Electronic Supplementary Material for CrystEngComm

Table of chemical groups used by *RPluto* for processing of H-bond contacts.

The groups are defined as atom centred fragments, with atom 1 in the centre, optionally connected to 4 atoms, numbered 2 - 5. Each atom has two defined attributes, nt is the total number of covalent bonds, nh is the number of hydrogens connected to the atom.

Gp	gp-name	at1	nt1	nh1	at2	nt2	nh2	at3	nt3	nh3	at4	nt4	nh4	at5	nt5	nh5
01	NO3-	N	3	0	O	1	0	O	1	0	O	1	0			
02	H3PO4	P	4	0	O	1	0	O	2	1	O	2	1	O	2	1
03	H2PO4-	P	4	0	O	1	0	O	1	0	O	2	1	O	2	1
04	HPO42-	P	4	0	O	1	0	O	1	0	O	1	0	O	2	1
05	HSO4-	S	4	0	O	1	0	O	1	0	O	1	0	O	2	1
06	SO42-	S	4	0	O	1	0	O	1	0	O	1	0	O	1	0
07	HCONH2	C	3	1	O	1	0	N	3	2						
08	SCS	C	2	0	S	1	0	S	1	0						
09	OH3+	O	3	3												
10	OH2	O	2	2												
11	NH4+	N	4	4												
12	HOCH3	O	2	1	C	4	3									
13	HOCH2CH3	C	4	2	O	2	1	C	4	3						
14	CH3CHOHCH3	C	4	1	O	2	1	C	4	3	C	4	3			
15	CCl4	C	4	0	Cl	1	0	Cl	1	0	Cl	1	0	Cl	1	0
16	HCCl3	C	4	1	Cl	1	0	Cl	1	0	Cl	1	0			
17	H2CCl2	C	4	2	Cl	1	0	Cl	1	0						
18	CBr4	C	4	0	Br	1	0	Br	1	0	Br	1	0	Br	1	0
19	F-	F	0	0												
20	Cl-	Cl	0	0												
21	Br-	Br	0	0												
22	I-	I	0	0												
23	H2N-CO-NH2	C	3	0	O	1	0	N	3	2	N	3	2			
24	H2N-CS-NH2	C	3	0	S	1	0	N	3	2	N	3	2			
25	H2N-CO-NHR	C	3	0	O	1	0	N	3	1	N	3	2			
26	RHN-CO-NHR	C	3	0	O	1	0	N	3	1	N	3	1			
27	H2N-CS-NHR	C	3	0	S	1	0	N	3	1	N	3	2			
28	RHN-CS-NHR	C	3	0	S	1	0	N	3	1	N	3	1			
29	RPO32-	P	4	0	O	1	0	O	1	0	O	1	0			
30	RHPO3-	P	4	0	O	1	0	O	1	0	O	2	1			
31	RH2PO3	P	4	0	O	1	0	O	2	1	O	2	1			
32	RRPO2-	P	4	0	O	1	0	O	1	0						
33	RRHPO2	P	4	0	O	1	0	O	2	1						
34	C3PO	P	4	0	O	1	0	C	*	*	C	*	*	C	*	*
35	R2NHPO	P	4	0	O	1	0	N	3	1						
36	R3PO	P	4	0	O	1	0									
37	R2SPOH	P	4	0	O	2	1	S	1	0						
38	RSO3-	S	4	0	O	1	0	O	1	0	O	1	0			
39	RHSO3	S	4	0	O	1	0	O	1	0	O	2	1			
40	RRSO2	S	4	0	O	1	0	O	1	0						
41	PS2	P	4	0	S	1	0	S	1	0						
42	PS2H	P	4	0	S	1	0	S	2	1						
43	SO2NH2	S	4	0	O	1	0	O	1	0	N	3	2			
44	SO2NH	S	4	0	O	1	0	O	1	0	N	3	1			
45	-O-CO-NH2	C	3	0	O	1	0	O	2	0	N	3	2			
46	CONH2	C	3	0	O	1	0	N	3	2						
47	CSNH2	C	3	0	S	1	0	N	3	2						
48	-O-CO-NH-	C	3	0	O	1	0	O	2	0	N	3	1			
49	HCONH	C	3	1	O	1	0	N	3	1						
50	CONH	C	3	0	O	1	0	N	3	1						
51	CSNH	C	3	0	S	1	0	N	3	1						
52	COOH	C	3	0	O	1	0	O	2	1						
53	COO-	C	3	0	O	1	0	O	1	0						
54	CSS-	C	3	0	S	1	0	S	1	0						
55	NO2	N	3	0	O	1	0	O	1	0	C	*	*			
56	C=N-NH2	N	2	0	N	3	2	C	3	*						
57	C=N-NH	N	2	0	N	3	1	C	3	*						

