Electronic Supplementary Information, Part I: 3 Compounds of Haloperidol type.

Note: In all Tables the non-revised output of the XD program (ref. 9) was used. With respect to the significance of the given data we refer to Grabowsky et al., Acta Cryst. 2009, B65, 488 , where transferability indices were derived as 0.09 e Å^{-3} and 2.8 e Å^{-5} for the ED's and Laplacians at the bond critical points and 0.7 Å^{3} and 0.11 e for the atomic volumes and charges. These quantities can serve as an estimate of the significance of the listed data.

Table S1. CRITICAL POINT SEARCH FOR **1a**-HCl

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Quantities are in e/Ang^x
Using ANALYTICAL derivatives

Searching internuclear distances between 1.200 and 1.750 Angstroms

Bond		ρ	Δρ	Rij d1 d2	
				Hessian Eigenvalues	ellip
CL(2)	-C(10)	1.316	-2.217	1.7351 0.9614 0.7737	
				-7.75 -7.33 12.86	0.06
F(1)	-C(24)	1.913	-16.513	1.3409 0.8326 0.5083	
				-15.43 -15.36 14.28	0.00
O(1)	-C(1)	1.807	-12.673	1.4272 0.8255 0.6017	
				-14.25 -13.67 15.25	0.04
O(2)	-C(20)	2.951	-32.901	1.2130 0.7619 0.4511	
				-27.76 -25.42 20.28	0.09
N(1)	-C(14)	1.819	-11.979	1.4961 0.8358 0.6604	
				-13.59 -13.43 15.05	0.01
N(1)	-C(15)	1.813	-11.826	1.4982 0.8364 0.6619	
				-13.53 -13.38 15.08	0.01
N(1)	-C(17)	1.801	-11.549	1.5023 0.8374 0.6649	
				-13.45 -13.24 15.14	0.02
C(1)	-C(7)	1.730	-11.883	1.5233 0.7625 0.7608	
				-12.52 -11.87 12.51	0.05
C(1)	-C(13)	1.706	-11.821	1.5342 0.7801 0.7541	
				-12.25 -11.69 12.12	0.05
C(1)	-C(16)	1.713	-11.996	1.5327 0.7793 0.7534	
				-12.33 -11.77 12.10	0.05
C(7)	-C(8)	2.140	-17.617	1.3902 0.6968 0.6934	
				-16.69 -13.82 12.89	0.21
C(7)	-C(12)	2.145	-17.987	1.3872 0.6953 0.6919	
				-16.75 -13.98 12.74	0.20
C(8)	-C(9)	2.098	-17.635	1.3856 0.7036 0.6820	
				-16.29 -13.80 12.45	0.18
C(9)	-C(10)	2.181	-18.640	1.3877 0.6812 0.7065	
				-17.32 -13.96 12.64	0.24
C(10)	-C(11)	2.201	-19.917	1.3729 0.7091 0.6638	
				-17.48 -14.40 11.97	0.21
C(11)	-C(12)	2.115	-17.200	1.3906 0.6924 0.6982	
				-16.41 -13.69 12.90	0.20
C(13)	-C(14)	1.682	-11.388	1.5274 0.7589 0.7685	
				-11.93 -11.53 12.06	0.03
C(15)	-C(16)	1.706	-11.845	1.5184 0.7640 0.7543	
				-12.14 -11.74 12.03	0.03
C(17)	-C(18)	1.713	-11.990	1.5149 0.7621 0.7528	

				-12.27	-11.74	12.02	0.04
C(18)	-C(19)	1.666	-10.997	1.5243	0.7621	0.7622	
				-11.60	-11.43	12.03	0.01
C(19)	-C(20)	1.799	-13.343	1.4953	0.7289	0.7663	
				-13.30	-12.50	12.45	0.06
C(20)	-C(21)	1.821	-13.110	1.4891	0.7528	0.7363	
				-13.71	-12.43	13.03	0.10
C(21)	-C(22)	2.122	-17.337	1.3949	0.6979	0.6970	
				-16.48	-13.79	12.93	0.20
C(21)	-C(26)	2.109	-16.922	1.3994	0.7014	0.6980	
				-16.40	-13.57	13.05	0.21
C(22)	-C(23)	2.154	-18.120	1.3789	0.6897	0.6892	
				-16.87	-13.97	12.71	0.21
C(23)	-C(24)	2.210	-19.629	1.3774	0.6656	0.7119	
				-17.88	-14.34	12.59	0.25
C(24)	-C(25)	2.196	-19.290	1.3819	0.7144	0.6675	
				-17.73	-14.23	12.67	0.25
C(25)	-C(26)	2.101	-16.844	1.3952	0.6973	0.6979	
				-16.33	-13.52	13.01	0.21

TABLE S2. BOND CRITICAL POINT SEARCH FOR **1a**-HPic

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Quantities are in e/Ang^x
Using ANALYTICAL derivatives

Searching internuclear distances between 1.200 and 1.750 Angstroms

Bond		ρ	Δρ	Rij	d1	d2	
				Hessian Eigenvalues			ellip
CL(1A)	-C(19A)	1.302	-2.038	1.7414	0.9640	0.7774	
				-7.65	-7.23	12.84	0.06
F(1A)	-C(4A)	1.915	-16.630	1.3397	0.8331	0.5066	
				-15.46	-15.39	14.22	0.00
O(2A)	-C(13A)	1.828	-13.435	1.4196	0.8251	0.5945	
				-14.44	-13.90	14.90	0.04
O(11A)	-C(7A)	3.413	-0.115	1.2455	0.8550	0.3905	
				-35.48	-31.19	66.55	0.14
O(11B)	-C(7A)	3.413	-0.115	1.2240	0.8335	0.3905	
				-35.48	-31.19	66.55	0.14
O(1B)	-C(1B)	2.796	-31.677	1.2423	0.7648	0.4775	
				-25.10	-23.25	16.68	0.08
O(1B)	-H(1N)	0.236	3.854	1.7258	1.1229	0.6029	
				-1.39	-1.36	6.60	0.03
O(21B)	-N(2B)	3.499	-14.020	1.2205	0.6438	0.5767	
				-33.54	-30.69	50.21	0.09
O(22B)	-N(2B)	3.489	-14.093	1.2223	0.6446	0.5777	
				-33.56	-30.63	50.09	0.10
O(41B)	-N(4B)	3.299	-8.176	1.2190	0.6223	0.5967	
				-29.48	-27.39	48.70	0.08
O(42B)	-N(4B)	3.507	-14.773	1.2181	0.6444	0.5737	
				-33.72	-30.81	49.76	0.09
O(61B)	-N(6B)	3.196	-6.365	1.2343	0.6277	0.6066	
				-28.35	-26.31	48.30	0.08
O(62B)	-N(6B)	3.542	-15.684	1.2128	0.6430	0.5698	
				-34.15	-31.23	49.69	0.09
N(1A)	-C(10A)	1.809	-10.991	1.5052	0.8340	0.6713	
				-13.39	-13.22	15.62	0.01
N(1A)	-C(11A)	1.852	-11.913	1.4912	0.8303	0.6609	
				-13.79	-13.59	15.46	0.01
N(1A)	-C(15A)	1.808	-10.953	1.5061	0.8343	0.6718	
				-13.38	-13.18	15.61	0.02
N(2B)	-C(2B)	1.782	-13.037	1.4588	0.8671	0.5917	
				-13.39	-11.94	12.29	0.12
N(4B)	-C(4B)	2.077	-16.624	1.4543	0.8225	0.6318	
				-17.18	-14.87	15.43	0.16
N(6B)	-C(6B)	1.840	-14.424	1.4383	0.8662	0.5720	
				-14.20	-11.82	11.59	0.20
C(1A)	-C(2A)	2.125	-17.070	1.3969	0.6976	0.6993	
				-16.49	-13.67	13.10	0.21
C(1A)	-C(6A)	2.139	-17.475	1.3926	0.6946	0.6980	
				-16.56	-13.89	12.97	0.19
C(1A)	-C(7A)	1.777	-11.925	1.5013	0.7422	0.7591	
				-13.04	-12.11	13.22	0.08
C(2A)	-C(3A)	2.149	-18.071	1.3797	0.6965	0.6832	

				-16.68 -14.06 12.67	0.19
C(3A)	-C(4A)	2.191	-18.255	1.3916 0.6818 0.7099	
				-17.62 -13.91 13.28	0.27
C(4A)	-C(5A)	2.203	-19.159	1.3821 0.7115 0.6706	
				-17.73 -14.24 12.81	0.25
C(5A)	-C(6A)	2.170	-18.015	1.3791 0.6892 0.6899	
				-16.88 -14.03 12.89	0.20
C(7A)	-C(8A)	1.739	-11.516	1.5130 0.7696 0.7434	
				-12.59 -11.83 12.90	0.06
C(8A)	-C(9A)	1.696	-10.989	1.5216 0.7610 0.7606	
				-11.65 -11.61 12.27	0.00
C(9A)	-C(10A)	1.720	-11.512	1.5212 0.7556 0.7656	
				-12.19 -11.64 12.32	0.05
C(11A)	-C(12A)	1.732	-11.714	1.5178 0.7642 0.7536	
				-12.22 -11.80 12.31	0.04
C(12A)	-C(13A)	1.704	-11.515	1.5406 0.7606 0.7800	
				-12.17 -11.62 12.27	0.05
C(13A)	-C(14A)	1.733	-12.059	1.5282 0.7734 0.7548	
				-12.43 -11.86 12.23	0.05
C(13A)	-C(16A)	1.716	-11.607	1.5285 0.7654 0.7631	
				-12.53 -11.61 12.53	0.08
C(14A)	-C(15A)	1.724	-11.585	1.5206 0.7551 0.7655	
				-12.16 -11.74 12.32	0.04
C(16A)	-C(17A)	2.136	-17.439	1.3931 0.6950 0.6981	
				-16.54 -13.87 12.97	0.19
C(16A)	-C(21A)	2.119	-16.917	1.3986 0.6988 0.6999	
				-16.42 -13.62 13.12	0.21
C(17A)	-C(18A)	2.128	-17.161	1.3904 0.6972 0.6933	
				-16.45 -13.73 13.02	0.20
C(18A)	-C(19A)	2.178	-19.023	1.3828 0.6715 0.7113	
				-17.17 -14.17 12.31	0.21
C(19A)	-C(20A)	2.171	-18.881	1.3840 0.7112 0.6728	
				-17.12 -14.10 12.34	0.21
C(20A)	-C(21A)	2.110	-16.757	1.3958 0.6960 0.6998	
				-16.28 -13.58 13.11	0.20
C(1B)	-C(2B)	1.893	-14.011	1.4554 0.7169 0.7385	
				-15.04 -12.05 13.08	0.25
C(1B)	-C(6B)	1.908	-14.449	1.4493 0.7138 0.7355	
				-15.30 -12.18 13.03	0.26
C(2B)	-C(3B)	2.165	-18.606	1.3565 0.6798 0.6767	
				-16.99 -13.83 12.21	0.23
C(3B)	-C(4B)	2.079	-15.790	1.4030 0.6867 0.7163	
				-15.95 -13.08 13.24	0.22
C(4B)	-C(5B)	2.177	-18.226	1.3723 0.7015 0.6708	
				-16.96 -13.89 12.62	0.22
C(5B)	-C(6B)	2.068	-16.238	1.3867 0.6920 0.6947	
				-16.04 -13.05 12.85	0.23

TABLE S3. BOND CRITICAL POINT SEARCH FOR **1b**-HCl

****

Quantities are in e/Ang^x
Using ANALYTICAL derivatives

Searching internuclear distances between 1.200 and 1.900 Angstroms

Bond		ρ	Δρ	Rij / Hessian Eigenvalues	d1	d2	ellip
CL(2)	-C(10)	1.350	-2.631	1.7208	0.9553	0.7655	
				-7.99	-7.55	12.91	0.06
SI	-O(1)	1.011	17.252	1.6232	0.6760	0.9472	
				-7.23	-6.74	31.22	0.07
SI	-C(7)	0.878	4.095	1.8575	0.7198	1.1377	
				-4.98	-4.61	13.68	0.08
SI	-C(13)	0.846	3.982	1.8616	0.7237	1.1379	
				-4.70	-4.37	13.05	0.08
SI	-C(16)	0.870	3.588	1.8732	0.7229	1.1503	
				-4.71	-4.61	12.91	0.02
F	-C(24)	1.933	-16.812	1.3346	0.8329	0.5017	
				-15.63	-15.49	14.31	0.01
O(2)	-C(20)	2.954	-32.858	1.2124	0.7619	0.4505	
				-27.81	-25.47	20.42	0.09
N	-C(14)	1.829	-11.407	1.4984	0.8321	0.6663	
				-13.59	-13.37	15.56	0.02
N	-C(15)	1.818	-11.178	1.5019	0.8330	0.6689	
				-13.49	-13.28	15.58	0.02
N	-C(17)	1.836	-11.550	1.4967	0.8317	0.6650	
				-13.66	-13.42	15.53	0.02
C(7)	-C(8)	2.143	-17.662	1.3823	0.6825	0.6998	
				-16.22	-13.97	12.53	0.16
C(7)	-C(12)	2.125	-17.391	1.3869	0.6858	0.7011	
				-16.09	-13.88	12.58	0.16
C(8)	-C(9)	2.125	-17.913	1.3832	0.7016	0.6816	
				-16.39	-14.01	12.49	0.17
C(9)	-C(10)	2.213	-19.140	1.3812	0.6801	0.7011	
				-17.56	-14.18	12.60	0.24
C(10)	-C(11)	2.213	-19.126	1.3814	0.7012	0.6802	
				-17.55	-14.19	12.61	0.24
C(11)	-C(12)	2.138	-18.085	1.3794	0.6788	0.7006	
				-16.47	-14.07	12.45	0.17
C(13)	-C(14)	1.709	-10.904	1.5105	0.7429	0.7677	
				-11.93	-11.24	12.27	0.06
C(15)	-C(16)	1.690	-10.473	1.5191	0.7714	0.7476	
				-11.74	-11.04	12.31	0.06
C(17)	-C(18)	1.745	-11.983	1.5116	0.7609	0.7507	
				-12.42	-11.85	12.29	0.05
C(18)	-C(19)	1.704	-11.157	1.5183	0.7592	0.7591	
				-11.75	-11.67	12.27	0.01
C(19)	-C(20)	1.779	-12.590	1.5067	0.7385	0.7682	
				-13.04	-12.23	12.68	0.07
C(20)	-C(21)	1.831	-13.334	1.4857	0.7507	0.7350	
				-13.81	-12.54	13.01	0.10
C(21)	-C(22)	2.175	-18.456	1.3807	0.6899	0.6909	

				-16.97	-14.19	12.70	0.20
C(21)	-C(26)	2.153	-17.649	1.3892	0.6940	0.6952	
				-16.74	-13.89	12.98	0.21
C(22)	-C(23)	2.137	-17.097	1.3900	0.6963	0.6938	
				-16.51	-13.75	13.16	0.20
C(23)	-C(24)	2.271	-20.873	1.3624	0.6592	0.7032	
				-18.43	-14.80	12.36	0.24
C(24)	-C(25)	2.263	-20.602	1.3653	0.7043	0.6611	
				-18.32	-14.72	12.45	0.24
C(25)	-C(26)	2.197	-18.632	1.3714	0.6856	0.6858	
				-17.14	-14.24	12.75	0.20

Table S8. Atomic charges q [e] and volumes V [Å^3] for **1a**-HCl

Atom	q	V_{tot}
CL(2)	-0.22308093	33.13906219
CL(1)	-1.18457530	35.40431444
F(1)	-0.58011751	17.51093358
O(1)	-0.92790504	15.93699935
O(2)	-0.91477987	16.75010101
N(1)	-0.90896941	8.36858255
C(1)	0.31279039	5.77583634
C(7)	-0.05808697	10.35175528
C(8)	-0.07986192	13.78676560
C(9)	0.00747384	11.95548860
C(10)	-0.00641145	10.25221686
C(11)	0.00711319	11.50887056
C(12)	-0.07050013	12.01023867
C(13)	-0.05327866	8.64707395
C(14)	0.16961123	7.85184284
C(15)	0.17672029	7.64826386
C(16)	-0.05544994	7.96428888
C(17)	0.15895570	8.09158501
C(18)	-0.04732827	8.24476956
C(19)	-0.05394924	8.74645283
C(20)	0.78093319	7.93940341
C(21)	-0.04369219	11.42616325
C(22)	-0.06985211	12.18834721
C(23)	-0.03072293	13.98820756
C(24)	0.42925546	8.88238026
C(25)	-0.03139200	11.82193572
C(26)	-0.06450641	12.50199003
H(1)	0.61619475	1.62798706
H(N)	0.60329291	1.37267409
H(8)	0.13359359	6.80662220
H(9)	0.13354332	7.59847087
H(11)	0.13384068	6.83029345
H(12)	0.12815539	5.48448581
H(13A)	0.08655756	6.62271130
H(13B)	0.08417040	9.58884503
H(14A)	0.06869291	6.92414156
H(14B)	0.07090974	7.16880245
H(15A)	0.06537592	7.86691406
H(15B)	0.07195823	5.84507280
H(16A)	0.08504294	6.60549708
H(16B)	0.08200500	6.54186941
H(17A)	0.06652586	6.47613104
H(17B)	0.07760306	6.15672894
H(18A)	0.09037167	6.62209334
H(18B)	0.08683581	6.88840329
H(19A)	0.08468391	6.82210113
H(19B)	0.08573112	6.32211535
H(22)	0.13125165	5.95086514
H(23)	0.13623041	6.77276620

H(25)	0.13481622	7.10505547
H(26)	0.12859188	7.77562375
sum:	0.02436796	492.47014021

V_{tot} values calculated by integration over the basins enclosed by the zero-flux surfaces of the ED gradient vector field in the crystal according to Bader's formalism.

Table S9. Atomic charges q [e] and volumes V [Å^3] for **1a**-HPic

Atom	q	V_{tot}
CL(1A)	-0.21776148	34.02187201
F(1A)	-0.57685565	18.49317283
O(2A)	-0.93462857	16.72821947
O(11A)	-0.52112835	13.08991391
N(1A)	-0.89023167	8.17245638
C(1A)	-0.01521034	9.81677680
C(2A)	-0.04410693	11.87426924
C(3A)	-0.00291316	10.90961069
C(4A)	0.45509133	7.89745201
C(5A)	-0.00635118	12.20732781
C(6A)	-0.03829504	11.94868910
C(7A)	1.06317994	6.65634155
C(8A)	-0.01037653	8.50165695
C(9A)	-0.00749188	7.57304051
C(10A)	0.19920156	7.60904988
C(11A)	0.21374698	6.91820779
C(12A)	-0.02565381	8.00564467
C(13A)	0.30976661	6.13227906
C(14A)	-0.01613784	7.55915934
C(15A)	0.19387550	7.72679218
C(16A)	-0.04902923	9.80542322
C(17A)	-0.04387295	11.70790943
C(18A)	0.03545197	10.35651392
C(19A)	-0.01117197	9.76549342
C(20A)	0.02947211	12.79147041
C(21A)	-0.04002232	12.52688712
H(2O)	0.58010308	2.19401631
H(1N)	0.49903580	1.99475868
H(2A)	0.10091634	7.36242121
H(3A)	0.11693592	6.75927724
H(5A)	0.10887735	8.28549076
H(6A)	0.10388369	6.29524042
H(81A)	0.06527092	6.71780172
H(81B)	0.06919834	6.80276166
H(91A)	0.06709861	6.36504599
H(91B)	0.06477823	7.85255123
H(10A)	0.05068597	7.12242004
H(10B)	0.04970871	6.58244990
H(11A)	0.04896396	5.64547290
H(11B)	0.04650239	7.89273177
H(12A)	0.06699682	7.71962300
H(12B)	0.06450155	6.85386669
H(14A)	0.07010317	6.19739190
H(14B)	0.07024859	5.93820947
H(15A)	0.05099945	7.03388395
H(15B)	0.04803332	6.70122783
H(17A)	0.10579151	7.91164062
H(18A)	0.10493665	6.52108700

H(20A)	0.10355331	8.21320611
H(21A)	0.09906689	6.81654750
O(1B)	-0.86282506	17.75114362
O(21B)	-0.40661362	18.56071294
O(22B)	-0.40747408	18.13190237
O(41B)	-0.41092857	18.66184334
O(42B)	-0.40465856	19.73022463
O(61B)	-0.41210601	16.35204133
O(62B)	-0.41558789	15.92335533
N(2B)	0.37744944	7.84748954
N(4B)	0.29726467	7.30082450
N(6B)	0.31673020	8.36610147
C(1B)	0.81874590	8.65127921
C(2B)	0.25832718	10.00644161
C(3B)	0.08605709	10.14040516
C(4B)	0.15317361	8.16657881
C(5B)	0.08929724	9.38576216
C(6B)	0.26620172	9.89980072
H(3B)	-0.20470264	7.84461546
H(5B)	-0.19871572	6.94698253
sum:	0.74437259	666.24225838

V_{tot} values calculated by integration over the basins enclosed by the zero-flux surfaces of the ED gradient vector field in the crystal according to Bader's formalism.

