

Deposited materials of the paper: “On the Transferability of QTAIMC Descriptors Derived from X-ray Diffraction Data and DFT Calculations: Substituted Hydropyrimidine Derivatives”

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Synopsis

The electron density features of substituted hydropyrimidine derivatives are characterized using the QTAIMC descriptors derived from the X-ray experimental electron density and DFT calculations. The application of these descriptors as transferable quantities suitable for prediction of the chemical properties of the molecular systems is discussed.

Abstract

The combined study of electron-density features in three substituted hydropyrimidines of the Biginelli compound family derived from low-temperature X-ray diffraction measurements and DFT B3LYP/6-311++G** calculations are described. The experimentally derived atomic and bond characteristics determined within the quantum-topological theory of atoms in molecules and crystals (QTAIMC) were demonstrated to be fully transferable within chemically similar structures such as the Biginelli compounds. However, for the certain covalent bonds they differ significantly from the theoretical results due to insufficient flexibility of the atom-centered multipole electron-density model. It was concluded that currently the analysis of the theoretical electron density provides a more reliable basis for the determination of the transferability of QTAIMC descriptors for molecular structures. Empirical corrections making the experimentally-derived QTAIMC bond descriptors more transferable are proposed.

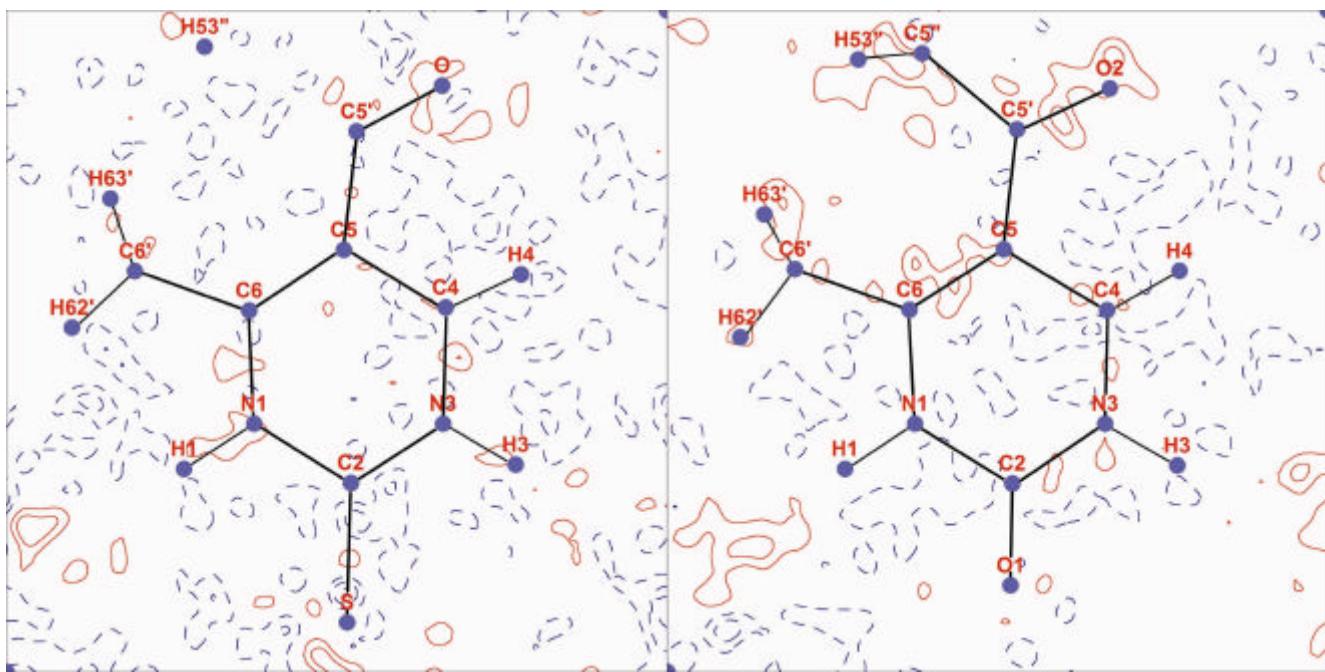


Figure 1S. Residual density map for compounds **(1)** and **(2)** Positive values correspond to red solid lines, negative contours are blue dashed lines. Contour intervals are $0.05 \text{ e}\text{\AA}^{-3}$

