Supplementary Information

Unraveling Nature of Hydrogen Bonds of "Proton Sponges" based on Car-Parrinello and metadynamics approaches

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11. XYZ coordinates.

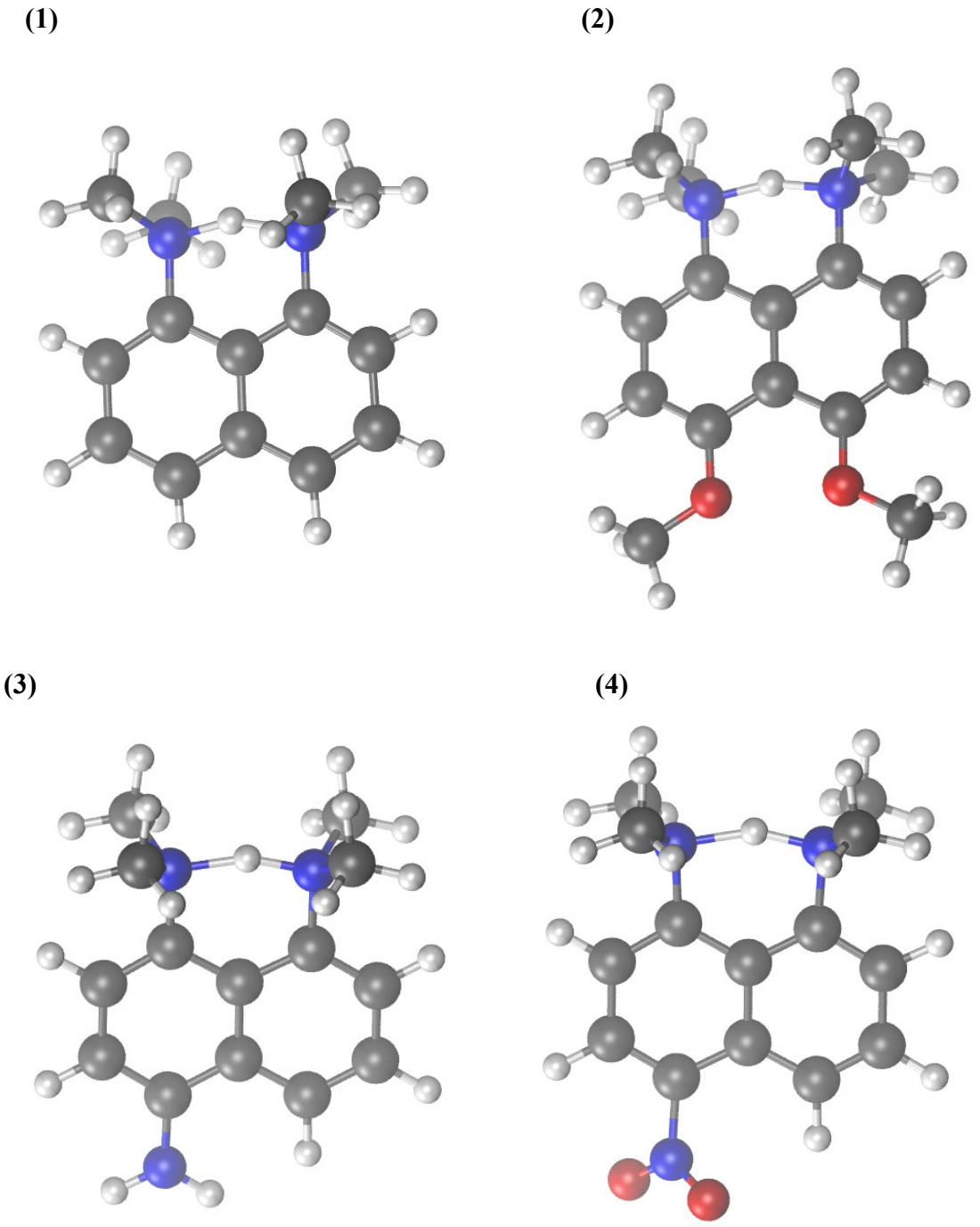

Figure S1. Molecular structures of the studied protonated form of 1,8-bis(dimethylamino)naphthalene ($DMANH^+$) and its derivatives obtained as a result of CPMD geometry optimization with PBE functional. Color coding: red - oxygen; blue - nitrogen; gray - carbon; white - hydrogen. The solid line between nitrogen atoms indicates the presence of intramolecular hydrogen bonding (HB).

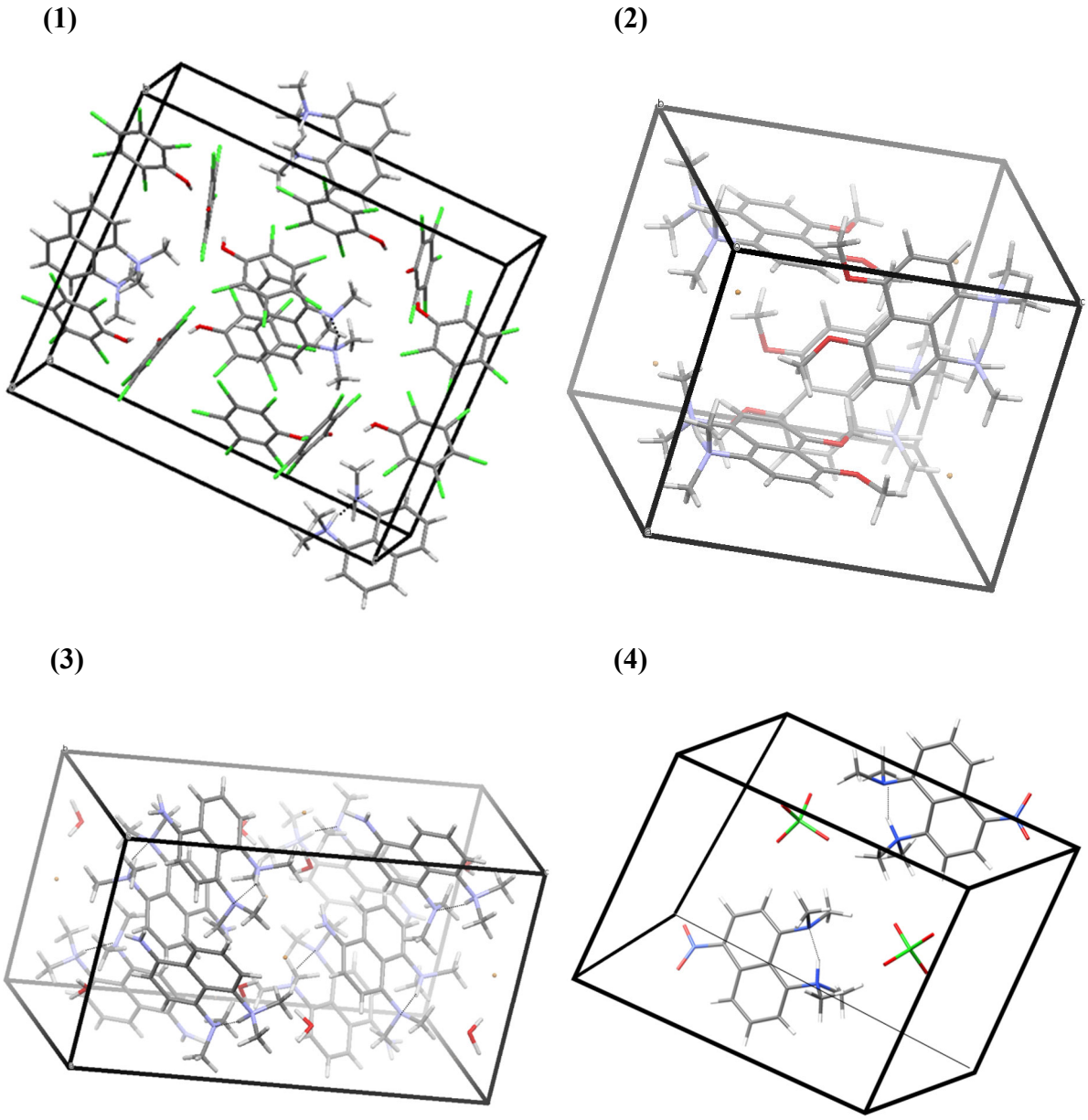

Figure S2. Crystal unit cells of the studied compounds (suitable references are included in the manuscript). The dotted lines indicate the presence of intramolecular hydrogen bridges. The data were used to construct CPMD models for crystalline phase simulations. Color coding: red - oxygen; blue - nitrogen; gray - carbon; white – hydrogen, green – chlorine, orange – bromine.

