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Supporting information for article:

Crystal structures of four δ -keto esters and a Cambridge Structural Database analysis of cyano...halogen interactions

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Table S1 Refcodes and parameters ANG1 (\angle C-X...N), ANG2 (\angle C-N...X) and d (N...X) for the 485 independent N...halogen interactions retrieved from the CSD. (Search criteria: no polymers, no ions, no errors and only organic compounds.)

<i>Refcode</i>	<i>ANG1 (°)</i>	<i>ANG2 (°)</i>	<i>d (Å)</i>
ACOKEI	164.614	164.433	3.155
ACOKIM	167.283	167.288	3.117
ADULEQ01	167.456	131.004	3.05
ADULEQ02	140.082	156.676	3.272
ADULEQ02	171.088	128.713	3.024
ADULEQ03	161.607	134.02	3.127
ADULEQ04	170.246	129.299	3.068
ADULEQ04	161.569	132.373	3.015
ADULEQ04	169.261	133.208	2.962
AFIBAT	166.93	123.076	3.142
APAVUJ	178.313	129.166	3.009
ASOKOJ	162.082	101.833	3.298
ATIXIK	167.987	113.218	3.064
AVAHHEL	162.499	98.975	3.193
AZUXAV	145.091	125.123	3.335
BAFJOH	177.466	176.899	3.031
BAGMIG	171.267	136.847	3.255
BAGMIG	171.498	124.312	3.397
BAGYAJ	172.49	111.558	3.283
BAHBAP	171.347	151.346	3.106
BAHBAP	149.249	103.601	3.165
BAHBET	135.144	123.808	2.832
BALQOV	157.397	128.017	3.194
BAQPAL	157.773	128.833	3.151
BAQPAL	169.837	114.624	3.35
BAQPAL	176.483	135.327	3.267
BAWMUH01	170.339	129.246	3.028
BAWMUH01	165.275	139.732	3
BAWMUH01	162.374	142.514	3.116
BAWNIW02	174.69	124.099	3.168
BAWNIW02	173.986	121.614	3.201
BAWNIW02	148.796	160.065	3.281
BAWNIW02	144.563	159.554	3.297
BAWNIW02	151.209	160.781	3.28
BAWNIW02	175.001	117.932	3.194
BAWNIW02	168.506	134.812	3.116
BAWNIW02	172.067	137.347	3.104
BAWNIW02	163.021	133.332	3.149
BAWNIW05	167.028	136.626	3.094
BAWNIW05	176.758	121.226	3.036
BAWNOC01	168.334	134.993	3.08

BCACEN	177.23	179.566	2.978
BCCANT10	172.413	141.167	3.104
BIBVUF	164.217	140.364	3.175
BILLOZ	147.291	88.065	3.242
BIYFAO10	173.532	142.492	3.148
BIYFEU10	159.232	122.518	3.184
BODBUT	176.738	107.354	3.048
BOSNUU	90.786	124.528	3.297
BOTRUX	171.433	122.305	3.215
BOZKAD	176.014	119.174	3.125
BRBNIT01	168.911	168.763	3.249
BRBZNT	168.923	130.127	3.067
BRCYBP	163.009	167.708	3.239
BRCYBP	171.203	169.482	3.185
BRMALN	168.193	108.238	3.264
BTCYME	163.087	156.95	3.031
BYMBPY	170.909	119.216	3.287
BZPCBQ	140.584	124.002	3.298
BZSALT	154.489	103.187	3.268
CAHZIW	166.124	142.408	3.279
CAJLOO	178.846	127.718	3.357
CAZGEP10	165.111	121.947	3.261
CBOXAZ10	170.265	162.664	3.294
CCACEN	178.252	178.279	2.984
CEBZEO	164.22	91.598	2.978
CEKFUU	174.834	161.688	3.002
CEKFUU	174.38	151.71	3.073
CETNEW	175.208	147.231	2.938
CIDPAI	163.456	171.36	3.185
CIMPBR	175.473	157.995	2.912
CIQQEA	163.195	172.567	3.251
CIRLIA	161.813	113.47	3.234
CIYDIY	172.72	129.323	3.147
CIZFIC	173.101	141.922	3.16
CLBECN03	176.108	119.905	3.153
CLCYBQ	166.042	151.972	3.207
CLPCPN	169.304	91.5	3.283
CMTBZN	172.278	113.819	3.295
CMTIPH	170.228	117.44	3.21
CMTIPH	171.495	113.648	3.279
CMTIPH	171.575	128.733	3.002
CMTIPH	172.817	124.638	2.995
COCGIL	138.421	109.764	3.366
CODBOM	168.701	90.088	3.353
COGBIL	175.108	137.152	3.052
COHYUU	176.735	159.416	2.932