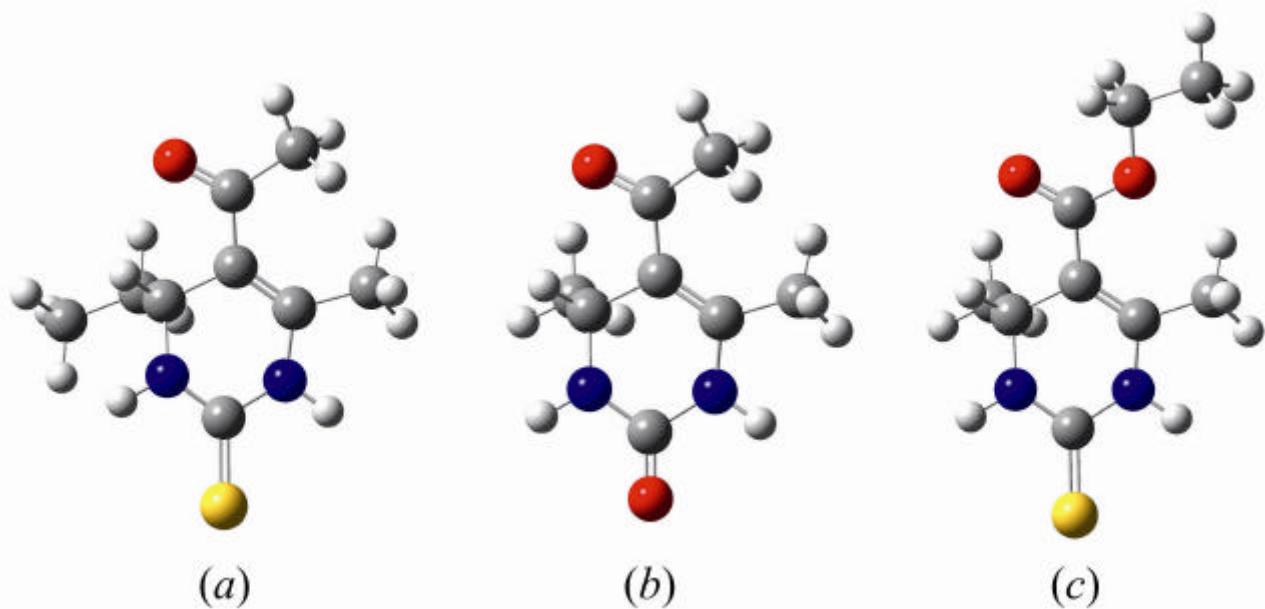


Figure 2S. Optimized structures of monomers of (1) (a), (2) (b) and (3) (c). Color correspondence: yellow – sulfur, red – oxygen, blue – nitrogen, gray – carbon, white –hydrogen

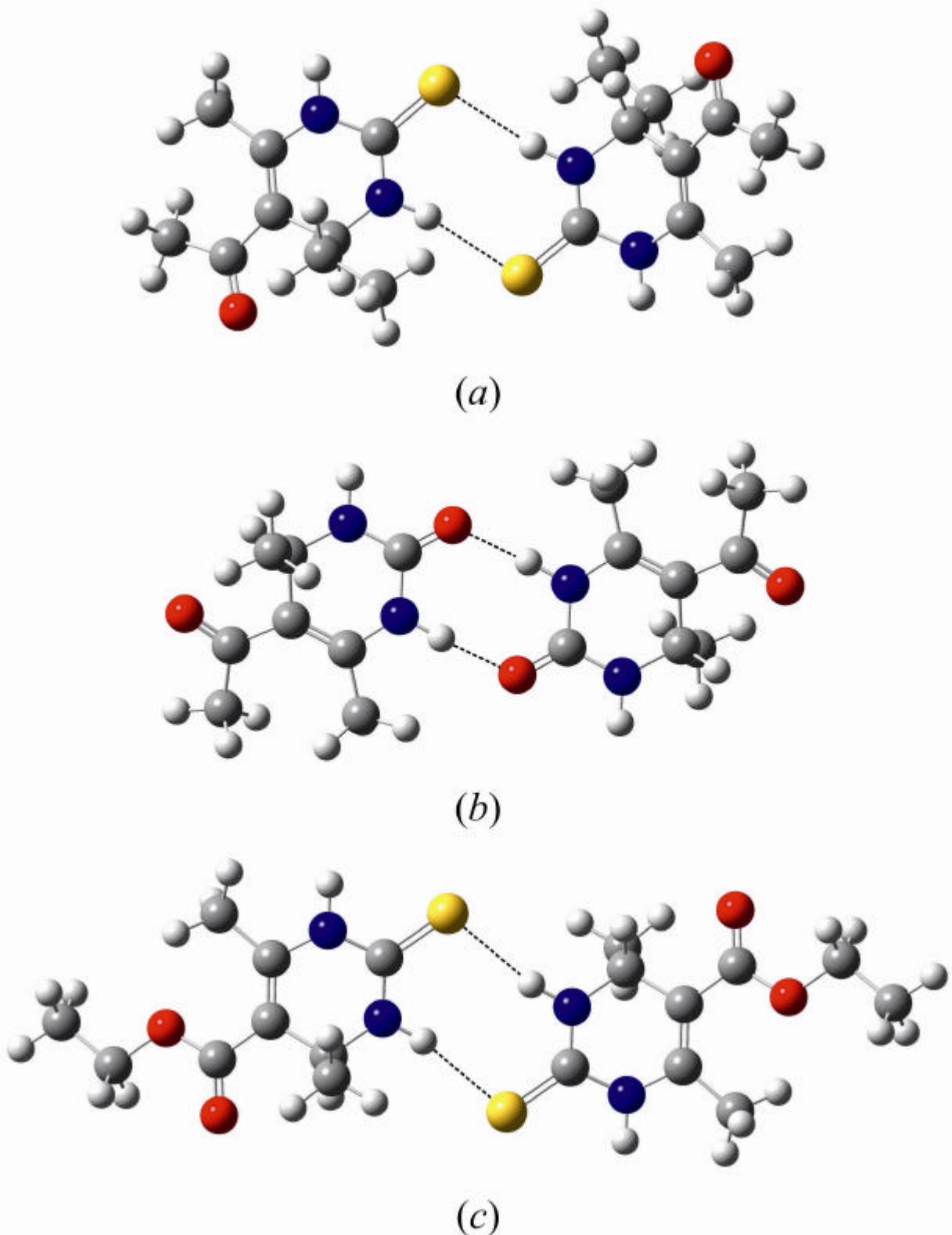


Figure 3S. Optimized structures of dimers of (1) (a), (2) (b) and (3) (c). Colors are the same as in the Figure 2S