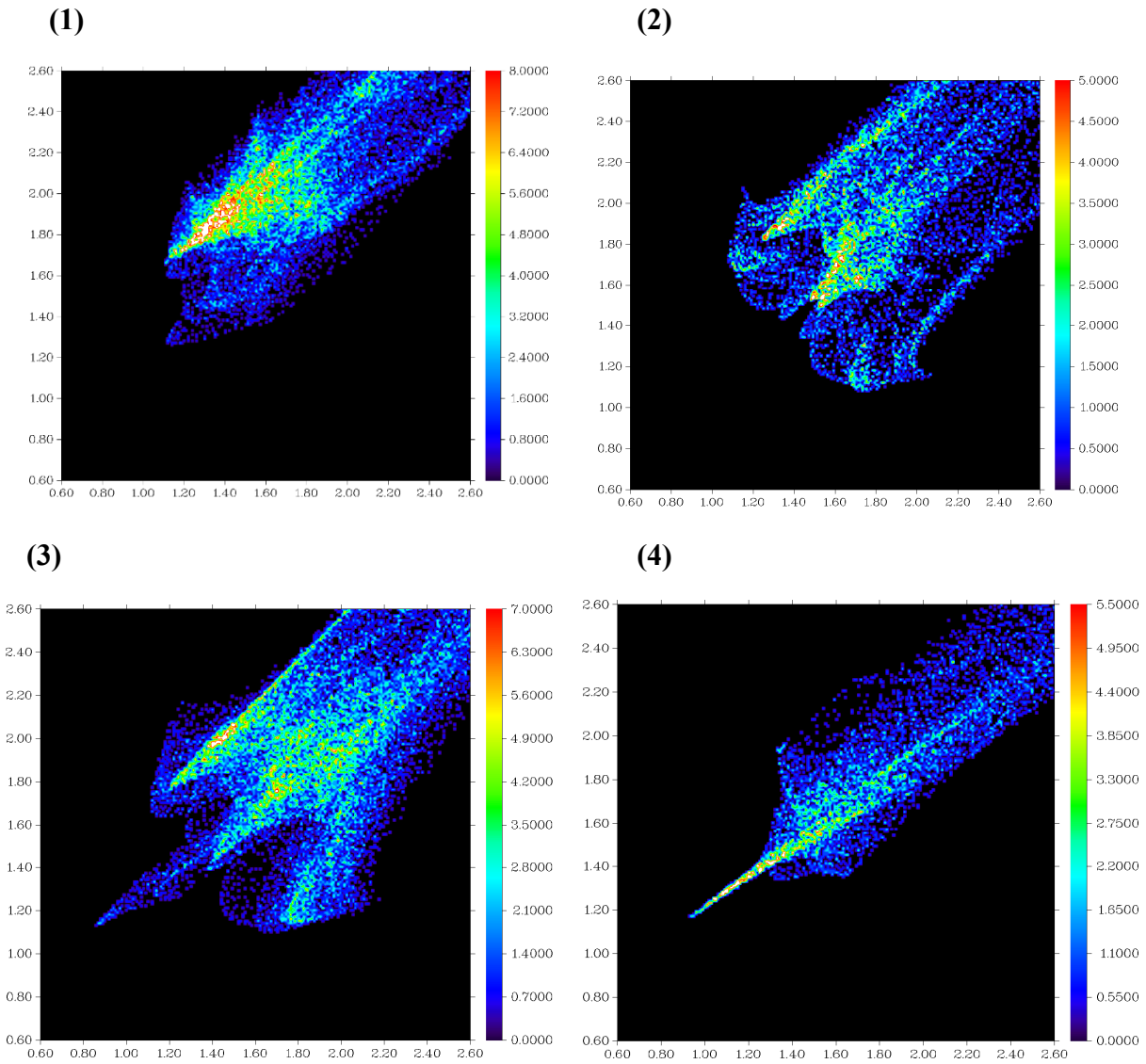

Figure S3. Complete 2-D fingerprint plot based on Hirshfeld surface of the studied compounds (1)-(4) calculated from their experimental crystal structures. The X and Y axes correspond respectively to d_i and d_e, where d_i (d_e) is the distance from a point on the surface to the nearest nucleus inside (outside) the surface. The color scale shows the values of the d_{norm} Hirshfeld normalized contact distance.

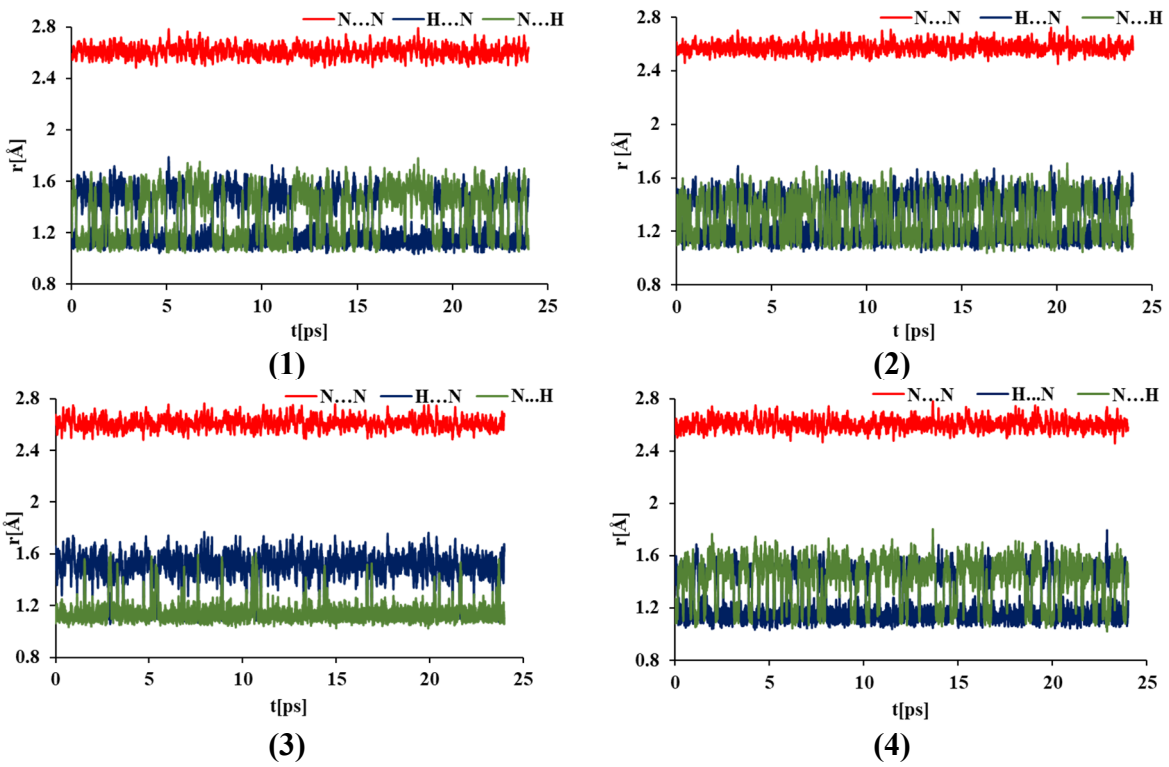

Figure S4. Time-evolution of metric parameters of atoms involved in the intramolecular hydrogen bond N-H···N. The CPMD results in the gas phase at 100 K for $DMANH^+$ and its derivatives. The calculations were carried out using the OLYP functional.

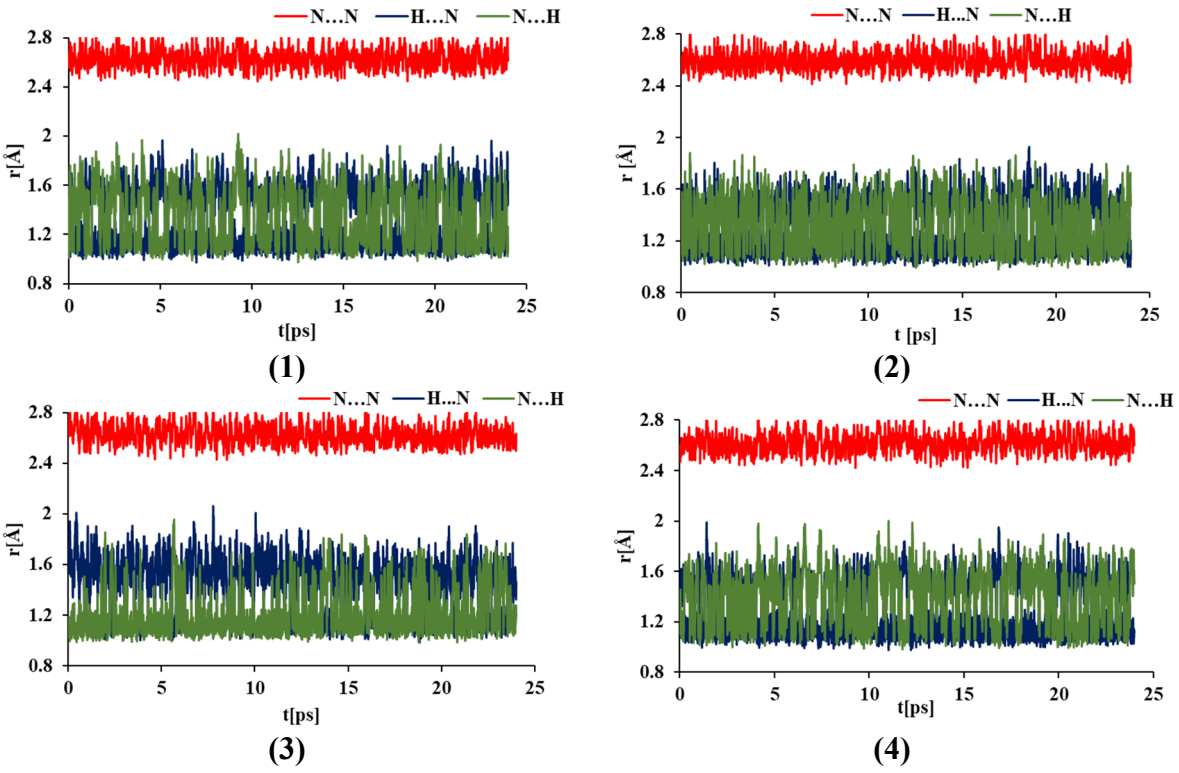

Figure S5. Time-evolution of metric parameters of atoms involved in the intramolecular hydrogen bond N-H···N. The CPMD results in the gas phase at 300 K for $DMANH^+$ and its derivatives. The calculations were carried out using the OLYP functional.

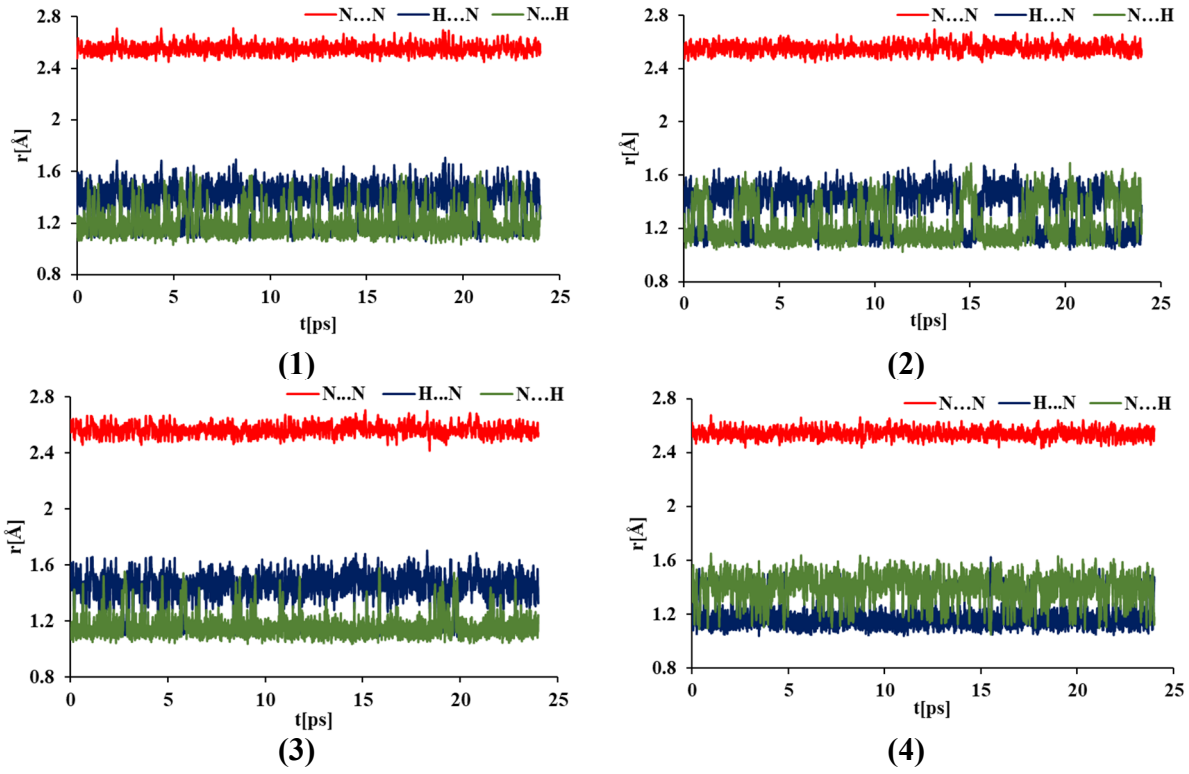

Figure S6. Time-evolution of metric parameters of atoms involved in the intramolecular hydrogen bond N-H···N. The CPMD results in the crystalline phase at 100 K for $DMANH^{+}$ and its derivatives. The calculations were carried out using the OLYP functional.

