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Supporting Information

Role of Hydrogen Bonding in the Formation of Glasses by Small Molecules: A Triazine Case Study

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Additional Crystal Structure Data for Compound 1

Table 1. Crystal data and structure refinement for ol03a

Identification code	ol03a	
Empirical formula	C20 H23 N5 O	
Formula weight	349.43	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 14.389(6) Å	α= 90°.
	b = 18.111(8) Å	β= 94.301(5)°.
	c = 15.870(7) Å	γ = 90°.
Volume	4124(3) $Å^3$	
Z	8	
Density (calculated)	1.126 Mg/m^3	
Absorption coefficient	0.073 mm^{-1}	
F(000)	1488	
Crystal size	0.30 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.81 to 25.00°.	
Index ranges	-17<=h<=17, -21<=k<=21, -18<=l<=18	
Reflections collected	19043	
Independent reflections	3636 [R(int) = 0.0955]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9928 and 0.9785	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3636 / 0 / 234	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0792, wR2 = 0.2006	
R indices (all data)	R1 = 0.1528, wR2 = 0.2581	
Extinction coefficient	0.0042(8)	
Largest diff. peak and hole	0.454 and -0.436 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ol03a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1295(2)	3746(2)	1252(2)	58(1)
N(1)	2542(2)	3048(2)	929(2)	42(1)
N(2)	3988(2)	3146(2)	1780(2)	42(1)
N(3)	2642(2)	3819(2)	2156(2)	41(1)
N(4)	3846(2)	2474(2)	517(2)	47(1)
N(5)	4018(2)	3772(2)	3034(2)	47(1)
C(1)	2212(3)	3534(2)	1466(3)	41(1)
C(2)	3462(3)	2900(2)	1107(2)	39(1)
C(3)	3524(3)	3579(2)	2312(2)	39(1)
C(4)	934(4)	4310(4)	1680(4)	86(2)
C(5)	4783(3)	2232(2)	508(3)	47(1)
C(6)	5181(3)	2232(3)	-283(3)	56(1)
C(7)	6082(4)	1976(3)	-345(4)	71(2)
C(8)	6587(4)	1725(3)	374(4)	76(2)
C(9)	6223(4)	1731(3)	1162(4)	68(2)
C(10)	5307(3)	1975(3)	1213(3)	57(1)
C(11)	6490(5)	1969(5)	-1206(4)	121(2)
C(12)	6788(4)	1473(4)	1952(4)	97(2)
C(13)	3728(3)	4201(2)	3723(3)	44(1)
C(14)	4183(3)	4072(2)	4513(2)	45(1)
C(15)	3950(3)	4470(3)	5228(3)	50(1)
C(16)	3250(4)	4980(3)	5128(3)	71(2)
C(17)	2780(5)	5117(4)	4351(4)	91(2)
C(18)	3036(4)	4727(3)	3645(3)	74(2)
C(19)	4456(4)	4316(3)	6083(3)	69(2)
C(20)	1959(5)	5658(5)	4270(4)	121(2)

Table 3. Bond lengths [Å] and angles [°] for ol03a.