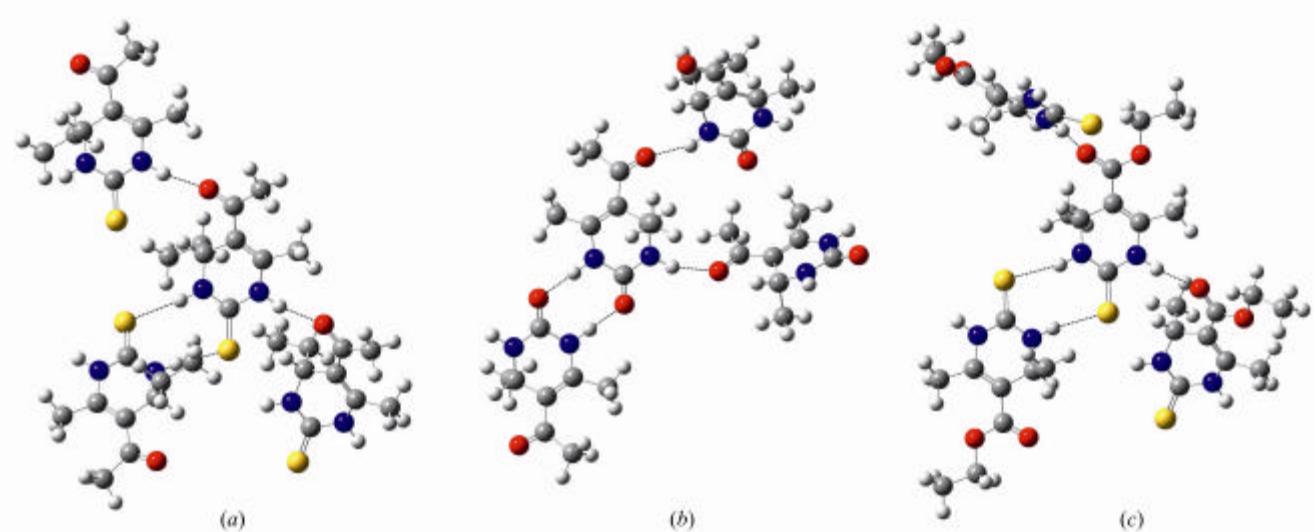


Figure 4S. Optimized structures of tetramers of (1) (a), (2) (b) and (3) (c). Colors are the same as in the Figure 2S

Table S1

Results of the Hirshfeld rigid-bond test for molecules (1), (2) and (3)

(1)		(2)		(3)	
Bond	? , Å ²	Bond	? , Å ²	Bond	? , Å ²
S – C2	0.0003	O1 – C2	0.0001	C2 – S	0.0003
O – C5'	0.0001	O2 – C5'	0.0004	O1 – C5'	0.0003
N1 – C2	0.0002	N1 – C2	0.0002	O2 – C5'	0.0003
N1 – C6	0.0000	N1 – C6	0.0003	N1 – C2	0.0004
N3 – C2	0.0001	N3 – C2	0.0002	C2 – N3	0.0005
N3 – C4	0.0004	N3 – C4	0.0004	N3 – C4	0.0002
C4 – C4'	0.0000	C4 – C4'	0.0001	C4 – C5	0.0003
C4' – C4''	0.0001	C4 – C5	0.0003	C5 – C6	0.0001
C4 – C5	0.0001	C5 – C6	0.0000	C6 – N1	0.0003
C5 – C6	0.0000	C6 – C6'	0.0004	C4 – C4'	0.0004
C6 – C6'	0.0005	C5 – C5'	0.0004	C5 – C5'	0.0000
C5 – C5'	0.0002	C5' – C5''	0.0003	C6 – C6'	0.0003
C5' – C5''	0.0004			O2 – C7	0.0009
				C7 – C8	0.0003

Table S2Characteristics of intramolecular bonds in molecule (**1**)

Experimental results are given in the first line for each bond. Non-empirical calculation results for the monomer in the gas-phase are presented in the second line, for the dimer – in the third line, for the tetramer – in the fourth line, calculations with periodic boundary conditions in the program TOPOND are listed in the fifth line, and the calculations in the WinXPRO program for the crystal are given in the sixth line.

Bond	R (Å)	$r(\mathbf{r})$, a.u.	$\nabla^2 r(\mathbf{r})$, a.u.
S – C2	1.689	0.212(7)	-0.32
	1.673	0.213	-0.09
	1.689	0.210	-0.19
	1.697	0.208	-0.23
	1.689	0.213	-0.15
	1.689	0.210	-0.27
O – C5'	1.238	0.402(3)	-1.28
	1.226	0.397	-0.18
	1.225	0.398	-0.17
	1.234	0.387	-0.18
	1.238	0.386	0.28
	1.238	0.404	-1.08
N1 – C2	1.374	0.342(4)	-0.93
	1.386	0.305	-0.89
	1.386	0.305	-0.90
	1.383	0.308	-0.92
	1.374	0.319	-1.03
	1.374	0.356	-1.04
N1 – C6	1.391	0.302(0)	-0.72
	1.390	0.297	-0.80
	1.393	0.295	-0.80
	1.384	0.302	-0.83
	1.391	0.304	-0.86
	1.391	0.305	-0.69
N3 – C2	1.327	0.366(0)	-1.20
	1.342	0.334	-0.98
	1.328	0.344	-1.00
	1.327	0.345	-1.00
	1.327	0.350	-0.95
	1.327	0.356	-1.04
N3 – C4	1.468	0.244(4)	-0.38
	1.473	0.249	-0.62
	1.474	0.248	-0.62
	1.475	0.247	-0.61
	1.468	0.258	-0.71
	1.468	0.255	-0.43
C4 – C4'	1.538	0.245(4)	-0.40
	1.544	0.239	-0.53
	1.544	0.238	-0.53
	1.544	0.238	-0.53
	1.538	0.240	-0.53
	1.538	0.238	-0.43
C4' – C4"	1.526	0.254(3)	-0.45
	1.531	0.239	-0.53
	1.531	0.239	-0.53
	1.531	0.239	-0.53
	1.526	0.240	-0.53
	1.526	0.236	-0.41
C4 – C5	1.515	0.269(4)	-0.54
	1.522	0.248	-0.57
	1.522	0.248	-0.57
	1.522	0.248	-0.57
	1.515	0.252	-0.58
	1.515	0.247	-0.45