Table S10. Atomic charges q [e] and volumes V [Å^3] for **1b**–HCl

Atom	q	V_{tot}
CL(2)	-0.22879194	41.72557135
CL(1)	-1.00900319	34.94734925
SI	2.98708812	3.97145414
F	-0.58504423	19.77133019
O(1)	-1.35631238	20.46618978
O(2)	-0.91363099	18.44353758
N	-0.90700237	8.56683211
C(7)	-0.83311405	15.96885713
C(8)	-0.03957503	13.18635304
C(9)	0.02563726	12.17073957
C(10)	0.02181306	11.98771465
C(11)	0.02338508	12.68048071
C(12)	-0.03584337	12.69037696
C(13)	-0.70099112	11.44654986
C(14)	0.18483682	7.41777234
C(15)	0.19623189	7.35538071
C(16)	-0.80355796	12.57552153
C(17)	0.20773876	7.20951467
C(18)	-0.01436849	8.10412683
C(19)	-0.01652465	8.35025110
C(20)	0.79055686	7.95110352
C(21)	-0.03679711	10.45300672
C(22)	-0.03721426	13.12006638
C(23)	-0.00974326	14.01283619
C(24)	0.42501617	10.31249504
C(25)	-0.00767501	14.13364077
C(26)	-0.03836692	12.27464532
H(1)	0.59106890	2.08293112
H(N)	0.48487242	2.29050472
H(8)	0.09386629	8.54682143
H(9)	0.10375810	8.64985181
H(11)	0.09840860	7.70583413
H(12)	0.09786470	6.77986488
H(13A)	0.06801466	7.49099476
H(13B)	0.07419131	6.54261403
H(14A)	0.04407943	5.62010444
H(14B)	0.04718550	5.81963845
H(15A)	0.04475857	8.36848350
H(15B)	0.04527482	6.18508853
H(16A)	0.06914446	6.42233211
H(16B)	0.06405771	7.34457290
H(17A)	0.04671421	6.89555422
H(17B)	0.04705630	6.44004619
H(18A)	0.06630382	7.20105948
H(18B)	0.06290749	6.77075843
H(19A)	0.06200352	8.70727633
H(19B)	0.06183908	5.85558264
H(22)	0.09803779	8.06933004
H(23)	0.10784006	8.87100729

H(25)	0.10923946	9.87157333
H(26)	0.09872684	7.96466538
sum:	-0.02403823	537.79018759

V_{tot} values calculated by integration over the basins enclosed by the zero-flux surfaces of the ED gradient vector field in the crystal according to Bader's formalism.

Tables S15 – S17 for 1a-HCl

Table S15. Atomic coordinates for **1a**-HCl

```
loop_
    _atom_site_label
    _atom_site_type_symbol
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
```

Cl(2)	Cl	1.09649(3)	1.52858(5)	-0.16167(3)	0.039	1	4
Cl(1)	Cl	0.32642(2)	0.90799(4)	0.38060(2)	0.026	1	4
F(1)	F	0.01711(7)	1.11928(12)	0.04620(10)	0.063	1	4
O(1)	O	0.66000(6)	1.39695(10)	-0.30969(6)	0.025	1	4
O(2)	O	0.41881(7)	1.09674(14)	0.09491(8)	0.047	1	4
N(1)	N	0.57344(7)	1.35310(11)	-0.11753(8)	0.02	1	4
C(1)	C	0.71633(9)	1.40969(14)	-0.19935(9)	0.02	1	4
C(7)	C	0.81195(9)	1.44285(13)	-0.18901(10)	0.022	1	4
C(8)	C	0.85052(10)	1.36880(16)	-0.24844(11)	0.032	1	4
C(9)	C	0.93718(10)	1.39498(17)	-0.24221(11)	0.034	1	4
C(10)	C	0.98673(9)	1.49608(16)	-0.17417(11)	0.029	1	4
C(11)	C	0.95013(10)	1.57072(17)	-0.11470(13)	0.039	1	4
C(12)	C	0.86279(10)	1.54416(17)	-0.12247(12)	0.035	1	4
C(13)	C	0.71473(9)	1.27944(14)	-0.13822(10)	0.022	1	4
C(14)	C	0.61859(9)	1.24109(14)	-0.15297(11)	0.023	1	4
C(15)	C	0.57747(9)	1.48435(14)	-0.17114(10)	0.023	1	4
C(16)	C	0.67370(9)	1.52081(14)	-0.15454(10)	0.022	1	4
C(17)	C	0.47718(9)	1.32098(15)	-0.13636(10)	0.024	1	4
C(18)	C	0.46692(9)	1.21782(16)	-0.05862(11)	0.026	1	4
C(19)	C	0.36851(9)	1.21014(15)	-0.07152(9)	0.023	1	4
C(20)	C	0.35545(9)	1.14136(14)	0.02040(10)	0.024	1	4
C(21)	C	0.26332(9)	1.13195(14)	0.02187(10)	0.023	1	4
C(22)	C	0.25507(11)	1.08803(16)	0.11612(12)	0.032	1	4
C(23)	C	0.17232(12)	1.08200(18)	0.12508(14)	0.043	1	4
C(24)	C	0.09786(11)	1.12030(18)	0.03801(15)	0.042	1	4
C(25)	C	0.10218(10)	1.16137(18)	-0.05794(14)	0.042	1	4
C(26)	C	0.18633(9)	1.16848(17)	-0.06579(11)	0.033	1	4
H(1)	H	0.66728(6)	1.30702(10)	-0.33226(6)	0.028(5)	1	4
H(N)	H	0.60709(7)	1.36590(11)	-0.03716(8)	0.031(5)	1	4
H(8)	H	0.81202(10)	1.28924(16)	-0.30080(11)	0.067(6)	1	4
H(9)	H	0.96587(10)	1.33716(17)	-0.28979(11)	0.048(5)	1	4
H(11)	H	0.98891(10)	1.65015(17)	-0.06243(13)	0.062(6)	1	4
H(12)	H	0.83407(10)	1.60337(17)	-0.07565(12)	0.061(6)	1	4
H(13A)	H	0.74515(9)	1.19711(14)	-0.16723(10)	0.037(4)	1	4
H(13B)	H	0.75456(9)	1.29395(14)	-0.05308(10)	0.036(4)	1	4
H(14A)	H	0.58008(9)	1.21802(14)	-0.23767(11)	0.031(4)	1	4
H(14B)	H	0.61984(9)	1.14967(14)	-0.10599(11)	0.042(5)	1	4
H(15A)	H	0.54835(9)	1.56515(14)	-0.13822(10)	0.038(4)	1	4
H(15B)	H	0.53745(9)	1.47650(14)	-0.25733(10)	0.036(4)	1	4
H(16A)	H	0.71283(9)	1.53366(14)	-0.06903(10)	0.028(4)	1	4
H(16B)	H	0.67484(9)	1.61662(14)	-0.19460(10)	0.039(4)	1	4
H(17A)	H	0.44389(9)	1.28256(15)	-0.21837(10)	0.035(4)	1	4

H(17B)	H	0.44283(9)	1.41475(15)	-0.12965(10)	0.043(5)	1	4
H(18A)	H	0.50828(9)	1.24696(16)	0.02343(11)	0.046(5)	1	4
H(18B)	H	0.48960(9)	1.11870(16)	-0.07447(11)	0.063(6)	1	4
H(19A)	H	0.34106(9)	1.31264(15)	-0.07970(9)	0.041(5)	1	4
H(19B)	H	0.33084(9)	1.15500(15)	-0.14508(9)	0.054(6)	1	4
H(22)	H	0.31460(11)	1.05829(16)	0.18336(12)	0.066(7)	1	4
H(23)	H	0.16609(12)	1.04838(18)	0.19840(14)	0.077(7)	1	4
H(25)	H	0.04177(10)	1.18749(18)	-0.12533(14)	0.069(7)	1	4
H(26)	H	0.19212(9)	1.20205(17)	-0.13936(11)	0.031(4)	1	4

Table S16. Anisotropic displacement parameters for **1a**-HCl

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
Cl(2) 0.02908(19) 0.0411(2) 0.0547(2) -0.00679(17) 0.02596(17) -0.00306(18)
Cl(1) 0.03089(18) 0.02503(18) 0.02197(15)-0.00076(15) 0.00819(12) -0.00138(13)
F(1) 0.0440(6) 0.0483(7) 0.1206(9) -0.0142(5) 0.0576(6) -0.0240(6)
O(1) 0.0264(5) 0.0269(5) 0.0211(4) -0.0008(4) 0.0096(4) -0.0007(4)
O(2) 0.0236(6) 0.0775(9) 0.0397(6) 0.0054(6) 0.0103(4) 0.0301(6)
N(1) 0.0199(5) 0.0212(6) 0.0201(5) 0.0006(5) 0.0102(4) 0.0013(4)
C(1) 0.0229(6) 0.0187(7) 0.0207(6) -0.0013(6) 0.0106(5) -0.0011(5)
C(7) 0.0228(7) 0.0207(7) 0.0262(6) -0.0043(6) 0.0140(5) -0.0033(5)
C(8) 0.0278(8) 0.0366(9) 0.0358(7) -0.0065(7) 0.0183(6) -0.0144(6)
C(9) 0.0295(8) 0.0408(9) 0.0395(8) -0.0045(7) 0.0216(6) -0.0121(7)
C(10) 0.0270(7) 0.0283(8) 0.0386(8) -0.0032(6) 0.0187(6) -0.0009(6)
C(11) 0.0288(8) 0.0364(10) 0.0609(10) -0.0128(7) 0.0263(7) -0.0213(7)
C(12) 0.0276(8) 0.0351(9) 0.0499(9) -0.0096(7) 0.0223(7) -0.0201(7)
C(13) 0.0222(6) 0.0201(7) 0.0263(6) 0.0012(6) 0.0130(5) 0.0024(5)
C(14) 0.0243(7) 0.0183(7) 0.0314(7) 0.0006(6) 0.0160(5) -0.0004(5)
C(15) 0.0244(7) 0.0193(7) 0.0269(6) 0.0020(6) 0.0129(5) 0.0032(5)
C(16) 0.0235(7) 0.0193(7) 0.0257(6) -0.0009(6) 0.0128(5) -0.0018(5)
C(17) 0.0185(6) 0.0287(8) 0.0268(6) -0.0001(6) 0.0114(5) 0.0028(5)
C(18) 0.0216(7) 0.0290(8) 0.0327(7) 0.0016(6) 0.0147(5) 0.0075(6)
C(19) 0.0215(7) 0.0260(8) 0.0231(6) -0.0009(6) 0.0118(5) 0.0016(5)
C(20) 0.0199(7) 0.0286(8) 0.0244(6) 0.0004(6) 0.0083(5) 0.0051(5)
C(21) 0.0211(7) 0.0250(7) 0.0276(7) -0.0023(6) 0.0127(5) 0.0010(5)
C(22) 0.0373(8) 0.0307(8) 0.0385(8) -0.0027(7) 0.0251(6) 0.0041(6)
C(23) 0.0458(10) 0.0373(10) 0.0615(10) -0.0044(8) 0.0388(8) 0.0011(8)
C(24) 0.0375(9) 0.0316(9) 0.0733(12) -0.0115(8) 0.0389(9) -0.0132(8)
C(25) 0.0206(8) 0.0452(10) 0.0571(10) -0.0027(7) 0.0110(7) -0.0121(8)
C(26) 0.0212(7) 0.0412(9) 0.0347(8) -0.0003(6) 0.0098(6) -0.0016(6)
```

Table S17. Multipole parameters for **1a**-HCl

```
loop_
    _atom_rho_multipole_atom_label
    _atom_rho_multipole_coeff_Pv
    _atom_rho_multipole_coeff_P00
    _atom_rho_multipole_coeff_P11
    _atom_rho_multipole_coeff_P1-1
```

```
    _atom_rho_multipole_coeff_P10
    _atom_rho_multipole_coeff_P20
    _atom_rho_multipole_coeff_P21
    _atom_rho_multipole_coeff_P2-1
    _atom_rho_multipole_coeff_P22
    _atom_rho_multipole_coeff_P2-2
    _atom_rho_multipole_coeff_P30
    _atom_rho_multipole_coeff_P31
    _atom_rho_multipole_coeff_P3-1
    _atom_rho_multipole_coeff_P32
    _atom_rho_multipole_coeff_P3-2
    _atom_rho_multipole_coeff_P33
    _atom_rho_multipole_coeff_P3-3
    _atom_rho_multipole_coeff_P40
    _atom_rho_multipole_coeff_P41
    _atom_rho_multipole_coeff_P4-1
    _atom_rho_multipole_coeff_P42
    _atom_rho_multipole_coeff_P4-2
    _atom_rho_multipole_coeff_P43
    _atom_rho_multipole_coeff_P4-3
    _atom_rho_multipole_coeff_P44
    _atom_rho_multipole_coeff_P4-4
    _atom_rho_multipole_kappa
    _atom_rho_multipole_kappa_prime0
    _atom_rho_multipole_kappa_prime1
    _atom_rho_multipole_kappa_prime2
    _atom_rho_multipole_kappa_prime3
    _atom_rho_multipole_kappa_prime4
Cl(2) 7.1278 0
0 0 -0.0316
-0.142 0 0 0 0
0.1018 0 0 0 0 0 0
0.0311 0 0 0 0 0 0 0 0
1.003934 0.98084 0.98084 0.98084 0.98084 0.98084


Cl(1) 8 0
0 0 0
0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.010613 1 1 1 1 1


F(1) 7.1283 0
0 0 -0.0492
-0.0902 0 0 0 0
0.0342 0 0 0 0 0 0
0.0065 0 0 0 0 0 0 0 0
1.002244 1.3624 1.3624 1.3624 1.3624 1.3624


O(1) 6.0788 0
-0.0536 -0.0866 0
0.1041 0 0 -0.028 0.042
0 -0.0147 -0.0263 0 0 0.065 -0.0215
0.0106 0 0 0.0042 0.0027 0 0 0.0149 0.0153
1.001632 1.113461 1.113461 1.113461 1.113461 1.113461
```

O(2) 6.1166 0
0 0 -0.0675
0.0293 0 0 -0.1531 0
0.0283 0 0 0.0172 0 0 0
-0.0118 0 0 0.0113 0 0 0 -0.0026 0
1.003017 1.109004 1.109004 1.109004 1.109004 1.109004

N(1) 5.0916 0
0 0 -0.005
0.0107 0 0 0 0
0.2234 0 0 0 0 0.176 0
0.066 0 0 0 0 -0.0509 0 0 0
0.997716 0.890138 0.890138 0.890138 0.890138 0.890138

C(1) 4.0474 0
-0.0538 -0.007 0
0.0477 0 0 -0.064 -0.0005
0 -0.1435 -0.1945 0 0 0.194 -0.0361
0.0369 0 0 -0.0505 0.0714 0 0 0.0428 0.0297
1.004815 1 1 1 1 1

C(7) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1

C(8) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(9) 3.9213 0
0.001 0.0319 0
-0.1622 0 0 -0.0042 -0.0155
0 0.0084 0.0245 0 0 0.2229 -0.0076
0.0242 0 0 0.0013 -0.0129 0 0 -0.0003 -0.001
1.017714 1 1 1 1 1

C(10) 4.1025 0
0 0 -0.0872
-0.0375 0 0 -0.1635 0
0.2348 0 0 0.1308 0 0 0
0.0148 0 0 -0.0125 0 0 0 0.0021 0
1.005708 1 1 1 1 1

C(11) 3.9213 0
0.001 0.0319 0
-0.1622 0 0 -0.0042 -0.0155
0 0.0084 0.0245 0 0 0.2229 -0.0076
0.0242 0 0 0.0013 -0.0129 0 0 -0.0003 -0.001
1.017714 1 1 1 1 1

C(12) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(13) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(14) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(15) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(16) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(17) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(18) 3.9428 0
0 0 0.0068

-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(19) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(20) 3.9937 0
0.0588 -0.0014 0
-0.2542 0 0 0.066 0.0001
0 0.0173 0.0063 0 0 0.2777 0.0024
0.0152 0 0 0.0131 0.0001 0 0 -0.0174 0.0025
1.016945 1 1 1 1 1

C(21) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1

C(22) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(23) 3.9654 0
0.0094 0.0348 0
-0.1568 0 0 -0.0015 -0.0186
0 0.0079 0.0255 0 0 0.222 -0.0068
0.0211 0 0 0.0022 -0.0107 0 0 0.0035 0.0023
1.018878 1 1 1 1 1

C(24) 3.9709 0
0 0 -0.1242
-0.0582 0 0 -0.1752 0
0.2702 0 0 0.1226 0 0 0
0.0391 0 0 -0.007 0 0 0 -0.0002 0
1.016611 1 1 1 1 1

C(25) 3.9654 0
0.0094 0.0348 0
-0.1568 0 0 -0.0015 -0.0186
0 0.0079 0.0255 0 0 0.222 -0.0068

0.0211 0 0 0.0022 -0.0107 0 0 0.0035 0.0023
1.018878 1 1 1 1 1

C(26) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

H(1) 0.9197 0
0 0 0.2069
0.0951 0 0 0 0
0.0171 0 0 0 0 0 0
-0.0278 0 0 0 0 0 0 0 0
1.119673 1.2 1.2 1.2 1.2 1.2

H(N) 0.7475 0
0 0 0.1685
0.0719 0 0 0 0
0.0004 0 0 0 0 0 0
-0.0157 0 0 0 0 0 0 0 0
1.197464 1.2 1.2 1.2 1.2 1.2

H(8) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(9) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(11) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(12) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(13A) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(13B) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(14A) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(14B) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(15A) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(15B) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(16A) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(16B) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(17A) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(17B) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(18A) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(18B) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(19A) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(19B) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(22) 0.951 0
0 0 0.1546

```
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

```
H(23) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

```
H(25) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

```
H(26) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

Tables S18 – S20 for 1a-HPic

Table S18. Atomic coordinates for **1a**-HPic