O(1)-C(4)	1.352(6)	C(14)-C(15)	1.405(6)
O(1)-C(1)	1.392(5)	C(14)-H(14A)	0.9500
N(1)-C(1)	1.337(5)	C(15)-C(16)	1.367(7)
N(1)-C(2)	1.359(5)	C(15)-C(19)	1.517(6)
N(2)-C(2)	1.338(5)	C(16)-C(17)	1.383(7)
N(2)-C(3)	1.363(5)	C(16)-H(16A)	0.9500
N(3)-C(1)	1.322(5)	C(17)-C(18)	1.398(7)
N(3)-C(3)	1.346(5)	C(17)-C(20)	1.533(8)
N(4)-C(2)	1.363(5)	C(18)-H(18A)	0.9500
N(4)-C(5)	1.419(5)	C(19)-H(19A)	0.9800
N(4)-H(4A)	0.8800	C(19)-H(19B)	0.9800
N(5)-C(3)	1.349(5)	C(19)-H(19C)	0.9800
N(5)-C(13)	1.428(5)	C(20)-H(20A)	0.9800
N(5)-H(5A)	0.8800	C(20)-H(20B)	0.9800
C(4)-H(4B)	0.9800	C(20)-H(20C)	0.9800
C(4)-H(4C)	0.9800		
C(4)-H(4D)	0.9800	C(4)-O(1)-C(1)	118.5(4)
C(5)-C(10)	1.382(6)	C(1)-N(1)-C(2)	112.6(3)
C(5)-C(6)	1.418(6)	C(2)-N(2)-C(3)	114.3(3)
C(6)-C(7)	1.387(7)	C(1)-N(3)-C(3)	113.7(3)
C(6)-H(6A)	0.9500	C(2)-N(4)-C(5)	128.1(4)
C(7)-C(8)	1.381(8)	C(2)-N(4)-H(4A)	116.0
C(7)-C(11)	1.528(8)	C(5)-N(4)-H(4A)	116.0
C(8)-C(9)	1.392(7)	C(3)-N(5)-C(13)	128.8(4)
C(8)-H(8A)	0.9500	C(3)-N(5)-H(5A)	115.6
C(9)-C(10)	1.397(6)	C(13)-N(5)-H(5A)	115.6
C(9)-C(12)	1.517(8)	N(3)-C(1)-N(1)	128.2(4)
C(10)-H(10A)	0.9500	N(3)-C(1)-O(1)	118.2(4)
C(11)-H(11A)	0.9800	N(1)-C(1)-O(1)	113.6(4)
C(11)-H(11B)	0.9800	N(2)-C(2)-N(1)	125.8(4)
C(11)-H(11C)	0.9800	N(2)-C(2)-N(4)	120.2(4)
C(12)-H(12A)	0.9800	N(1)-C(2)-N(4)	114.1(4)
C(12)-H(12B)	0.9800	N(3)-C(3)-N(5)	120.1(4)
C(12)-H(12C)	0.9800	N(3)-C(3)-N(2)	124.8(4)
C(13)-C(18)	1.378(6)	N(5)-C(3)-N(2)	115.1(4)
C(13)-C(14)	1.390(6)	O(1)-C(4)-H(4B)	109.5
		O(1)-C(4)-H(4C)	109.5
		H(4B)-C(4)-H(4C)	109.5