C5 – C6	1.366	0.336(0)	-0.91
	1.362	0.324	-0.91
	1.361	0.325	-0.91
	1.367	0.322	-0.90
	1.366	0.330	-0.93
	1.366	0.328	-0.78
C6 – C6'	1.503	0.266(7)	-0.54
	1.506	0.252	-0.60
	1.506	0.252	-0.60
	1.507	0.252	-0.60
	1.503	0.250	-0.58
	1.503	0.247	-0.47
C5 – C5'	1.466	0.274(4)	-0.60
	1.477	0.268	-0.66
	1.478	0.268	-0.66
	1.462	0.276	-0.69
	1.466	0.277	-0.69
	1.466	0.274	-0.57
C5' – C5"	1.506	0.262(1)	-0.51
	1.521	0.250	-0.59
	1.521	0.249	-0.59
	1.520	0.250	-0.59
	1.506	0.253	-0.59
	1.506	0.251	-0.50
N1 – H1	1.010	0.310(3)	-1.23
	1.009	0.342	-1.72
	1.010	0.342	-1.71
	1.018	0.333	-1.77
	1.010	0.343	-1.89
	1.010	0.327	-1.53
N3 – H3	1.010	0.319(3)	-1.08
	1.009	0.341	-1.69
	1.023	0.327	-1.68
	1.024	0.326	-1.68
	1.010	0.342	-1.87
	1.010	0.328	-1.49
C4 – H4	1.090	0.273	-0.72
	1.091	0.286	-0.99
	1.090	0.287	-0.99
	1.091	0.288	-1.00
	1.090	0.293	-1.09
	1.090	0.287	-0.93
C4' – H41	1.090	0.261	-0.60
	1.093	0.277	-0.93
	1.094	0.277	-0.93
	1.094	0.276	-0.92
	1.090	0.285	-1.01
	1.090	0.278	-0.93
C4' – H42	1.090	0.260	-0.61
	1.096	0.274	-0.91
	1.096	0.274	-0.91
	1.096	0.274	-0.90
	1.090	0.284	-0.99
	1.090	0.279	-0.84
C4" – H43	1.060	0.263	-0.65
	1.095	0.272	-0.90
	1.094	0.273	-0.90
	1.093	0.274	-0.91
	1.060	0.296	-1.10
	1.060	0.291	-0.92
C4" – H44	1.060	0.273	-0.67
	1.093	0.273	-0.91
	1.093	0.273	-0.90

	1.093	0.273	-0.90
	1.060	0.297	-1.09
	1.060	0.292	-0.94
C4'' – H45	1.060	0.276	-0.65
	1.094	0.273	-0.90
	1.093	0.275	-0.91
	1.093	0.275	-0.91
	1.060	0.296	-1.07
	1.060	0.292	-0.93
C6' – H61	1.060	0.268	-0.61
	1.095	0.272	-0.89
	1.095	0.271	-0.89
	1.095	0.271	-0.89
	1.060	0.297	-1.11
	1.060	0.292	-0.95
C6' – H62	1.060	0.268	-0.64
	1.093	0.274	-0.91
	1.093	0.274	-0.91
	1.090	0.279	-0.94
	1.060	0.299	-1.13
	1.060	0.294	-0.95
C6' – H63	1.060	0.268	-0.62
	1.085	0.280	-0.95
	1.085	0.280	-0.95
	1.087	0.278	-0.94
	1.060	0.299	-1.11
	1.060	0.294	-0.95
C5'' – H51	1.060	0.264	-0.61
	1.089	0.278	-0.94
	1.089	0.278	-0.94
	1.089	0.277	-0.93
	1.060	0.298	-1.12
	1.060	0.291	-0.94
C5'' – H52	1.060	0.270	-0.62
	1.091	0.274	-0.91
	1.091	0.274	-0.91
	1.090	0.275	-0.92
	1.060	0.298	-1.13
	1.060	0.293	-0.95
C5'' – H53	1.060	0.264	-0.58
	1.094	0.270	-0.88
	1.094	0.270	-0.88
	1.094	0.270	-0.88
	1.060	0.295	-1.09
	1.060	0.290	-0.93

Table S3

Characteristics of intramolecular bonds in molecule (2)

Experimental results are given in the first line for each bond. Non-empirical calculation results for the monomer in the gas-phase are presented in the second line, for the dimer – in the third line, for the tetramer – in the fourth line, calculations with periodic boundary conditions in the program TOPOND are listed in the fifth line, and the calculations in the WinXPRO program for the crystal are given in the sixth line.

Bond	R (Å)	$\mathbf{r}(\mathbf{r})$, a.u.	$\nabla^2 \mathbf{r}(\mathbf{r})$, a.u.
O1 – C2	1.245	0.417(2)	-1.46
	1.219	0.411	-0.39
	1.237	0.394	-0.46
	1.235	0.394	-0.45
	1.245	0.387	-0.06
	1.245	0.402	-1.17
O2 – C5'	1.236	0.443(2)	-1.49
	1.227	0.397	-0.18
	1.228	0.395	-0.19
	1.236	0.386	-0.19
	1.236	0.389	0.28
	1.236	0.409	-1.14
N1 – C2	1.384	0.334(1)	-0.94
	1.406	0.295	-0.86
	1.385	0.311	-0.95
	1.398	0.302	-0.90
	1.384	0.314	-1.06
	1.384	0.316	-0.82
N1 – C6	1.387	0.306(1)	-0.72
	1.387	0.299	-0.82
	1.387	0.300	-0.83
	1.376	0.308	-0.86
	1.387	0.307	-0.87
	1.387	0.308	-0.69
N3 – C2	1.337	0.374(4)	-1.24
	1.357	0.329	-1.01
	1.350	0.333	-1.03
	1.341	0.340	-1.05
	1.337	0.346	-1.07
	1.337	0.350	-1.00
N3 – C4	1.463	0.254(4)	-0.41
	1.471	0.251	-0.63
	1.471	0.249	-0.62
	1.467	0.253	-0.65
	1.463	0.261	-0.73
	1.463	0.258	-0.44
C4 – C4'	1.534	0.241(2)	-0.40
	1.538	0.240	-0.54
	1.538	0.240	-0.54
	1.538	0.240	-0.54
	1.534	0.239	-0.53
	1.534	0.237	-0.43
C4 – C5	1.517	0.263(1)	-0.48
	1.524	0.247	-0.57
	1.523	0.247	-0.57
	1.523	0.247	-0.57
	1.517	0.251	-0.58
	1.517	0.247	-0.45
C5 – C6	1.367	0.349(2)	-0.93
	1.363	0.323	-0.90
	1.365	0.323	-0.90
	1.371	0.320	-0.89
	1.367	0.328	-0.92