```
loop_
    _atom_site_label
    _atom_site_type_symbol
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
```

Cl(1A)	Cl	1.34760(3)	0.42143(3)	0.45279	0.03	1	4
F(1A)	F	0.37133(6)	0.23186(7)	1.20783(8)	0.047	1	4
O(2A)	O	1.06234(7)	0.08932(7)	0.66086(8)	0.024	1	4
O(11A)	O	0.7338(5)	0.3306(7)	0.9985(6)	0.052	0.72	4
O(11B)	O	0.7082(13)	0.3273(18)	0.9763(15)	0.041	0.28	4
O(1B)	O	0.94476(6)	0.41259(7)	0.84643(8)	0.027	1	4
O(21B)	O	1.11754(7)	0.49130(8)	0.85856(10)	0.039	1	4
O(22B)	O	1.09787(8)	0.58465(8)	0.98204(9)	0.04	1	4
O(41B)	O	0.93163(7)	0.90438(7)	0.86420(9)	0.035	1	4
O(42B)	O	0.80483(7)	0.87696(7)	0.79756(10)	0.038	1	4
O(61B)	O	0.71033(7)	0.52970(7)	0.72826(9)	0.029	1	4
O(62B)	O	0.78684(7)	0.39134(7)	0.76247(9)	0.033	1	4
N(1A)	N	0.90797(8)	0.20736(8)	0.80697(9)	0.018	1	4
N(2B)	N	1.07407(9)	0.55203(9)	0.90655(12)	0.027	1	4
N(4B)	N	0.87480(9)	0.84587(9)	0.83149(10)	0.025	1	4
N(6B)	N	0.77735(8)	0.48697(8)	0.76171(10)	0.018	1	4
C(1A)	C	0.61168(11)	0.24008(11)	1.07123(12)	0.026	1	4
C(2A)	C	0.57169(12)	0.33400(12)	1.10181(13)	0.03	1	4
C(3A)	C	0.49102(12)	0.33232(12)	1.14838(13)	0.032	1	4
C(4A)	C	0.44972(12)	0.23463(12)	1.16274(13)	0.031	1	4
C(5A)	C	0.48691(12)	0.14053(12)	1.13209(13)	0.031	1	4
C(6A)	C	0.56872(11)	0.14378(11)	1.08784(12)	0.028	1	4
C(7A)	C	0.70029(12)	0.24689(12)	1.02264(13)	0.033	1	4
C(8A)	C	0.75691(11)	0.14769(11)	1.01574(13)	0.028	1	4
C(9A)	C	0.84449(11)	0.16554(12)	0.96416(13)	0.03	1	4
C(10A)	C	0.83107(10)	0.16023(11)	0.86033(11)	0.021	1	4
C(11A)	C	0.89472(10)	0.18708(11)	0.70662(12)	0.021	1	4
C(12A)	C	0.96800(10)	0.23886(10)	0.64958(12)	0.022	1	4
C(13A)	C	1.06166(10)	0.20004(10)	0.67922(12)	0.019	1	4
C(14A)	C	1.07280(10)	0.21909(10)	0.78260(12)	0.023	1	4
C(15A)	C	0.99818(9)	0.16711(11)	0.83799(13)	0.022	1	4
C(16A)	C	1.13360(9)	0.25728(10)	0.62297(11)	0.019	1	4
C(17A)	C	1.18430(10)	0.20206(11)	0.55810(12)	0.024	1	4
C(18A)	C	1.24958(10)	0.25302(11)	0.50586(13)	0.025	1	4
C(19A)	C	1.26338(10)	0.36080(11)	0.51719(12)	0.023	1	4
C(20A)	C	1.21369(10)	0.41852(12)	0.58028(12)	0.026	1	4
C(21A)	C	1.14957(11)	0.36604(11)	0.63357(13)	0.026	1	4
C(1B)	C	0.92641(10)	0.50837(10)	0.83841(11)	0.018	1	4
C(2B)	C	0.98816(10)	0.58953(10)	0.87110(11)	0.02	1	4
C(3B)	C	0.97231(10)	0.69558(11)	0.87241(11)	0.022	1	4
C(4B)	C	0.89194(10)	0.73220(10)	0.83346(12)	0.02	1	4
C(5B)	C	0.82955(10)	0.66298(10)	0.79848(12)	0.019	1	4
C(6B)	C	0.84532(10)	0.55450(10)	0.80060(11)	0.017	1	4

H(2O)	H	1.11717(7)	0.05886(7)	0.68348(8)	0.020(5)	1	4
H(1N)	H	0.90698(8)	0.28759(8)	0.81705(9)	0.035(6)	1	4
H(2A)	H	0.59967(12)	0.39868(12)	1.09038(13)	0.037(5)	1	4
H(3A)	H	0.46485(12)	0.39470(12)	1.16970(13)	0.049(6)	1	4
H(5A)	H	0.45719(12)	0.07642(12)	1.14103(13)	0.039(6)	1	4
H(6A)	H	0.59568(11)	0.08082(11)	1.06898(12)	0.034(5)	1	4
H(81A)	H	0.72275(11)	0.09313(11)	0.98421(13)	0.040(5)	1	4
H(81B)	H	0.77012(11)	0.12210(11)	1.07733(13)	0.078(8)	1	4
H(91A)	H	0.86864(11)	0.23453(12)	0.98053(13)	0.034(5)	1	4
H(91B)	H	0.88768(11)	0.11196(12)	0.98255(13)	0.066(7)	1	4
H(10A)	H	0.82340(10)	0.08666(11)	0.84218(11)	0.027(4)	1	4
H(10B)	H	0.77651(10)	0.19805(11)	0.84455(11)	0.037(5)	1	4
H(11A)	H	0.83688(10)	0.21483(11)	0.68773(12)	0.037(5)	1	4
H(11B)	H	0.89485(10)	0.11117(11)	0.69527(12)	0.030(5)	1	4
H(12A)	H	0.96462(10)	0.31531(10)	0.65692(12)	0.035(5)	1	4
H(12B)	H	0.95878(10)	0.22256(10)	0.58493(12)	0.030(5)	1	4
H(14A)	H	1.13022(10)	0.19082(10)	0.80225(12)	0.038(5)	1	4
H(14B)	H	1.07279(10)	0.29485(10)	0.79469(12)	0.020(4)	1	4
H(15A)	H	1.00096(9)	0.09071(11)	0.82997(13)	0.022(4)	1	4
H(15B)	H	1.00631(9)	0.18262(11)	0.90295(13)	0.043(6)	1	4
H(17A)	H	1.17451(10)	0.12977(11)	0.54968(12)	0.040(5)	1	4
H(18A)	H	1.28360(10)	0.21504(11)	0.46344(13)	0.035(5)	1	4
H(20A)	H	1.22291(10)	0.49114(12)	0.58701(12)	0.031(5)	1	4
H(21A)	H	1.11654(11)	0.40423(11)	0.67667(13)	0.031(5)	1	4
H(3B)	H	1.01341(10)	0.74243(11)	0.89830(11)	0.070(6)	1	4
H(5B)	H	0.77665(10)	0.68885(10)	0.77298(12)	0.065(6)	1	4

Table S19. Anisotropic displacement parameters for **1a**-HPic

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
Cl(1A) 0.0239(2) 0.0344(2) 0.0324(2) -0.00286(17) 0.0034(2) 0.0033(2)
F(1A) 0.0311(6) 0.0462(6) 0.0635(8) 0.0092(4) 0.0082(6) 0.0030(6)
O(2A) 0.0212(6) 0.0150(4) 0.0366(7) 0.0010(4) -0.0036(5) -0.0024(5)
O(11A) 0.060(4) 0.0231(14) 0.073(5) -0.012(2) 0.027(3) -0.000(2)
O(11B) 0.057(9) 0.022(5) 0.044(8) -0.002(5) 0.022(6) 0.020(5)
O(1B) 0.0270(6) 0.0118(5) 0.0433(8) -0.0016(4) -0.0153(6) -0.0000(5)
O(21B) 0.0250(7) 0.0365(6) 0.0561(10) 0.0061(5) -0.0144(7) -0.0067(7)
O(22B) 0.0495(8) 0.0250(5) 0.0454(9) -0.0037(5) -0.0305(7) 0.0011(6)
O(41B) 0.0392(7) 0.0132(5) 0.0525(9) -0.0048(5) -0.0048(7) -0.0035(6)
O(42B) 0.0315(7) 0.0146(5) 0.0685(10) 0.0052(5) -0.0079(7) 0.0002(6)
O(61B) 0.0276(7) 0.0205(5) 0.0383(8) -0.0020(5) -0.0150(6) 0.0004(5)
O(62B) 0.0224(6) 0.0131(5) 0.0621(9) -0.0034(4) -0.0134(6) -0.0041(5)
N(1A) 0.0180(7) 0.0140(6) 0.0212(8) -0.0013(5) -0.0044(6) 0.0014(6)
N(2B) 0.0292(9) 0.0158(6) 0.0368(10) -0.0057(6) -0.0164(8) 0.0029(6)
N(4B) 0.0276(8) 0.0118(6) 0.0343(9) -0.0014(6) 0.0021(7) -0.0017(6)
N(6B) 0.0179(7) 0.0141(6) 0.0225(7) -0.0017(5) -0.0016(6) -0.0014(6)
C(1A) 0.0394(11) 0.0176(8) 0.0212(10) -0.0018(7) 0.0032(8) -0.0010(7)
C(2A) 0.0440(12) 0.0196(8) 0.0278(11) 0.0006(8) -0.0002(9) 0.0003(8)
C(3A) 0.0408(12) 0.0249(9) 0.0316(12) 0.0098(8) -0.0043(10) 0.0008(8)
C(4A) 0.0324(11) 0.0279(9) 0.0315(11) 0.0050(8) -0.0056(9) 0.0019(8)
```

C(5A) 0.0318(11) 0.0255(8) 0.0368(12) -0.0053(8) -0.0012(10) -0.0000(8)
C(6A) 0.0382(11) 0.0201(8) 0.0267(11) 0.0001(8) -0.0000(9) -0.0035(8)
C(7A) 0.0502(12) 0.0209(8) 0.0294(11) -0.0055(8) 0.0122(10) 0.0001(8)
C(8A) 0.0320(10) 0.0285(8) 0.0249(11) -0.0078(7) 0.0005(9) 0.0022(8)
C(9A) 0.0285(9) 0.0357(9) 0.0267(11) -0.0098(8) -0.0039(9) 0.0013(9)
C(10A) 0.0209(9) 0.0204(8) 0.0222(10) -0.0032(6) -0.0035(8) 0.0015(7)
C(11A) 0.0192(9) 0.0215(8) 0.0231(10) -0.0005(6) -0.0058(8) -0.0004(7)
C(12A) 0.0210(9) 0.0220(8) 0.0235(11) 0.0036(6) -0.0021(8) 0.0021(7)
C(13A) 0.0168(9) 0.0171(7) 0.0238(10) 0.0022(6) -0.0029(7) 0.0008(7)
C(14A) 0.0190(9) 0.0179(8) 0.0320(11) -0.0008(6) -0.0055(8) 0.0020(7)
C(15A) 0.0172(9) 0.0197(8) 0.0284(11) -0.0003(6) -0.0071(8) 0.0055(7)
C(16A) 0.0161(8) 0.0139(7) 0.0283(10) 0.0015(6) -0.0023(7) 0.0005(7)
C(17A) 0.0263(10) 0.0186(8) 0.0268(10) 0.0013(6) -0.0020(8) -0.0016(7)
C(18A) 0.0231(9) 0.0258(8) 0.0266(11) 0.0048(7) 0.0011(8) -0.0018(8)
C(19A) 0.0186(9) 0.0255(8) 0.0249(10) 0.0027(6) -0.0027(8) -0.0003(8)
C(20A) 0.0261(9) 0.0166(8) 0.0360(11) 0.0004(7) 0.0067(9) 0.0017(8)
C(21A) 0.0257(9) 0.0176(7) 0.0345(11) 0.0036(7) 0.0075(9) 0.0006(8)
C(1B) 0.0220(9) 0.0125(7) 0.0204(9) -0.0021(6) -0.0041(7) 0.0002(7)
C(2B) 0.0234(9) 0.0124(7) 0.0233(9) -0.0034(6) -0.0049(7) 0.0002(7)
C(3B) 0.0242(9) 0.0178(7) 0.0229(10) -0.0047(6) -0.0026(8) -0.0011(7)
C(4B) 0.0208(9) 0.0102(7) 0.0290(10) -0.0005(6) -0.0004(8) -0.0027(7)
C(5B) 0.0224(9) 0.0145(7) 0.0214(9) -0.0007(6) 0.0021(8) -0.0001(7)
C(6B) 0.0191(8) 0.0132(7) 0.0195(8) -0.0012(6) 0.0013(7) 0.0005(6)

Table S20. Multipole parameters for **1a**-HPic

```
loop_
    _atom_rho_multipole_atom_label
    _atom_rho_multipole_coeff_Pv
    _atom_rho_multipole_coeff_P00
    _atom_rho_multipole_coeff_P11
    _atom_rho_multipole_coeff_P1-1
    _atom_rho_multipole_coeff_P10
    _atom_rho_multipole_coeff_P20
    _atom_rho_multipole_coeff_P21
    _atom_rho_multipole_coeff_P2-1
    _atom_rho_multipole_coeff_P22
    _atom_rho_multipole_coeff_P2-2
    _atom_rho_multipole_coeff_P30
    _atom_rho_multipole_coeff_P31
    _atom_rho_multipole_coeff_P3-1
    _atom_rho_multipole_coeff_P32
    _atom_rho_multipole_coeff_P3-2
    _atom_rho_multipole_coeff_P33
    _atom_rho_multipole_coeff_P3-3
    _atom_rho_multipole_coeff_P40
    _atom_rho_multipole_coeff_P41
    _atom_rho_multipole_coeff_P4-1
    _atom_rho_multipole_coeff_P42
    _atom_rho_multipole_coeff_P4-2
    _atom_rho_multipole_coeff_P43
    _atom_rho_multipole_coeff_P4-3
    _atom_rho_multipole_coeff_P44
    _atom_rho_multipole_coeff_P4-4
    _atom_rho_multipole_kappa
    _atom_rho_multipole_kappa_prime0
    _atom_rho_multipole_kappa_prime1
```

```
    _atom_rho_multipole_kappa_prime2
    _atom_rho_multipole_kappa_prime3
    _atom_rho_multipole_kappa_prime4
Cl(1A) 7.1278 0
0 0 -0.0316
-0.142 0 0 0 0
0.1018 0 0 0 0 0 0
0.0311 0 0 0 0 0 0 0 0
1.003934 0.98084 0.98084 0.98084 0.98084 0.98084


F(1A) 7.1283 0
0 0 -0.0492
-0.0902 0 0 0 0
0.0342 0 0 0 0 0 0
0.0065 0 0 0 0 0 0 0 0
1.002244 1.3624 1.3624 1.3624 1.3624 1.3624


O(2A) 6.0788 0
-0.0536 -0.0866 0
0.1041 0 0 -0.028 0.042
0 -0.0147 -0.0263 0 0 0.065 -0.0215
0.0106 0 0 0.0042 0.0027 0 0 0.0149 0.0153
1.001632 1.113461 1.113461 1.113461 1.113461 1.113461


O(11A) 4.404 0
0 0 -0.0486
0.0211 0 0 -0.1102 0
0.0204 0 0 0.0124 0 0 0
-0.0085 0 0 0.0081 0 0 0 -0.0019 0
1.003017 1.109004 1.109004 1.109004 1.109004 1.109004


O(11B) 1.7126 0
0 0 -0.0189
0.0082 0 0 -0.0429 0
0.0079 0 0 0.0048 0 0 0
-0.0033 0 0 0.0032 0 0 0 -0.0007 0
1.003017 1.109004 1.109004 1.109004 1.109004 1.109004


O(1B) 6.1783 0
-0.0681 -0.0001 0
-0.0983 0 0 -0.0621 -0.0011
0 -0.0091 0.0004 0 0 0.034 0.0016
-0.0066 0 0 0.0027 -0.0002 0 0 0.0103 0.005
0.999014 1.147181 1.147181 1.147181 1.147181 1.147181


O(21B) 6.1187 0
-0.0977 -0.0056 0
-0.193 0 0 -0.112 -0.007
0 -0.0143 0.0015 0 0 0.0647 0.0035
-0.0159 0 0 0.0077 0.0024 0 0 0.0066 -0.0035
1.003886 1.086474 1.086474 1.086474 1.086474 1.086474
```

O(22B) 6.1187 0
-0.0977 -0.0056 0
-0.193 0 0 -0.112 -0.007
0 -0.0143 0.0015 0 0 0.0647 0.0035
-0.0159 0 0 0.0077 0.0024 0 0 0.0066 -0.0035
1.003886 1.086474 1.086474 1.086474 1.086474 1.086474

O(41B) 6.1471 0
0 0 -0.1094
-0.1112 0 0 -0.1097 0
0.0375 0 0 0.0102 0 0 0
-0.0019 0 0 0.0043 0 0 0 -0.0014 0
1.000254 1.037783 1.037783 1.037783 1.037783 1.037783

O(42B) 6.1187 0
-0.0977 -0.0056 0
-0.193 0 0 -0.112 -0.007
0 -0.0143 0.0015 0 0 0.0647 0.0035
-0.0159 0 0 0.0077 0.0024 0 0 0.0066 -0.0035
1.003886 1.086474 1.086474 1.086474 1.086474 1.086474

O(61B) 6.1471 0
0 0 -0.1094
-0.1112 0 0 -0.1097 0
0.0375 0 0 0.0102 0 0 0
-0.0019 0 0 0.0043 0 0 0 -0.0014 0
1.000254 1.037783 1.037783 1.037783 1.037783 1.037783

O(62B) 6.1187 0
-0.0977 -0.0056 0
-0.193 0 0 -0.112 -0.007
0 -0.0143 0.0015 0 0 0.0647 0.0035
-0.0159 0 0 0.0077 0.0024 0 0 0.0066 -0.0035
1.003886 1.086474 1.086474 1.086474 1.086474 1.086474

N(1A) 5.0916 0
0 0 -0.005
0.0107 0 0 0 0
0.2234 0 0 0 0 0.176 0
0.066 0 0 0 0 -0.0509 0 0 0
0.997716 0.890138 0.890138 0.890138 0.890138 0.890138

N(2B) 4.9998 0
-0.008 -0.0145 0
-0.2057 0 0 0.0224 -0.0298
0 -0.0003 -0.0013 0 0 0.3358 0.0423
0.017 0 0 0.0081 -0.0093 0 0 -0.0172 -0.0362
0.999556 0.842726 0.842726 0.842726 0.842726 0.842726

N(4B) 5.0066 0

0 0 0.0263
0.0813 0 0 -0.1755 0
0.2912 0 0 0.226 0 0 0
0.0354 0 0 0.0098 0 0 0 0.0094 0
0.998662 0.839998 0.839998 0.839998 0.839998 0.839998

N(6B) 5.0066 0
0 0 0.0263
0.0813 0 0 -0.1755 0
0.2912 0 0 0.226 0 0 0
0.0354 0 0 0.0098 0 0 0 0.0094 0
0.998662 0.839998 0.839998 0.839998 0.839998 0.839998

C(1A) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1

C(2A) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(3A) 3.9654 0
0.0094 0.0348 0
-0.1568 0 0 -0.0015 -0.0186
0 0.0079 0.0255 0 0 0.222 -0.0068
0.0211 0 0 0.0022 -0.0107 0 0 0.0035 0.0023
1.018878 1 1 1 1 1

C(4A) 3.9709 0
0 0 -0.1242
-0.0582 0 0 -0.1752 0
0.2702 0 0 0.1226 0 0 0
0.0391 0 0 -0.007 0 0 0 -0.0002 0
1.016611 1 1 1 1 1

C(5A) 3.9654 0
0.0094 0.0348 0
-0.1568 0 0 -0.0015 -0.0186
0 0.0079 0.0255 0 0 0.222 -0.0068
0.0211 0 0 0.0022 -0.0107 0 0 0.0035 0.0023
1.018878 1 1 1 1 1

C(6A) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246

0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(7A) 3.9937 0
0.0588 -0.0014 0
-0.2542 0 0 0.066 0.0001
0 0.0173 0.0063 0 0 0.2777 0.0024
0.0152 0 0 0.0131 0.0001 0 0 -0.0174 0.0025
1.016945 1 1 1 1 1

C(8A) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(9A) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(10A) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(11A) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(12A) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(13A) 4.0474 0
-0.0538 -0.007 0
0.0477 0 0 -0.064 -0.0005
0 -0.1435 -0.1945 0 0 0.194 -0.0361
0.0369 0 0 -0.0505 0.0714 0 0 0.0428 0.0297

1.004815 1 1 1 1 1

C(14A) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(15A) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(16A) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1

C(17A) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(18A) 3.9213 0
0.001 0.0319 0
-0.1622 0 0 -0.0042 -0.0155
0 0.0084 0.0245 0 0 0.2229 -0.0076
0.0242 0 0 0.0013 -0.0129 0 0 -0.0003 -0.001
1.017714 1 1 1 1 1

C(19A) 4.1025 0
0 0 -0.0872
-0.0375 0 0 -0.1635 0
0.2348 0 0 0.1308 0 0 0
0.0148 0 0 -0.0125 0 0 0 0.0021 0
1.005708 1 1 1 1 1