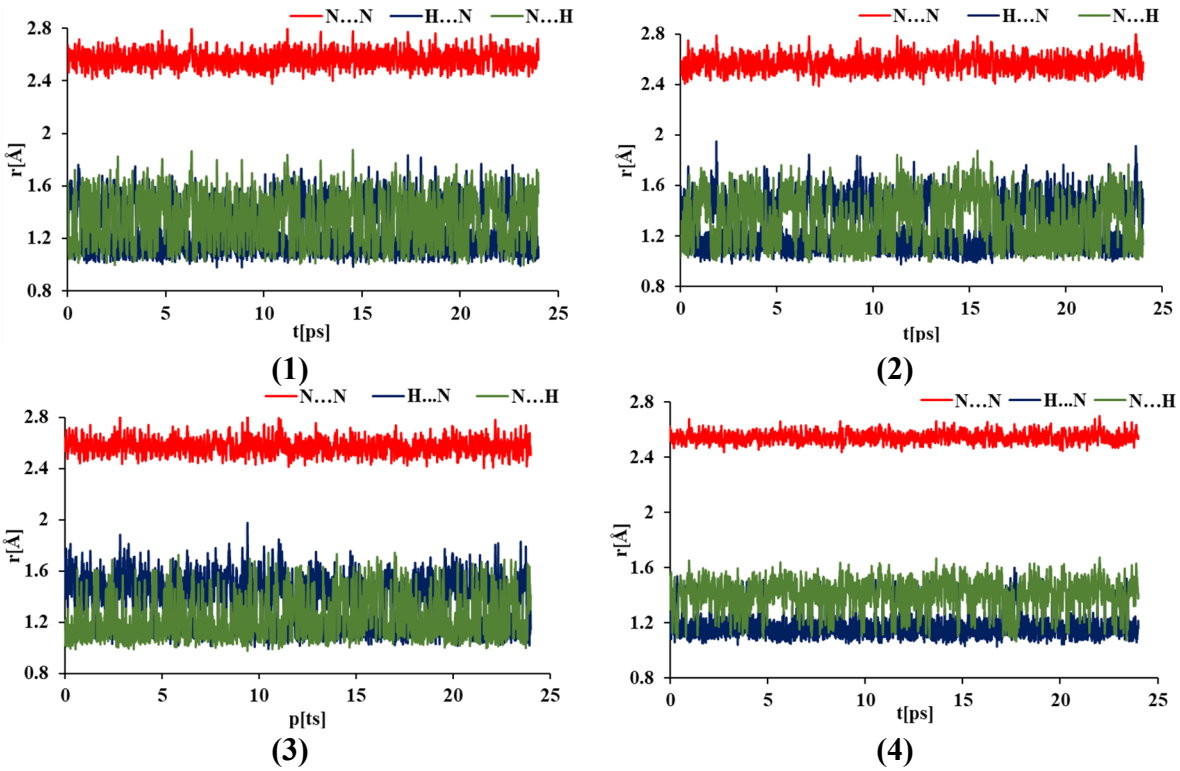

Figure S7. Time-evolution of metric parameters of atoms involved in the intramolecular hydrogen bond N-H···N. The CPMD results in the crystalline phase at 300 K for $DMANH^{+}$ and its derivatives. The calculations were carried out using the OLYP functional.

Table S1. The proton possession percentage during the CPMD simulation of the $DMANH^+$ and its derivatives. The reference nitrogen atoms are those at the position 1 of the aromatic system, i.e. the left-side amine functions in Figure 1 in the manuscript. The calculations were carried out using the OLYP functional. The main manuscript body contains corresponding data for the PBE functional.

Compound	Proton possession (%)			
	Gas phase		Crystalline phase	
	100 K	300 K	100 K	300 K
(1)	44.0	48.4	76.9	59.5
(2)	48.6	47.9	33.4	54.7
(3)	93.7	75.0	91.6	66.0
(4)	26.4	38.2	14.6	15.1

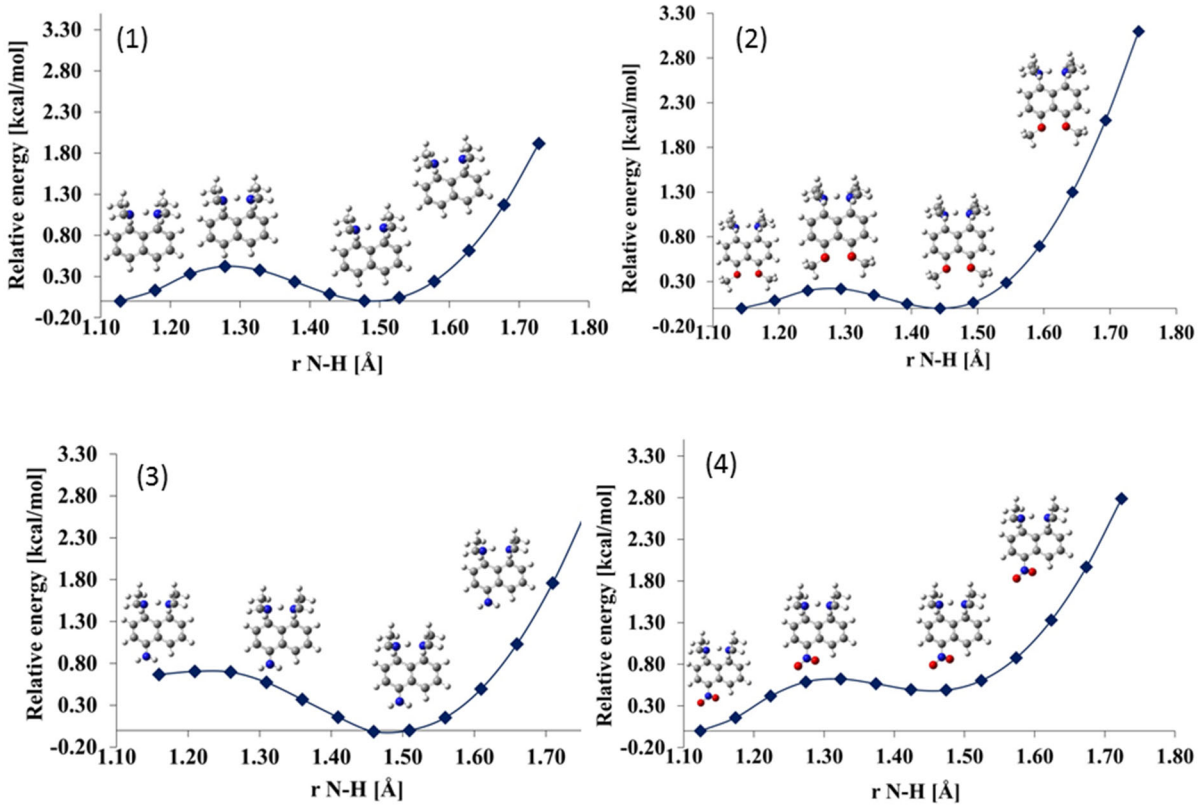

Figure S8. Potential energy profile obtained as a result of a scan with optimization method for the investigated "proton sponges". The simulations were performed at the PBE0-D3/def2-TZVP level of theory.

Table S2. QTAIM parameters for BCPs of N···H and H···N interactions (presented one above the other in single table cell) within studied compounds in the gas phase. All QTAIM data are given in a.u.

Compound	Snapshot time [ps]	100 K						300 K					
		ρ	$\nabla^2\rho$	ε	H	V	G	ρ	$\nabla^2\rho$	ε	H	V	G
(1)	**0**	0.228 0.103	-0.779 0.023	0.005 0.019	-0.253 -0.049	-0.312 -0.105	0.059 0.055	0.121 0.202	-0.026 -0.511	0.016 0.004	-0.067 -0.187	-0.127 -0.247	0.060 0.060
	8	0.229 0.090	-0.798 0.033	0.006 0.019	-0.253 -0.039	-0.307 -0.087	0.053 0.048	0.308 0.080	-1.670 0.099	0.004 0.025	-0.478 -0.029	-0.539 -0.082	0.061 0.054
	16	0.140 0.199	-0.079 -0.479	0.013 0.005	-0.087 -0.187	-0.155 -0.254	0.067 0.067	0.080 0.266	0.062 -1.173	0.021 0.006	-0.031 -0.349	-0.077 -0.405	0.046 0.056
	24	0.208 0.132	-0.564 -0.053	0.009 0.010	-0.208 -0.078	-0.276 -0.143	0.067 0.065	0.091 0.237	0.041 -0.867	0.017 0.007	-0.039 -0.272	-0.089 -0.328	0.050 0.056
(2)	**0**	0.104 0.225	0.018 -0.752	0.019 0.008	-0.050 -0.247	-0.104 -0.306	0.054 0.059	0.104 0.225	0.018 -0.752	0.019 0.008	-0.050 -0.247	-0.104 -0.305	0.054 0.058
	8	0.231 0.111	-0.795 0.014	0.005 0.021	-0.261 -0.056	-0.324 -0.116	0.063 0.060	0.111 0.210	-0.003 -0.610	0.027 0.006	-0.057 -0.210	-0.113 -0.268	0.056 0.058
	16	0.211 0.125	-0.591 -0.028	0.006 0.015	-0.213 -0.070	-0.278 -0.133	0.065 0.063	0.210 0.133	-0.581 -0.048	0.004 0.015	-0.214 -0.079	-0.283 -0.146	0.069 0.067
	24	0.139 0.171	-0.122 -0.298	0.014 0.012	-0.088 -0.135	-0.146 -0.196	0.058 0.061	0.206 0.150	-0.516 -0.103	0.011 0.016	-0.202 -0.101	-0.276 -0.175	0.073 0.075
(3)	**0**	0.163 0.171	-0.211 -0.267	0.008 0.011	-0.122 -0.135	-0.191 -0.203	0.069 0.068	0.116 0.226	0.003 -0.745	0.015 0.010	-0.061 -0.250	-0.123 -0.314	0.062 0.064
	8	0.159 0.159	-0.203 -0.210	0.010 0.011	-0.114 -0.114	-0.178 -0.177	0.063 0.062	0.163 0.129	-0.273 -0.105	0.013 0.020	-0.124 -0.077	-0.180 -0.129	0.056 0.051
	16	0.090 0.241	0.044 -0.922	0.019 0.005	-0.039 -0.286	-0.089 -0.342	0.050 0.056	0.153 0.168	-0.169 -0.259	0.010 0.015	-0.106 -0.129	-0.170 -0.193	0.064 0.064
	24	0.107 0.217	0.011 -0.675	0.022 0.004	-0.053 -0.227	-0.109 -0.285	0.056 0.058	0.058 0.287	0.078 -1.400	0.030 0.003	-0.016 -0.400	-0.051 -0.450	0.035 0.050
(4)	**0**	0.103 0.229	0.022 -0.781	0.019 0.006	-0.050 -0.254	-0.105 -0.313	0.055 0.059	0.216 0.130	-0.612 -0.033	0.004 0.018	-0.222 -0.075	-0.291 -0.141	0.069 0.066
	8	0.097 0.238	0.034 -0.886	0.025 0.006	-0.044 -0.280	-0.097 -0.338	0.052 0.058	0.108 0.242	0.030 -0.911	0.017 0.008	-0.054 -0.291	-0.114 -0.355	0.060 0.064
	16	0.112 0.213	-0.007 -0.635	0.011 0.009	-0.058 -0.219	-0.115 -0.279	0.057 0.060	0.252 0.087	-1.024 0.055	0.001 0.028	-0.312 -0.036	-0.368 -0.085	0.056 0.050
	24	0.227 0.092	-0.788 0.031	0.004 0.016	-0.251 -0.041	-0.305 -0.090	0.054 0.049	0.064 0.305	0.092 -1.627	0.020 0.004	-0.019 -0.461	-0.060 -0.515	0.042 0.054