COLDOY	77.584	138.362	2.975
COLLUM	176.441	167.227	2.946
COMJUL	166.692	109.34	3.212
CURQUC	166.2	115.978	3.093
CYBISX	169.313	130.096	3.355
CYMEBF20	166.558	153.39	3.168
CYMEBF20	172.086	149.901	3.235
CYTMNQ	165.635	88.688	3.224
CYVHZM	161.02	146.129	3.259
DAGVAJ	170.757	145.572	3.25
DAJMOR	170.146	112.799	3.099
DAQNAK	166.661	96.778	3.205
DAQNAK	168.821	117.972	3.138
DATWAX	167.595	156.046	3.121
DATWAX	151.105	122.122	3.124
DATWEB	173.477	157.23	3.135
DBIBZN	152.11	117.332	3.275
DBIBZN	171.943	162.606	3.153
DBPHCN	166.921	158.744	3.288
DBPHCN	170.813	160.567	3.146
DETVII	144.228	111.622	3.262
DICXIX	138.627	98.091	3.251
DIRLEX	171.431	119.541	2.991
DIRLEX	167.615	134.557	3.099
DIWGEW	160.259	159.086	3.356
DIWGIA	163.848	160.828	3.316
DOCGAF	141.409	102.03	3.243
DORLIH	170.289	122.305	3.24
DOVWAN	165.653	157.105	3.214
EBIHIH	176.175	169.348	2.981
EBIHON	174.03	149.725	3.012
EBIHUT	176.46	155.98	3.002
EBIJAB	176.634	149.746	3.046
EBIJEF	174.582	171.238	2.966
EBIJJ	176.978	159.138	2.967
EBIJOP	177.535	143.121	3.023
EHAHOM	154.264	105.563	3.237
EHICII	87.083	151.911	2.989
EHICOO	131.769	102.149	2.917
EJUZEP	168.825	138.999	3.003
EMODOA	171.599	140.91	3.079
ENABEB	158.396	122.33	3.275
ENABEB	150.458	111.883	3.292
ERIVEG	172.043	135.678	3.19
ERIVEG	178.832	124.743	3.1
ERIVEG	169.087	138.893	3.057