C(20A) 3.9213 0
0.001 0.0319 0
-0.1622 0 0 -0.0042 -0.0155
0 0.0084 0.0245 0 0 0.2229 -0.0076
0.0242 0 0 0.0013 -0.0129 0 0 -0.0003 -0.001
1.017714 1 1 1 1 1

C(21A) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(1B) 3.9458 0
0 0 0.0569
0.1723 0 0 -0.1358 0
0.2321 0 0 0.1649 0 0 0
-0.0303 0 0 -0.0335 0 0 0 0.009 0
1.014762 1 1 1 1 1

C(2B) 3.8847 0
0.0434 0.1 0
-0.0592 0 0 0.0514 -0.0979
0 -0.0048 0.0191 0 0 0.2028 0.0145
0.021 0 0 -0.0004 -0.0068 0 0 -0.0049 -0.0002
1.021809 1 1 1 1 1

C(3B) 3.9673 0
0 0 0.0363
0.0263 0 0 -0.0964 0
-0.2017 0 0 -0.1155 0 0 0
0.0163 0 0 -0.0147 0 0 0 0.0092 0
1.019947 1 1 1 1 1

C(4B) 4.0611 0
0 0 -0.0578
0.0419 0 0 -0.1762 0
0.2267 0 0 0.1248 0 0 0
0.0212 0 0 0.0043 0 0 0 0.0002 0
1.01374 1 1 1 1 1

C(5B) 3.9673 0
0 0 0.0363
0.0263 0 0 -0.0964 0
-0.2017 0 0 -0.1155 0 0 0
0.0163 0 0 -0.0147 0 0 0 0.0092 0
1.019947 1 1 1 1 1

C(6B) 3.8847 0
0.0434 0.1 0
-0.0592 0 0 0.0514 -0.0979
0 -0.0048 0.0191 0 0 0.2028 0.0145
0.021 0 0 -0.0004 -0.0068 0 0 -0.0049 -0.0002
1.021809 1 1 1 1 1

H(2O) 0.9197 0

0 0 0.2069
0.0951 0 0 0 0
0.0171 0 0 0 0 0 0
-0.0278 0 0 0 0 0 0 0 0
1.119673 1.2 1.2 1.2 1.2 1.2

H(1N) 0.7475 0
0 0 0.1685
0.0719 0 0 0 0
0.0004 0 0 0 0 0 0
-0.0157 0 0 0 0 0 0 0 0
1.197464 1.2 1.2 1.2 1.2 1.2

H(2A) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(3A) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(5A) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(6A) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(81A) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(81B) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0

```
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(91A) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(91B) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(10A) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2


H(10B) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2


H(11A) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2


H(11B) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2


H(12A) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
```

1.127115 1.2 1.2 1.2 1.2 1.2

H(12B) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(14A) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(14B) 0.9768 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(15A) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(15B) 1.0102 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(17A) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(18A) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

```
H(20A) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

```
H(21A) 0.951 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

```
H(3B) 1.1644 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

```
H(5B) 1.1644 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

Tables S21 – S23 for 1b-HCl

Table S21. Atomic coordinates for **1b**-HCl

```
loop_
    _atom_site_label
    _atom_site_type_symbol
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
```

Cl(2)	Cl	0.61468(18)	1.21664(15)	0.46445(5)	0.14	1	2
Cl(1)	Cl	0.69192(6)	0.77111(7)	0.07676(3)	0.038	1	2
Si	Si	0.16229(7)	0.88757(7)	0.19608(3)	0.033	1	2
F	F	0.0634(3)	0.2997(3)	-0.46766(9)	0.131	1	2
O(1)	O	-0.06255(18)	0.89170(19)	0.21316(8)	0.048	1	2
O(2)	O	0.0149(2)	0.6921(2)	-0.17651(8)	0.056	1	2
N	N	0.26493(18)	0.73267(18)	0.04038(8)	0.025	1	2
C(7)	C	0.2921(3)	0.9774(3)	0.27654(11)	0.041	1	2
C(8)	C	0.2018(4)	1.0219(3)	0.33976(13)	0.063	1	2
C(9)	C	0.2991(5)	1.0937(4)	0.39842(15)	0.082	1	2
C(10)	C	0.4913(5)	1.1237(4)	0.39296(16)	0.079	1	2
C(11)	C	0.5873(4)	1.0786(4)	0.33117(17)	0.076	1	2
C(12)	C	0.4862(3)	1.0055(3)	0.27405(14)	0.056	1	2
C(13)	C	0.2246(3)	0.9919(2)	0.11160(11)	0.037	1	2
C(14)	C	0.1758(2)	0.8954(2)	0.04283(10)	0.029	1	2
C(15)	C	0.1936(2)	0.6234(2)	0.09757(10)	0.031	1	2
C(16)	C	0.2493(3)	0.6802(3)	0.17440(11)	0.036	1	2
C(17)	C	0.2356(3)	0.6546(3)	-0.03334(10)	0.034	1	2
C(18)	C	0.3441(3)	0.7364(3)	-0.09206(10)	0.042	1	2
C(19)	C	0.3432(3)	0.6371(3)	-0.16253(11)	0.042	1	2
C(20)	C	0.1543(3)	0.6315(3)	-0.20277(11)	0.04	1	2
C(21)	C	0.1385(3)	0.5455(3)	-0.27452(11)	0.045	1	2
C(22)	C	0.2801(4)	0.4473(3)	-0.30043(13)	0.064	1	2
C(23)	C	0.2548(5)	0.3627(4)	-0.36619(15)	0.085	1	2
C(24)	C	0.0892(6)	0.3813(4)	-0.40467(15)	0.087	1	2
C(25)	C	-0.0516(5)	0.4806(4)	-0.38157(15)	0.085	1	2
C(26)	C	-0.0266(4)	0.5626(4)	-0.31630(13)	0.061	1	2
H(1)	H	-0.14460(18)	0.85490(19)	0.17371(8)	0.036(7)	1	2
H(N)	H	0.40833(18)	0.74377(18)	0.04871(8)	0.034(6)	1	2
H(8)	H	0.0721(4)	1.0020(3)	0.34283(13)	0.085(10)	1	2
H(9)	H	0.2359(5)	1.1212(4)	0.44073(15)	0.104(12)	1	2
H(11)	H	0.7171(4)	1.0975(4)	0.32811(17)	0.103(12)	1	2
H(12)	H	0.5497(3)	0.9741(3)	0.23232(14)	0.088(10)	1	2
H(13A)	H	0.1584(3)	1.0935(2)	0.11035(11)	0.050(7)	1	2
H(13B)	H	0.3599(3)	1.0151(2)	0.11301(11)	0.042(6)	1	2
H(14A)	H	0.0390(2)	0.8825(2)	0.03865(10)	0.050(6)	1	2
H(14B)	H	0.2169(2)	0.9547(2)	0.00121(10)	0.037(6)	1	2
H(15A)	H	0.2435(2)	0.5166(2)	0.08885(10)	0.048(6)	1	2
H(15B)	H	0.0562(2)	0.6164(2)	0.09336(10)	0.042(6)	1	2
H(16A)	H	0.3866(3)	0.6796(3)	0.17976(11)	0.051(7)	1	2
H(16B)	H	0.1983(3)	0.6061(3)	0.20893(11)	0.063(8)	1	2
H(17A)	H	0.1012(3)	0.6548(3)	-0.04620(10)	0.054(7)	1	2

H(17B)	H	0.2755(3)	0.5435(3)	-0.03131(10)	0.060(8)	1	2
H(18A)	H	0.4741(3)	0.7552(3)	-0.07521(10)	0.059(7)	1	2
H(18B)	H	0.2872(3)	0.8398(3)	-0.10122(10)	0.058(8)	1	2
H(19A)	H	0.4377(3)	0.6807(3)	-0.19429(11)	0.074(9)	1	2
H(19B)	H	0.3800(3)	0.5282(3)	-0.15152(11)	0.077(9)	1	2
H(22)	H	0.3928(4)	0.4379(3)	-0.27356(13)	0.083(11)	1	2
H(23)	H	0.3489(5)	0.2949(4)	-0.38343(15)	0.100(12)	1	2
H(25)	H	-0.1616(5)	0.4927(4)	-0.40981(15)	0.124(15)	1	2
H(26)	H	-0.1214(4)	0.6302(4)	-0.29955(13)	0.095(12)	1	2

Table S22. Anisotropic displacement parameters for **1b**-HCl

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
Cl(2) 0.2038(12) 0.1238(10) 0.0882(6) -0.0566(8) -0.0790(7) -0.0070(6)
Cl(1) 0.0179(2) 0.0362(3) 0.0582(3) -0.00159(19) -0.0037(2) 0.0025(3)
Si 0.0249(3) 0.0377(4) 0.0370(3) -0.0005(2) 0.0042(2) -0.0045(3)
F 0.183(2) 0.153(2) 0.0528(11) -0.0162(16) -0.0097(11) -0.0456(13)
O(1) 0.0292(7) 0.0648(11) 0.0494(9) -0.0007(7) 0.0095(7) -0.0092(8)
O(2) 0.0568(9) 0.0621(12) 0.0491(9) 0.0214(8) -0.0085(7) -0.0137(9)
N 0.0182(7) 0.0201(9) 0.0351(8) -0.0008(6) -0.0017(6) -0.0003(7)
C(7) 0.0349(10) 0.0453(14) 0.0423(12) -0.0003(9) 0.0004(9) -0.0047(11)
C(8) 0.0558(16) 0.090(2) 0.0426(14) 0.0071(13) -0.0008(11) -0.0163(14)
C(9) 0.106(2) 0.095(3) 0.0445(17) 0.0041(19) -0.0132(16) -0.0201(17)
C(10) 0.105(2) 0.069(2) 0.0607(18) -0.0189(17) -0.0375(17) -0.0004(16)
C(11) 0.0674(18) 0.080(2) 0.078(2) -0.0254(15) -0.0337(15) 0.0085(17)
C(12) 0.0367(11) 0.0666(18) 0.0628(16) -0.0072(11) -0.0077(11) -0.0081(14)
C(13) 0.0332(10) 0.0269(12) 0.0500(13) 0.0037(8) 0.0061(9) -0.0058(10)
C(14) 0.0235(9) 0.0224(11) 0.0412(11) 0.0044(7) 0.0013(8) 0.0051(9)
C(15) 0.0249(9) 0.0234(11) 0.0433(12) -0.0012(8) 0.0003(8) 0.0037(9)
C(16) 0.0325(10) 0.0377(13) 0.0382(11) -0.0008(9) 0.0010(8) 0.0039(10)
C(17) 0.0329(10) 0.0306(13) 0.0373(12) -0.0069(9) -0.0009(8) -0.0048(10)
C(18) 0.0445(12) 0.0418(15) 0.0389(12) -0.0098(10) 0.0036(9) -0.0024(11)
C(19) 0.0445(12) 0.0432(16) 0.0391(12) -0.0004(10) 0.0030(10) -0.0017(11)
C(20) 0.0517(12) 0.0345(13) 0.0348(11) 0.0058(10) -0.0037(9) -0.0031(10)
C(21) 0.0623(13) 0.0402(15) 0.0322(12) -0.0006(10) -0.0016(10) -0.0000(11)
C(22) 0.095(2) 0.0597(19) 0.0369(13) 0.0182(15) -0.0012(14) -0.0114(13)
C(23) 0.129(3) 0.079(2) 0.0450(17) 0.019(2) 0.0047(18) -0.0205(17)
C(24) 0.128(3) 0.092(3) 0.0381(15) -0.008(2) -0.0050(18) -0.0163(17)
C(25) 0.099(2) 0.115(3) 0.0395(16) -0.025(2) -0.0125(16) -0.0062(17)
C(26) 0.0716(16) 0.076(2) 0.0352(13) -0.0067(15) -0.0075(12) 0.0046(13)
```

Table S23 Multipole parameters for **1b**-HCl

```
loop_
    _atom_rho_multipole_atom_label
    _atom_rho_multipole_coeff_Pv
    _atom_rho_multipole_coeff_P00
    _atom_rho_multipole_coeff_P11
    _atom_rho_multipole_coeff_P1-1
```

```
    _atom_rho_multipole_coeff_P10
    _atom_rho_multipole_coeff_P20
    _atom_rho_multipole_coeff_P21
    _atom_rho_multipole_coeff_P2-1
    _atom_rho_multipole_coeff_P22
    _atom_rho_multipole_coeff_P2-2
    _atom_rho_multipole_coeff_P30
    _atom_rho_multipole_coeff_P31
    _atom_rho_multipole_coeff_P3-1
    _atom_rho_multipole_coeff_P32
    _atom_rho_multipole_coeff_P3-2
    _atom_rho_multipole_coeff_P33
    _atom_rho_multipole_coeff_P3-3
    _atom_rho_multipole_coeff_P40
    _atom_rho_multipole_coeff_P41
    _atom_rho_multipole_coeff_P4-1
    _atom_rho_multipole_coeff_P42
    _atom_rho_multipole_coeff_P4-2
    _atom_rho_multipole_coeff_P43
    _atom_rho_multipole_coeff_P4-3
    _atom_rho_multipole_coeff_P44
    _atom_rho_multipole_coeff_P4-4
    _atom_rho_multipole_kappa
    _atom_rho_multipole_kappa_prime0
    _atom_rho_multipole_kappa_prime1
    _atom_rho_multipole_kappa_prime2
    _atom_rho_multipole_kappa_prime3
    _atom_rho_multipole_kappa_prime4
Cl(2) 7.1278 0
0 0 -0.0316
-0.142 0 0 0 0
0.1018 0 0 0 0 0 0
0.0311 0 0 0 0 0 0 0 0
1.003934 0.98084 0.98084 0.98084 0.98084 0.98084


Cl(1) 8 0
0 0 0
0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.010613 1 1 1 1 1


Si 4.6313 0
0.0422 0.0029 -0.0048
-0.0305 -0.0463 -0.0158 -0.034 -0.0192
0.717 0.0053 -0.0983 -0.0221 0.0244 0.0021 -0.5586
0.2182 0.003 -0.0309 0.0681 -0.0225 0.0185 0.2464 0.0102 -0.0052
0.940235 0.747749 0.747749 0.747749 0.747749 0.747749


F 7.1283 0
0 0 -0.0492
-0.0902 0 0 0 0
0.0342 0 0 0 0 0 0
0.0065 0 0 0 0 0 0 0 0
1.002244 1.3624 1.3624 1.3624 1.3624 1.3624
```

O(1) 5.9236 0
-0.0686 -0.0463 0
0.0485 0 0 -0.0489 0.0107
0 -0.024 -0.0061 0 0 0.0469 -0.0031
0.0033 0 0 -0.0089 -0.0055 0 0 0.0162 -0.0008
1.008424 1.095759 1.095759 1.095759 1.095759 1.095759

O(2) 6.1166 0
0 0 -0.0675
0.0293 0 0 -0.1531 0
0.0283 0 0 0.0172 0 0 0
-0.0118 0 0 0.0113 0 0 0 -0.0026 0
1.003017 1.109004 1.109004 1.109004 1.109004 1.109004

N 5.0916 0
0 0 -0.005
0.0107 0 0 0 0
0.2234 0 0 0 0 0.176 0
0.066 0 0 0 0 -0.0509 0 0 0
0.997716 0.890138 0.890138 0.890138 0.890138 0.890138

C(7) 3.9617 0
0 0 -0.0065
0.087 0 0 -0.147 0
0.1693 0 0 0.1248 0 0 0
-0.0075 0 0 -0.02 0 0 0 0.0002 0
1.015453 1 1 1 1 1

C(8) 3.9596 0
0.0166 0.0354 0
-0.1753 0 0 0.013 -0.0221
0 0.0108 0.022 0 0 0.2313 0.007
0.0164 0 0 0.008 -0.0146 0 0 0.0014 0
1.015464 1 1 1 1 1

C(9) 3.9213 0
0.001 0.0319 0
-0.1622 0 0 -0.0042 -0.0155
0 0.0084 0.0245 0 0 0.2229 -0.0076
0.0242 0 0 0.0013 -0.0129 0 0 -0.0003 -0.001
1.017714 1 1 1 1 1

C(10) 4.1025 0
0 0 -0.0872
-0.0375 0 0 -0.1635 0
0.2348 0 0 0.1308 0 0 0
0.0148 0 0 -0.0125 0 0 0 0.0021 0
1.005708 1 1 1 1 1

C(11) 3.9213 0
0.001 0.0319 0
-0.1622 0 0 -0.0042 -0.0155
0 0.0084 0.0245 0 0 0.2229 -0.0076
0.0242 0 0 0.0013 -0.0129 0 0 -0.0003 -0.001
1.017714 1 1 1 1 1

C(12) 3.9596 0
0.0166 0.0354 0
-0.1753 0 0 0.013 -0.0221
0 0.0108 0.022 0 0 0.2313 0.007
0.0164 0 0 0.008 -0.0146 0 0 0.0014 0
1.015464 1 1 1 1 1

C(13) 3.7949 0
0.0181 0.0134 0
-0.016 0 0 0.0247 0.0048
0 -0.0824 -0.1728 0 0 0.1346 -0.0198
0.0007 0 0 -0.0288 0.0575 0 0 0.0067 0.0155
1.01596 1 1 1 1 1

C(14) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(15) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(16) 3.7949 0
0.0181 0.0134 0
-0.016 0 0 0.0247 0.0048
0 -0.0824 -0.1728 0 0 0.1346 -0.0198
0.0007 0 0 -0.0288 0.0575 0 0 0.0067 0.0155
1.01596 1 1 1 1 1

C(17) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(18) 3.9428 0
0 0 0.0068

-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(19) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(20) 3.9937 0
0.0588 -0.0014 0
-0.2542 0 0 0.066 0.0001
0 0.0173 0.0063 0 0 0.2777 0.0024
0.0152 0 0 0.0131 0.0001 0 0 -0.0174 0.0025
1.016945 1 1 1 1 1

C(21) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1

C(22) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(23) 3.9654 0
0.0094 0.0348 0
-0.1568 0 0 -0.0015 -0.0186
0 0.0079 0.0255 0 0 0.222 -0.0068
0.0211 0 0 0.0022 -0.0107 0 0 0.0035 0.0023
1.018878 1 1 1 1 1

C(24) 3.9709 0
0 0 -0.1242
-0.0582 0 0 -0.1752 0
0.2702 0 0 0.1226 0 0 0
0.0391 0 0 -0.007 0 0 0 -0.0002 0
1.016611 1 1 1 1 1

C(25) 3.9654 0
0.0094 0.0348 0
-0.1568 0 0 -0.0015 -0.0186
0 0.0079 0.0255 0 0 0.222 -0.0068

0.0211 0 0 0.0022 -0.0107 0 0 0.0035 0.0023
1.018878 1 1 1 1 1

C(26) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

H(1) 0.887 0
0 0 0.2158
0.1007 0 0 0 0
0.0194 0 0 0 0 0 0
-0.0224 0 0 0 0 0 0 0 0
1.122351 1.2 1.2 1.2 1.2 1.2

H(N) 0.7484 0
0 0 0.1685
0.0719 0 0 0 0
0.0004 0 0 0 0 0 0
-0.0157 0 0 0 0 0 0 0 0
1.197464 1.2 1.2 1.2 1.2 1.2

H(8) 0.9519 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(9) 0.9519 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(11) 0.9519 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(12) 0.9519 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(13A) 0.9831 0
0 0 0.1502
0.068 0 0 0 0
0.024 0 0 0 0 0 0
0.0082 0 0 0 0 0 0 0 0
1.117466 1.2 1.2 1.2 1.2 1.2

H(13B) 0.9831 0
0 0 0.1502
0.068 0 0 0 0
0.024 0 0 0 0 0 0
0.0082 0 0 0 0 0 0 0 0
1.117466 1.2 1.2 1.2 1.2 1.2

H(14A) 1.0111 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(14B) 1.0111 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(15A) 1.0111 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(15B) 1.0111 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(16A) 0.9831 0
0 0 0.1502
0.068 0 0 0 0
0.024 0 0 0 0 0 0
0.0082 0 0 0 0 0 0 0 0
1.117466 1.2 1.2 1.2 1.2 1.2

H(16B) 0.9831 0
0 0 0.1502
0.068 0 0 0 0
0.024 0 0 0 0 0 0
0.0082 0 0 0 0 0 0 0 0
1.117466 1.2 1.2 1.2 1.2 1.2

H(17A) 1.0111 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(17B) 1.0111 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(18A) 0.9777 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(18B) 0.9777 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(19A) 0.9777 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(19B) 0.9777 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(22) 0.9519 0
0 0 0.1546

```
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(23) 0.9519 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(25) 0.9519 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(26) 0.9519 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

Electronic Supplementary Information Part II: 4 Compounds of Venlafaxine type.