XYZ coordinates

The models for CPMD and DFT simulations were prepared based on X-ray data. The xyz experimental coordinates are provided below for the studied compounds. Suitable references for the crystal structures are cited in the manuscript.

Compound (1) CCDC identifiers: TAPCES (1266338)

XYZ for single molecule:

35

TAPCES

N	0.384524	0.462592	6.779898
H	-0.386342	-0.336855	6.849551
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C	1.210160	1.920241	8.599202
C	1.355606	2.201732	9.968706
C	0.836317	1.356426	10.900391
C	-0.414749	-0.680214	11.492341
C	-1.111301	-1.791336	11.128642
C	-1.380604	-2.035973	9.768073
C	-0.922676	-1.182162	8.802881
C	-0.121584	-0.056365	9.133479
C	0.103403	0.208283	10.522884
C	-0.052270	1.566210	5.903651
C	1.627182	-0.175432	6.276284
C	-0.993126	-2.696509	6.859908
C	-2.725984	-0.991388	7.191115
H	1.636272	2.474718	7.988774
H	1.818080	2.931641	10.253004
H	0.943129	1.582552	11.824766
H	-0.227260	-0.453587	12.425853
H	-1.443101	-2.396341	11.806490
H	-1.874895	-2.841590	9.491492
H	-0.874951	1.941086	6.213942
H	-0.181808	1.200672	5.015829
H	0.636328	2.227914	5.864662
H	2.340778	0.473598	6.220034
H	1.931710	-0.928853	6.884073
H	1.443101	-0.565316	5.387447
H	-1.590820	-3.381893	7.261783

H	-1.272656	-2.689839	5.933705
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H	-2.897565	-0.001668	7.479068
H	-3.408900	-1.614237	7.631371
H	-2.931654	-1.023906	6.244402

XYZ for crystal:

292

TAPCES

N	11.747524	17.138592	6.779898
H	10.976658	16.339145	6.849551
N	10.059096	15.321575	7.393169
C	11.860699	17.503797	8.204231
C	12.573160	18.596241	8.599202
C	12.718606	18.877732	9.968706
C	12.199317	18.032426	10.900391
C	10.948251	15.995786	11.492341
C	10.251699	14.884664	11.128642
C	9.982396	14.640027	9.768073
C	10.440324	15.493838	8.802881
C	11.241416	16.619635	9.133479
C	11.466403	16.884283	10.522884
C	11.310730	18.242210	5.903651
C	12.990182	16.500568	6.276284
C	10.369874	13.979491	6.859908
C	8.637016	15.684612	7.191115
H	12.999272	19.150718	7.988774
H	13.181080	19.607641	10.253004
H	12.306129	18.258552	11.824766
H	11.135740	16.222413	12.425853
H	9.919899	14.279659	11.806490
H	9.488105	13.834410	9.491492
H	10.488049	18.617086	6.213942
H	11.181192	17.876672	5.015829
H	11.999328	18.903914	5.864662
H	13.703778	17.149598	6.220034
H	13.294710	15.747147	6.884073
H	12.806101	16.110684	5.387447
H	9.772180	13.294107	7.261783
H	10.090344	13.986161	5.933705

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H	**4.408844**	**11.027839**	**14.373295**
H	**5.704226**	**11.179590**	**13.276717**
H	**2.783935**	**8.339668**	**12.827932**
H	**2.272600**	**9.952237**	**12.675629**
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N	**1.303904**	**6.983575**	**2.760331**
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C	**-0.836317**	**9.694426**	**-0.746891**
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C	**1.111301**	**6.546664**	**-0.975142**
C	**1.380605**	**6.302027**	**0.385427**
C	**0.922676**	**7.155838**	**1.350619**
C	**0.121584**	**8.281635**	**1.020021**
C	**-0.103403**	**8.546283**	**-0.369384**
C	**0.052270**	**9.904210**	**4.249849**
C	**-1.627182**	**8.162568**	**3.877216**
C	**0.993126**	**5.641491**	**3.293592**
C	**2.725984**	**7.346612**	**2.962385**
H	**-1.636272**	**10.812718**	**2.164726**
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H	**0.227260**	**7.884413**	**-2.272353**
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H	**1.874895**	**5.496410**	**0.662008**
H	**0.874951**	**10.279086**	**3.939558**
H	**0.181808**	**9.538672**	**5.137671**
H	**-0.636328**	**10.565914**	**4.288838**
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H	**-1.931710**	**7.409147**	**3.269427**
H	**-1.443101**	**7.772684**	**4.766053**
H	**1.590820**	**4.956107**	**2.891717**
H	**1.272656**	**5.648161**	**4.219795**
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N	**6.985404**	**1.354425**	**17.546669**
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C	**5.733770**	**-1.566210**	**16.057151**
C	**4.054318**	**0.175432**	**16.429784**
C	**6.674626**	**2.696509**	**17.013408**
C	**8.407484**	**0.991388**	**17.344615**
H	**4.045228**	**-2.474718**	**18.142274**
H	**3.863420**	**-2.931641**	**20.406504**
H	**4.738371**	**-1.582552**	**21.978266**
H	**5.908760**	**0.453587**	**22.579353**
H	**7.124601**	**2.396341**	**21.959990**
H	**7.556395**	**2.841590**	**19.644992**
H	**6.556451**	**-1.941086**	**16.367442**
H	**5.863308**	**-1.200672**	**15.169329**
H	**5.045172**	**-2.227914**	**16.018162**
H	**3.340722**	**-0.473598**	**16.373534**
H	**3.749790**	**0.928853**	**17.037573**
H	**4.238399**	**0.565316**	**15.540947**
H	**7.272320**	**3.381893**	**17.415283**
H	**6.954156**	**2.689839**	**16.087205**
H	**5.658774**	**2.841590**	**17.183783**
H	**8.579065**	**0.001668**	**17.632568**
H	**9.090400**	**1.614237**	**17.784871**
H	**8.613154**	**1.023906**	**16.397902**
O	**9.100172**	**3.940205**	**4.941708**
C	**7.816608**	**3.867331**	**5.105586**
C	**7.032561**	**4.951771**	**5.561478**
C	**5.655365**	**4.899075**	**5.684132**
C	**4.973926**	**3.721249**	**5.393742**
C	**5.705362**	**2.604458**	**5.005472**
C	**7.079149**	**2.686504**	**4.845047**
Cl	**7.878763**	**6.409421**	**5.969649**
Cl	**4.761665**	**6.297858**	**6.165408**
Cl	**3.248795**	**3.652044**	**5.514772**
Cl	**4.894612**	**1.097614**	**4.770520**

Cl	**7.986144**	**1.308566**	**4.317471**
O	**3.418672**	**4.397795**	**15.365292**
C	**2.135108**	**4.470669**	**15.201414**
C	**1.351061**	**3.386229**	**14.745522**
C	**-0.026135**	**3.438925**	**14.622868**
C	**-0.707574**	**4.616751**	**14.913258**
C	**0.023862**	**5.733542**	**15.301528**
C	**1.397649**	**5.651496**	**15.461953**
Cl	**2.197263**	**1.928579**	**14.337351**
Cl	**-0.919835**	**2.040142**	**14.141592**
Cl	**-2.432705**	**4.685956**	**14.792228**
Cl	**-0.786888**	**7.240386**	**15.536480**
Cl	**2.304644**	**7.029434**	**15.989529**
O	**2.262828**	**12.278205**	**5.211792**
C	**3.546392**	**12.205331**	**5.047914**
C	**4.330439**	**13.289771**	**4.592022**
C	**5.707635**	**13.237075**	**4.469368**
C	**6.389074**	**12.059249**	**4.759758**
C	**5.657638**	**10.942458**	**5.148028**
C	**4.283851**	**11.024504**	**5.308453**
Cl	**3.484237**	**14.747421**	**4.183851**
Cl	**6.601335**	**14.635858**	**3.988092**
Cl	**8.114205**	**11.990044**	**4.638728**
Cl	**6.468388**	**9.435614**	**5.382980**
Cl	**3.376856**	**9.646566**	**5.836029**
O	**7.944328**	**12.735795**	**15.095208**
C	**9.227892**	**12.808669**	**15.259086**
C	**10.011939**	**11.724229**	**15.714978**
C	**11.389135**	**11.776925**	**15.837632**
C	**12.070574**	**12.954751**	**15.547242**
C	**11.339138**	**14.071542**	**15.158972**
C	**9.965351**	**13.989496**	**14.998547**
Cl	**9.165737**	**10.266579**	**16.123149**
Cl	**12.282835**	**10.378142**	**16.318908**
Cl	**13.795705**	**13.023956**	**15.668272**
Cl	**12.149888**	**15.578386**	**14.924020**
Cl	**9.058356**	**15.367434**	**14.470971**
O	**10.845529**	**2.822413**	**3.274504**
H	**10.181248**	**3.176778**	**3.529357**
C	**11.016429**	**2.765214**	**1.948863**