	1.367	0.325	-0.77
C6 – C6'	1.505	0.271(0)	-0.55
	1.507	0.252	-0.60
	1.508	0.251	-0.60
	1.509	0.251	-0.60
	1.505	0.250	-0.58
	1.505	0.246	-0.45
C5 – C5'	1.468	0.273(2)	-0.57
	1.475	0.269	-0.66
	1.474	0.270	-0.66
	1.460	0.276	-0.69
	1.468	0.276	-0.68
	1.468	0.272	-0.55
C5' – C5''	1.509	0.266(1)	-0.52
	1.522	0.249	-0.58
	1.521	0.250	-0.59
	1.520	0.250	-0.59
	1.509	0.251	-0.59
	1.509	0.248	-0.47
N1 – H1	1.009	0.313	-1.17
	1.009	0.341	-1.68
	1.028	0.323	-1.71
	1.027	0.324	-1.71
	1.009	0.342	-1.86
	1.009	0.340	-1.58
N3 – H3	1.009	0.319	-1.21
	1.010	0.339	-1.64
	1.010	0.339	-1.64
	1.021	0.327	-1.70
	1.009	0.342	-1.86
	1.009	0.341	-1.53
C4 – H4	1.093	0.277	-0.69
	1.090	0.287	-1.00
	1.090	0.287	-1.00
	1.090	0.287	-1.00
	1.093	0.290	-1.06
	1.093	0.290	-0.94
C4' – H41	1.058	0.288	-0.74
	1.094	0.272	-0.90
	1.095	0.272	-0.90
	1.093	0.274	-0.91
	1.058	0.296	-0.94
	1.058	0.299	-1.11
C4' – H42	1.058	0.261	-0.59
	1.091	0.276	-0.92
	1.091	0.276	-0.92
	1.092	0.275	-0.92
	1.058	0.299	-1.12
	1.058	0.296	-0.95
C4' – H43	1.058	0.270	-0.64
	1.094	0.273	-0.90
	1.094	0.273	-0.90
	1.093	0.273	-0.90
	1.058	0.300	-1.12
	1.058	0.297	-0.96
C6' – H61	1.058	0.266	-0.56
	1.095	0.271	-0.89
	1.094	0.271	-0.89
	1.094	0.271	-0.89
	1.058	0.298	-1.12
	1.058	0.295	-0.93
C6' – H62	1.058	0.277	-0.64
	1.093	0.274	-0.91

	1.091	0.278	-0.93
	1.090	0.278	-0.94
	1.058	0.301	-1.14
	1.058	0.298	-0.95
C6' – H63	1.058	0.267	-0.59
	1.085	0.280	-0.95
	1.087	0.278	-0.94
	1.087	0.278	-0.93
	1.058	0.299	-1.13
	1.058	0.296	-0.94
C5" – H51	1.058	0.273	-0.62
	1.089	0.278	-0.94
	1.089	0.278	-0.94
	1.089	0.278	-0.94
	1.058	0.300	-1.14
	1.058	0.297	-0.94
C5" – H52	1.058	0.280	-0.64
	1.091	0.274	-0.91
	1.091	0.274	-0.91
	1.091	0.274	-0.91
	1.058	0.297	-1.11
	1.058	0.293	-0.91
C5" – H53	1.058	0.260	-0.53
	1.094	0.270	-0.88
	1.094	0.270	-0.88
	1.094	0.271	-0.89
	1.058	0.298	-1.11
	1.058	0.295	-0.93

Table S4

Characteristics of intramolecular bonds in molecule (3)

Experimental results are given in the first line for each bond. Non-empirical calculation results for the monomer in the gas-phase are presented in the second line, for the dimer – in the third line, for the tetramer – in the fourth line, calculations with periodic boundary conditions in the program TOPOND are listed in the fifth line, and the calculations in the WinXPRO program for the crystal are given in the sixth line.

Bond	R (Å)	$\mathbf{r}(\mathbf{r})$, a.u.	$\nabla^2 \mathbf{r}(\mathbf{r})$, a.u.
C2 – S	1.689	0.212(5)	-0.20
	1.673	0.213	-0.09
	1.690	0.209	-0.19
	1.699	0.211	-0.24
	1.689	0.212	-0.14
	1.689	0.211	-0.27
O1 – C5'	1.225	0.440(0)	-1.63
	1.217	0.410	-0.27
	1.216	0.410	-0.26
	1.227	0.398	-0.31
	1.225	0.401	0.22
	1.225	0.413	-0.94
O2 – C5'	1.334	0.327(4)	-1.00
	1.355	0.296	-0.50
	1.356	0.295	-0.50
	1.342	0.305	-0.48
	1.334	0.313	-0.37
	1.334	0.322	-0.95
N1 – C2	1.369	0.332(3)	-0.90
	1.384	0.306	-0.90
	1.384	0.307	-0.91
	1.378	0.311	-0.93
	1.369	0.322	-1.03
	1.369	0.321	-0.82
C2 – N3	1.328	0.357(3)	-1.02
	1.344	0.333	-0.98
	1.329	0.343	-1.00
	1.328	0.343	-0.99
	1.328	0.347	-0.92
	1.328	0.350	-0.99
N3 – C4	1.468	0.250(4)	-0.37
	1.473	0.250	-0.63
	1.473	0.250	-0.63
	1.470	0.251	-0.64
	1.468	0.258	-0.72
	1.468	0.254	-0.40
C4 – C5	1.515	0.248(1)	-0.42
	1.520	0.249	-0.58
	1.520	0.249	-0.58
	1.518	0.250	-0.58
	1.515	0.252	-0.59
	1.515	0.244	-0.42
C5 – C6	1.361	0.328(1)	-0.79
	1.359	0.326	-0.92
	1.358	0.327	-0.92
	1.361	0.326	-0.92
	1.361	0.333	-0.94
	1.361	0.329	-0.80
C6 – N1	1.391	0.306(2)	-0.70
	1.390	0.297	-0.80
	1.392	0.295	-0.80
	1.388	0.299	-0.82
	1.391	0.304	-0.88