O(1)-C(4)-H(4D)	109.5
H(4B)-C(4)-H(4D)	109.5
H(4C)-C(4)-H(4D)	109.5
C(10)-C(5)-C(6)	119.0(4)
C(10)-C(5)-N(4)	123.8(4)
C(6)-C(5)-N(4)	117.1(4)
C(7)-C(6)-C(5)	120.3(5)
C(7)-C(6)-H(6A)	119.9
C(5)-C(6)-H(6A)	119.9
C(8)-C(7)-C(6)	119.2(5)
C(8)-C(7)-C(11)	121.5(5)
C(6)-C(7)-C(11)	119.3(6)
C(7)-C(8)-C(9)	121.9(5)
C(7)-C(8)-H(8A)	119.0
C(9)-C(8)-H(8A)	119.0
C(8)-C(9)-C(10)	118.3(5)
C(8)-C(9)-C(12)	121.7(5)
C(10)-C(9)-C(12)	119.9(5)
C(5)-C(10)-C(9)	121.2(5)
C(5)-C(10)-H(10A)	119.4
C(9)-C(10)-H(10A)	119.4
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	119.1(4)
C(18)-C(13)-N(5)	123.9(4)
C(14)-C(13)-N(5)	117.1(4)
C(13)-C(14)-C(15)	121.2(4)
C(13)-C(14)-H(14A)	119.4
C(15)-C(14)-H(14A)	119.4
C(16)-C(15)-C(14)	118.1(4)
C(16)-C(15)-C(19)	121.9(4)
C(14)-C(15)-C(19)	120.0(4)
C(15)-C(16)-C(17)	122.1(5)
C(15)-C(16)-H(16A)	119.0
C(17)-C(16)-H(16A)	119.0
C(16)-C(17)-C(18)	118.9(5)
C(16)-C(17)-C(20)	120.8(5)
C(18)-C(17)-C(20)	120.2(5)
C(13)-C(18)-C(17)	120.6(5)
C(13)-C(18)-H(18A)	119.7
C(17)-C(18)-H(18A)	119.7
C(15)-C(19)-H(19A)	109.5
C(15)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(15)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for ol03a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	60(2)	67(2)	45(2)	-8(2)	-14(2)	-4(2)
N(1)	48(2)	50(2)	28(2)	-3(2)	8(2)	3(2)
N(2)	45(2)	54(2)	28(2)	-6(2)	7(2)	-2(2)
N(3)	44(2)	50(2)	31(2)	-3(2)	8(2)	-2(2)
N(4)	50(2)	61(2)	30(2)	-12(2)	7(2)	-2(2)
N(5)	49(2)	60(2)	31(2)	-13(2)	3(2)	6(2)
C(1)	42(2)	48(3)	35(2)	-1(2)	10(2)	-6(2)
C(2)	44(2)	46(3)	28(2)	0(2)	9(2)	-2(2)
C(3)	49(3)	45(2)	25(2)	-3(2)	8(2)	-3(2)
C(4)	60(4)	120(5)	78(4)	-8(4)	4(3)	19(3)
C(5)	50(3)	51(3)	40(3)	-11(2)	13(2)	-6(2)
C(6)	62(3)	68(3)	40(3)	-19(2)	16(2)	-11(2)
C(7)	59(3)	91(4)	64(4)	-39(3)	24(3)	-14(3)
C(8)	55(3)	92(4)	81(4)	-36(3)	18(3)	9(3)
C(9)	60(3)	77(4)	67(4)	-11(3)	6(3)	14(3)
C(10)	61(3)	65(3)	46(3)	-6(2)	11(2)	6(2)
C(11)	119(4)	163(5)	81(3)	-54(3)	11(3)	44(4)
C(12)	80(4)	114(5)	95(5)	7(4)	1(4)	36(4)
C(13)	52(3)	47(3)	34(2)	-8(2)	2(2)	0(2)
C(14)	53(3)	50(3)	32(2)	-1(2)	3(2)	-1(2)
C(15)	62(3)	57(3)	32(2)	-6(2)	5(2)	-8(2)
C(16)	87(4)	81(4)	43(3)	-24(3)	-4(3)	21(3)
C(17)	110(5)	96(5)	64(4)	-41(3)	-20(3)	48(4)
C(18)	101(4)	79(4)	39(3)	-19(3)	-16(3)	35(3)
C(19)	102(4)	76(4)	29(3)	0(2)	2(3)	-6(3)
C(20)	119(4)	163(5)	81(3)	-54(3)	11(3)	44(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ol03a.

	x	y	z	U(eq)
H(4A)	3466	2331	88	56
H(5A)	4596	3612	3089	56
H(4B)	334	4457	1397	129
H(4C)	1364	4730	1695	129
H(4D)	843	4152	2258	129
H(6A)	4829	2407	-773	68
H(8A)	7201	1544	328	91
H(10A)	5040	1964	1742	68
H(11A)	7126	1774	-1145	181
H(11B)	6500	2473	-1430	181
H(11C)	6105	1656	-1596	181
H(12A)	6382	1207	2317	145
H(12B)	7061	1902	2256	145
H(12C)	7287	1145	1794	145
H(14A)	4660	3709	4572	54
H(16A)	3080	5248	5608	85
H(18A)	2729	4826	3105	89
H(19A)	4257	4674	6497	104
H(19B)	5130	4360	6040	104
H(19C)	4308	3815	6265	104
H(20A)	1659	5675	4804	181
H(20B)	1507	5494	3816	181
H(20C)	2187	6151	4137	181

Table 6. Torsion angles [°] for ol03a.

