SUPPORTING INFORMATION

Halogen bonds as a tool in the design of high energetic materials: evidence from crystal structures and quantum chemical calculations

Aleksandra B. Đunović[b], Dušan Ž. Veljković [a*]

I Cambridge Structural Databank search

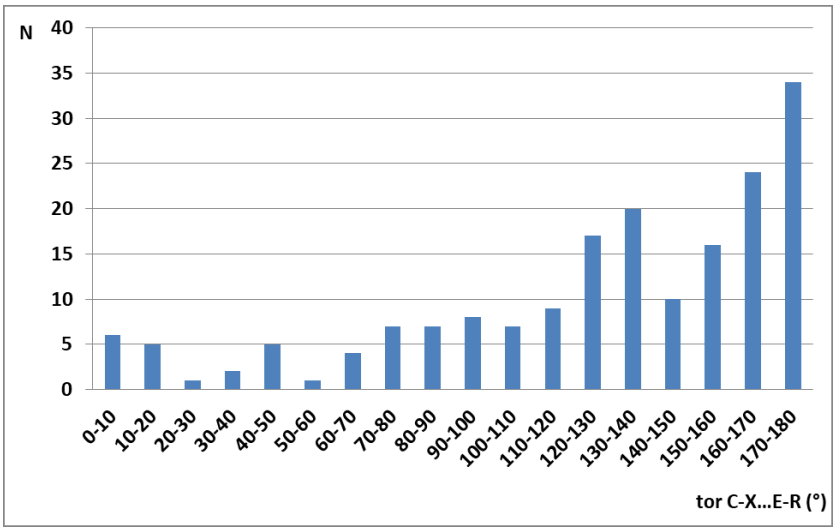

Figure S1. Distribution of torsion angle defined by atoms C, X, E, and R in fragments of crystal structures containing halogen bonds.

Peaks in the interval 160 - 180° (58 contacts) indicates that in the majority of contacts mutual orientation of C-X and E-R fragments is antiparallel. This also indicates the existence of contacts between halogen atom (X) and electron-rich atom (E) since in this orientation X and E are orientated towards each other. The number of interactions with the parallel orientation of C-X and E-R fragments (torsion angle values in the interval 0 - 10° is significantly lower (6 contacts).

II Optimized geometries of model systems A-C

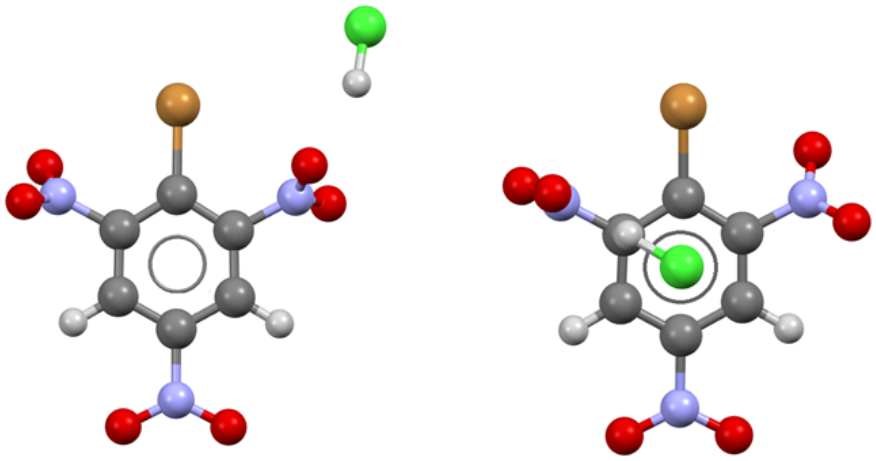

Figure S2. Optimized geometries for the distances in the geometries A-C with the strongest interactions. Geometry optimizations for the structures A and B resulted in the same optimized geometry with Cl-H···O interaction (a) while geometry optimization for model system C resulted in geometry with Cl-H···O and Cl···π interactions (b).

III Geometries of model systems

Table S1: Geometries of model systems used for quantum chemical calculations - model system A

Br	-1.747569	-0.000789	-0.018287
C	0.129798	-0.005005	-0.008175
C	0.850866	-1.185090	0.000729
N	0.133497	-2.478398	0.049150
O	-0.157002	-2.959950	-1.016039
O	-0.028104	-2.969342	1.069847
C	2.226002	-1.199915	0.011718
H	2.697890	-2.001728	0.025285
C	2.874583	-0.002413	0.000292
N	4.354256	0.011158	0.043150
O	4.898660	-1.022298	-0.345498
O	4.920654	1.019040	0.377342
C	2.217882	1.205964	-0.015946
H	2.684172	2.010401	-0.014633
C	0.849824	1.172183	-0.037163
N	0.148573	2.466492	-0.050636
O	-0.074686	2.972053	-1.087658
O	-0.122692	2.968250	0.991633
Cl	-5.147552	0.000758	-0.028789
H	-5.151476	0.028369	1.245906

Table S2: Geometries of model systems used for quantum chemical calculations - model system B

Br	1.694653	-0.002896	-0.001688
C	-0.182744	-0.005656	-0.000015
C	-0.904769	-1.185182	-0.004283
N	-0.188720	-2.479050	-0.057085
O	0.108086	-2.960734	1.006304
O	-0.033910	-2.970210	-1.078730
C	-2.279958	-1.198940	-0.006638
H	-2.752542	-2.000388	-0.017169
C	-2.927525	-0.000935	0.008747
N	-4.407427	0.013781	-0.024823
O	-4.950182	-1.019218	0.367330
O	-4.975130	1.022073	-0.355548
C	-2.269798	1.206934	0.020750
H	-2.735463	2.011733	0.022288
C	-0.901661	1.172094	0.033382
N	-0.199335	2.465858	0.042332
O	0.030821	2.971338	1.077885
O	0.065771	2.967314	-1.001666
Cl	5.294648	0.002397	-0.004894
H	6.569646	0.004272	-0.006030

Table S3: Geometries of model systems used for quantum chemical calculations - model system C

Br	1.986939	0.033703	-1.090648
C	0.192738	0.019016	-0.538150
C	-0.502110	1.191635	-0.304120
N	0.190719	2.491376	-0.446490
O	0.157798	2.988626	-1.543106
O	0.637623	2.971562	0.490879
C	-1.815364	1.192569	0.104173
H	-2.268033	1.989399	0.265164
C	-2.432229	-0.011136	0.263450
N	-3.836161	-0.040026	0.732060
O	-4.475982	0.992546	0.532366
O	-4.275553	-1.057482	1.201138
C	-1.800945	-1.212600	0.040601
H	-2.242022	-2.021619	0.165048
C	-0.497721	-1.164882	-0.374733
N	0.177531	-2.451853	-0.609057
O	0.094400	-2.942608	-1.673529
O	0.741693	-2.963410	0.302920
Cl	3.046753	-0.052374	2.348739
H	3.422104	-0.082859	3.566855