C	**10.302832**	**3.529475**	**1.023473**
C	**10.580089**	**3.437257**	**-0.343594**
C	**11.534581**	**2.546258**	**-0.803954**
C	**12.252723**	**1.782831**	**0.107424**
C	**12.019781**	**1.914572**	**1.466572**
Cl	**9.094150**	**4.601075**	**1.616640**
Cl	**9.729228**	**4.458495**	**-1.451747**
Cl	**11.841155**	**2.399343**	**-2.498979**
Cl	**13.423907**	**0.642360**	**-0.446145**
Cl	**12.970524**	**1.040249**	**2.607825**
O	**5.164029**	**5.515587**	**17.032496**
H	**4.499748**	**5.161222**	**16.777643**
C	**5.334929**	**5.572786**	**18.358137**
C	**4.621332**	**4.808525**	**19.283527**
C	**4.898589**	**4.900743**	**20.650594**
C	**5.853081**	**5.791742**	**21.110954**
C	**6.571223**	**6.555169**	**20.199576**
C	**6.338281**	**6.423428**	**18.840428**
Cl	**3.412650**	**3.736925**	**18.690360**
Cl	**4.047728**	**3.879505**	**21.758747**
Cl	**6.159655**	**5.938657**	**22.805979**
Cl	**7.742407**	**7.695640**	**20.753145**
Cl	**7.289024**	**7.297751**	**17.699175**
O	**0.517471**	**11.160413**	**6.878996**
H	**1.181752**	**11.514778**	**6.624143**
C	**0.346572**	**11.103214**	**8.204637**
C	**1.060168**	**11.867475**	**9.130027**
C	**0.782911**	**11.775257**	**10.497094**
C	**-0.171581**	**10.884258**	**10.957454**
C	**-0.889723**	**10.120831**	**10.046076**
C	**-0.656781**	**10.252572**	**8.686928**
Cl	**2.268850**	**12.939075**	**8.536860**
Cl	**1.633772**	**12.796495**	**11.605247**
Cl	**-0.478155**	**10.737343**	**12.652479**
Cl	**-2.060907**	**8.980360**	**10.599645**
Cl	**-1.607524**	**9.378249**	**7.545675**
O	**6.198971**	**13.853587**	**13.428004**
H	**6.863252**	**13.499222**	**13.682857**
C	**6.028072**	**13.910786**	**12.102363**
C	**6.741668**	**13.146525**	**11.176973**

C	**6.464411**	**13.238743**	**9.809906**
C	**5.509919**	**14.129742**	**9.349546**
C	**4.791777**	**14.893169**	**10.260924**
C	**5.024719**	**14.761428**	**11.620072**
Cl	**7.950350**	**12.074925**	**11.770140**
Cl	**7.315272**	**12.217505**	**8.701753**
Cl	**5.203345**	**14.276657**	**7.654521**
Cl	**3.620593**	**16.033640**	**9.707355**
Cl	**4.073976**	**15.635751**	**12.761325**
C	**11.010747**	**5.356498**	**7.638478**
O	**10.893367**	**5.101689**	**6.339033**
H	**10.203974**	**4.754328**	**6.083977**
C	**11.932286**	**6.346719**	**8.021671**
C	**12.170909**	**6.649722**	**9.353404**
C	**11.492538**	**5.968007**	**10.357585**
C	**10.574408**	**4.983956**	**10.009930**
C	**10.317604**	**4.697129**	**8.671089**
Cl	**12.755990**	**7.197028**	**6.766902**
Cl	**13.319709**	**7.871072**	**9.756295**
Cl	**11.753660**	**6.363728**	**12.016464**
Cl	**9.780248**	**4.080617**	**11.243986**
Cl	**9.134375**	**3.518136**	**8.242408**
C	**5.329247**	**2.981502**	**12.668522**
O	**5.211867**	**3.236311**	**13.967967**
H	**4.522474**	**3.583672**	**14.223023**
C	**6.250786**	**1.991281**	**12.285329**
C	**6.489409**	**1.688278**	**10.953596**
C	**5.811038**	**2.369993**	**9.949415**
C	**4.892908**	**3.354044**	**10.297070**
C	**4.636104**	**3.640871**	**11.635911**
Cl	**7.074490**	**1.140972**	**13.540098**
Cl	**7.638209**	**0.466928**	**10.550705**
Cl	**6.072160**	**1.974272**	**8.290536**
Cl	**4.098748**	**4.257383**	**9.063014**
Cl	**3.452875**	**4.819864**	**12.064592**
C	**0.352253**	**13.694498**	**2.515022**
O	**0.469633**	**13.439689**	**3.814467**
H	**1.159026**	**13.092328**	**4.069523**
C	**-0.569286**	**14.684719**	**2.131829**
C	**-0.807909**	**14.987722**	**0.800096**

C	-0.129538	14.306007	-0.204085
C	0.788592	13.321956	0.143570
C	1.045396	13.035129	1.482411
Cl	-1.392990	15.535028	3.386598
Cl	-1.956709	16.209072	0.397205
Cl	-0.390660	14.701728	-1.862964
Cl	1.582752	12.418617	-1.090486
Cl	2.228625	11.856136	1.911092
C	6.033753	11.319502	17.791978
O	6.151133	11.574311	16.492533
H	6.840526	11.921672	16.237477
C	5.112214	10.329281	18.175171
C	4.873591	10.026278	19.506904
C	5.551962	10.707993	20.511085
C	6.470092	11.692044	20.163430
C	6.726896	11.978871	18.824589
Cl	4.288510	9.478972	16.920402
Cl	3.724791	8.804928	19.909795
Cl	5.290840	10.312272	22.169964
Cl	7.264252	12.595383	21.397486
Cl	7.910125	13.157864	18.395908

Compound (2) CCDC identifiers: RISBEA (122006)

XYZ for single molecule:

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odorf4

C	4.108741	2.852500	9.664674
C	5.266856	2.852500	8.987372
C	5.281689	2.852500	7.578952
C	4.104177	2.852500	6.888525
C	2.852500	2.852500	7.560576
C	2.852500	2.852500	9.009686
N	4.128138	2.852500	11.136098
O	4.050550	2.852500	5.531296
C	4.744278	1.631630	11.690016
C	5.280548	2.852500	4.810679
H	2.852500	2.852500	11.248982
H	6.138580	2.852500	9.490098
H	6.195630	2.852500	7.061788
H	4.643870	1.540350	12.600960

H	4.153240	0.855750	11.445872
H	5.796280	1.506120	11.590258
H	5.921790	1.939700	5.119140
H	5.100270	2.852500	3.977178
C	1.596259	2.852500	9.664674
C	0.438144	2.852500	8.987372
C	0.423311	2.852500	7.578952
C	1.600823	2.852500	6.888525
N	1.576862	2.852500	11.136098
O	1.654450	2.852500	5.531296
C	0.960722	4.073370	11.690016
C	0.424452	2.852500	4.810679
H	-0.433580	2.852500	9.490098
H	-0.490630	2.852500	7.061788
H	1.061130	4.164650	12.600960
H	1.551760	4.849250	11.445872
H	-0.091280	4.198880	11.590258
H	-0.216790	3.765300	5.119140
H	0.604730	2.852500	3.977178
C	4.744278	4.073370	11.690016
H	4.643870	4.164650	12.600960
H	4.153240	4.849250	11.445872
H	5.796280	4.198880	11.590258
H	5.921790	3.765300	5.119140
C	0.960722	1.631630	11.690016
H	1.061130	1.540350	12.600960
H	1.551760	0.855750	11.445872
H	-0.091280	1.506120	11.590258
H	-0.216790	1.939700	5.119140

XYZ for crystal:

132

odorf4

Br	2.852500	2.852500	1.702442
Br	8.557500	2.852500	11.423558
Br	2.852500	8.557500	11.423558
C	4.108741	2.852500	9.664674
C	5.266856	2.852500	8.987372
C	5.281689	2.852500	7.578952
C	4.104177	2.852500	6.888525

C	**2.852500**	**2.852500**	**7.560576**
C	**2.852500**	**2.852500**	**9.009686**
N	**4.128138**	**2.852500**	**11.136098**
O	**4.050550**	**2.852500**	**5.531296**
C	**4.744278**	**1.631630**	**11.690016**
C	**5.280548**	**2.852500**	**4.810679**
H	**2.852500**	**2.852500**	**11.248982**
H	**6.138580**	**2.852500**	**9.490098**
H	**6.195630**	**2.852500**	**7.061788**
H	**4.643870**	**1.540350**	**12.600960**
H	**4.153240**	**0.855750**	**11.445872**
H	**5.796280**	**1.506120**	**11.590258**
H	**5.921790**	**1.939700**	**5.119140**
H	**5.100270**	**2.852500**	**3.977178**
C	**1.596259**	**2.852500**	**9.664674**
C	**0.438144**	**2.852500**	**8.987372**
C	**0.423311**	**2.852500**	**7.578952**
C	**1.600823**	**2.852500**	**6.888525**
N	**1.576862**	**2.852500**	**11.136098**
O	**1.654450**	**2.852500**	**5.531296**
C	**0.960722**	**4.073370**	**11.690016**
C	**0.424452**	**2.852500**	**4.810679**
H	**-0.433580**	**2.852500**	**9.490098**
H	**-0.490630**	**2.852500**	**7.061788**
H	**1.061130**	**4.164650**	**12.600960**
H	**1.551760**	**4.849250**	**11.445872**
H	**-0.091280**	**4.198880**	**11.590258**
H	**-0.216790**	**3.765300**	**5.119140**
H	**0.604730**	**2.852500**	**3.977178**
C	**4.744278**	**4.073370**	**11.690016**
H	**4.643870**	**4.164650**	**12.600960**
H	**4.153240**	**4.849250**	**11.445872**
H	**5.796280**	**4.198880**	**11.590258**
H	**5.921790**	**3.765300**	**5.119140**
C	**0.960722**	**1.631630**	**11.690016**
H	**1.061130**	**1.540350**	**12.600960**
H	**1.551760**	**0.855750**	**11.445872**
H	**-0.091280**	**1.506120**	**11.590258**
H	**-0.216790**	**1.939700**	**5.119140**
C	**8.557500**	**4.108741**	**3.461326**

