00165600	0.00002700
C	-4.40312500	0.61032200	1.21234500
H	-2.78896200	-0.47894900	-2.15126400
H	-2.78887200	-0.47886100	2.15128700
H	-4.85359400	0.91415900	-2.15371300
H	-4.85350400	0.91424700	2.15376500
H	-5.88418800	1.60962600	0.00003400

$(CBr_4)_2$ (180,180)

C	0.000000	0.000000	0.000000
Br	0.000000	0.000000	1.944556
Br	1.833618	0.000000	-0.647410
Br	-0.917258	1.587701	-0.647410
Br	-0.918439	-1.589745	-0.648244
Br	-2.556611	-4.426339	-1.805124
C	-3.474483	-6.016281	-2.453688
Br	-5.307717	-6.014922	-1.805190
Br	-3.473544	-6.016628	-4.398243
Br	-2.557320	-7.603453	-1.804849

$(CHBr_3)_2$ (180,180)

C	0.000000	0.000000	0.000000
Br	0.000000	0.000000	1.939200
Br	1.816000	0.000000	-0.680400
H	-0.517400	0.896200	-0.355700
Br	-0.907600	-1.572100	-0.681000
Br	-2.558000	-4.431700	-1.920000
C	-3.465100	-6.003900	-2.601300
Br	-5.293100	-6.067200	-1.957000
Br	-3.500400	-5.982600	-4.540100
H	-2.932600	-6.897400	-2.261000

$(CH_2Br_2)_2$ (180,180)

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.095800
H	1.039100	0.000000	-0.347900
Br	-0.868900	1.578600	-0.697100
Br	-0.885300	-1.608300	-0.614600
Br	-2.514000	-4.568500	-1.746200
C	-3.398700	-6.177000	-2.361100
H	-4.426900	-6.174900	-1.982000
H	-3.414000	-6.168500	-3.456800
Br	-2.513200	-7.758800	-1.692800