Note: In all Tables the non-revised output of the XD program (ref. 12) was used. With respect to the significance of the given data we refer to Grabowsky et al., Acta Cryst. 2009, B65, 488 , where transferability indices were derived as 0.09 e Å^{-3} and 2.8 e Å^{-5} for the ED's and Laplacians at the bond critical points and 0.7 Å^{3} and 0.11 e for the atomic volumes and charges. These quantities can serve as an estimate of the significance of the listed data.

TABLE S4 BOND CRITICAL POINT SEARCH FOR **2a**

****

Quantities are in e/Ang^x
Using ANALYTICAL derivatives

Searching internuclear distances between 1.200 and 1.600 Angstroms

Bond		ρ	Δρ	Rij d1 d2	
				Hessian Eigenvalues	ellip
O(1)	-C(5)	1.765	-11.853	1.4378 0.8296 0.6082	
				-13.72 -13.31 15.17	0.03
O(2)	-C(14)	2.058	-17.791	1.3646 0.8107 0.5538	
				-17.43 -15.92 15.56	0.10
O(2)	-C(17)	1.804	-11.986	1.4195 0.8279 0.5916	
				-13.87 -13.65 15.54	0.02
N(1)	-C(1)	1.708	-6.280	1.4687 0.7999 0.6689	
				-12.36 -10.69 16.77	0.16
N(1)	-C(2)	1.709	-6.320	1.4684 0.7997 0.6687	
				-12.38 -10.70 16.76	0.16
N(1)	-C(3)	1.684	-6.087	1.4769 0.8030 0.6740	
				-12.22 -10.54 16.68	0.16
C(3)	-C(4)	1.632	-10.411	1.5426 0.7759 0.7667	
				-11.54 -11.04 12.16	0.05
C(4)	-C(5)	1.630	-10.450	1.5608 0.7670 0.7937	
				-11.59 -11.06 12.20	0.05
C(4)	-C(11)	1.652	-10.222	1.5235 0.7504 0.7731	
				-11.50 -11.23 12.51	0.02
C(5)	-C(6)	1.700	-11.834	1.5376 0.7814 0.7562	
				-12.17 -11.72 12.05	0.04
C(5)	-C(10)	1.711	-12.048	1.5337 0.7797 0.7540	
				-12.27 -11.82 12.04	0.04
C(6)	-C(7)	1.637	-10.416	1.5365 0.7683 0.7681	
				-11.28 -11.20 12.06	0.01
C(7)	-C(8)	1.668	-11.019	1.5240 0.7619 0.7621	
				-11.56 -11.47 12.02	0.01
C(8)	-C(9)	1.657	-10.800	1.5285 0.7644 0.7641	
				-11.46 -11.37 12.03	0.01
C(9)	-C(10)	1.637	-10.421	1.5365 0.7681 0.7684	
				-11.28 -11.19 12.06	0.01
C(11)	-C(12)	2.086	-16.376	1.4059 0.7041 0.7018	
				-16.17 -13.37 13.17	0.21
C(11)	-C(16)	2.119	-17.391	1.3949 0.6989 0.6960	
				-16.49 -13.76 12.86	0.20
C(12)	-C(13)	2.100	-17.461	1.3920 0.7021 0.6899	
				-16.46 -13.63 12.63	0.21

C(13)	-C(14)	2.136	-17.279	1.4013	0.6882	0.7130	
				-16.87	-13.59	13.19	0.24
C(14)	-C(15)	2.133	-17.834	1.3943	0.7142	0.6800	
				-16.93	-13.73	12.83	0.23
C(15)	-C(16)	2.091	-16.461	1.3985	0.6973	0.7012	
				-16.16	-13.37	13.07	0.21

TABLE S5 BOND CRITICAL POINT SEARCH FOR **2a**-HCl-ortho

****

Quantities are in e/Ang^x
Using ANALYTICAL derivatives

Searching internuclear distances between 1.200 and 1.600 Angstroms

Bond		ρ	Δρ	Rij d1 d2	
				Hessian Eigenvalues	ellip
O(1)	-C(4)	2.065	-17.915	1.3631 0.8105 0.5526	
				-17.48 -15.98 15.54	0.09
O(1)	-C(17)	1.899	-12.909	1.3985 0.8194 0.5791	
				-14.49 -14.27 15.85	0.02
O(2)	-C(8)	1.813	-13.515	1.4198 0.8280 0.5919	
				-14.20 -13.76 14.45	0.03
N(1)	-C(14)	1.826	-11.398	1.4990 0.8323 0.6667	
				-13.58 -13.37 15.55	0.02
N(1)	-C(15)	1.818	-10.529	1.5057 0.8310 0.6747	
				-13.31 -13.22 16.00	0.01
N(1)	-C(16)	1.870	-11.642	1.4882 0.8258 0.6624	
				-13.78 -13.72 15.85	0.00
C(1)	-C(2)	2.172	-18.393	1.3816 0.6903 0.6913	
				-16.93 -14.17 12.71	0.20
C(1)	-C(6)	2.143	-17.417	1.3916 0.6950 0.6967	
				-16.63 -13.80 13.02	0.21
C(1)	-C(7)	1.706	-11.048	1.5066 0.7641 0.7425	
				-11.88 -11.70 12.53	0.02
C(2)	-C(3)	2.093	-16.049	1.4026 0.7034 0.6992	
				-16.04 -13.32 13.32	0.20
C(3)	-C(4)	2.156	-18.075	1.3888 0.6794 0.7094	
				-17.07 -13.87 12.87	0.23
C(4)	-C(5)	2.183	-18.830	1.3871 0.7098 0.6773	
				-17.44 -14.12 12.73	0.23
C(5)	-C(6)	2.176	-18.047	1.3771 0.6881 0.6890	
				-16.87 -13.99 12.82	0.21
C(7)	-C(8)	1.613	-10.007	1.5708 0.7739 0.7969	
				-11.34 -10.94 12.27	0.04
C(7)	-C(14)	1.641	-10.108	1.5470 0.7671 0.7799	
				-11.42 -11.08 12.39	0.03
C(8)	-C(9)	1.758	-12.612	1.5210 0.7699 0.7511	
				-12.61 -12.14 12.13	0.04
C(8)	-C(13)	1.745	-12.374	1.5250 0.7718 0.7532	
				-12.49 -12.03 12.15	0.04
C(9)	-C(10)	1.700	-11.008	1.5209 0.7607 0.7601	
				-11.69 -11.59 12.27	0.01
C(10)	-C(11)	1.718	-11.348	1.5136 0.7574 0.7562	
				-11.86 -11.74 12.24	0.01
C(11)	-C(12)	1.661	-10.290	1.5352 0.7679 0.7674	
				-11.35 -11.25 12.32	0.01
C(12)	-C(13)	1.693	-10.888	1.5234 0.7614 0.7620	
				-11.63 -11.53 12.28	0.01

TABLE S6. BOND CRITICAL POINT SEARCH FOR **2a**-HCl-mono

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Quantities are in e/Ang^x
Using ANALYTICAL derivatives

Searching internuclear distances between 1.200 and 1.600 Angstroms

Bond		**ρ**	**Δρ**	Rij / Hessian Eigenvalues	d1	d2	ellip
O(1)	-C(4)	2.112	-19.996	1.3479	0.8122	0.5357	
				-17.98	-16.51	14.49	0.09
O(1)	-C(17)	1.840	-10.994	1.4188	0.8207	0.5980	
				-13.97	-13.74	16.71	0.02
O(2)	-C(8)	1.777	-12.228	1.4327	0.8283	0.6043	
				-13.86	-13.42	15.06	0.03
N(1)	-C(14)	1.828	-11.389	1.4975	0.8316	0.6659	
				-13.58	-13.37	15.56	0.02
N(1)	-C(15)	1.868	-11.534	1.4888	0.8260	0.6628	
				-13.73	-13.67	15.86	0.00
N(1)	-C(16)	1.882	-11.806	1.4822	0.8238	0.6584	
				-13.86	-13.80	15.85	0.00
C(1)	-C(2)	2.124	-16.989	1.3975	0.6980	0.6995	
				-16.46	-13.65	13.12	0.21
C(1)	-C(6)	2.158	-17.944	1.3866	0.6914	0.6952	
				-16.75	-14.05	12.85	0.19
C(1)	-C(7)	1.685	-10.658	1.5141	0.7673	0.7469	
				-11.72	-11.50	12.56	0.02
C(2)	-C(3)	2.144	-18.029	1.3834	0.6980	0.6854	
				-16.76	-13.92	12.65	0.20
C(3)	-C(4)	2.146	-17.194	1.4013	0.6902	0.7111	
				-16.87	-13.63	13.31	0.24
C(4)	-C(5)	2.184	-18.742	1.3804	0.7052	0.6751	
				-17.35	-14.10	12.70	0.23
C(5)	-C(6)	2.145	-17.352	1.3860	0.6921	0.6939	
				-16.59	-13.75	12.99	0.21
C(7)	-C(8)	1.640	-10.509	1.5611	0.7691	0.7920	
				-11.59	-11.18	12.26	0.04
C(7)	-C(14)	1.662	-10.484	1.5386	0.7626	0.7760	
				-11.60	-11.27	12.39	0.03
C(8)	-C(9)	1.744	-12.374	1.5260	0.7724	0.7536	
				-12.49	-12.03	12.15	0.04
C(8)	-C(13)	1.730	-12.064	1.5308	0.7745	0.7563	
				-12.35	-11.89	12.18	0.04
C(9)	-C(10)	1.668	-10.412	1.5334	0.7668	0.7666	
				-11.41	-11.31	12.31	0.01
C(10)	-C(11)	1.725	-11.500	1.5112	0.7555	0.7557	
				-11.92	-11.80	12.23	0.01
C(11)	-C(12)	1.688	-10.776	1.5256	0.7628	0.7627	
				-11.58	-11.48	12.29	0.01
C(12)	-C(13)	1.715	-11.296	1.5151	0.7575	0.7577	
				-11.83	-11.72	12.25	0.01

TABLE S7. BOND CRITICAL POINT SEARCH FOR **2b**-HCl

****

Quantities are in e/Ang^x
Using ANALYTICAL derivatives
Searching internuclear distances between 1.200 and 1.990 Angstroms

Bond		**ρ**	**Δρ**	Rij	d1	d2	
				Hessian Eigenvalues			ellip
SI	-O(1)	0.995	16.810	1.6285	0.6775	0.9510	
				-6.95	-6.84	30.60	0.02
SI	-C(1)	0.874	4.280	1.8574	0.7192	1.1381	
				-4.88	-4.67	13.83	0.05
SI	-C(5)	0.865	3.987	1.8641	0.7214	1.1427	
				-4.77	-4.55	13.31	0.05
SI	-C(6)	0.833	2.447	1.9082	0.7309	1.1773	
				-4.47	-4.30	11.22	0.04
O(2)	-C(13)	2.076	-18.456	1.3593	0.8110	0.5484	
				-17.60	-16.10	15.25	0.09
O(2)	-C(16)	1.849	-11.284	1.4154	0.8203	0.5951	
				-14.05	-13.82	16.59	0.02
N	-C(7)	1.802	-10.715	1.5045	0.8328	0.6717	
				-13.27	-13.15	15.71	0.01
N	-C(8)	1.880	-11.858	1.4850	0.8250	0.6600	
				-13.87	-13.80	15.81	0.01
N	-C(9)	1.852	-11.180	1.4937	0.8272	0.6665	
				-13.58	-13.52	15.92	0.00
C(1)	-C(2)	1.617	-9.086	1.5398	0.7628	0.7770	
				-10.86	-10.46	12.23	0.04
C(2)	-C(3)	1.688	-10.845	1.5246	0.7622	0.7625	
				-11.60	-11.51	12.27	0.01
C(3)	-C(4)	1.687	-10.845	1.5247	0.7626	0.7621	
				-11.60	-11.51	12.26	0.01
C(4)	-C(5)	1.598	-8.840	1.5454	0.7802	0.7652	
				-10.73	-10.35	12.24	0.04
C(6)	-C(7)	1.698	-10.764	1.5175	0.7469	0.7705	
				-11.59	-11.39	12.22	0.02
C(6)	-C(10)	1.681	-10.168	1.5160	0.7464	0.7696	
				-11.80	-10.87	12.50	0.08
C(10)	-C(11)	2.159	-18.084	1.3855	0.6921	0.6934	
				-16.81	-14.06	12.78	0.20
C(10)	-C(15)	2.110	-16.648	1.4018	0.7002	0.7016	
				-16.31	-13.53	13.19	0.21
C(11)	-C(12)	2.120	-16.673	1.3944	0.6992	0.6951	
				-16.31	-13.54	13.18	0.20
C(12)	-C(13)	2.164	-18.263	1.3866	0.6784	0.7082	
				-17.15	-13.94	12.82	0.23
C(13)	-C(14)	2.159	-17.550	1.3970	0.7090	0.6881	
				-17.03	-13.75	13.22	0.24
C(14)	-C(15)	2.144	-18.028	1.3834	0.6856	0.6979	
				-16.76	-13.92	12.65	0.20

Table S11. Atomic charges q [e] and volumes V [Å^3] for **2a**

Atom	q	V_{tot}
O(1)	-0.92559837	14.52555795
O(2)	-0.91380486	16.49428144
N(1)	-0.81057091	9.87766316
C(1)	0.22385028	8.94395838
C(2)	0.22011276	8.93318125
C(3)	0.22655904	6.94037590
C(4)	0.00891146	6.77867091
C(5)	0.29249116	5.59781546
C(6)	-0.04434796	7.71418307
C(7)	-0.04480180	8.82246325
C(8)	-0.04415940	8.66977349
C(9)	-0.03311147	8.42950047
C(10)	-0.05410476	8.29127915
C(11)	-0.04191079	9.04513739
C(12)	-0.06770643	11.09731374
C(13)	-0.06312423	12.61931004
C(14)	0.36790682	8.65147560
C(15)	-0.05245304	12.10122338
C(16)	-0.06131412	11.91659261
C(17)	0.33836622	9.68322895
H(1)	0.53518518	2.16229824
H(1A)	0.02292403	8.22064180
H(1B)	0.02489771	7.09768108
H(1C)	0.02170372	8.52555166
H(2A)	0.02279507	6.55431310
H(2B)	0.02637248	8.98444643
H(2C)	0.02319805	7.38076357
H(3A)	0.01877950	5.46176652
H(3B)	0.01270497	6.80172647
H(4)	0.03176334	7.06210713
H(6A)	0.03150051	6.36312512
H(6B)	0.04031261	6.57942660
H(7A)	0.03362135	7.12324765
H(7B)	0.03474593	6.89773464
H(8A)	0.03532404	8.77581828
H(8B)	0.03377119	7.85595043
H(9A)	0.03575097	7.40460551
H(9B)	0.03714844	7.05888174
H(10A)	0.03269455	7.09398459
H(10B)	0.03609770	8.66087275
H(12)	0.08188354	5.72387551
H(13)	0.08444923	7.12376709
H(15)	0.08098308	7.34067221
H(16)	0.08042835	7.63882997
H(17A)	0.03973513	6.91880435
H(17B)	0.04136513	7.82159038
H(17C)	0.04225142	9.10183234
sum :	0.06357678	388.86730077

V_{tot} values calculated by integration over the basins enclosed by the zero-flux surfaces of the ED gradient vector field in the crystal according to Bader's formalism.

Table S12. Atomic charges q [e] and volumes V [Å^3] for **2a**-HCl-ortho

Atom	q	V_{tot}
CL(1)	-1.00927143	38.27744590
O(1)	-0.93115563	14.56300817
O(2)	-0.94141659	14.63618521
N(1)	-0.86751035	8.42658566
C(1)	-0.03048425	8.61469555
C(2)	-0.03075401	12.12146271
C(3)	-0.02237320	13.36448462
C(4)	0.36765291	8.97905254
C(5)	-0.02758256	11.87329192
C(6)	-0.03262619	11.86567467
C(7)	0.02046041	6.66077763
C(8)	0.32311184	5.36868927
C(9)	-0.01442892	7.32613598
C(10)	-0.00536948	7.78325176
C(11)	-0.01734586	8.71895120
C(12)	-0.00623775	8.35060930
C(13)	-0.01583101	7.55195247
C(14)	0.20945850	7.18381017
C(15)	0.19964204	9.81641546
C(16)	0.19111133	9.52326537
C(17)	0.39232419	9.54556038
H(2B)	0.55674063	2.23229504
H(1A)	0.47583083	2.25994480
H(2A)	0.07808446	7.37819243
H(3A)	0.07874756	7.05861127
H(5A)	0.07978735	9.58244844
H(6A)	0.07744182	6.73659436
H(7A)	0.04848126	5.90091332
H(9A)	0.04320289	7.76086752
H(9B)	0.04215035	7.76097659
H(10A)	0.04403828	8.52627990
H(10B)	0.04422373	7.14329383
H(11A)	0.04425976	8.12540090
H(11B)	0.04326769	8.92279591
H(12A)	0.04665198	8.28566015
H(12B)	0.04873484	8.15155808
H(15A)	0.04469330	6.52834566
H(15B)	0.04308511	8.96505316
H(14A)	0.02638945	6.07175822
H(14B)	0.03086253	5.95130916
H(15C)	0.04023759	8.00821362
H(15D)	0.04067909	9.97833835
H(15E)	0.03986016	9.13799589
H(16B)	0.04130524	8.37016332
H(16C)	0.04171796	7.36892740
H(16D)	0.04325695	6.51854667
H(17A)	0.05168273	8.89224861
H(17B)	0.05378076	7.62159502

H(17C)	0.05292691	8.50844583
sum:	0.05349519	438.29807937

V_{tot} values calculated by integration over the basins enclosed by the zero-flux surfaces of the ED gradient vector field in the crystal according to Bader's formalism.

Table S13. Atomic charges q [e] and volumes V [Å^3] for **2a**-HCl-mono

Atom	q	V_{tot}
CL(1)	-1.00074280	37.36182124
O(1)	-0.93444914	16.18645069
O(2)	-0.92776924	14.89330236
N(1)	-0.89065670	8.64167448
C(1)	-0.02936110	9.01931573
C(2)	-0.03701436	12.73305492
C(3)	-0.02832322	13.60526721
C(4)	0.40563647	9.21671874
C(5)	-0.02506029	12.56072404
C(6)	-0.03638985	11.79351071
C(7)	0.02525801	6.46905737
C(8)	0.30933519	5.38807809
C(9)	-0.02325736	7.77939203
C(10)	0.00187100	7.86795038
C(11)	-0.02256638	8.94248573
C(12)	-0.01173806	8.09914596
C(13)	-0.01186010	7.52928292
C(14)	0.21308255	7.14084112
C(15)	0.20730398	9.65759403
C(16)	0.21353002	8.60592545
C(17)	0.37570856	8.36864437
H(27)	0.55677378	2.38733452
H(28)	0.46780157	2.45579327
H(1)	0.07861615	7.52519956
H(2)	0.07953887	7.41575934
H(3)	0.07864662	6.82132954
H(4)	0.07697926	6.75249219
H(5)	0.05006674	5.53500534
H(6)	0.04232906	9.94181336
H(7)	0.04216773	6.76612664
H(8)	0.04377279	9.95645898
H(9)	0.04284549	7.30664079
H(10)	0.04336334	8.22065902
H(11)	0.04632951	7.08563162
H(12)	0.04587548	6.98006206
H(13)	0.04466905	7.60055350
H(14)	0.04270294	8.10616524
H(15)	0.04513911	6.25425528
H(16)	0.02599247	5.91683336
H(17)	0.03245003	5.74047528
H(18)	0.04262644	8.32629708
H(19)	0.04167050	8.67522691
H(20)	0.04190679	7.75551098
H(21)	0.04268692	7.00876347
H(22)	0.04104703	8.77513867
H(23)	0.03940025	7.21508336
H(24)	0.05273226	8.84347992

H(25)	0.05233252	8.20415203
H(26)	0.05272415	7.78688785
sum:	0.06572403	433.21936675

V_{tot} values calculated by integration over the basins enclosed by the zero-flux surfaces of the ED gradient vector field in the crystal according to Bader's formalism.