C	**8.557500**	**5.266856**	**4.138628**
C	**8.557500**	**5.281689**	**5.547048**
C	**8.557500**	**4.104177**	**6.237475**
C	**8.557500**	**2.852500**	**5.565424**
C	**8.557500**	**2.852500**	**4.116314**
N	**8.557500**	**4.128138**	**1.989902**
O	**8.557500**	**4.050550**	**7.594704**
C	**9.778370**	**4.744278**	**1.435984**
C	**8.557500**	**5.280548**	**8.315321**
H	**8.557500**	**2.852500**	**1.877018**
H	**8.557500**	**6.138580**	**3.635902**
H	**8.557500**	**6.195630**	**6.064212**
H	**9.869650**	**4.643870**	**0.525040**
H	**10.554250**	**4.153240**	**1.680128**
H	**9.903880**	**5.796280**	**1.535742**
H	**9.470300**	**5.921790**	**8.006860**
H	**8.557500**	**5.100270**	**9.148822**
C	**8.557500**	**1.596259**	**3.461326**
C	**8.557500**	**0.438144**	**4.138628**
C	**8.557500**	**0.423311**	**5.547048**
C	**8.557500**	**1.600823**	**6.237475**
N	**8.557500**	**1.576862**	**1.989902**
O	**8.557500**	**1.654450**	**7.594704**
C	**7.336630**	**0.960722**	**1.435984**
C	**8.557500**	**0.424452**	**8.315321**
H	**8.557500**	**-0.433580**	**3.635902**
H	**8.557500**	**-0.490630**	**6.064212**
H	**7.245350**	**1.061130**	**0.525040**
H	**6.560750**	**1.551760**	**1.680128**
H	**7.211120**	**-0.091280**	**1.535742**
H	**7.644700**	**-0.216790**	**8.006860**
H	**8.557500**	**0.604730**	**9.148822**
C	**7.336630**	**4.744278**	**1.435984**
H	**7.245350**	**4.643870**	**0.525040**
H	**6.560750**	**4.153240**	**1.680128**
H	**7.211120**	**5.796280**	**1.535742**
H	**7.644700**	**5.921790**	**8.006860**
C	**9.778370**	**0.960722**	**1.435984**
H	**9.869650**	**1.061130**	**0.525040**
H	**10.554250**	**1.551760**	**1.680128**

H	**9.903880**	**-0.091280**	**1.535742**
H	**9.470300**	**-0.216790**	**8.006860**
C	**2.852500**	**7.301259**	**3.461326**
C	**2.852500**	**6.143144**	**4.138628**
C	**2.852500**	**6.128311**	**5.547048**
C	**2.852500**	**7.305823**	**6.237475**
C	**2.852500**	**8.557500**	**5.565424**
C	**2.852500**	**8.557500**	**4.116314**
N	**2.852500**	**7.281862**	**1.989902**
O	**2.852500**	**7.359450**	**7.594704**
C	**1.631630**	**6.665722**	**1.435984**
C	**2.852500**	**6.129452**	**8.315321**
H	**2.852500**	**8.557500**	**1.877018**
H	**2.852500**	**5.271420**	**3.635902**
H	**2.852500**	**5.214370**	**6.064212**
H	**1.540350**	**6.766130**	**0.525040**
H	**0.855750**	**7.256760**	**1.680128**
H	**1.506120**	**5.613720**	**1.535742**
H	**1.939700**	**5.488210**	**8.006860**
H	**2.852500**	**6.309730**	**9.148822**
C	**2.852500**	**9.813741**	**3.461326**
C	**2.852500**	**10.971856**	**4.138628**
C	**2.852500**	**10.986689**	**5.547048**
C	**2.852500**	**9.809177**	**6.237475**
N	**2.852500**	**9.833138**	**1.989902**
O	**2.852500**	**9.755550**	**7.594704**
C	**4.073370**	**10.449278**	**1.435984**
C	**2.852500**	**10.985548**	**8.315321**
H	**2.852500**	**11.843580**	**3.635902**
H	**2.852500**	**11.900630**	**6.064212**
H	**4.164650**	**10.348870**	**0.525040**
H	**4.849250**	**9.858240**	**1.680128**
H	**4.198880**	**11.501280**	**1.535742**
H	**3.765300**	**11.626790**	**8.006860**
H	**2.852500**	**10.805270**	**9.148822**
C	**4.073370**	**6.665722**	**1.435984**
H	**4.164650**	**6.766130**	**0.525040**
H	**4.849250**	**7.256760**	**1.680128**
H	**4.198880**	**5.613720**	**1.535742**
H	**3.765300**	**5.488210**	**8.006860**

C	1.631630	10.449278	1.435984
H	1.540350	10.348870	0.525040
H	0.855750	9.858240	1.680128
H	1.506120	11.501280	1.535742
H	1.939700	11.626790	8.006860

Compound (3) CCDC identifiers: XUCKAH (170012)

XYZ for single molecule:

37

brom

N	6.868125	-0.872809	7.632716
N	8.264594	0.976447	6.535100
N	4.820869	0.833660	2.052970
C	5.976222	-0.893167	6.484306
C	4.912783	-1.741490	6.438672
H	4.726012	-2.294843	7.162677
C	4.104064	-1.779785	5.304151
H	3.391371	-2.375988	5.273794
C	4.333426	-0.971038	4.246019
H	3.778545	-1.022145	3.501974
C	5.656047	0.848750	3.145427
C	6.693551	1.712448	3.216260
H	6.846176	2.299114	2.509913
C	7.536921	1.743341	4.316456
H	8.253205	2.337551	4.321416
C	7.346926	0.931319	5.383714
C	6.264553	0.005694	5.398198
C	5.408362	-0.043420	4.253956
C	6.190314	-0.439892	8.891244
H	6.835930	-0.384372	9.599178
H	5.512297	-1.077665	9.124973
H	5.787323	0.421386	8.757911
C	7.576674	-2.163730	7.790652
H	8.180658	-2.108352	8.535689
H	8.071697	-2.357482	6.990059
H	6.937363	-2.862860	7.948389
C	8.256635	2.295270	7.249780
H	8.837713	2.249288	8.011881
H	7.364048	2.496994	7.539660
H	8.563919	2.983866	6.654742

C	9.639365	0.538121	6.174982
H	10.172490	0.468364	6.970218
H	10.035044	1.178741	5.579349
H	9.598763	-0.317463	5.742047
H	7.561197	-0.024201	7.329344
H	4.872382	1.383739	1.523805
H	4.208140	0.000000	1.914677

XYZ for crystal:

342

brom

Br	4.110120	3.559427	19.659089
Br	4.174684	10.677427	10.102728
Br	5.140416	10.676573	0.182122
Br	5.075852	3.558573	9.738483
Br	0.000000	0.000000	0.000000
Br	-1.931464	0.000000	19.841211
Br	0.000000	14.236000	0.000000
Br	-1.931464	14.236000	19.841211
Br	11.182000	0.000000	0.000000
Br	9.250536	0.000000	19.841211
Br	11.182000	14.236000	0.000000
Br	9.250536	14.236000	19.841211
Br	-0.965732	7.118000	9.920606
Br	10.216268	7.118000	9.920606
Br	0.000000	7.118000	0.000000
Br	-1.931464	7.118000	19.841211
Br	11.182000	7.118000	0.000000
Br	9.250536	7.118000	19.841211
Br	-0.965732	0.000000	9.920606
Br	-0.965732	14.236000	9.920606
Br	10.216268	0.000000	9.920606
Br	10.216268	14.236000	9.920606
O	2.807740	12.935114	1.310115
H	3.370620	12.351154	0.765871
H	1.995325	13.135557	0.684522
O	7.408528	5.817114	8.610491
H	6.845648	5.233154	9.154735
H	8.220943	6.017557	9.236084
O	6.442796	1.300886	18.531096

H	**5.879917**	**1.884846**	**19.075341**
H	**7.255211**	**1.100443**	**19.156690**
O	**1.842009**	**8.418886**	**11.230721**
H	**2.404888**	**9.002846**	**10.686476**
H	**1.029593**	**8.218443**	**10.605128**
O	**8.593044**	**5.193578**	**1.381742**
H	**9.297527**	**5.613255**	**0.853172**
H	**8.190540**	**4.595381**	**0.680554**
O	**1.623224**	**12.311578**	**8.538864**
H	**0.918741**	**12.731255**	**9.067434**
H	**2.025729**	**11.713381**	**9.240052**
O	**0.657492**	**9.042422**	**18.459470**
H	**-0.046991**	**8.622745**	**18.988039**
H	**1.059997**	**9.640619**	**19.160658**
O	**7.627312**	**1.924422**	**11.302348**
H	**8.331795**	**1.504745**	**10.773778**
H	**7.224808**	**2.522619**	**10.601159**
N	**6.868125**	**-0.872809**	**7.632716**
N	**8.264594**	**0.976447**	**6.535100**
N	**4.820869**	**0.833660**	**2.052970**
C	**5.976222**	**-0.893167**	**6.484306**
C	**4.912783**	**-1.741490**	**6.438672**
H	**4.726012**	**-2.294843**	**7.162677**
C	**4.104064**	**-1.779785**	**5.304151**
H	**3.391371**	**-2.375988**	**5.273794**
C	**4.333426**	**-0.971038**	**4.246019**
H	**3.778545**	**-1.022145**	**3.501974**
C	**5.656047**	**0.848750**	**3.145427**
C	**6.693551**	**1.712448**	**3.216260**
H	**6.846176**	**2.299114**	**2.509913**
C	**7.536921**	**1.743341**	**4.316456**
H	**8.253205**	**2.337551**	**4.321416**
C	**7.346926**	**0.931319**	**5.383714**
C	**6.264553**	**0.005694**	**5.398198**
C	**5.408362**	**-0.043420**	**4.253956**
C	**6.190314**	**-0.439892**	**8.891244**
H	**6.835930**	**-0.384372**	**9.599178**
H	**5.512297**	**-1.077665**	**9.124973**
H	**5.787323**	**0.421386**	**8.757911**
C	**7.576674**	**-2.163730**	**7.790652**

