Table S1. Geometries (in Å) of all electron donors as well as electron acceptors taken from X-ray crystal structures or optimisation.

DTCA...I_2				**DTCA…Br_2**			
13				13			
				S	6.278000	3.020000	-2.261000
C	5.183000	2.499000	-1.062000	C	5.183000	2.499000	-1.062000
C	3.823000	3.619000	-2.928000	S	3.538000	2.850000	-1.411000
C	5.102000	3.708000	-3.318000	C	3.823000	3.619000	-2.928000
C	5.623000	4.347000	-4.535000	C	5.102000	3.708000	-3.318000
O	4.696000	4.759000	-5.354000	S	5.747000	1.719000	0.303000
O	6.832000	4.439000	-4.703000	C	5.623000	4.347000	-4.535000
S	5.747000	1.719000	0.303000	O	6.832000	4.439000	-4.703000
S	3.538000	2.850000	-1.411000	O	4.696000	4.759000	-5.354000
S	6.278000	3.020000	-2.261000	H	2.983000	4.010000	-3.496000
H	2.983000	4.010000	-3.496000	H	5.052000	5.192000	-6.166000
H	5.052000	5.192000	-6.166000	Br	3.516000	1.070000	1.741000
I	1.342000	0.350000	3.385000	Br	1.725000	0.477000	3.095000
I	3.516000	1.070000	1.741000				
DTCA…Cl_2				**DTCA...N_2**			
13				13			
S	6.278000	3.020000	-2.261000	S	6.278000	3.020000	-2.261000
C	5.183000	2.499000	-1.062000	C	5.183000	2.499000	-1.062000

S	3.538000	2.850000	-1.411000	S	3.538000	2.850000	-1.411000
C	3.823000	3.619000	-2.928000	C	3.823000	3.619000	-2.928000
C	5.102000	3.708000	-3.318000	C	5.102000	3.708000	-3.318000
S	5.747000	1.719000	0.303000	S	5.747000	1.719000	0.303000
C	5.623000	4.347000	-4.535000	C	5.623000	4.347000	-4.535000
O	6.832000	4.439000	-4.703000	O	6.832000	4.439000	-4.703000
O	4.696000	4.759000	-5.354000	O	4.696000	4.759000	-5.354000
H	2.983000	4.010000	-3.496000	H	2.983000	4.010000	-3.496000
H	5.052000	5.192000	-6.166000	H	5.052000	5.192000	-6.166000
Cl	3.516000	1.070000	1.741000	N	3.516000	1.070000	1.741000
Cl	1.964000	0.556000	2.915000	N	2.655000	0.785000	2.392000
DTCA...IF				**DTCA...ICH$_3$**			
13				16			
S	6.278000	3.020000	-2.261000	S	6.278000	3.020000	-2.261000
C	5.183000	2.499000	-1.062000	C	5.183000	2.499000	-1.062000
S	3.538000	2.850000	-1.411000	S	3.538000	2.850000	-1.411000
C	3.823000	3.619000	-2.928000	C	3.823000	3.619000	-2.928000
C	5.102000	3.708000	-3.318000	C	5.102000	3.708000	-3.318000
S	5.747000	1.719000	0.303000	S	5.747000	1.719000	0.303000
C	5.623000	4.347000	-4.535000	C	5.623000	4.347000	-4.535000
O	6.832000	4.439000	-4.703000	O	6.832000	4.439000	-4.703000
O	4.696000	4.759000	-5.354000	O	4.696000	4.759000	-5.354000
H	2.983000	4.010000	-3.496000	H	2.983000	4.010000	-3.496000
H	5.052000	5.192000	-6.166000	H	5.052000	5.192000	-6.166000

I 3.516000 1.070000 1.741000 F 1.806000 0.504000 3.034000	I 3.516000 1.070000 1.741000 C 1.817000 0.507000 3.026000 H 0.903000 0.664000 2.444000 H 1.946000 -0.546000 3.295000 H 1.846000 1.154000 3.909000
DABCO...I_2 22 I 7.108000 0.340000 0.900000 I 8.305000 2.629000 -0.311000 N 6.152000 -1.548000 1.959000 N 5.055000 -3.560000 3.111000 C 5.706000 -2.529000 0.940000 H 6.597000 -2.841000 0.378000 H 5.038000 -2.002000 0.246000 C 4.975000 -1.089000 2.741000 H 4.274000 -0.625000 2.035000 H 5.322000 -0.314000 3.437000 C 5.006000 -3.713000 1.655000 H 3.951000 -3.781000 1.354000 H 5.488000 -4.666000 1.392000 C 7.135000 -2.204000 2.868000 H 7.440000 -1.455000 3.610000 H 8.014000 -2.465000 2.264000	**DABCO…Br_2** 22 C 6.466000 -3.447000 3.517000 N 5.055000 -3.560000 3.111000 C 5.006000 -3.713000 1.655000 C 5.706000 -2.529000 0.940000 N 6.152000 -1.548000 1.959000 C 7.135000 -2.204000 2.868000 C 4.362000 -2.316000 3.474000 C 4.975000 -1.089000 2.741000 H 6.597000 -2.841000 0.378000 H 5.038000 -2.002000 0.246000 H 4.274000 -0.625000 2.035000 H 5.322000 -0.314000 3.437000 H 3.951000 -3.781000 1.354000 H 5.488000 -4.666000 1.392000 H 7.440000 -1.455000 3.610000 H 8.014000 -2.465000 2.264000