Table S14. Atomic charges q [e] and volumes V [Å^3] for **2b**-HCl

Atom	q	V_{tot}
CL	-1.00040029	37.10116422
SI	3.02088112	3.70498136
O(1)	-1.37228998	18.75588723
O(2)	-0.91901817	15.51565913
N	-0.88876333	8.41578079
C(1)	-0.80805684	12.11686933
C(2)	-0.02433874	8.52346546
C(3)	-0.02567017	8.45583946
C(4)	-0.01692102	8.93057514
C(5)	-0.81029741	12.29848426
C(6)	-0.78335385	10.25615878
C(7)	0.19044243	7.26050811
C(8)	0.20004786	9.78345358
C(9)	0.20080366	8.71750338
C(10)	-0.04940198	9.39256381
C(11)	-0.03501334	13.35708107
C(12)	-0.03000029	12.06332572
C(13)	0.38748250	8.63552579
C(14)	-0.03069236	11.56124067
C(15)	-0.04589295	11.49611096
C(16)	0.37337885	9.36852070
H(O)	0.58696416	2.00805100
H(N)	0.47560316	2.81781853
H(1A)	0.05447311	8.62549914
H(1B)	0.05032280	9.26371113
H(2A)	0.04868650	9.30091072
H(2B)	0.05085463	6.87628583
H(3A)	0.04738796	7.90014051
H(3B)	0.05039584	8.05379302
H(4A)	0.05003333	8.69755782
H(4B)	0.04868552	7.26162580
H(5A)	0.05584081	6.89309850
H(5B)	0.04630016	8.05363086
H(6)	0.06191857	6.43914087
H(7A)	0.03536516	5.62695800
H(7B)	0.02952236	6.46312960
H(8A)	0.04829271	7.45304467
H(8B)	0.04644026	8.89645559
H(8C)	0.04681274	7.08562135
H(9A)	0.04746094	6.20438163
H(9B)	0.04691154	6.53702827
H(9C)	0.04904177	8.84994940
H(11)	0.08269932	8.07195150
H(12)	0.08618258	5.94971853
H(14)	0.08657388	7.80367675
H(15)	0.08478053	5.73072510
H(16A)	0.06006318	8.45258378
H(16B)	0.05885197	7.86587930

H(16C)	0.06036371	6.77047374
sum:	0.02975489	445.66353991

V_{tot} values calculated by integration over the basins enclosed by the zero-flux surfaces of the ED gradient vector field in the crystal according to Bader's formalism.

Tables S24 – S26 for (2a)

Table S24. Atomic coordinates for **2a**

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loop_
    _atom_site_label
    _atom_site_type_symbol
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
O(1)     O   0.68504(8)    -0.15161(6)     0.18894(3)     0.02       1       4
O(2)     O   0.35814(9)     0.64131(6)     0.05869(3)     0.026      1       4
N(1)     N   0.50199(9)    -0.03989(8)     0.28044(4)     0.019      1       4
C(1)     C   0.52132(13)   -0.00093(10)    0.34675(4)     0.025      1       4
C(2)     C   0.34708(12)   -0.11875(11)    0.26953(5)     0.027      1       4
C(3)     C   0.50601(12)    0.10181(9)     0.24397(4)     0.019      1       4
C(4)     C   0.52295(11)    0.07633(9)     0.17355(4)     0.018      1       4
C(5)     C   0.68270(11)   -0.00724(9)     0.15791(4)     0.016      1       4
C(6)     C   0.83561(11)    0.08207(9)     0.17803(5)     0.02       1       4
C(7)     C   0.99031(12)   -0.00102(10)    0.16006(5)     0.023      1       4
C(8)     C   0.98969(13)   -0.02974(11)    0.09014(5)     0.027      1       4
C(9)     C   0.83966(12)   -0.12018(10)    0.06911(5)     0.025      1       4
C(10)    C   0.68341(12)   -0.04098(10)    0.08792(4)     0.021      1       4
C(11)    C   0.49167(11)    0.22575(9)     0.13970(4)     0.018      1       4
C(12)    C   0.55407(11)    0.36497(9)     0.16151(4)     0.019      1       4
C(13)    C   0.51011(12)    0.50168(9)     0.13333(4)     0.019      1       4
C(14)    C   0.40106(12)    0.50236(9)     0.08177(4)     0.019      1       4
C(15)    C   0.34190(12)    0.36555(9)     0.05787(5)     0.022      1       4
C(16)    C   0.38694(12)    0.22976(9)     0.08727(4)     0.022      1       4
C(17)    C   0.24636(13)    0.64560(10)    0.00691(5)     0.028      1       4
H(1)     H   0.63981(8)    -0.13308(6)     0.22873(3)     0.032(3)   1       4
H(1A)    H   0.42645(13)    0.07886(10)    0.35964(4)     0.043(3)   1       4
H(1B)    H   0.64055(13)    0.05123(10)    0.35553(4)     0.052(4)   1       4
H(1C)    H   0.51253(13)   -0.10453(10)    0.37466(4)     0.055(4)   1       4
H(2A)    H   0.34181(12)   -0.21643(11)    0.30099(5)     0.053(4)   1       4
H(2B)    H   0.33820(12)   -0.15810(11)    0.22108(5)     0.051(4)   1       4
H(2C)    H   0.24616(12)   -0.04173(11)    0.27819(5)     0.048(3)   1       4
H(3A)    H   0.60867(12)    0.17071(9)     0.26159(4)     0.042(3)   1       4
H(3B)    H   0.39474(12)    0.16669(9)     0.25111(4)     0.044(3)   1       4
H(4)     H   0.42396(11)    0.00062(9)     0.15880(4)     0.034(3)   1       4
H(6A)    H   0.83189(11)    0.19373(9)     0.15594(5)     0.030(3)   1       4
H(6B)    H   0.83794(11)    0.09875(9)     0.22848(5)     0.040(3)   1       4
H(7A)    H   1.09610(12)    0.06717(10)    0.17397(5)     0.042(3)   1       4
H(7B)    H   0.99898(12)   -0.10912(10)    0.18486(5)     0.041(3)   1       4
H(8A)    H   1.09863(13)   -0.09260(11)    0.07870(5)     0.051(3)   1       4
H(8B)    H   0.99087(13)    0.07851(11)    0.06538(5)     0.044(3)   1       4
H(9A)    H   0.84560(12)   -0.23310(10)    0.09005(5)     0.040(3)   1       4
H(9B)    H   0.83776(12)   -0.13370(10)    0.01851(5)     0.049(3)   1       4
```

H(10A)	H	0.66980(12)	0.06530(10)	0.06207(4)	0.039(3)	1	4
H(10B)	H	0.57978(12)	-0.11307(10)	0.07510(4)	0.040(3)	1	4
H(12)	H	0.63849(11)	0.36589(9)	0.20127(4)	0.034(3)	1	4
H(13)	H	0.56000(12)	0.60715(9)	0.15118(4)	0.036(3)	1	4
H(15)	H	0.26175(12)	0.36436(9)	0.01685(5)	0.040(3)	1	4
H(16)	H	0.33891(12)	0.12425(9)	0.06872(4)	0.031(3)	1	4
H(17A)	H	0.29859(13)	0.58799(10)	-0.03271(5)	0.058(4)	1	4
H(17B)	H	0.22005(13)	0.76361(10)	-0.00548(5)	0.052(3)	1	4
H(17C)	H	0.13426(13)	0.58851(10)	0.01896(5)	0.048(3)	1	4

Table S25. Anisotropic displacement parameters for **2a**

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
O(1) 0.0239(4) 0.0138(3) 0.0226(4) 0.0028(3) 0.0024(3) 0.0034(3)
O(2) 0.0330(5) 0.0169(3) 0.0284(4) 0.0043(3) -0.0010(3) 0.0060(3)
N(1) 0.0184(5) 0.0177(4) 0.0215(5) 0.0012(3) 0.0010(4) 0.0033(3)
C(1) 0.0273(7) 0.0273(6) 0.0214(6) 0.0041(4) 0.0034(5) 0.0008(4)
C(2) 0.0228(6) 0.0274(5) 0.0323(7) -0.0065(4) 0.0009(5) 0.0075(5)
C(3) 0.0205(6) 0.0170(5) 0.0207(6) 0.0019(4) 0.0030(4) 0.0016(4)
C(4) 0.0167(6) 0.0151(5) 0.0222(6) 0.0012(4) -0.0000(4) 0.0026(4)
C(5) 0.0178(6) 0.0133(5) 0.0176(5) -0.0003(4) 0.0000(4) -0.0005(4)
C(6) 0.0186(6) 0.0162(5) 0.0237(6) -0.0009(4) -0.0013(4) -0.0019(4)
C(7) 0.0197(6) 0.0205(5) 0.0295(6) 0.0008(4) 0.0012(5) -0.0013(4)
C(8) 0.0261(7) 0.0261(5) 0.0300(7) 0.0014(4) 0.0076(5) 0.0007(4)
C(9) 0.0323(7) 0.0221(5) 0.0212(6) 0.0023(4) 0.0044(5) -0.0025(4)
C(10) 0.0265(6) 0.0184(5) 0.0178(6) 0.0003(4) -0.0005(5) -0.0008(4)
C(11) 0.0192(6) 0.0125(5) 0.0208(6) 0.0005(4) -0.0022(5) 0.0012(4)
C(12) 0.0195(6) 0.0156(5) 0.0220(6) 0.0005(4) -0.0021(4) 0.0011(4)
C(13) 0.0212(6) 0.0150(5) 0.0221(6) 0.0000(4) -0.0006(5) 0.0004(4)
C(14) 0.0207(6) 0.0157(5) 0.0208(6) 0.0024(4) 0.0001(5) 0.0035(4)
C(15) 0.0250(6) 0.0161(5) 0.0241(6) 0.0017(4) -0.0057(5) 0.0027(4)
C(16) 0.0247(6) 0.0146(5) 0.0250(6) 0.0011(4) -0.0064(5) 0.0014(4)
C(17) 0.0312(7) 0.0258(6) 0.0274(6) 0.0091(5) 0.0010(5) 0.0098(5)
```

Table S26 Multipole parameters for **2a**

```
loop_
    _atom_rho_multipole_atom_label
    _atom_rho_multipole_coeff_Pv
    _atom_rho_multipole_coeff_P00
    _atom_rho_multipole_coeff_P11
    _atom_rho_multipole_coeff_P1-1
    _atom_rho_multipole_coeff_P10
    _atom_rho_multipole_coeff_P20
    _atom_rho_multipole_coeff_P21
    _atom_rho_multipole_coeff_P2-1
    _atom_rho_multipole_coeff_P22
    _atom_rho_multipole_coeff_P2-2
    _atom_rho_multipole_coeff_P30
```

```
    _atom_rho_multipole_coeff_P31
    _atom_rho_multipole_coeff_P3-1
    _atom_rho_multipole_coeff_P32
    _atom_rho_multipole_coeff_P3-2
    _atom_rho_multipole_coeff_P33
    _atom_rho_multipole_coeff_P3-3
    _atom_rho_multipole_coeff_P40
    _atom_rho_multipole_coeff_P41
    _atom_rho_multipole_coeff_P4-1
    _atom_rho_multipole_coeff_P42
    _atom_rho_multipole_coeff_P4-2
    _atom_rho_multipole_coeff_P43
    _atom_rho_multipole_coeff_P4-3
    _atom_rho_multipole_coeff_P44
    _atom_rho_multipole_coeff_P4-4
    _atom_rho_multipole_kappa
    _atom_rho_multipole_kappa_prime0
    _atom_rho_multipole_kappa_prime1
    _atom_rho_multipole_kappa_prime2
    _atom_rho_multipole_kappa_prime3
    _atom_rho_multipole_kappa_prime4
O(1) 6.0788 0
-0.0536 -0.0866 0
0.1041 0 0 -0.028 0.042
0 -0.0147 -0.0263 0 0 0.065 -0.0215
0.0106 0 0 0.0042 0.0027 0 0 0.0149 0.0153
1.001632 1.113461 1.113461 1.113461 1.113461 1.113461


O(2) 6.1892 0
-0.0409 -0.0776 0
0.0709 0 0 -0.0249 0.0465
0 -0.0099 -0.023 0 0 0.0675 -0.0052
0.0027 0 0 0.0004 -0.0002 0 0 0.0118 0.0025
0.999544 1.195553 1.195553 1.195553 1.195553 1.195553


N(1) 5.1519 0
0 0 -0.0943
0.1166 0 0 0 0
-0.0742 0 0 0 0 0 -0.1282
-0.0124 0 0 0 0 0 -0.0427 0 0
0.998012 1.047518 1.047518 1.047518 1.047518 1.047518


C(1) 3.7963 0
0 0 -0.0134
-0.0353 0 0 0 0
0.2419 0 0 0 0 0 -0.1632
0.0404 0 0 0 0 0 0.0723 0 0
1.009611 1 1 1 1 1


C(2) 3.7963 0
0 0 -0.0134
-0.0353 0 0 0 0
0.2419 0 0 0 0 0 -0.1632
0.0404 0 0 0 0 0 0.0723 0 0
```

1.009611 1 1 1 1 1

C(3) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(4) 3.939 0
-0.0028 -0.0063 0
-0.0017 0 0 -0.0091 0.0044
0 -0.1364 -0.1687 0 0 0.1441 -0.0628
0.0216 0 0 -0.0135 0.06 0 0 0.0264 0.02
1.015244 1 1 1 1 1

C(5) 4.0663 0
0 0 -0.0564
-0.0884 0 0 0 0
0.2577 0 0 0 0 0.1963 0
0.083 0 0 0 0 -0.0794 0 0 0
1.002523 1 1 1 1 1

C(6) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(7) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(8) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(9) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(10) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(11) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1

C(12) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(13) 3.9952 0
0.0117 0.0383 0
-0.1447 0 0 0.0015 -0.0224
0 0.0075 0.0255 0 0 0.2238 0.0024
0.0214 0 0 0.0044 -0.0117 0 0 0.0099 0.0005
1.016678 1 1 1 1 1

C(14) 4.0021 0
0 0 -0.0816
0.005 0 0 -0.1763 0
0.2647 0 0 0.1301 0 0 0
0.0371 0 0 0.0102 0 0 0 0.0041 0
1.01558 1 1 1 1 1

C(15) 3.9952 0
0.0117 0.0383 0
-0.1447 0 0 0.0015 -0.0224
0 0.0075 0.0255 0 0 0.2238 0.0024
0.0214 0 0 0.0044 -0.0117 0 0 0.0099 0.0005
1.016678 1 1 1 1 1

C(16) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(17) 3.8259 0

```
0 0 -0.0464
-0.078 0 0 0 0
0.2666 0 0 0 0 0.176 0
0.059 0 0 0 0 -0.0796 0 0 0
1.006075 1 1 1 1 1


H(1) 0.9608 0
0 0 0.2069
0.0951 0 0 0 0
0.0171 0 0 0 0 0 0
-0.0278 0 0 0 0 0 0 0 0
1.119673 1.2 1.2 1.2 1.2 1.2


H(1A) 1.0458 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(1B) 1.0458 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(1C) 1.0458 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(2A) 1.0458 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(2B) 1.0458 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(2C) 1.0458 0
0 0 0.1518
0.0722 0 0 0 0
```

```
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(3A) 1.0513 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2


H(3B) 1.0513 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2


H(4) 1.0297 0
0 0 0.1521
0.076 0 0 0 0
0.0258 0 0 0 0 0 0
0.003 0 0 0 0 0 0 0 0
1.130049 1.2 1.2 1.2 1.2 1.2


H(6A) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(6B) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(7A) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(7B) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
```

```
1.127115 1.2 1.2 1.2 1.2 1.2


H(8A) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(8B) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(9A) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(9B) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(10A) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(10B) 1.0179 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(12) 0.9921 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

H(13) 0.9921 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(15) 0.9921 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(16) 0.9921 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(17A) 1.0149 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2

H(17B) 1.0149 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2

H(17C) 1.0149 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2

Tables S27 – S29 for (2a-HCl-ortho)

Table S27. Atomic coordinates for **2a**-HCl-ortho