	1.391	0.303	-0.68
C4 – C4'	1.532	0.239(3)	-0.37
	1.537	0.240	-0.54
	1.537	0.240	-0.54
	1.538	0.240	-0.54
	1.532	0.240	-0.53
	1.532	0.233	-0.38
C5 – C5'	1.466	0.279(5)	-0.58
	1.468	0.273	-0.69
	1.470	0.272	-0.69
	1.462	0.276	-0.71
	1.466	0.276	-0.69
	1.466	0.272	-0.58
C6 – C6'	1.499	0.257(1)	-0.49
	1.504	0.253	-0.61
	1.504	0.253	-0.61
	1.505	0.252	-0.60
	1.499	0.252	-0.60
	1.499	0.246	-0.44
O2 – C7	1.451	0.242(4)	-0.30
	1.450	0.230	-0.32
	1.449	0.231	-0.33
	1.455	0.225	-0.29
	1.451	0.232	-0.31
	1.451	0.237	-0.30
C7 – C8	1.509	0.253(1)	-0.48
	1.515	0.251	-0.60
	1.515	0.251	-0.60
	1.514	0.251	-0.60
	1.509	0.249	-0.58
	1.509	0.243	-0.43
N1 – H1	1.010	0.322	-1.30
	1.009	0.342	-1.73
	1.009	0.342	-1.72
	1.018	0.333	-1.77
	1.010	0.343	-1.89
	1.010	0.351	-1.79
N3 – H3	1.010	0.319	-1.32
	1.009	0.340	-1.68
	1.024	0.326	-1.68
	1.023	0.327	-1.68
	1.010	0.343	-1.87
	1.010	0.353	-1.82
C4 – H4	1.090	0.265	-0.72
	1.091	0.287	-0.99
	1.090	0.287	-1.00
	1.090	0.287	-1.00
	1.090	0.293	-1.09
	1.090	0.293	-0.95
C4' – H41	1.060	0.260	-0.65
	1.092	0.275	-0.92
	1.092	0.275	-0.92
	1.092	0.275	-0.91
	1.060	0.299	-1.12
	1.060	0.296	-0.93
C4' – H42	1.060	0.261	-0.66
	1.094	0.273	-0.90
	1.093	0.274	-0.91
	1.093	0.274	-0.91
	1.060	0.298	-1.12
	1.060	0.296	-0.93
C4' – H43	1.060	0.260	-0.63
	1.093	0.274	-0.91

	1.093	0.274	-0.91
	1.093	0.274	-0.91
	1.060	0.297	-1.10
	1.060	0.294	-0.91
C6' – H61	1.060	0.265	-0.61
	1.094	0.272	-0.90
	1.094	0.272	-0.90
	1.092	0.273	-0.91
	1.060	0.297	-1.12
	1.060	0.296	-0.95
C6' – H62	1.060	0.273	-0.71
	1.093	0.274	-0.91
	1.093	0.273	-0.91
	1.089	0.279	-0.94
	1.060	0.301	-1.14
	1.060	0.300	-0.98
C6' – H63	1.060	0.258	-0.61
	1.086	0.281	-0.96
	1.085	0.281	-0.96
	1.089	0.277	-0.93
	1.060	0.299	-1.13
	1.060	0.298	-0.95
C7 – H71	1.090	0.275	-0.76
	1.092	0.285	-0.98
	1.092	0.285	-0.98
	1.091	0.287	-1.00
	1.090	0.290	-1.07
	1.090	0.291	-0.95
C7 – H72	1.090	0.269	-0.72
	1.092	0.284	-0.98
	1.092	0.284	-0.98
	1.093	0.284	-0.98
	1.090	0.290	-1.06
	1.090	0.290	-0.94
C8 – H81	1.060	0.271	-0.71
	1.092	0.274	-0.91
	1.092	0.274	-0.91
	1.092	0.275	-0.92
	1.060	0.299	-1.12
	1.060	0.296	-0.94
C8 – H82	1.060	0.257	-0.64
	1.093	0.274	-0.91
	1.093	0.274	-0.91
	1.093	0.274	-0.91
	1.060	0.298	-1.11
	1.060	0.297	-0.94
C8 – H83	1.057	0.258	-0.65
	1.093	0.273	-0.90
	1.093	0.273	-0.90
	1.093	0.296	-0.91
	1.057	0.298	-1.11
	1.057	0.296	-0.93

Table S5Characteristics of non-covalent bonds in molecule (**1**)

Experimental results are given in the first line for each bond. Non-empirical calculation results for the monomer in the gas-phase are presented in the second line, for the dimer – in the third line, for the tetramer – in the fourth line, calculations with periodic boundary conditions in the program TOPOND are listed in the fifth line, and the calculations in the WinXPRO program for the crystal are given in the sixth line.

Bond	R (Å)	$\mathbf{r}(\mathbf{r})$, a.u.	$\nabla^2 \mathbf{r}(\mathbf{r})$, a.u.
C5" ...H63	2.193	0.011	0.04
	2.563	0.011	0.04
	2.558	0.011	0.04
	2.616	0.011	0.04
	2.193	0.010	0.04
	2.193	0.009	0.04
	2.333	0.015	0.07
	-	-	-
	2.419	0.019	0.04
	2.409	0.019	0.04
S ...H3	2.333	0.023	0.05
	2.333	0.024	0.04
	1.869	0.019	0.12
	-	-	-
	-	-	-
O ...H1	1.958	0.021	0.09
	1.869	0.027	0.09
	1.869	0.029	0.09

Table S6Characteristics of non-covalent bonds in molecule (**2**)

Experimental results are given in the first line for each bond. Non-empirical calculation results for the monomer in the gas-phase are presented in the second line, for the dimer – in the third line, for the tetramer – in the fourth line, calculations with periodic boundary conditions in the program TOPOND are listed in the fifth line, and the calculations in the WinXPRO program for the crystal are given in the sixth line.