H	**8.180658**	**-2.108352**	**8.535689**
H	**8.071697**	**-2.357482**	**6.990059**
H	**6.937363**	**-2.862860**	**7.948389**
C	**8.256635**	**2.295270**	**7.249780**
H	**8.837713**	**2.249288**	**8.011881**
H	**7.364048**	**2.496994**	**7.539660**
H	**8.563919**	**2.983866**	**6.654742**
C	**9.639365**	**0.538121**	**6.174982**
H	**10.172490**	**0.468364**	**6.970218**
H	**10.035044**	**1.178741**	**5.579349**
H	**9.598763**	**-0.317463**	**5.742047**
H	**7.561197**	**-0.024201**	**7.329344**
H	**4.872382**	**1.383739**	**1.523805**
H	**4.208140**	**0.000000**	**1.914677**
N	**3.348143**	**6.245191**	**2.287890**
N	**1.951674**	**8.094447**	**3.385506**
N	**5.395399**	**7.951660**	**7.867636**
C	**4.240046**	**6.224833**	**3.436299**
C	**5.303485**	**5.376510**	**3.481934**
H	**5.490257**	**4.823157**	**2.757928**
C	**6.112204**	**5.338215**	**4.616455**
H	**6.824897**	**4.742012**	**4.646812**
C	**5.882842**	**6.146962**	**5.674586**
H	**6.437723**	**6.095855**	**6.418632**
C	**4.560221**	**7.966750**	**6.775178**
C	**3.522717**	**8.830448**	**6.704345**
H	**3.370092**	**9.417114**	**7.410692**
C	**2.679347**	**8.861341**	**5.604150**
H	**1.963064**	**9.455551**	**5.599190**
C	**2.869342**	**8.049319**	**4.536891**
C	**3.951716**	**7.123694**	**4.522407**
C	**4.807907**	**7.074580**	**5.666650**
C	**4.025954**	**6.678108**	**1.029362**
H	**3.380338**	**6.733628**	**0.321428**
H	**4.703972**	**6.040335**	**0.795633**
H	**4.428945**	**7.539386**	**1.162695**
C	**2.639595**	**4.954270**	**2.129954**
H	**2.035610**	**5.009648**	**1.384917**
H	**2.144571**	**4.760518**	**2.930547**
H	**3.278905**	**4.255140**	**1.972216**

C	**1.959633**	**9.413270**	**2.670825**
H	**1.378555**	**9.367288**	**1.908725**
H	**2.852220**	**9.614994**	**2.380945**
H	**1.652349**	**10.101866**	**3.265863**
C	**0.576903**	**7.656121**	**3.745624**
H	**0.043779**	**7.586364**	**2.950388**
H	**0.181224**	**8.296741**	**4.341257**
H	**0.617505**	**6.800537**	**4.178559**
H	**2.655071**	**7.093799**	**2.591262**
H	**5.343887**	**8.501739**	**8.396801**
H	**6.008128**	**7.118000**	**8.005929**
N	**2.382411**	**15.108809**	**12.208496**
N	**0.985942**	**13.259553**	**13.306112**
N	**4.429667**	**13.402340**	**17.788241**
C	**3.274314**	**15.129167**	**13.356905**
C	**4.337753**	**15.977490**	**13.402540**
H	**4.524525**	**16.530843**	**12.678534**
C	**5.146472**	**16.015785**	**14.537060**
H	**5.859165**	**16.611988**	**14.567417**
C	**4.917110**	**15.207038**	**15.595192**
H	**5.471991**	**15.258145**	**16.339238**
C	**3.594489**	**13.387250**	**16.695784**
C	**2.556985**	**12.523552**	**16.624951**
H	**2.404360**	**11.936886**	**17.331298**
C	**1.713615**	**12.492659**	**15.524756**
H	**0.997332**	**11.898449**	**15.519796**
C	**1.903610**	**13.304681**	**14.457497**
C	**2.985984**	**14.230306**	**14.443013**
C	**3.842175**	**14.279420**	**15.587256**
C	**3.060222**	**14.675892**	**10.949968**
H	**2.414607**	**14.620372**	**10.242033**
H	**3.738240**	**15.313665**	**10.716238**
H	**3.463213**	**13.814614**	**11.083301**
C	**1.673863**	**16.399730**	**12.050560**
H	**1.069878**	**16.344352**	**11.305522**
H	**1.178839**	**16.593482**	**12.851153**
H	**2.313173**	**17.098860**	**11.892822**
C	**0.993901**	**11.940730**	**12.591431**
H	**0.412823**	**11.986712**	**11.829330**
H	**1.886488**	**11.739006**	**12.301551**

H	**0.686618**	**11.252134**	**13.186469**
C	**-0.388829**	**13.697879**	**13.666230**
H	**-0.921953**	**13.767636**	**12.870994**
H	**-0.784508**	**13.057259**	**14.261863**
H	**-0.348227**	**14.553463**	**14.099165**
H	**1.689339**	**14.260201**	**12.511868**
H	**4.378155**	**12.852261**	**18.317406**
H	**5.042396**	**14.236000**	**17.926535**
N	**5.902393**	**7.990809**	**17.553321**
N	**7.298862**	**6.141553**	**16.455706**
N	**3.855138**	**6.284340**	**11.973576**
C	**5.010490**	**8.011167**	**16.404912**
C	**3.947052**	**8.859490**	**16.359277**
H	**3.760280**	**9.412843**	**17.083283**
C	**3.138332**	**8.897785**	**15.224757**
H	**2.425639**	**9.493988**	**15.194400**
C	**3.367694**	**8.089038**	**14.166625**
H	**2.812814**	**8.140145**	**13.422580**
C	**4.690316**	**6.269250**	**13.066033**
C	**5.727819**	**5.405552**	**13.136866**
H	**5.880444**	**4.818886**	**12.430519**
C	**6.571189**	**5.374659**	**14.237061**
H	**7.287473**	**4.780449**	**14.242022**
C	**6.381195**	**6.186681**	**15.304320**
C	**5.298821**	**7.112306**	**15.318804**
C	**4.442630**	**7.161420**	**14.174561**
C	**5.224583**	**7.557892**	**18.811849**
H	**5.870198**	**7.502372**	**19.519784**
H	**4.546565**	**8.195665**	**19.045579**
H	**4.821592**	**6.696614**	**18.678516**
C	**6.610942**	**9.281730**	**17.711257**
H	**7.214926**	**9.226352**	**18.456295**
H	**7.105965**	**9.475482**	**16.910665**
H	**5.971631**	**9.980860**	**17.868995**
C	**7.290904**	**4.822730**	**17.170386**
H	**7.871981**	**4.868712**	**17.932487**
H	**6.398316**	**4.621006**	**17.460266**
H	**7.598187**	**4.134134**	**16.575348**
C	**8.673634**	**6.579879**	**16.095588**
H	**9.206758**	**6.649636**	**16.890823**

H	**9.069312**	**5.939259**	**15.499954**
H	**8.633031**	**7.435463**	**15.662652**
H	**6.595465**	**7.142201**	**17.249949**
H	**3.906650**	**5.734261**	**11.444411**
H	**3.242408**	**7.118000**	**11.835283**
N	**1.395501**	**4.416007**	**7.694025**
N	**2.732783**	**2.590525**	**6.502560**
N	**-0.861841**	**2.820294**	**2.156541**
C	**0.471159**	**4.468538**	**6.543433**
C	**-0.563698**	**5.344906**	**6.548790**
H	**-0.694117**	**5.903669**	**7.279740**
C	**-1.434003**	**5.410961**	**5.461095**
H	**-2.152238**	**6.001898**	**5.476174**
C	**-1.233479**	**4.610756**	**4.377566**
H	**-1.801761**	**4.685068**	**3.644831**
C	**0.003920**	**2.796520**	**3.210506**
C	**1.041529**	**1.895950**	**3.234316**
H	**1.157120**	**1.313983**	**2.517850**
C	**1.920956**	**1.840430**	**4.308717**
H	**2.620760**	**1.228567**	**4.287686**
C	**1.787543**	**2.653733**	**5.392048**
C	**0.715911**	**3.594305**	**5.453555**
C	**-0.183329**	**3.672461**	**4.341455**
C	**0.758921**	**3.910629**	**8.928744**
H	**0.071044**	**4.519930**	**9.206322**
H	**1.419481**	**3.836602**	**9.621003**
H	**0.372806**	**3.047928**	**8.759895**
C	**2.109887**	**5.696962**	**7.916048**
H	**2.813603**	**5.564852**	**8.555530**
H	**1.493680**	**6.353527**	**8.249976**
H	**2.484651**	**6.001898**	**7.087281**
C	**2.762027**	**1.288927**	**7.167042**
H	**3.290292**	**1.349573**	**7.966246**
H	**3.148181**	**0.637773**	**6.577362**
H	**1.867851**	**1.024992**	**7.392835**
C	**4.089137**	**3.025150**	**6.089268**
H	**4.459293**	**2.383106**	**5.480143**
H	**4.653420**	**3.093483**	**6.863075**
H	**4.032841**	**3.880734**	**5.656729**
H	**1.904416**	**3.687124**	**7.545613**

H	**-0.882272**	**2.049984**	**1.367059**
H	**-1.369767**	**3.581778**	**2.009915**
N	**8.820767**	**11.534007**	**2.226581**
N	**7.483485**	**9.708525**	**3.418045**
N	**11.078110**	**9.938294**	**7.764064**
C	**9.745109**	**11.586538**	**3.377173**
C	**10.779966**	**12.462906**	**3.371815**
H	**10.910386**	**13.021669**	**2.640865**
C	**11.650272**	**12.528961**	**4.459511**
H	**12.368506**	**13.119898**	**4.444431**
C	**11.449747**	**11.728756**	**5.543039**
H	**12.018029**	**11.803068**	**6.275775**
C	**10.212348**	**9.914520**	**6.710099**
C	**9.174739**	**9.013950**	**6.686290**
H	**9.059148**	**8.431983**	**7.402756**
C	**8.295312**	**8.958430**	**5.611888**
H	**7.595508**	**8.346567**	**5.632920**
C	**8.428725**	**9.771733**	**4.528558**
C	**9.500357**	**10.712305**	**4.467050**
C	**10.399597**	**10.790461**	**5.579150**
C	**9.457347**	**11.028629**	**0.991862**
H	**10.145224**	**11.637930**	**0.714284**
H	**8.796787**	**10.954602**	**0.299602**
H	**9.843462**	**10.165928**	**1.160711**
C	**8.106381**	**12.814962**	**2.004558**
H	**7.402665**	**12.682852**	**1.365075**
H	**8.722588**	**13.471527**	**1.670630**
H	**7.731617**	**13.119898**	**2.833325**
C	**7.454241**	**8.406927**	**2.753563**
H	**6.925976**	**8.467573**	**1.954359**
H	**7.068087**	**7.755773**	**3.343244**
H	**8.348417**	**8.142992**	**2.527770**
C	**6.127131**	**10.143150**	**3.831338**
H	**5.756975**	**9.501106**	**4.440463**
H	**5.562848**	**10.211483**	**3.057531**
H	**6.183427**	**10.998734**	**4.263876**
H	**8.311852**	**10.805124**	**2.374993**
H	**11.098540**	**9.167984**	**8.553546**
H	**11.586035**	**10.699778**	**7.910691**
N	**7.855035**	**9.819993**	**12.147186**