ESAFIO	171.634	167.884	3.29
ETEYIM	166.633	147.147	3.206
ETEYIM	170.859	142.783	3.229
EVIBOB	175.025	129.43	3.169
FAKFII	177.195	153.248	3.007
FAKFOO	177.214	152.676	3.001
FEMREW	169.17	116.856	3.204
FEQQUN	162.535	138.882	3.102
FEQQUN	170.621	145.901	3.005
FEVGUK	174.333	120.776	3.16
FEWBAM	170.401	159.484	3.13
FEWLAW	98.197	94.567	2.92
FIZRAH	167.059	129.891	3.228
FOCBAB	174.551	116.219	3.151
FODYUU	162.774	124.117	3.239
FOMRAB	166.045	133.175	3.049
FOMWIN	166.244	121.128	3.232
FUBXIK	176.023	124.096	3.116
FUQJIK01	163.416	107.06	3.341
FUWMOA	168.997	112.463	3.246
GEDCEY	164.977	161.992	3.284
GEDTOZ	164.405	112.019	3.293
GIDJUY	177.329	114.445	3.075
GIVMIJ	172.053	105.648	3.147
GODQOH	146.256	101.381	2.957
GOKJIB	126.103	111.867	2.852
GUWKIT	159.636	138.162	3.101
HAHVOC	143.294	123.825	2.215
HAHVOC	66.785	169.172	3.265
HASZEI	158.212	112.912	3.135
HEJCOQ	176.936	147.13	3.026
HEJCOQ	175.15	109.22	3.181
HELGUC	148.341	93.655	3.413
HELGUC	141.1	94.54	3.487
HELHAJ	174.303	157.647	3.038
HELHEN	175.481	127.769	3.08
HELHIR	175.001	150.02	3.056
HEYRIN	164.445	97.777	3.277
HIBJAF	176.591	112.23	3.121
HIBJAF	165.633	115.213	3.123
HILSIF	171.813	133.304	3.205
HISKEB	83.529	111.098	2.945
HOFMUK	173.687	167.831	3.077
HOHHES	129.614	105.491	3.015
HOLTOS	142.637	121.033	3.296
HOQBEU	175.924	122.372	3.175

HUMLOQ	172.573	143.355	3.061
HUMYAQ	168.612	153.576	2.921
HURZEZ	158.681	156.589	3.23
HUXGEN	163.587	111.582	3.054
HUXGEN	163.984	111.666	3.083
IBIRAN	132.632	110.558	3.009
ICACEN	177.278	178.617	2.932
ICIMEM	166.098	108.244	3.134
ICIMIQ	161.858	100.8	3.35
INULIN	150.509	119.119	3.048
INULIN	160.863	96.764	3.171
IOBNIT01	180	180	3.127
ISUQIW	168.31	110.173	3.25
IYERUA	166.501	145.773	3.242
IYERUA	165.365	81.56	3.393
IYURAV	88.542	97.58	3.002
JEGWEX	177.959	100.412	2.833
JELGEM	162.062	129.171	3.289
JIXBEX	166.827	169.774	3.243
JIXBEX	174.79	173.406	3.18
JIXBEX01	167.432	170.903	3.19
JIXBEX01	174.52	172.164	3.142
JIYVUI	79.286	165.386	2.974
JIYVUI	95.24	166.585	3.012
JIYVUI	176.755	124.527	3.162
JUBKIA01	132.201	111.683	3.01
JUSTIA	168.594	115.642	3.185
JUSTIA	161.04	118.22	3.044
KABBIA	151.891	132.436	3.241
KABBIA	150.569	135.698	3.281
KATCOX	150.514	100.225	3.327
KECGUU	176.569	117.729	3.305
KELGEO03	163.72	148.543	3.207
KEMDEM	174.731	115.021	3.196
KEMDEM	176.259	116.404	3.129
KEVVUE	170.53	123.531	3.088
KIMLAV	161.866	106.269	3.11
KITDEY	167.32	129.777	3.302
KIWVAO	171.658	129.089	3.081
KIXZIB	163.576	153.391	3.172
KUCBAM	178.603	148.315	3.057
KUCBEQ	160.082	141.393	3.205
KUCBEQ	164.191	143.09	3.191
KUXBEL	169.718	130.02	3.202
LAGMOV	158.883	137.499	3.101
LALMEQ	177.89	179.652	3.147