Bond	R (Å)	$\mathbf{r}(\mathbf{r})$, a.u.	$\nabla^2 \mathbf{r}(\mathbf{r})$, a.u.
C5" ...H63	2.190	0.011	0.04
	2.547	0.012	0.04
	2.629	0.011	0.04
	2.648	0.011	0.04
	2.190	0.010	0.04
	2.190	0.010	0.04
	1.826	0.028	0.15
	-	-	-
	1.828	0.033	0.11
	1.791	0.036	0.12
O1...H1	1.826	0.034	0.10
	1.826	0.037	0.08
	1.935	0.022	0.11
	-	-	-
	-	-	-
O2...H3	1.948	0.022	0.09
	1.935	0.026	0.08
	1.935	0.026	0.08

Table S7
Characteristics of non-covalent bonds in molecule (**3**)

Experimental results are given in the first line for each bond. Non-empirical calculation results for the monomer in the gas-phase are presented in the second line, for the dimer – in the third line, for the tetramer – in the fourth line, calculations with periodic boundary conditions in the program TOPOND are listed in the fifth line, and the calculations in the WinXPRO program for the crystal are given in the sixth line.

Bond	R (Å)	$\mathbf{r}(\mathbf{r})$, a.u.	$\nabla^2 \mathbf{r}(\mathbf{r})$, a.u.
O2…H63	2.373	0.017	0.07
	2.333	0.015	0.06
	2.309	0.016	0.06
	2.466	0.014	0.06
	2.373	0.015	0.06
	2.373	0.015	0.06
S…H3	2.369	0.017	0.06
	-	-	-
	2.412	0.019	0.04
	2.416	0.019	0.04
	2.369	0.022	0.04
	2.369	0.024	0.03
O1…H1	1.951	0.016	0.10
	-	-	-
	-	-	-
	1.940	0.023	0.09
	1.951	0.022	0.07
	1.951	0.026	0.06

Table S8Atomic properties for molecule (**1**)

Experimental results are given in the first line for each bond. Non-empirical calculations for the monomer in the gas-phase are presented in the second line, dimer results are in the third line, tetramer – in the fourth line, and calculations with periodic boundary conditions are listed in the fifth line.

Atom	$O (\text{\AA}^3)$	$Q (\text{e})$
S	34.540	-0.29
	37.354	-0.01
	36.303	-0.08
	35.900	-0.11
	35.988	-0.23
O	18.773	-1.08
	19.404	-1.11
	19.413	-1.10
	18.391	-1.15
	18.494	-1.07
N1	14.836	-1.08
	13.867	-1.13
	13.827	-1.12
	13.897	-1.15
	13.836	-1.03
N3	14.475	-1.08
	13.492	-1.11
	13.579	-1.14
	13.560	-1.14
	13.662	-1.01
C2	7.773	0.60
	8.462	0.59
	8.205	0.66
	8.191	0.69
	8.098	0.56
C4	6.508	0.24
	6.480	0.36
	6.502	0.36
	6.528	0.35
	6.671	0.21
C4'	8.449	0.07
	8.481	0.05
	8.463	0.05
	8.457	0.05
	8.935	-0.06
C4"	9.307	0.02
	10.263	0.02
	10.305	0.02
	10.306	0.02
	10.025	-0.06
C5	11.474	-0.09
	10.728	-0.03
	10.670	-0.03
	10.661	-0.03
	11.792	-0.09
C5'	7.595	0.87
	7.528	0.94

	7.516	0.94
	7.523	0.92
	8.147	0.85
C5"	10.393	0.08
	10.266	-0.01
	10.258	-0.01
	10.177	0.00
	10.874	-0.14
C6	9.469	0.26
	9.181	0.37
	9.197	0.37
	9.021	0.39
	10.139	0.27
C6'	11.006	0.09
	10.055	0.03
	10.068	0.03
	10.080	0.02
	10.617	-0.12
H1	2.315	0.55
	4.387	0.41
	4.388	0.41
	2.822	0.47
	2.200	0.53
H3	3.338	0.44
	4.495	0.41
	3.473	0.44
	3.439	0.46
	2.593	0.50
H4	5.596	0.12
	6.375	0.05
	6.419	0.06
	6.343	0.08
	5.661	0.11
H41	6.402	0.04
	7.056	0.02
	7.113	0.01
	7.130	0.00
	6.308	0.09
H42	8.566	0.01
	7.483	-0.01
	7.476	-0.02
	7.552	-0.02
	7.380	0.07
H43	6.310	0.06
	7.617	-0.01
	7.678	0.00
	7.912	0.01
	6.560	0.06
H44	7.136	0.01
	7.524	0.00
	7.596	-0.01
	7.632	-0.01
	6.622	0.05
H45	7.689	-0.14
	7.459	-0.01
	7.517	0.00

	7.390	0.00
	8.009	0.02
H51	8.259	0.04
	7.021	0.05
	7.026	0.04
	7.134	0.04
	8.728	0.09
H52	6.542	0.03
	7.103	0.01
	7.115	0.01
	6.952	0.02
	5.886	0.09
H53	6.528	-0.01
	7.185	0.01
	7.199	0.01
	7.180	0.02
	6.256	0.08
H61	5.932	0.10
	7.227	0.03
	7.249	0.03
	7.181	0.03
	5.476	0.10
H62	6.007	0.04
	7.148	0.02
	7.172	0.02
	6.181	0.06
	6.612	0.10
H63	6.560	-0.01
	6.485	0.03
	6.475	0.03
	6.712	0.02
	6.465	0.08
S	251.772	0.02
	260.124	0.00
	258.197	0.00
	254.252	0.00
	252.033	0.01

Table S9Atomic properties for molecule (**2**)

Experimental results are given in the first line for each bond. Non-empirical calculations for the monomer in the gas-phase are presented in the second line, dimer results are in the third line, tetramer – in the fourth line, and calculations with periodic boundary conditions are listed in the fifth line.