```
loop_
    _atom_site_label
    _atom_site_type_symbol
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
```

Cl(1)	Cl	0.47896(4)	0.33870(15)	0.101798	0.055	1	4
O(1)	O	0.32126(10)	0.9491(4)	0.7728(2)	0.059	1	4
O(2)	O	0.38451(9)	0.5010(3)	0.2544(2)	0.039	1	4
N(1)	N	0.49049(10)	1.0328(5)	0.3149(3)	0.041	1	4
C(1)	C	0.37657(12)	0.9123(6)	0.4311(3)	0.035	1	4
C(2)	C	0.34965(12)	1.1020(6)	0.4665(3)	0.04	1	4
C(3)	C	0.32987(13)	1.1227(6)	0.5799(3)	0.043	1	4
C(4)	C	0.33731(13)	0.9479(6)	0.6595(3)	0.042	1	4
C(5)	C	0.36320(12)	0.7546(6)	0.6235(3)	0.044	1	4
C(6)	C	0.38250(14)	0.7376(6)	0.5119(3)	0.041	1	4
C(7)	C	0.39763(11)	0.8992(5)	0.3088(3)	0.033	1	4
C(8)	C	0.36849(13)	0.7260(5)	0.2285(3)	0.033	1	4
C(9)	C	0.31143(12)	0.7353(7)	0.2517(4)	0.048	1	4
C(10)	C	0.28121(16)	0.5830(9)	0.1696(4)	0.061	1	4
C(11)	C	0.29154(16)	0.6413(10)	0.0430(4)	0.07	1	4
C(12)	C	0.34890(14)	0.6286(8)	0.0173(4)	0.058	1	4
C(13)	C	0.37842(14)	0.7820(6)	0.1004(3)	0.045	1	4
C(14)	C	0.45477(11)	0.8342(6)	0.3084(4)	0.039	1	4
C(15)	C	0.54467(13)	0.9495(9)	0.3073(5)	0.067	1	4
C(16)	C	0.48233(18)	1.1800(7)	0.4190(4)	0.058	1	4
C(17)	C	0.3018(2)	1.1512(7)	0.8193(4)	0.074	1	4
H(2B)	H	0.41300(9)	0.4522(3)	0.2081(2)	0.057(14)	1	4
H(1A)	H	0.48333(10)	1.1322(5)	0.2437(3)	0.09(2)	1	4
H(2A)	H	0.34506(12)	1.2204(6)	0.4137(3)	0.050(12)	1	4
H(3A)	H	0.31067(13)	1.2493(6)	0.6007(3)	0.090(17)	1	4
H(5A)	H	0.36749(12)	0.6356(6)	0.6760(3)	0.046(11)	1	4
H(6A)	H	0.39956(14)	0.6056(6)	0.4902(3)	0.047(12)	1	4
H(7A)	H	0.39444(11)	1.0503(5)	0.2735(3)	0.046(11)	1	4
H(9A)	H	0.29964(12)	0.8908(7)	0.2434(4)	0.067(14)	1	4
H(9B)	H	0.30492(12)	0.6875(7)	0.3314(4)	0.065(14)	1	4
H(10A)	H	0.29062(16)	0.4256(9)	0.1830(4)	0.072(15)	1	4
H(10B)	H	0.24500(16)	0.5983(9)	0.1848(4)	0.053(12)	1	4
H(11A)	H	0.27967(16)	0.7947(10)	0.0277(4)	0.13(3)	1	4
H(11B)	H	0.27331(16)	0.5385(10)	-0.0084(4)	0.13(2)	1	4
H(12A)	H	0.36030(14)	0.4725(8)	0.0256(4)	0.100(19)	1	4
H(12B)	H	0.35582(14)	0.6773(8)	-0.0621(4)	0.065(14)	1	4
H(15A)	H	0.41468(14)	0.7694(6)	0.0851(3)	0.057(12)	1	4
H(15B)	H	0.36864(14)	0.9387(6)	0.0864(3)	0.059(12)	1	4
H(14A)	H	0.46157(11)	0.7368(6)	0.3750(4)	0.078(16)	1	4
H(14B)	H	0.46211(11)	0.7476(6)	0.2383(4)	0.078(15)	1	4
H(15C)	H	0.56761(13)	1.0767(9)	0.3090(5)	0.25(4)	1	4

H(15D)	H	0.54923(13)	0.8670(9)	0.2358(5)	0.10(2)	1	4
H(15E)	H	0.55168(13)	0.8513(9)	0.3723(5)	0.14(3)	1	4
H(16B)	H	0.50762(18)	1.2980(7)	0.4201(4)	0.082(16)	1	4
H(16C)	H	0.48585(18)	1.0873(7)	0.4876(4)	0.069(15)	1	4
H(16D)	H	0.44896(18)	1.2471(7)	0.4177(4)	0.33(5)	1	4
H(17A)	H	0.2988(2)	1.1344(7)	0.9024(4)	0.088(18)	1	4
H(17B)	H	0.2689(2)	1.1827(7)	0.7864(4)	0.19(4)	1	4
H(17C)	H	0.3246(2)	1.2744(7)	0.8020(4)	0.075(17)	1	4

Table S28. Anisotropic displacement parameters for **2a**-HCl-ortho

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
Cl(1) 0.0615(6) 0.0535(5) 0.0494(5) 0.0176(5) 0.0164(6) 0.0079(6)
O(1) 0.075(2) 0.0580(16) 0.0441(16) 0.0024(16) 0.0116(14) 0.0004(14)
O(2) 0.0363(14) 0.0332(11) 0.0464(13) -0.0006(11) 0.0010(12) 0.0043(11)
N(1) 0.0311(18) 0.0471(17) 0.0458(17) -0.0076(15) 0.0009(14) 0.0037(17)
C(1) 0.034(2) 0.0329(17) 0.0383(18) 0.0005(16) 0.0007(16) 0.0026(16)
C(2) 0.043(2) 0.0378(19) 0.0408(19) 0.0057(18) 0.0065(17) 0.0025(18)
C(3) 0.046(2) 0.0412(19) 0.043(2) 0.0093(18) 0.0080(18) 0.0023(18)
C(4) 0.040(2) 0.046(2) 0.040(2) 0.0012(19) 0.0010(17) -0.0021(19)
C(5) 0.044(2) 0.043(2) 0.045(2) 0.0020(18) -0.0003(17) 0.0085(19)
C(6) 0.042(2) 0.0371(19) 0.045(2) 0.0045(18) -0.0008(18) 0.0024(18)
C(7) 0.0247(17) 0.0340(17) 0.0405(18) 0.0024(15) 0.0034(16) 0.0017(16)
C(8) 0.0273(19) 0.0326(16) 0.0384(19) -0.0004(16) 0.0001(16) 0.0010(16)
C(9) 0.024(2) 0.055(2) 0.064(3) 0.0019(19) -0.0001(19) -0.004(2)
C(10) 0.036(3) 0.070(3) 0.077(3) -0.009(2) -0.004(2) -0.010(3)
C(11) 0.048(3) 0.092(4) 0.071(3) 0.001(3) -0.023(3) -0.011(3)
C(12) 0.065(3) 0.064(3) 0.046(2) -0.004(3) -0.015(2) -0.001(2)
C(13) 0.045(2) 0.047(2) 0.042(2) -0.0016(18) -0.002(2) 0.010(2)
C(14) 0.0265(18) 0.0399(18) 0.050(2) -0.0023(16) 0.0015(18) -0.004(2)
C(15) 0.030(2) 0.086(3) 0.085(4) 0.003(3) 0.004(2) 0.009(4)
C(16) 0.069(3) 0.048(2) 0.058(3) -0.016(2) -0.010(3) -0.009(2)
C(17) 0.107(5) 0.066(3) 0.048(3) 0.007(3) 0.026(3) -0.006(3)
```

Table S29. Multipole parameters for **2a**-HCl-ortho

```
loop_
    _atom_rho_multipole_atom_label
    _atom_rho_multipole_coeff_Pv
    _atom_rho_multipole_coeff_P00
    _atom_rho_multipole_coeff_P11
    _atom_rho_multipole_coeff_P1-1
    _atom_rho_multipole_coeff_P10
    _atom_rho_multipole_coeff_P20
    _atom_rho_multipole_coeff_P21
    _atom_rho_multipole_coeff_P2-1
    _atom_rho_multipole_coeff_P22
    _atom_rho_multipole_coeff_P2-2
    _atom_rho_multipole_coeff_P30
```

```
    _atom_rho_multipole_coeff_P31
    _atom_rho_multipole_coeff_P3-1
    _atom_rho_multipole_coeff_P32
    _atom_rho_multipole_coeff_P3-2
    _atom_rho_multipole_coeff_P33
    _atom_rho_multipole_coeff_P3-3
    _atom_rho_multipole_coeff_P40
    _atom_rho_multipole_coeff_P41
    _atom_rho_multipole_coeff_P4-1
    _atom_rho_multipole_coeff_P42
    _atom_rho_multipole_coeff_P4-2
    _atom_rho_multipole_coeff_P43
    _atom_rho_multipole_coeff_P4-3
    _atom_rho_multipole_coeff_P44
    _atom_rho_multipole_coeff_P4-4
    _atom_rho_multipole_kappa
    _atom_rho_multipole_kappa_prime0
    _atom_rho_multipole_kappa_prime1
    _atom_rho_multipole_kappa_prime2
    _atom_rho_multipole_kappa_prime3
    _atom_rho_multipole_kappa_prime4
Cl(1) 8 0
0 0 0
0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.010613 1 1 1 1 1


O(1) 6.1892 0
-0.0409 -0.0776 0
0.0709 0 0 -0.0249 0.0465
0 -0.0099 -0.023 0 0 0.0675 -0.0052
0.0027 0 0 0.0004 -0.0002 0 0 0.0118 0.0025
0.999544 1.195553 1.195553 1.195553 1.195553 1.195553


O(2) 6.0788 0
-0.0536 -0.0866 0
0.1041 0 0 -0.028 0.042
0 -0.0147 -0.0263 0 0 0.065 -0.0215
0.0106 0 0 0.0042 0.0027 0 0 0.0149 0.0153
1.001632 1.113461 1.113461 1.113461 1.113461 1.113461


N(1) 5.0916 0
0 0 -0.005
0.0107 0 0 0 0
0.2234 0 0 0 0 0.176 0
0.066 0 0 0 0 -0.0509 0 0 0
0.997716 0.890138 0.890138 0.890138 0.890138 0.890138


C(1) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
```

1.014566 1 1 1 1 1

C(2) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(3) 3.9952 0
0.0117 0.0383 0
-0.1447 0 0 0.0015 -0.0224
0 0.0075 0.0255 0 0 0.2238 0.0024
0.0214 0 0 0.0044 -0.0117 0 0 0.0099 0.0005
1.016678 1 1 1 1 1

C(4) 4.0021 0
0 0 -0.0816
0.005 0 0 -0.1763 0
0.2647 0 0 0.1301 0 0 0
0.0371 0 0 0.0102 0 0 0 0.0041 0
1.01558 1 1 1 1 1

C(5) 3.9952 0
0.0117 0.0383 0
-0.1447 0 0 0.0015 -0.0224
0 0.0075 0.0255 0 0 0.2238 0.0024
0.0214 0 0 0.0044 -0.0117 0 0 0.0099 0.0005
1.016678 1 1 1 1 1

C(6) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(7) 3.939 0
-0.0028 -0.0063 0
-0.0017 0 0 -0.0091 0.0044
0 -0.1364 -0.1687 0 0 0.1441 -0.0628
0.0216 0 0 -0.0135 0.06 0 0 0.0264 0.02
1.015244 1 1 1 1 1

C(8) 4.0663 0
0 0 -0.0564
-0.0884 0 0 0 0
0.2577 0 0 0 0 0.1963 0
0.083 0 0 0 0 -0.0794 0 0 0
1.002523 1 1 1 1 1

C(9) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(10) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(11) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(12) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(13) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(14) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(15) 3.7963 0
0 0 -0.0134
-0.0353 0 0 0 0
0.2419 0 0 0 0 0 -0.1632
0.0404 0 0 0 0 0 0.0723 0 0
1.009611 1 1 1 1 1

C(16) 3.7963 0

0 0 -0.0134
-0.0353 0 0 0 0
0.2419 0 0 0 0 0 -0.1632
0.0404 0 0 0 0 0 0.0723 0 0
1.009611 1 1 1 1 1

C(17) 3.8259 0
0 0 -0.0464
-0.078 0 0 0 0
0.2666 0 0 0 0 0.176 0
0.059 0 0 0 0 -0.0796 0 0 0
1.006075 1 1 1 1 1

H(2B) 0.9348 0
0 0 0.2069
0.0951 0 0 0 0
0.0171 0 0 0 0 0 0
-0.0278 0 0 0 0 0 0 0 0
1.119673 1.2 1.2 1.2 1.2 1.2

H(1A) 0.7626 0
0 0 0.1685
0.0719 0 0 0 0
0.0004 0 0 0 0 0 0
-0.0157 0 0 0 0 0 0 0 0
1.197464 1.2 1.2 1.2 1.2 1.2

H(2A) 0.9661 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(3A) 0.9661 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(5A) 0.9661 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(6A) 0.9661 0
0 0 0.1546
0.0629 0 0 0 0

0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(7A) 1.0037 0
0 0 0.1521
0.076 0 0 0 0
0.0258 0 0 0 0 0 0
0.003 0 0 0 0 0 0 0 0
1.130049 1.2 1.2 1.2 1.2 1.2

H(9A) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(9B) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(10A) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(10B) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(11A) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(11B) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0

1.127115 1.2 1.2 1.2 1.2 1.2

H(12A) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(12B) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(15A) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(15B) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(14A) 1.0253 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(14B) 1.0253 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(15C) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2

```
H(15D) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(15E) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(16B) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(16C) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(16D) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(17A) 0.9889 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2


H(17B) 0.9889 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2
```

```
H(17C) 0.9889 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2
```

Tables S30 – S32 for (2a-HCl-mono)

Table S30. Atomic coordinates for **2a**-HCl-mono

```
loop_
    _atom_site_label
    _atom_site_type_symbol
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
```

Cl(1)	Cl	0.3865(2)	0.77715(5)	0.75688(11)	0.058	1	4
O(1)	O	0.4907(6)	0.93547(15)	0.0839(3)	0.065	1	4
O(2)	O	1.1457(5)	0.86869(13)	0.5936(3)	0.049	1	4
N(1)	N	0.6132(7)	0.75620(14)	0.5482(4)	0.048	1	4
C(1)	C	0.6675(8)	0.87039(17)	0.4127(4)	0.044	1	4
C(2)	C	0.4612(8)	0.89848(19)	0.3777(4)	0.054	1	4
C(3)	C	0.4071(9)	0.91972(19)	0.2678(4)	0.056	1	4
C(4)	C	0.5583(8)	0.91317(19)	0.1885(4)	0.05	1	4
C(5)	C	0.7592(9)	0.88441(18)	0.2219(4)	0.052	1	4
C(6)	C	0.8128(9)	0.86354(18)	0.3324(4)	0.051	1	4
C(7)	C	0.7280(7)	0.84997(16)	0.5355(4)	0.041	1	4
C(8)	C	0.9189(8)	0.88238(16)	0.6158(4)	0.042	1	4
C(9)	C	0.8877(10)	0.93962(18)	0.5905(4)	0.058	1	4
C(10)	C	1.0625(12)	0.9723(2)	0.6747(5)	0.073	1	4
C(11)	C	1.0496(15)	0.9611(2)	0.7998(5)	0.078	1	4
C(12)	C	1.0836(11)	0.90398(19)	0.8256(4)	0.062	1	4
C(13)	C	0.9064(9)	0.87244(18)	0.7432(4)	0.049	1	4
C(14)	C	0.8063(8)	0.79350(16)	0.5408(4)	0.044	1	4
C(15)	C	0.7133(12)	0.7036(2)	0.5661(7)	0.077	1	4
C(16)	C	0.4222(10)	0.7576(3)	0.4449(6)	0.076	1	4
C(17)	C	0.6398(12)	0.9295(3)	0.0016(5)	0.074	1	4
H(27)	H	1.2304(5)	0.84673(13)	0.6527(3)	0.042(15)	1	4
H(28)	H	0.5587(7)	0.76379(14)	0.6244(4)	0.11(3)	1	4
H(1)	H	0.3587(8)	0.90305(19)	0.4292(4)	0.09(2)	1	4
H(2)	H	0.2693(9)	0.93844(19)	0.2462(4)	0.056(15)	1	4
H(3)	H	0.8596(9)	0.87901(18)	0.1697(4)	0.09(2)	1	4
H(4)	H	0.9496(9)	0.84444(18)	0.3533(4)	0.063(17)	1	4
H(5)	H	0.5847(7)	0.85172(16)	0.5685(4)	0.075(17)	1	4
H(6)	H	0.7292(10)	0.94965(18)	0.5964(4)	0.11(3)	1	4
H(7)	H	0.9085(10)	0.94628(18)	0.5116(4)	0.10(2)	1	4
H(8)	H	1.2201(12)	0.9654(2)	0.6619(5)	0.09(2)	1	4
H(9)	H	1.0295(12)	1.0083(2)	0.6587(5)	0.10(2)	1	4
H(10)	H	0.8987(15)	0.9721(2)	0.8156(5)	0.13(3)	1	4
H(11)	H	1.1711(15)	0.9803(2)	0.8503(5)	0.10(3)	1	4
H(12)	H	1.2410(11)	0.89387(19)	0.8179(4)	0.10(2)	1	4
H(13)	H	1.0659(11)	0.89725(19)	0.9049(4)	0.066(16)	1	4
H(14)	H	0.7498(9)	0.88064(18)	0.7558(4)	0.09(2)	1	4
H(15)	H	0.9341(9)	0.83631(18)	0.7602(4)	0.08(2)	1	4
H(16)	H	0.8714(8)	0.78580(16)	0.4723(4)	0.09(2)	1	4
H(17)	H	0.9301(8)	0.78880(16)	0.6081(4)	0.057(16)	1	4
H(18)	H	0.5930(12)	0.6801(2)	0.5784(7)	0.13(3)	1	4
H(19)	H	0.8378(12)	0.7035(2)	0.6327(7)	0.13(4)	1	4
H(20)	H	0.7739(12)	0.6934(2)	0.4987(7)	0.12(3)	1	4
H(21)	H	0.3428(10)	0.7900(3)	0.4416(6)	0.09(2)	1	4

H(22)	H	0.3127(10)	0.7305(3)	0.4502(6)	0.09(2)	1	4
H(23)	H	0.4871(10)	0.7531(3)	0.3759(6)	0.15(4)	1	4
H(24)	H	0.6457(12)	0.8939(3)	-0.0190(5)	0.13(3)	1	4
H(25)	H	0.7949(12)	0.9411(3)	0.0349(5)	0.07(2)	1	4
H(26)	H	0.5801(12)	0.9493(3)	-0.0665(5)	0.12(3)	1	4

Table S31. Anisotropic displacement parameters for **2a**-HCl-mono

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
Cl(1) 0.0563(7) 0.0682(8) 0.0554(7) 0.0125(7) 0.0261(6) 0.0161(7)
O(1) 0.068(2) 0.078(3) 0.052(2) 0.012(2) 0.0145(17) 0.0116(19)
O(2) 0.0406(17) 0.058(2) 0.0528(19) -0.0056(16) 0.0222(15) 0.0007(18)
N(1) 0.054(2) 0.038(2) 0.057(2) -0.0085(18) 0.025(2) -0.0034(18)
C(1) 0.043(3) 0.045(3) 0.046(2) 0.009(2) 0.016(2) 0.004(2)
C(2) 0.051(3) 0.059(3) 0.056(3) 0.016(2) 0.020(2) 0.015(2)
C(3) 0.045(3) 0.065(3) 0.060(3) 0.021(3) 0.016(2) 0.013(3)
C(4) 0.053(3) 0.056(3) 0.043(3) 0.006(2) 0.014(2) 0.004(2)
C(5) 0.058(3) 0.057(3) 0.044(3) 0.008(2) 0.018(2) -0.002(2)
C(6) 0.050(3) 0.058(3) 0.049(3) 0.018(2) 0.022(2) 0.004(2)
C(7) 0.040(2) 0.039(3) 0.047(3) 0.0016(19) 0.017(2) 0.0056(19)
C(8) 0.050(3) 0.038(3) 0.041(3) 0.003(2) 0.017(2) 0.0031(19)
C(9) 0.080(4) 0.041(3) 0.054(3) -0.004(3) 0.019(3) 0.006(2)
C(10) 0.111(5) 0.045(3) 0.066(4) -0.015(3) 0.025(3) 0.003(3)
C(11) 0.121(6) 0.048(3) 0.065(4) -0.007(4) 0.018(4) -0.007(3)
C(12) 0.086(4) 0.054(3) 0.045(3) 0.001(3) 0.015(3) -0.002(2)
C(13) 0.065(3) 0.045(3) 0.041(3) 0.004(2) 0.023(2) 0.007(2)
C(14) 0.048(3) 0.034(2) 0.052(3) -0.000(2) 0.013(2) 0.002(2)
C(15) 0.087(5) 0.041(3) 0.112(6) -0.001(3) 0.043(5) 0.003(3)
C(16) 0.054(3) 0.088(5) 0.085(5) -0.015(4) 0.012(3) -0.025(3)
C(17) 0.087(5) 0.090(5) 0.046(3) -0.001(4) 0.014(3) 0.004(3)
```

Table S32. Multipole parameters for **2a**-HCl-mono

```
loop_
    _atom_rho_multipole_atom_label
    _atom_rho_multipole_coeff_Pv
    _atom_rho_multipole_coeff_P00
    _atom_rho_multipole_coeff_P11
    _atom_rho_multipole_coeff_P1-1
    _atom_rho_multipole_coeff_P10
    _atom_rho_multipole_coeff_P20
    _atom_rho_multipole_coeff_P21
    _atom_rho_multipole_coeff_P2-1
    _atom_rho_multipole_coeff_P22
    _atom_rho_multipole_coeff_P2-2
    _atom_rho_multipole_coeff_P30
    _atom_rho_multipole_coeff_P31
    _atom_rho_multipole_coeff_P3-1
    _atom_rho_multipole_coeff_P32
```

```
    _atom_rho_multipole_coeff_P3-2
    _atom_rho_multipole_coeff_P33
    _atom_rho_multipole_coeff_P3-3
    _atom_rho_multipole_coeff_P40
    _atom_rho_multipole_coeff_P41
    _atom_rho_multipole_coeff_P4-1
    _atom_rho_multipole_coeff_P42
    _atom_rho_multipole_coeff_P4-2
    _atom_rho_multipole_coeff_P43
    _atom_rho_multipole_coeff_P4-3
    _atom_rho_multipole_coeff_P44
    _atom_rho_multipole_coeff_P4-4
    _atom_rho_multipole_kappa
    _atom_rho_multipole_kappa_prime0
    _atom_rho_multipole_kappa_prime1
    _atom_rho_multipole_kappa_prime2
    _atom_rho_multipole_kappa_prime3
    _atom_rho_multipole_kappa_prime4
Cl(1) 8 0
0 0 0
0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.010613 1 1 1 1 1


O(1) 6.1892 0
-0.0409 -0.0776 0
0.0709 0 0 -0.0249 0.0465
0 -0.0099 -0.023 0 0 0.0675 -0.0052
0.0027 0 0 0.0004 -0.0002 0 0 0.0118 0.0025
0.999544 1.195553 1.195553 1.195553 1.195553 1.195553


O(2) 6.0788 0
-0.0536 -0.0866 0
0.1041 0 0 -0.028 0.042
0 -0.0147 -0.0263 0 0 0.065 -0.0215
0.0106 0 0 0.0042 0.0027 0 0 0.0149 0.0153
1.001632 1.113461 1.113461 1.113461 1.113461 1.113461