LALNUH	175.876	175.546	3.259
LANNUK	105.003	93.274	3.295
LANNUK	146.011	120.197	3.276
LAXJAW	151.923	114.08	3.27
LAXZOA	176.615	161.061	3.147
LEYVAN	167.432	88.048	3.268
LIRJAZ	167.52	131.383	3.273
LIRJED	175.581	128.585	3.102
LIRJIG01	167.513	124.366	3.194
LIYQAN	168.316	90.362	3.271
LIZMOY	165.979	101.635	3.19
MAYTOW	174.985	95.062	3.266
MBRMAD01	172.209	161.807	3.218
MDBADN	172.182	163.396	3.202
MDMBAD	175.465	97.473	3.257
MEFBEE	163.992	96.748	3.293
MIFXEE	173.291	123.048	3.111
MILVAG	122.279	101.844	3.277
MIQNAC	164.344	154.391	3.18
MIQNAC	166.941	111.774	3.156
MISSEM	157.162	89.18	3.337
MOCCEM	155.851	140.079	3.084
MOCCEM	158.563	141.87	3.047
MOCCOW	143.857	155.12	3.25
MOCCOW	143.709	155.401	3.243
MOCCOW	166.437	130.16	3.027
MOCCOW	166.486	129.504	3.031
MOCCOW	176.226	125.887	3.028
MOCCOW	175.869	125.815	3.02
MTBCEY	165.433	166.205	3.202
MUKMAH	169.103	131.041	3.041
MUMQUH	158.517	106.592	3.231
MUMRES	160.413	98.807	3.215
MUTZIK	168.977	162.169	3.169
MUTZOQ	160.138	167.832	3.272
NAKXEC	174.095	152.665	2.951
NAKXEC	157.517	141.272	3.167
NAXYIW	171.415	112.284	3.184
NAXYIW	173.103	169.647	3.269
NEFJOZ	107.003	137.77	3.225
NEFJOZ	106.506	137.611	3.231
NEGQAT	157.667	82.648	3.283
NELSOM	172.617	114.947	3.263
NELSOM	154.909	118.988	3.343
NEMPAY	156.626	106.819	3.321
NIXVUN	95.679	148.528	3.289

NOCGER	175.675	92.938	3.307
NOCGER	169.153	95.881	3.166
NOCGER	72.31	111.392	3.259
NOKDAS	163.848	128.513	3.273
NOKDEW	164.613	175.488	3.005
NOKDEW	175.339	166.72	3.026
NOKDEW	171.182	164.011	3.019
NUGRAJ	171.976	116.051	3.115
OCAWIA	176.273	126.424	3.222
OCIQUN	142.874	152.777	3.385
ODOTUX	153.872	106.67	2.997
OQUNYI	80.692	126.482	2.957
OTOKOY	153.378	124.598	3.137
OZEGUW	167.181	79.35	3.359
PABDOL	168.719	98.364	2.954
PALPAV	164.264	132.972	3.097
PALPAV	149.625	140.841	3.083
PARLID10	165.47	149.995	3.201
PEGGUF	135.371	85.871	3.193
PEJLOF	165.414	165.955	3.185
PEXGOO	168.477	174.438	3.095
PEXGOO	165.714	148.761	3.037
PIBZUX	164.587	116.579	3.177
PIDBOV	157.935	156.043	3.274
PIXCCP	80.368	149.412	2.966
PIXCCP	167.7	112.154	3.287
PIYGUZ	177.865	114.831	3.27
PORWIC	165.346	108.299	2.964
PORWIC	104.465	114.543	3.047
POXNIA	162.844	135.011	3.167
PUCJAY	142.234	93.026	3.146
PUWNAX	169.863	144.121	3.089
QAGPEV	71.728	126.453	3.285
QAGPEV	156.91	117.439	3.157
QAPROQ	159.947	141.833	3.031
QAPVOU	161.366	106.233	2.945
QATBEU	168.587	123.56	3.201
QECXED	158.234	107.693	3.261
QEKCUE	135.272	121.463	3.254
QEKDAL	174.636	153.121	3.095
QEKDAL	177.144	87.824	3.253
QEKDAL	152.765	103.944	3.286
QEWQIU	149.71	128.402	3.255
QINDOI02	176.252	158.865	2.957
QINDOI02	157.334	117.099	3.423
QINPEK02	174.443	160.56	3.05