Atom	O (Å ³)	Q (e)
O1	18.368	-1.05
	20.733	-1.16
	19.348	-1.19
	19.150	-1.19
	18.002	-1.15
O2	17.675	-1.16
	19.441	-1.11
	19.455	-1.11
	18.953	-1.15
	17.105	-1.07
N1	14.899	-1.22
	14.116	-1.12
	14.183	-1.17
	14.141	-1.17
	13.785	-1.00
N3	13.766	-1.18
	14.039	-1.10
	13.985	-1.11
	13.937	-1.15
	12.763	-0.98
C2	4.773	1.57
	4.892	1.78
	4.863	1.78
	4.859	1.78
	5.138	1.54
C4	6.761	0.23
	6.572	0.38
	6.577	0.37
	6.469	0.38
	6.534	0.26
C5	10.540	-0.06
	10.805	-0.03
	10.857	-0.04
	10.863	-0.04
	10.814	-0.11
C6	9.419	0.30
	9.138	0.38
	9.096	0.39
	8.972	0.41
	9.625	0.28
C4'	10.054	0.11
	10.123	0.02
	10.103	0.02
	10.115	0.02
	9.610	0.04
C6'	9.923	0.19
	10.063	0.02
	10.071	0.02

	10.070	0.02
	10.299	0.03
C5'	7.566	0.87
	7.539	0.94
	7.538	0.93
	7.579	0.91
	7.817	0.87
C5"	9.443	0.17
	10.246	-0.01
	10.236	-0.01
	10.194	0.00
	9.773	0.00
H1	2.402	0.52
	4.372	0.41
	2.500	0.49
	2.488	0.48
	2.207	0.50
H3	2.301	0.54
	4.501	0.40
	4.506	0.40
	2.960	0.47
	2.563	0.48
H4	5.296	0.09
	6.359	0.05
	6.365	0.05
	6.584	0.04
	5.617	0.05
H41	7.317	0.01
	7.622	-0.01
	7.661	-0.01
	7.581	0.01
	7.729	0.00
H42	7.185	0.02
	7.135	0.03
	7.093	0.03
	7.308	0.01
	7.192	0.01
H43	7.637	0.02
	7.571	0.00
	7.589	0.00
	7.590	-0.01
	7.689	0.01
H61	5.867	0.02
	7.249	0.03
	7.183	0.03
	7.125	0.03
	6.194	0.03
H62	6.985	0.00
	7.184	0.01
	6.640	0.05
	6.511	0.05
	7.068	0.04
H63	6.709	0.01
	6.468	0.03
	6.681	0.02
	6.727	0.02

	6.847	0.04
H51	8.160	-0.01
	7.025	0.04
	7.048	0.04
	7.078	0.04
	8.478	0.04
H52	6.342	-0.01
	7.101	0.01
	7.060	0.01
	6.978	0.01
	6.266	0.04
H53	6.305	0.02
	7.207	0.01
	7.185	0.01
	7.141	0.02
	6.406	0.04
S	205.690	0.01
	217.500	0.00
	213.823	0.00
	211.371	0.00
	205.518	0.01

Table S10Atomic properties for molecule (**3**)

Experimental results are given in the first line for each bond. Non-empirical calculations for the monomer in the gas-phase are presented in the second line, dimer results are in the third line, tetramer – in the fourth line, and calculations with periodic boundary conditions are listed in the fifth line.

Atom	O (Å ³)	Q (e)
S	34.640	-0.23
	37.362	-0.01
	36.312	-0.09
	35.716	-0.12
	37.185	-0.28
O1	15.607	-1.01
	19.117	-1.15
	19.122	-1.15
	18.101	-1.19
	16.572	-1.17
O2	13.222	-0.98
	14.099	-1.06
	14.102	-1.06
	13.964	-1.07
	13.353	-0.95
N1	13.520	-1.07
	13.934	-1.13
	13.920	-1.13
	14.034	-1.16
	13.120	-0.98
N3	12.983	-1.07
	13.747	-1.10
	13.800	-1.14
	13.722	-1.14
	12.593	-0.97
C2	7.208	0.71
	8.452	0.60
	8.185	0.67
	8.075	0.70
	7.308	0.62
C4	6.975	0.23
	6.610	0.37
	6.639	0.37
	6.613	0.38
	6.683	0.28
C4'	11.382	-0.20
	10.135	0.02
	10.142	0.02
	10.143	0.02
	9.890	0.05
C5	9.782	-0.05
	10.621	-0.01
	10.590	0.00
	10.581	0.00
	10.045	-0.08
C5'	5.905	1.33
	5.994	1.47
	5.999	1.47

	5.973	1.47
	5.688	1.45
C6	8.772	0.37
	9.047	0.39
	9.069	0.38
	8.960	0.40
	8.767	0.30
C6'	11.436	-0.03
	10.091	0.03
	10.112	0.03
	10.083	0.03
	10.347	0.06
C7	7.935	0.29
	7.715	0.45
	7.707	0.45
	7.857	0.42
	7.581	0.37
C8	10.872	0.02
	10.266	0.04
	10.262	0.04
	10.251	0.04
	10.067	0.06
H1	3.108	0.46
	4.377	0.41
	4.378	0.41
	2.791	0.47
	2.557	0.50
H3	3.083	0.46
	4.490	0.41
	3.515	0.44
	3.492	0.44
	2.773	0.47
H4	6.820	0.12
	6.455	0.05
	6.500	0.06
	6.527	0.05
	6.732	0.05
H41	6.971	0.07
	7.185	0.03
	7.228	0.02
	7.310	0.01
	7.157	0.02
H42	8.636	0.06
	7.578	0.00
	7.625	0.01
	7.657	0.01
	8.799	0.01
H43	8.339	0.08
	7.523	0.00
	7.563	0.00
	7.572	0.00
	8.740	0.00
H61	7.039	0.09
	7.187	0.04
	7.236	0.04
	6.987	0.04

	7.517	0.04
H62	5.619	0.07
	7.265	0.00
	7.291	0.00
	6.403	0.04
	5.832	0.04
H63	5.766	0.09
	6.407	0.06
	6.347	0.06
	6.807	0.04
	6.363	0.03
H71	6.114	0.05
	6.952	0.04
	6.958	0.04
	6.516	0.07
	6.050	0.03
H72	6.588	0.05
	6.994	0.03
	6.990	0.03
	7.045	0.02
	6.568	0.03
H81	8.125	0.05
	7.479	0.01
	7.480	0.01
	7.474	0.01
	7.993	0.02
H82	6.711	0.04
	7.533	0.00
	7.539	0.00
	7.579	0.00
	6.889	0.00
H83	8.065	0.03
	7.497	0.01
	7.508	0.01
	7.485	0.01
	8.331	0.01
S	261.222	0.02
	272.110	0.00
	270.119	0.00
	265.719	0.00
	261.303	-0.03