C	4.362000	-2.316000	3.474000	H	4.432000	-2.193000	4.564000
H	4.432000	-2.193000	4.564000	H	3.298000	-2.428000	3.218000
H	3.298000	-2.428000	3.218000	H	6.981000	-4.371000	3.217000
C	6.466000	-3.447000	3.517000	H	6.505000	-3.381000	4.614000
H	6.981000	-4.371000	3.217000	Br	7.108000	0.340000	0.900000
H	6.505000	-3.381000	4.614000	Br	8.082000	2.203000	-0.086000

DABCO…Cl_2				**DABCO…N_2**			
22				22			
C	4.975000	-1.089000	2.741000	C	6.466000	-3.447000	3.517000
N	6.152000	-1.548000	1.959000	N	5.055000	-3.560000	3.111000
C	5.706000	-2.529000	0.940000	C	5.006000	-3.713000	1.655000
C	5.006000	-3.713000	1.655000	C	5.706000	-2.529000	0.940000
N	5.055000	-3.560000	3.111000	N	6.152000	-1.548000	1.959000
C	4.362000	-2.316000	3.474000	C	7.135000	-2.204000	2.868000
C	7.135000	-2.204000	2.868000	C	4.362000	-2.316000	3.474000
C	6.466000	-3.447000	3.517000	C	4.975000	-1.089000	2.741000
H	6.597000	-2.841000	0.378000	H	6.597000	-2.841000	0.378000
H	5.038000	-2.002000	0.246000	H	5.038000	-2.002000	0.246000
H	4.274000	-0.625000	2.035000	H	4.274000	-0.625000	2.035000
H	5.322000	-0.314000	3.437000	H	5.322000	-0.314000	3.437000
H	3.951000	-3.781000	1.354000	H	3.951000	-3.781000	1.354000
H	5.488000	-4.666000	1.392000	H	5.488000	-4.666000	1.392000
H	7.440000	-1.455000	3.610000	H	7.440000	-1.455000	3.610000

H	8.014000	-2.465000	2.264000	H	8.014000	-2.465000	2.264000
H	4.432000	-2.193000	4.564000	H	4.432000	-2.193000	4.564000
H	3.298000	-2.428000	3.218000	H	3.298000	-2.428000	3.218000
H	6.981000	-4.371000	3.217000	H	6.981000	-4.371000	3.217000
H	6.505000	-3.381000	4.614000	H	6.505000	-3.381000	4.614000
Cl	7.108000	0.340000	0.900000	N	7.108000	0.340000	0.900000
Cl	7.952000	1.955000	0.045000	N	7.576000	1.235000	0.426000
DABCO…IF				**DABCO…ICH$_3$**			
22				25			
C	6.466000	-3.447000	3.517000	C	6.466000	-3.447000	3.517000
N	5.055000	-3.560000	3.111000	N	5.055000	-3.560000	3.111000
C	5.006000	-3.713000	1.655000	C	5.006000	-3.713000	1.655000
C	5.706000	-2.529000	0.940000	C	5.706000	-2.529000	0.940000
N	6.152000	-1.548000	1.959000	N	6.152000	-1.548000	1.959000
C	7.135000	-2.204000	2.868000	C	7.135000	-2.204000	2.868000
C	4.362000	-2.316000	3.474000	C	4.362000	-2.316000	3.474000
C	4.975000	-1.089000	2.741000	C	4.975000	-1.089000	2.741000
H	6.597000	-2.841000	0.378000	H	6.597000	-2.841000	0.378000
H	5.038000	-2.002000	0.246000	H	5.038000	-2.002000	0.246000
H	4.274000	-0.625000	2.035000	H	4.274000	-0.625000	2.035000
H	5.322000	-0.314000	3.437000	H	5.322000	-0.314000	3.437000
H	3.951000	-3.781000	1.354000	H	3.951000	-3.781000	1.354000
H	5.488000	-4.666000	1.392000	H	5.488000	-4.666000	1.392000
H	7.440000	-1.455000	3.610000	H	7.440000	-1.455000	3.610000

H	8.014000	-2.465000	2.264000
H	4.432000	-2.193000	4.564000
H	3.298000	-2.428000	3.218000
H	6.981000	-4.371000	3.217000
H	6.505000	-3.381000	4.614000
I	7.108000	0.340000	0.900000
F	7.945000	1.940000	0.054000

H	8.014000	-2.465000	2.264000
H	4.432000	-2.193000	4.564000
H	3.298000	-2.428000	3.218000
H	6.981000	-4.371000	3.217000
H	6.505000	-3.381000	4.614000
I	7.108000	0.340000	0.900000
C	8.032000	2.108000	-0.035000
H	7.597000	2.213000	-1.034000
H	7.800000	2.971000	0.597000
H	9.111000	1.925000	-0.085000