C(3)-N(3)-C(1)-N(1)	0.5(6)
C(3)-N(3)-C(1)-O(1)	179.8(3)
C(2)-N(1)-C(1)-N(3)	-6.3(6)
C(2)-N(1)-C(1)-O(1)	174.4(3)
C(4)-O(1)-C(1)-N(3)	9.7(6)
C(4)-O(1)-C(1)-N(1)	-170.9(4)
C(3)-N(2)-C(2)-N(1)	0.1(6)
C(3)-N(2)-C(2)-N(4)	178.7(4)
C(1)-N(1)-C(2)-N(2)	5.8(6)
C(1)-N(1)-C(2)-N(4)	-172.8(3)
C(5)-N(4)-C(2)-N(2)	0.3(6)
C(5)-N(4)-C(2)-N(1)	179.0(4)
C(1)-N(3)-C(3)-N(5)	-173.9(4)
C(1)-N(3)-C(3)-N(2)	6.7(6)
C(13)-N(5)-C(3)-N(3)	2.3(7)
C(13)-N(5)-C(3)-N(2)	-178.3(4)
C(2)-N(2)-C(3)-N(3)	-7.0(6)
C(2)-N(2)-C(3)-N(5)	173.7(4)
C(2)-N(4)-C(5)-C(10)	42.2(7)
C(2)-N(4)-C(5)-C(6)	-140.3(4)
C(10)-C(5)-C(6)-C(7)	0.1(7)
N(4)-C(5)-C(6)-C(7)	-177.6(4)
C(5)-C(6)-C(7)-C(8)	-0.3(8)
C(5)-C(6)-C(7)-C(11)	179.0(5)
C(6)-C(7)-C(8)-C(9)	-0.9(9)
C(11)-C(7)-C(8)-C(9)	179.8(6)
C(7)-C(8)-C(9)-C(10)	2.3(9)
C(7)-C(8)-C(9)-C(12)	-178.5(6)
C(6)-C(5)-C(10)-C(9)	1.3(7)
N(4)-C(5)-C(10)-C(9)	178.9(4)
C(8)-C(9)-C(10)-C(5)	-2.5(8)
C(12)-C(9)-C(10)-C(5)	178.2(5)
C(3)-N(5)-C(13)-C(18)	-26.7(7)
C(3)-N(5)-C(13)-C(14)	153.5(4)
C(18)-C(13)-C(14)-C(15)	-0.2(7)
N(5)-C(13)-C(14)-C(15)	179.6(4)
C(13)-C(14)-C(15)-C(16)	1.2(7)
C(13)-C(14)-C(15)-C(19)	179.8(4)
C(14)-C(15)-C(16)-C(17)	-0.8(9)
C(19)-C(15)-C(16)-C(17)	-179.4(6)
C(15)-C(16)-C(17)-C(18)	-0.6(10)
C(15)-C(16)-C(17)-C(20)	176.3(6)
C(14)-C(13)-C(18)-C(17)	-1.2(9)
N(5)-C(13)-C(18)-C(17)	178.9(5)
C(16)-C(17)-C(18)-C(13)	1.6(10)
C(20)-C(17)-C(18)-C(13)	-175.3(6)

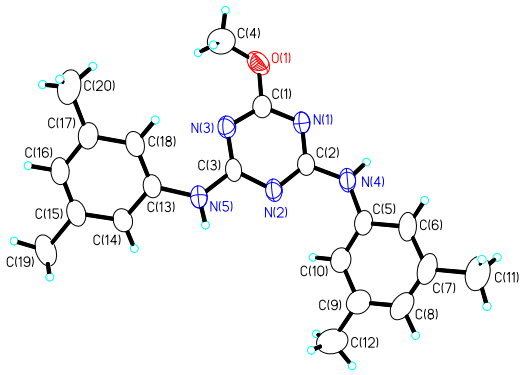
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for ol03a [Å and °].

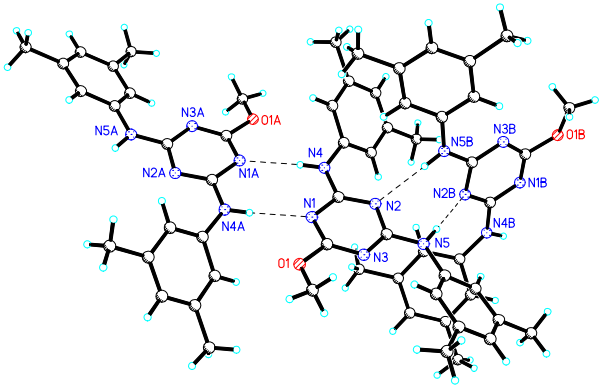
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4A)...N(1)#1	0.88	2.20	3.076(5)	176.6
N(5)-H(5A)...N(2)#2	0.88	2.20	3.078(5)	176.8