N	**6.517753**	**11.645475**	**13.338651**
N	**10.112378**	**11.415706**	**17.684670**
C	**8.779377**	**9.767462**	**13.297778**
C	**9.814234**	**8.891094**	**13.292421**
H	**9.944654**	**8.332331**	**12.561471**
C	**10.684540**	**8.825039**	**14.380116**
H	**11.402774**	**8.234102**	**14.365037**
C	**10.484015**	**9.625244**	**15.463645**
H	**11.052297**	**9.550932**	**16.196381**
C	**9.246616**	**11.439480**	**16.630705**
C	**8.209008**	**12.340050**	**16.606896**
H	**8.093416**	**12.922017**	**17.323362**
C	**7.329580**	**12.395570**	**15.532494**
H	**6.629776**	**13.007433**	**15.553526**
C	**7.462993**	**11.582267**	**14.449164**
C	**8.534625**	**10.641695**	**14.387656**
C	**9.433865**	**10.563539**	**15.499756**
C	**8.491615**	**10.325371**	**10.912468**
H	**9.179492**	**9.716070**	**10.634889**
H	**7.831056**	**10.399398**	**10.220208**
H	**8.877730**	**11.188072**	**11.081317**
C	**7.140649**	**8.539038**	**11.925163**
H	**6.436933**	**8.671148**	**11.285681**
H	**7.756856**	**7.882473**	**11.591236**
H	**6.765885**	**8.234102**	**12.753931**
C	**6.488509**	**12.947073**	**12.674169**
H	**5.960244**	**12.886427**	**11.874965**
H	**6.102355**	**13.598227**	**13.263850**
H	**7.382685**	**13.211008**	**12.448376**
C	**5.161399**	**11.210850**	**13.751944**
H	**4.791244**	**11.852894**	**14.361069**
H	**4.597116**	**11.142517**	**12.978136**
H	**5.217695**	**10.355266**	**14.184482**
H	**7.346120**	**10.548876**	**12.295599**
H	**10.132808**	**12.186016**	**18.474152**
H	**10.620303**	**10.654222**	**17.831297**
N	**0.429769**	**2.701993**	**17.614631**
N	**1.767051**	**4.527475**	**16.423166**
N	**-1.827573**	**4.297706**	**12.077147**
C	**-0.494573**	**2.649462**	**16.464039**

C	-1.529430	1.773094	16.469396
H	-1.659849	1.214331	17.200346
C	-2.399735	1.707039	15.381701
H	-3.117970	1.116102	15.396780
C	-2.199211	2.507244	14.298172
H	-2.767493	2.432932	13.565436
C	-0.961811	4.321480	13.131112
C	0.075797	5.222050	13.154922
H	0.191388	5.804017	12.438455
C	0.955224	5.277570	14.229323
H	1.655028	5.889433	14.208292
C	0.821811	4.464267	15.312653
C	-0.249821	3.523695	15.374161
C	-1.149061	3.445539	14.262061
C	-0.206811	3.207371	18.849349
H	-0.894688	2.598070	19.126928
H	0.453749	3.281398	19.541609
H	-0.592926	4.070072	18.680501
C	1.144155	1.421038	17.836654
H	1.847871	1.553148	18.476136
H	0.527948	0.764473	18.170581
H	1.518919	1.116102	17.007886
C	1.796296	5.829073	17.087648
H	2.324561	5.768427	17.886852
H	2.182449	6.480227	16.497967
H	0.902119	6.093008	17.313441
C	3.123405	4.092850	16.009874
H	3.493561	4.734894	15.400748
H	3.687689	4.024517	16.783681
H	3.067110	3.237266	15.577335
H	0.938684	3.430876	17.466218
H	-1.848004	5.068016	11.287665
H	-2.335499	3.536222	11.930520

Compound (4) CCDC identifiers: ZOSKEX (1315231)

XYZ for single molecule:

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Zostex

C	6.39533	5.88652	6.54964
C	7.04515	4.75785	7.04101

C	**8.14411**	**4.96402**	**7.83895**
C	**8.64055**	**6.17052**	**8.18531**
C	**8.42638**	**8.66718**	**8.11925**
C	**7.75765**	**9.78446**	**7.67638**
C	**6.64319**	**9.65707**	**6.83140**
C	**6.20355**	**8.41140**	**6.45309**
C	**6.83928**	**7.20808**	**6.88885**
C	**8.00059**	**7.36918**	**7.74319**
C	**5.57855**	**5.03161**	**4.40835**
C	**4.10938**	**5.03553**	**6.36339**
C	**5.28640**	**8.87533**	**4.20026**
C	**3.77660**	**8.85427**	**6.16304**
O	**10.56401**	**7.08916**	**9.21450**
O	**10.08288**	**4.97835**	**9.50593**
H	**4.92788**	**7.18627**	**5.46792**
H	**6.68939**	**3.75766**	**6.78189**
H	**9.29713**	**8.76625**	**8.76050**
H	**8.09447**	**10.77531**	**7.97838**
H	**6.13042**	**10.55401**	**6.48314**
H	**6.42768**	**5.53536**	**3.93306**
H	**5.84514**	**3.97567**	**4.57248**
H	**4.71139**	**5.06933**	**3.73819**
H	**3.85959**	**5.56835**	**7.28815**
H	**3.23916**	**5.03666**	**5.69535**
H	**4.35228**	**3.99139**	**6.61581**
H	**6.19134**	**8.41777**	**3.78841**
H	**4.42757**	**8.65589**	**3.55590**
H	**5.42650**	**9.95994**	**4.26704**
H	**2.93526**	**8.62541**	**5.49890**
H	**3.62027**	**8.38724**	**7.14078**
H	**3.85864**	**9.93945**	**6.28713**
H	**8.44419**	**4.26160**	**8.41577**
N	**5.23746**	**5.71094**	**5.68036**
N	**5.02815**	**8.30776**	**5.55805**
N	**9.85837**	**6.09866**	**9.03654**

XYZ for crystal:

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Zostex

O	**9.797701**	**9.324569**	**8.587165**
O	**9.331256**	**7.347575**	**9.261835**
N	**4.424457**	**7.886197**	**5.356292**
N	**4.199215**	**10.443096**	**5.228901**
N	**9.073052**	**8.365513**	**8.632422**
C	**5.604818**	**8.058296**	**6.192715**
C	**6.297469**	**6.950912**	**6.614279**
C	**7.430160**	**7.114729**	**7.438969**
C	**7.838767**	**8.331544**	**7.797675**
C	**7.551586**	**10.835759**	**7.816113**
C	**6.869531**	**11.926084**	**7.384492**
C	**5.767505**	**11.790336**	**6.541365**
C	**5.350096**	**10.565199**	**6.138239**
C	**6.024429**	**9.367024**	**6.557288**
C	**7.174842**	**9.522321**	**7.410473**
C	**4.735157**	**7.290954**	**4.042991**
C	**3.350457**	**7.169006**	**6.067838**
C	**4.523592**	**10.973890**	**3.866152**
C	**2.959249**	**11.033991**	**5.782047**
H	**4.127759**	**9.475353**	**5.036976**
H	**5.917675**	**6.137639**	**6.419840**
H	**8.419168**	**10.814674**	**8.556993**
H	**7.197729**	**12.788968**	**7.685370**
H	**5.380697**	**12.543310**	**6.243838**
H	**5.484578**	**7.595377**	**3.687637**
H	**4.832538**	**6.408725**	**4.131829**
H	**4.052497**	**7.702081**	**3.494874**
H	**3.094817**	**7.484871**	**7.023272**
H	**2.646250**	**7.368345**	**5.456026**
H	**3.661597**	**6.352375**	**6.336030**
H	**5.293487**	**10.514185**	**3.536779**
H	**3.813612**	**10.634574**	**3.310492**
H	**4.593514**	**11.832717**	**3.905542**
H	**2.387514**	**10.801517**	**4.860976**
H	**2.838227**	**10.646095**	**6.713175**
H	**3.113486**	**11.888323**	**5.774504**
O	**-4.556257**	**2.816268**	**-0.206172**

O	**-4.089812**	**4.793262**	**-0.880843**
N	**0.816987**	**4.254641**	**3.024700**
N	**1.042229**	**1.697741**	**3.152091**
N	**-3.831608**	**3.775324**	**-0.251430**
C	**-0.363375**	**4.082541**	**2.188277**
C	**-1.056025**	**5.189925**	**1.766713**
C	**-2.188716**	**5.026108**	**0.942024**
C	**-2.597324**	**3.809293**	**0.583317**
C	**-2.310142**	**1.305079**	**0.564879**
C	**-1.628088**	**0.214753**	**0.996500**
C	**-0.526061**	**0.350501**	**1.839628**
C	**-0.108653**	**1.575639**	**2.242754**
C	**-0.782985**	**2.773814**	**1.823704**
C	**-1.933398**	**2.618517**	**0.970519**
C	**0.506286**	**4.849884**	**4.338002**
C	**1.890987**	**4.971831**	**2.313154**
C	**0.717852**	**1.166947**	**4.514841**
C	**2.282195**	**1.106847**	**2.598946**
H	**1.113685**	**2.665484**	**3.344016**
H	**-0.676231**	**6.003198**	**1.961151**
H	**-3.177725**	**1.326164**	**-0.176001**
H	**-1.956285**	**-0.648130**	**0.695622**
H	**-0.139254**	**-0.402473**	**2.137153**
H	**-0.243134**	**4.545460**	**4.693356**
H	**0.408906**	**5.732112**	**4.249163**
H	**1.188946**	**4.438756**	**4.886119**
H	**2.146627**	**4.655967**	**1.357721**
H	**2.595194**	**4.772492**	**2.924966**
H	**1.579847**	**5.788463**	**2.044962**
H	**-0.052044**	**1.626653**	**4.844214**
H	**1.427831**	**1.506263**	**5.070500**
H	**0.647930**	**0.308120**	**4.475450**
H	**2.853930**	**1.339320**	**3.520017**
H	**2.403217**	**1.494743**	**1.667817**
H	**2.127957**	**0.252515**	**2.606489**
Cl	**0.562549**	**9.158448**	**3.130302**
O	**-0.114074**	**10.089131**	**3.922304**
O	**-0.118291**	**8.335442**	**2.288012**
O	**1.451305**	**9.971679**	**2.380202**
O	**1.115541**	**8.327844**	**4.081544**

Cl	**4.678895**	**2.982389**	**5.250692**
O	**5.355518**	**2.051706**	**4.458688**
O	**5.359734**	**3.805396**	**6.092981**
O	**3.790138**	**2.169159**	**6.000791**
O	**4.125901**	**3.812994**	**4.299448**
H	**8.090280**	**6.380725**	**7.851740**
H	**-2.848836**	**5.760113**	**0.529254**