QINPEK02	156.476	114.982	3.43
QIPFEC	159.906	95.281	3.388
QIYFUA	161.672	136.439	3.283
QOCTEJ	158.402	94.075	3.22
QORZED	172.065	176.235	3.261
QORZUT	175	171.656	2.994
QOSBIK	169.797	171.747	3.26
QOSBIK	173.042	163.714	3.188
QOSBIK	177.57	163.622	3.17
QOSCAD	172.462	175.817	3.042
QOSCOR	177.534	176.074	3.214
QOSCOR	176.531	173.766	3.142
QOVICIO	174.763	172.66	3.014
QOVICIO	175.824	171.277	3.152
QOWPAU	170.072	124.708	3.186
QUCWUH	151.946	106.117	3.329
QUCXAO	129.346	139.405	3.249
RECVUS	77.869	133.772	3.287
REFLOD01	118.205	119.198	2.973
REGJUJ	172.279	92.098	2.576
RENMAA	164.175	126.886	3.304
REQSAI	159.998	124.532	3.224
RIMZUI	95.535	108.478	3.241
RIMZUI	70.647	78.399	3.275
ROFFAU	167.272	118.183	3.218
ROFHUP	170.081	123.253	3.026
ROFKON	163.446	135.492	3.213
ROJKAE	159.613	123.093	3.231
ROJKEI	165.233	129.106	3.086
RONFOQ	163.815	137.128	3.053
RUXZIU	175.155	102.585	3.217
SAHFOY	175.259	132.013	3.245
SAKGUG	179.366	141.448	3.059
SAMSOQ	169.609	125.004	3.346
SAWZIA	163.318	123.365	3.344
SIBDUC	78.367	141.339	2.966
SIBPUP	170.576	95.341	3.292
SIDFIU	164.255	141.767	3.127
SILKED	177.857	125.371	3.024
SILKED	175.498	159.499	3.1
SILKED	175.665	126.844	3.014
SILMUW	153.203	105.349	3.159
SINCUP	158.832	121.388	3.231
SINCUP	155.994	125.533	3.254
SINGED	162.77	123.963	3.208
SOCGOI	167.195	144.249	2.991

SOCHUP	164.573	93.108	3.207
SOMKIO	170.014	146.874	3.156
SOYFUH	162.236	145.615	3.12
TAFNEV	162.141	89.899	3.228
TAGVEC02	156.149	140.306	3.116
TAGVEC02	160.082	137.115	3.138
TAGWON	170.026	153.434	3.147
TAHCEK	163.76	106.905	3.187
TAHFIR01	105.556	104.616	3.298
TAPGOH	126.497	119.653	3.008
TAPGOH	109.942	133.12	3.007
TAPNOO	175.96	149.039	3.406
TEHCAL	170.042	90.59	3.255
TEHNIF	167.009	95.017	2.946
TEQSUF	140.997	114.854	3.008
TEXLEP	166.84	116.484	3.06
TEXLEP	163.698	115.613	3.113
TIMLUY	127.435	149.129	2.98
TIMLUY	137.442	98.902	2.955
TIQDAY	173.232	130.211	3.102
TIWFOW	162.167	145.224	3.229
TIXTUQ01	170.623	147.559	3.034
TOLQER	91.713	125.007	2.963
TUMSEA	169.443	123.928	3.216
TUMSEA	159.837	120.668	3.238
TUXDEV	159.991	113.483	3.221
UFERUU	158.672	104.847	3.385
UFERUU	169.308	129.76	3.095
UHAHIU	158.641	106.744	3.27
USUKAV	154.578	105.044	3.221
UWETIA	173.011	107.396	2.974
VADFAI	165.1	131.686	3.173
VALNAZ	166.796	130.119	3.282
VAPQIO	159.143	152.462	3.296
VAWMUB	170.362	108.548	3.318
VAZVIC	169.284	100.421	3.226
VEDYOU	175.563	131.626	3.059
VEDYUA	178.186	147.823	3.163
VEDYUA	171.004	139.194	2.895
VEFGAQ	171.478	152.469	3.177
VEWHOW	109.442	109.288	3.016
VICGEU	164.131	166.282	3.257
VICSUX	146.053	134.326	3.305
VIFBAO	163.85	128.174	3.299
VOBXOB	76.309	131.006	3.261
VOBYAO	160.789	87.279	3.245