N(1) 5.0916 0
0 0 -0.005
0.0107 0 0 0 0
0.2234 0 0 0 0 0.176 0
0.066 0 0 0 0 -0.0509 0 0 0
0.997716 0.890138 0.890138 0.890138 0.890138 0.890138


C(1) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1
```

C(2) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(3) 3.9952 0
0.0117 0.0383 0
-0.1447 0 0 0.0015 -0.0224
0 0.0075 0.0255 0 0 0.2238 0.0024
0.0214 0 0 0.0044 -0.0117 0 0 0.0099 0.0005
1.016678 1 1 1 1 1

C(4) 4.0021 0
0 0 -0.0816
0.005 0 0 -0.1763 0
0.2647 0 0 0.1301 0 0 0
0.0371 0 0 0.0102 0 0 0 0.0041 0
1.01558 1 1 1 1 1

C(5) 3.9952 0
0.0117 0.0383 0
-0.1447 0 0 0.0015 -0.0224
0 0.0075 0.0255 0 0 0.2238 0.0024
0.0214 0 0 0.0044 -0.0117 0 0 0.0099 0.0005
1.016678 1 1 1 1 1

C(6) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(7) 3.939 0
-0.0028 -0.0063 0
-0.0017 0 0 -0.0091 0.0044
0 -0.1364 -0.1687 0 0 0.1441 -0.0628
0.0216 0 0 -0.0135 0.06 0 0 0.0264 0.02
1.015244 1 1 1 1 1

C(8) 4.0663 0
0 0 -0.0564
-0.0884 0 0 0 0
0.2577 0 0 0 0 0.1963 0
0.083 0 0 0 0 -0.0794 0 0 0
1.002523 1 1 1 1 1

C(9) 3.9428 0
0 0 0.0068

-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(10) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(11) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(12) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(13) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(14) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(15) 3.7963 0
0 0 -0.0134
-0.0353 0 0 0 0
0.2419 0 0 0 0 0 -0.1632
0.0404 0 0 0 0 0 0.0723 0 0
1.009611 1 1 1 1 1

C(16) 3.7963 0
0 0 -0.0134
-0.0353 0 0 0 0
0.2419 0 0 0 0 0 -0.1632

0.0404 0 0 0 0 0 0.0723 0 0
1.009611 1 1 1 1 1

C(17) 3.8259 0
0 0 -0.0464
-0.078 0 0 0 0
0.2666 0 0 0 0 0.176 0
0.059 0 0 0 0 -0.0796 0 0 0
1.006075 1 1 1 1 1

H(27) 0.9348 0
0 0 0.2069
0.0951 0 0 0 0
0.0171 0 0 0 0 0 0
-0.0278 0 0 0 0 0 0 0 0
1.119673 1.2 1.2 1.2 1.2 1.2

H(28) 0.7626 0
0 0 0.1685
0.0719 0 0 0 0
0.0004 0 0 0 0 0 0
-0.0157 0 0 0 0 0 0 0 0
1.197464 1.2 1.2 1.2 1.2 1.2

H(1) 0.9661 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(2) 0.9661 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(3) 0.9661 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(4) 0.9661 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(5) 1.0037 0
0 0 0.1521
0.076 0 0 0 0
0.0258 0 0 0 0 0 0
0.003 0 0 0 0 0 0 0 0
1.130049 1.2 1.2 1.2 1.2 1.2

H(6) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(7) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(8) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(9) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(10) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(11) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(12) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(13) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(14) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(15) 0.9919 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(16) 1.0253 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(17) 1.0253 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2

H(18) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2

H(19) 1.0198 0
0 0 0.1518

```
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(20) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(21) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(22) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(23) 1.0198 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(24) 0.9889 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2


H(25) 0.9889 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2


H(26) 0.9889 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
```

```
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2
```

Tables S33 – S35 for (2b-HCl)

Table S33. Atomic coordinates for **2b**-HCl

```
loop_
    _atom_site_label
    _atom_site_type_symbol
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
```

Cl	Cl	-0.10768(3)	-0.05727(3)	0.48119	0.032	1	4
Si	Si	0.14903(2)	0.30381(2)	0.22998(6)	0.017	1	4
O(1)	O	0.12525(8)	0.26619(8)	0.07623(13)	0.036	1	4
O(2)	O	-0.34737(6)	0.25833(7)	0.30479(13)	0.031	1	4
N	N	0.09731(8)	0.04944(8)	0.43940(11)	0.017	1	4
C(1)	C	0.09062(10)	0.42308(9)	0.24248(18)	0.028	1	4
C(2)	C	0.15527(11)	0.49427(11)	0.15968(19)	0.03	1	4
C(3)	C	0.26963(10)	0.49742(10)	0.20167(19)	0.033	1	4
C(4)	C	0.32951(10)	0.40706(11)	0.17174(18)	0.029	1	4
C(5)	C	0.29132(9)	0.32209(9)	0.25646(16)	0.023	1	4
C(6)	C	0.09140(9)	0.22077(9)	0.36292(16)	0.018	1	4
C(7)	C	0.13742(9)	0.12341(9)	0.34300(16)	0.018	1	4
C(8)	C	0.11580(11)	0.07247(11)	0.58513(16)	0.026	1	4
C(9)	C	0.14468(11)	-0.04321(10)	0.40293(18)	0.027	1	4
C(10)	C	-0.02646(9)	0.22559(8)	0.35527(15)	0.017	1	4
C(11)	C	-0.08310(9)	0.27765(10)	0.44898(16)	0.023	1	4
C(12)	C	-0.19049(10)	0.29022(10)	0.43705(16)	0.025	1	4
C(13)	C	-0.24353(10)	0.24945(9)	0.32908(16)	0.022	1	4
C(14)	C	-0.18839(9)	0.19425(9)	0.23583(18)	0.023	1	4
C(15)	C	-0.08177(9)	0.18285(9)	0.24868(15)	0.02	1	4
C(16)	C	-0.40779(11)	0.30975(14)	0.39982(19)	0.04	1	4
H(O)	H	0.12481(8)	0.20033(8)	0.05510(13)	0.042(6)	1	4
H(N)	H	0.01915(8)	0.03751(8)	0.43030(11)	0.027(4)	1	4
H(1A)	H	0.01964(10)	0.42174(9)	0.20847(18)	0.054(5)	1	4
H(1B)	H	0.08872(10)	0.44258(9)	0.33725(18)	0.054(6)	1	4
H(2A)	H	0.15109(11)	0.47749(11)	0.06395(19)	0.061(7)	1	4
H(2B)	H	0.12508(11)	0.55643(11)	0.17020(19)	0.052(6)	1	4
H(3A)	H	0.27363(10)	0.51034(10)	0.29866(19)	0.066(7)	1	4
H(3B)	H	0.30315(10)	0.54908(10)	0.15417(19)	0.056(6)	1	4
H(4A)	H	0.40292(10)	0.41727(11)	0.19018(18)	0.042(5)	1	4
H(4B)	H	0.32241(10)	0.39221(11)	0.07563(18)	0.047(6)	1	4
H(5A)	H	0.30504(9)	0.33343(9)	0.35234(16)	0.049(6)	1	4
H(5B)	H	0.32899(9)	0.26593(9)	0.22940(16)	0.050(5)	1	4
H(6)	H	0.11270(9)	0.24339(9)	0.45313(16)	0.027(4)	1	4
H(7A)	H	0.12312(9)	0.10326(9)	0.25036(16)	0.040(5)	1	4
H(7B)	H	0.21249(9)	0.12743(9)	0.35312(16)	0.027(4)	1	4
H(8A)	H	0.09205(11)	0.02137(11)	0.64115(16)	0.079(8)	1	4
H(8B)	H	0.07835(11)	0.12868(11)	0.60858(16)	0.054(6)	1	4
H(8C)	H	0.18897(11)	0.08222(11)	0.59988(16)	0.050(5)	1	4
H(9A)	H	0.11482(11)	-0.09169(10)	0.45883(18)	0.056(6)	1	4
H(9B)	H	0.21860(11)	-0.04085(10)	0.41768(18)	0.049(6)	1	4
H(9C)	H	0.13095(11)	-0.05668(10)	0.30869(18)	0.048(6)	1	4
H(11)	H	-0.04837(9)	0.30525(10)	0.52199(16)	0.035(5)	1	4
H(12)	H	-0.22653(10)	0.32562(10)	0.50139(16)	0.037(5)	1	4

H(14)	H	-0.22356(9)	0.16531(9)	0.16428(18)	0.052(6)	1	4
H(15)	H	-0.04600(9)	0.14592(9)	0.18589(15)	0.041(5)	1	4
H(16A)	H	-0.47955(11)	0.30919(14)	0.37209(19)	0.065(7)	1	4
H(16B)	H	-0.38319(11)	0.37351(14)	0.40333(19)	0.075(8)	1	4
H(16C)	H	-0.40152(11)	0.28159(14)	0.48843(19)	0.073(7)	1	4

Table S34. Anisotropic displacement parameters for **2b**-HCl

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
Cl 0.02039(14) 0.0376(2) 0.0392(2) -0.00714(15) -0.00416(17) 0.01505(19)
Si 0.01907(14) 0.01550(15) 0.01775(18) -0.00143(13) -0.00072(17) 0.00274(16)
O(1) 0.0549(7) 0.0323(7) 0.0205(6) -0.0150(5) -0.0030(5) 0.0026(5)
O(2) 0.0189(4) 0.0354(6) 0.0393(7) 0.0035(4) 0.0027(4) 0.0047(5)
N 0.0168(5) 0.0144(6) 0.0205(7) -0.0008(4) 0.0004(5) 0.0013(4)
C(1) 0.0268(7) 0.0215(7) 0.0356(11) 0.0047(5) 0.0032(7) 0.0084(7)
C(2) 0.0368(8) 0.0192(8) 0.0339(10) 0.0034(6) 0.0022(7) 0.0087(6)
C(3) 0.0385(9) 0.0194(7) 0.0401(12) -0.0072(6) 0.0013(8) 0.0040(7)
C(4) 0.0255(7) 0.0261(8) 0.0360(10) -0.0056(6) 0.0043(6) 0.0053(7)
C(5) 0.0210(6) 0.0203(7) 0.0287(10) -0.0002(5) 0.0014(6) 0.0037(6)
C(6) 0.0193(6) 0.0182(7) 0.0176(7) 0.0005(5) 0.0002(5) 0.0009(5)
C(7) 0.0180(6) 0.0184(7) 0.0188(8) 0.0005(5) 0.0024(5) 0.0038(6)
C(8) 0.0304(7) 0.0268(8) 0.0210(8) -0.0015(6) 0.0010(7) 0.0030(6)
C(9) 0.0268(7) 0.0171(7) 0.0364(10) 0.0018(6) 0.0033(7) -0.0009(6)
C(10) 0.0177(6) 0.0157(6) 0.0189(7) 0.0003(5) 0.0008(6) 0.0003(5)
C(11) 0.0214(6) 0.0262(7) 0.0228(9) 0.0016(5) 0.0018(6) -0.0060(6)
C(12) 0.0230(6) 0.0264(8) 0.0269(8) 0.0034(6) 0.0057(6) -0.0036(6)
C(13) 0.0186(5) 0.0196(7) 0.0267(8) 0.0021(5) 0.0044(6) 0.0036(6)
C(14) 0.0202(5) 0.0249(6) 0.0231(7) -0.0012(5) 0.0001(7) -0.0015(7)
C(15) 0.0189(5) 0.0195(7) 0.0227(9) 0.0003(5) 0.0031(6) -0.0042(6)
C(16) 0.0230(7) 0.0508(12) 0.0468(12) 0.0141(7) 0.0125(7) 0.0158(9)
```

Table S35. Multipole parameters for **2b**-HCl

```
loop_
    _atom_rho_multipole_atom_label
    _atom_rho_multipole_coeff_Pv
    _atom_rho_multipole_coeff_P00
    _atom_rho_multipole_coeff_P11
    _atom_rho_multipole_coeff_P1-1
    _atom_rho_multipole_coeff_P10
    _atom_rho_multipole_coeff_P20
    _atom_rho_multipole_coeff_P21
    _atom_rho_multipole_coeff_P2-1
    _atom_rho_multipole_coeff_P22
    _atom_rho_multipole_coeff_P2-2
    _atom_rho_multipole_coeff_P30
    _atom_rho_multipole_coeff_P31
    _atom_rho_multipole_coeff_P3-1
    _atom_rho_multipole_coeff_P32
```

```
    _atom_rho_multipole_coeff_P3-2
    _atom_rho_multipole_coeff_P33
    _atom_rho_multipole_coeff_P3-3
    _atom_rho_multipole_coeff_P40
    _atom_rho_multipole_coeff_P41
    _atom_rho_multipole_coeff_P4-1
    _atom_rho_multipole_coeff_P42
    _atom_rho_multipole_coeff_P4-2
    _atom_rho_multipole_coeff_P43
    _atom_rho_multipole_coeff_P4-3
    _atom_rho_multipole_coeff_P44
    _atom_rho_multipole_coeff_P4-4
    _atom_rho_multipole_kappa
    _atom_rho_multipole_kappa_prime0
    _atom_rho_multipole_kappa_prime1
    _atom_rho_multipole_kappa_prime2
    _atom_rho_multipole_kappa_prime3
    _atom_rho_multipole_kappa_prime4
Cl 8 0
0 0 0
0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.010613 1 1 1 1 1


Si 4.6632 0
0 0 -0.0195
-0.0419 0 0 0 0
0.7059 0 0 0 0 0 -0.5532
0.2212 0 0 0 0 0 0.2505 0 0
0.936608 0.751918 0.751918 0.751918 0.751918 0.751918


O(1) 5.9426 0
-0.0643 -0.0436 0
0.0512 0 0 -0.0493 0.0123
0 -0.0269 -0.0073 0 0 0.0505 -0.0057
0.0049 0 0 -0.0088 -0.004 0 0 0.0154 0.0062
1.009092 1.099713 1.099713 1.099713 1.099713 1.099713


O(2) 6.1892 0
-0.0409 -0.0776 0
0.0709 0 0 -0.0249 0.0465
0 -0.0099 -0.023 0 0 0.0675 -0.0052
0.0027 0 0 0.0004 -0.0002 0 0 0.0118 0.0025
0.999544 1.195553 1.195553 1.195553 1.195553 1.195553


N 5.0916 0
0 0 -0.005
0.0107 0 0 0 0
0.2234 0 0 0 0 0.176 0
0.066 0 0 0 0 -0.0509 0 0 0
0.997716 0.890138 0.890138 0.890138 0.890138 0.890138
```

C(1) 3.8208 0
0.0233 0.0148 0
-0.0157 0 0 0.0274 0.0068
0 -0.0792 -0.1736 0 0 0.1338 -0.0115
-0.0001 0 0 -0.0274 0.0544 0 0 0.0037 0.021
1.013486 1 1 1 1 1

C(2) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(3) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(4) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1

C(5) 3.8208 0
0.0233 0.0148 0
-0.0157 0 0 0.0274 0.0068
0 -0.0792 -0.1736 0 0 0.1338 -0.0115
-0.0001 0 0 -0.0274 0.0544 0 0 0.0037 0.021
1.013486 1 1 1 1 1

C(6) 3.8961 0
0.0056 0.0047 0.0139
0.0233 0.0057 0.0004 0.0029 -0.0041
0.1654 0.0267 0.0095 0.0156 0.0217 -0.0435 -0.1729
0.0216 0.0035 0.0019 -0.0056 -0.0121 0.0146 0.0524 0.0047 0.0164
1.013724 1 1 1 1 1

C(7) 3.8671 0
-0.0199 0.011 0
0.0163 0 0 -0.0337 -0.0059
0 -0.1339 -0.172 0 0 0.1776 -0.0445
0.0086 0 0 -0.0279 0.0714 0 0 0.0321 0.023
1.009768 1 1 1 1 1

C(8) 3.7963 0
0 0 -0.0134

-0.0353 0 0 0 0
0.2419 0 0 0 0 0 -0.1632
0.0404 0 0 0 0 0 0.0723 0 0
1.009611 1 1 1 1 1

C(9) 3.7963 0
0 0 -0.0134
-0.0353 0 0 0 0
0.2419 0 0 0 0 0 -0.1632
0.0404 0 0 0 0 0 0.0723 0 0
1.009611 1 1 1 1 1

C(10) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1

C(11) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(12) 3.9952 0
0.0117 0.0383 0
-0.1447 0 0 0.0015 -0.0224
0 0.0075 0.0255 0 0 0.2238 0.0024
0.0214 0 0 0.0044 -0.0117 0 0 0.0099 0.0005
1.016678 1 1 1 1 1

C(13) 4.0021 0
0 0 -0.0816
0.005 0 0 -0.1763 0
0.2647 0 0 0.1301 0 0 0
0.0371 0 0 0.0102 0 0 0 0.0041 0
1.01558 1 1 1 1 1

C(14) 3.9952 0
0.0117 0.0383 0
-0.1447 0 0 0.0015 -0.0224
0 0.0075 0.0255 0 0 0.2238 0.0024
0.0214 0 0 0.0044 -0.0117 0 0 0.0099 0.0005
1.016678 1 1 1 1 1

C(15) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061

0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1

C(16) 3.8259 0
0 0 -0.0464
-0.078 0 0 0 0
0.2666 0 0 0 0 0.176 0
0.059 0 0 0 0 -0.0796 0 0 0
1.006075 1 1 1 1 1

H(O) 0.8962 0
0 0 0.2158
0.1007 0 0 0 0
0.0194 0 0 0 0 0 0
-0.0224 0 0 0 0 0 0 0 0
1.122351 1.2 1.2 1.2 1.2 1.2

H(N) 0.7576 0
0 0 0.1685
0.0719 0 0 0 0
0.0004 0 0 0 0 0 0
-0.0157 0 0 0 0 0 0 0 0
1.197464 1.2 1.2 1.2 1.2 1.2

H(1A) 0.9923 0
0 0 0.1502
0.068 0 0 0 0
0.024 0 0 0 0 0 0
0.0082 0 0 0 0 0 0 0 0
1.117466 1.2 1.2 1.2 1.2 1.2

H(1B) 0.9923 0
0 0 0.1502
0.068 0 0 0 0
0.024 0 0 0 0 0 0
0.0082 0 0 0 0 0 0 0 0
1.117466 1.2 1.2 1.2 1.2 1.2

H(2A) 0.9869 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(2B) 0.9869 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(3A) 0.9869 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(3B) 0.9869 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(4A) 0.9869 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(4B) 0.9869 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2

H(5A) 0.9923 0
0 0 0.1502
0.068 0 0 0 0
0.024 0 0 0 0 0 0
0.0082 0 0 0 0 0 0 0 0
1.117466 1.2 1.2 1.2 1.2 1.2

H(5B) 0.9923 0
0 0 0.1502
0.068 0 0 0 0
0.024 0 0 0 0 0 0
0.0082 0 0 0 0 0 0 0 0
1.117466 1.2 1.2 1.2 1.2 1.2

H(6) 0.9758 0
0 0 0.1499
0.0728 0 0 0 0
0.0275 0 0 0 0 0 0
0.0029 0 0 0 0 0 0 0 0
1.12968 1.2 1.2 1.2 1.2 1.2

```
H(7A) 1.0203 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2


H(7B) 1.0203 0
0 0 0.1508
0.0758 0 0 0 0
0.0308 0 0 0 0 0 0
0.0119 0 0 0 0 0 0 0 0
1.113134 1.2 1.2 1.2 1.2 1.2


H(8A) 1.0148 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(8B) 1.0148 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(8C) 1.0148 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(9A) 1.0148 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(9B) 1.0148 0
0 0 0.1518
0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2


H(9C) 1.0148 0
0 0 0.1518
```

0.0722 0 0 0 0
0.0313 0 0 0 0 0 0
0.017 0 0 0 0 0 0 0 0
1.112822 1.2 1.2 1.2 1.2 1.2

H(11) 0.9611 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(12) 0.9611 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(14) 0.9611 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(15) 0.9611 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2

H(16A) 0.9839 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2

H(16B) 0.9839 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2

H(16C) 0.9839 0
0 0 0.1455
0.0684 0 0 0 0
0.0292 0 0 0 0 0 0

```
0.0155 0 0 0 0 0 0 0 0
1.123015 1.2 1.2 1.2 1.2 1.2
```