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y+1/2,-z #2 -x+1,y,-z+1/2



a



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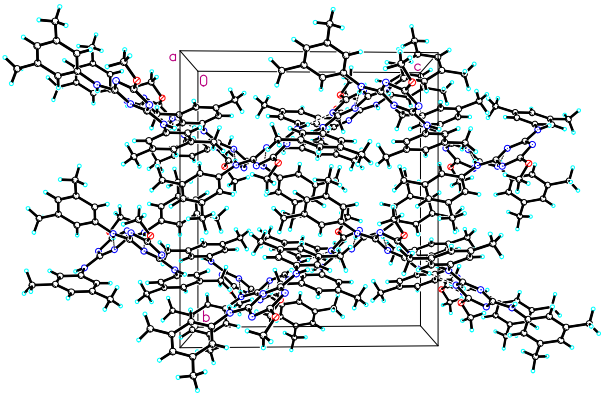


c

Figure S1. ORTEP plots of the crystal structure of compound **1**. Displacement ellipsoids for non-H atoms are shown at the 50% probability level and H atoms are represented by circles of arbitrary size. a) Single molecule of **1**. b) Hydrogen bonding pattern. c) Unit cell packing along the *a* axis.

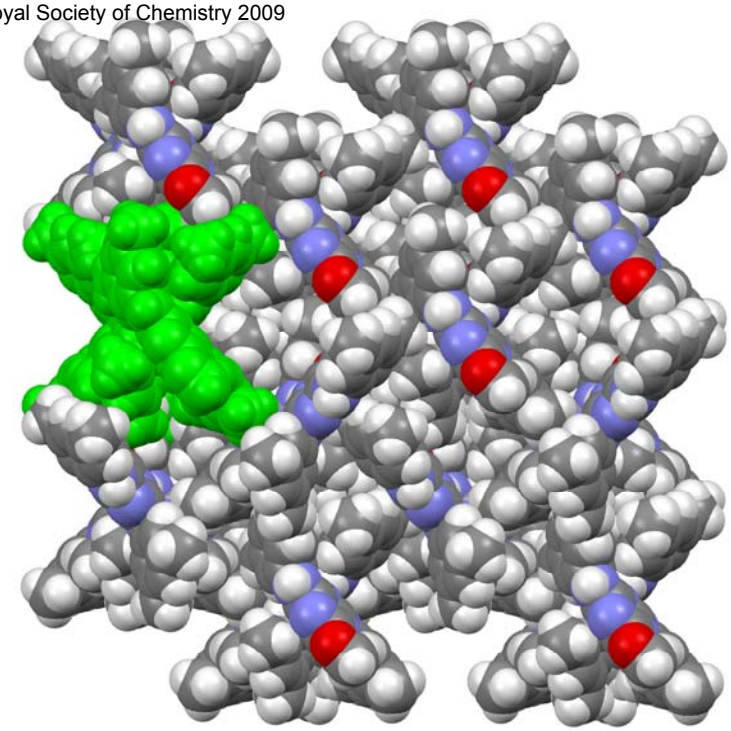


Figure S2. View along the *ac* diagonal of a 2 x 2 x 2 array of unit cells in the crystal structure of compound **1**. Carbon atoms are shown in grey, hydrogen atoms in white, nitrogen atoms in blue and oxygen atoms in red. One hydrogen-bonded ribbon with a hourglass-shaped cross-section is depicted in green for simplifying visualization.