58	C=N-OH	N	2	0	O	2	1	C	3	*			
59	C-NH-O-	N	3	1	O	2	0	C	*	*			
60	N--N+=N	N	2	0	N	1	0	N	2	0			
61	C-N+=N	N	2	0	N	1	0	C	*	*			
62	-N=C=O	C	2	0	O	1	0	N	2	0			
63	C-N=O	N	2	0	O	1	0	C	*	*			
64	X-N=O	N	2	0	O	1	0						
65	N=O	N	*	0	O	1	0						
66	COOR	C	3	0	O	1	0	O	2	0			
67	C-N=N-	N	2	0	N	2	0	C	*	*			
68	HOCH2R	O	2	1	C	4	2						
69	HOCHR2	O	2	1	C	4	1						
70	HOCR3	O	2	1	C	4	0						
71	HOPh	C	3	0	O	2	1	C	3	*	C	3	*
72	HOCHR	O	2	1	C	3	1						
73	HOCR2	O	2	1	C	3	0						
74	NH3+	N	4	3									
75	NH2R2+	N	4	2									
76	NHR3+	N	4	1									
77	H2NCH2R	N	3	2	C	4	2						
78	H2NCHR2	N	3	2	C	4	1						
79	H2NCR3	N	3	2	C	4	0						
80	H2NPh	C	3	0	N	3	2	C	3	*	C	3	*
81	H2NCHR	N	3	2	C	3	1						
82	H2NCR2	N	3	2	C	3	0						
83	4CNHC4	N	3	1	C	4	*	C	4	*			
84	4CNHC3	N	3	1	C	4	*	C	3	*			
85	3CNHC3	N	3	1	C	3	*	C	3	*			
86	CF3	C	4	0	F	1	0	F	1	0	F	1	0
87	CCl3	C	4	0	Cl	1	0	Cl	1	0	Cl	1	0
88	NH	N	3	1									
89	N3	N	3	0									
90	N2	N	2	0									
91	OH	O	2	1									
92	SH	S	2	1									
93	HCO	C	3	1	O	1	0						
94	CO	O	1	0	C	*	*						
95	HCS	C	3	1	S	1	0						
96	CS	S	1	0	C	*	*						
97	-O-	O	2	0									
98	-S-	S	2	0									
99	CN	N	1	0	C	*	*						
100	F-C	F	1	0	C	*	*						
101	Cl-C	Cl	1	0	C	*	*						
102	Br-C	Br	1	0	C	*	*						
103	I-C	I	1	0	C	*	*						
104	OH2-X	O	3	2									
105	F-X	F	1	0									
106	Cl-X	Cl	1	0									
107	Br-X	Br	1	0									
108	I-X	I	1	0									
109	O-nocon	O	0	0									
110	N-nocon	N	0	0									

* means any possibility allowed

Command file used by Pluto to generate contact data files.

```
COMDEF BATCH NOLAB
BATMAX   200  50
HOME
HNORM
HCAL  ALL KEEP
ASSIGN
VATM O  P=1.50 N=8000 NOCRYST NOPLOT
VATM N
VATM S
VATM F
VATM Cl
VATM Br
VATM I
CALC INTERX O 1.57 N 1.61 S 1.85 F 1.52 Cl 1.80 Br 1.90 I 2.03
HBTOT
PLOT NEXT
```