VOHVOD	169.082	115.756	3.31
VONNOC	153.006	109.216	3.257
VUCLOV	164.411	141.426	3.247
WALXIR	158.226	174.143	3.225
WALYIS	156.823	175.453	3.227
WAMQEH	133.19	103.371	3.017
WASDIF	167.464	101.657	3.157
WEFKUO	171.558	173.501	3.012
WEFLAV	174.456	174.28	2.986
WEFQAB	93.208	98.793	3.012
WEVROF	173.956	74.027	3.191
WEVSEW	170.477	90.458	3.327
WEVVIE	161.439	88.866	3.298
WITLUG	168.517	97.199	3.263
WIXQOK	149.075	88.314	2.871
WOCQUC	174.364	127.008	3.13
WOCQUC	166.643	134.239	3.159
WOJQIV	175.946	157.485	3.179
WOJQIV	173.159	134.119	3.116
WORTUS	153.584	138.527	3.002
WUDXOJ	153.483	126.538	3.234
WUDXOJ	169.313	143.097	3.217
WUKGAK	167.617	141.814	3.059
WUNKOF	109.833	97.187	2.905
WUNKOF	131.37	116.297	2.931
WUSJUP	128.604	128.61	2.952
XACVEE	150.502	101.182	3.179
XAFPAX	172.508	130.256	3.219
XAHFIV	122.272	160.54	2.922
XAPROV	161.483	118.513	3.38
XATFII	165.512	130.315	3.203
XINNIR01	125.391	103.66	3.228
XIZPON	174.487	103.99	3.332
XODQIS	164.755	81.778	3.202
XOKVUQ	154.439	96.72	3.01
XOKVUQ	154.445	135.433	3.093
XOPYAC	99.964	120.949	3.012
XOPYIK	131.254	126.705	2.939
XOXXIF	165.91	129.435	3.485
XOXLIG	165.543	125.925	3.163
XOXLIG	170.277	127.154	3.219
XOYYIU	176.384	158.053	2.897
YAGSEE	162.01	122.04	3.287
YATJUA	172.863	175.21	3.239
YEJCAT	164.932	141.6	3.036
YENVUI	120.383	145.034	3.254

YITKOB	157.5	128.06	3.153
YIZTAE	119.382	100.519	2.983
YOFNIS	145.249	123.585	2.997
YOJKAL	162.006	108.722	3.277
YOQZOU	154.234	88.822	3.015
YOSHOD10	169.21	119.148	3.061
YOSHOD10	176.452	117.945	3.099
YOSHOD10	168.326	167.809	3.241
YOSHOD10	166.359	167.245	3.271
YOTPED	157.266	151.415	3.345
YOXGOH	179.798	107.329	3.247
YOYHIE	176.427	132.248	3.267
YUNSAC	172.749	118.686	3.146
YUQJEA	155.709	105.861	3.292
YUQJEA	165.581	93.879	3.189
YUZBOL	127.793	87.996	3.395
YUZGUV	68.763	105.027	3.214
ZEQBAA	139.679	113.933	3.225
ZESGAH	134.095	89.71	2.524
ZIDVOZ	168.9	100.033	3.08
ZIDVOZ	176.441	94.904	3.014
ZIDVUF	163.472	170.375	3.261
ZIDVUF	159.005	125.85	3.15
ZIFBUN	167.486	154.757	3.123
ZITDOX	166.201	118.107	3.304
ZIZMAW	160.066	130.152	3.209
ZOBBEZ	177.256	163.848	2.934
ZOBBEZ01	176.348	171.577	2.949
ZOBBEZ01	176.253	172.101	2.933
ZUGPOI	172.333	139.096	3.06