Additional Crystal Structure Data for Compound 2

Table 1. Crystal data and structure refinement for ol01

Identification code	ol01	
Empirical formula	C20 H21 N3 O3	
Formula weight	351.40	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.4082(6) Å	α= 100.4910(10)°.
	b = 15.0816(11) Å	β= 100.3680(10)°.
	c = 16.0829(12) Å	γ = 106.0730(10)°.
Volume	1868.8(2) $Å^3$	
Z	4	
Density (calculated)	1.249 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	744	
Crystal size	0.37 x 0.35 x 0.11 mm^3	
Theta range for data collection	1.33 to 26.00°.	
Index ranges	-10<=h<=10, -18<=k<=18, -19<=l<=19	
Reflections collected	19775	
Independent reflections	7314 [R(int) = 0.0233]	
Completeness to theta = 26.00°	99.5 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9905 and 0.9694	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7314 / 0 / 480	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0401, wR2 = 0.1047	
R indices (all data)	R1 = 0.0635, wR2 = 0.1198	
Extinction coefficient	0.0082(10)	
Largest diff. peak and hole	0.177 and -0.158 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ol01. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2113(1)	8791(1)	8217(1)	57(1)
O(2)	6133(2)	8076(1)	9980(1)	62(1)
O(3)	7546(2)	10805(1)	9107(1)	58(1)
O(4)	-2882(2)	5438(1)	5602(1)	56(1)
O(5)	1790(2)	7307(1)	5011(1)	60(1)
O(6)	-1508(2)	4571(1)	3060(1)	61(1)
N(1)	4028(2)	8412(1)	9096(1)	47(1)
N(2)	6903(2)	9437(1)	9578(1)	49(1)
N(3)	4846(2)	9856(1)	8643(1)	47(1)
N(4)	-482(2)	6415(1)	5343(1)	49(1)
N(5)	-2222(2)	4945(1)	4357(1)	48(1)
N(6)	123(2)	5943(1)	3974(1)	50(1)
C(1)	3743(2)	9055(1)	8667(1)	44(1)
C(2)	5634(2)	8657(1)	9528(1)	46(1)
C(3)	6411(2)	10002(1)	9119(1)	45(1)
C(12)	1532(2)	9338(1)	7678(1)	47(1)
C(17)	1628(2)	10262(1)	8016(1)	54(1)
C(16)	901(2)	10738(1)	7476(1)	55(1)
C(15)	89(2)	10255(1)	6620(1)	59(1)
C(14)	-24(2)	9317(1)	6283(1)	55(1)
C(13)	735(2)	8859(1)	6833(1)	51(1)
C(19)	969(3)	11751(2)	7810(2)	82(1)
C(18)	-989(3)	8801(2)	5365(1)	80(1)
C(4)	4883(2)	7242(1)	10010(1)	53(1)
C(9)	4650(2)	6409(1)	9421(1)	58(1)
C(8)	3477(2)	5574(1)	9465(1)	60(1)
C(7)	2602(3)	5620(1)	10111(1)	63(1)
C(6)	2855(2)	6462(2)	10714(1)	63(1)
C(5)	4020(2)	7285(1)	10654(1)	59(1)
C(11)	3173(3)	4647(2)	8817(2)	86(1)
C(10)	1869(3)	6492(2)	11408(2)	99(1)
C(20)	9243(2)	11044(2)	9648(2)	76(1)
C(22)	433(2)	6512(1)	4749(1)	47(1)
C(21)	-1796(2)	5624(1)	5090(1)	45(1)

C(23)	-1221(2)	5162(1)	3829(1)	47(1)
C(32)	2927(2)	7512(1)	4467(1)	48(1)
C(33)	3205(2)	8377(1)	4270(1)	57(1)
C(34)	4366(2)	8651(1)	3776(1)	59(1)
C(35)	5214(2)	8031(1)	3506(1)	59(1)
C(36)	4943(2)	7159(1)	3718(1)	56(1)
C(37)	3787(2)	6904(1)	4215(1)	53(1)
C(38)	4689(4)	9601(2)	3535(2)	98(1)
C(39)	5889(3)	6500(2)	3411(2)	91(1)
C(24)	-2609(2)	6124(1)	6385(1)	48(1)
C(29)	-1818(2)	5990(1)	7149(1)	56(1)
C(28)	-1578(2)	6643(1)	7923(1)	59(1)
C(27)	-2184(2)	7401(1)	7896(1)	56(1)
C(26)	-3014(2)	7529(1)	7123(1)	52(1)
C(25)	-3230(2)	6872(1)	6355(1)	51(1)
C(31)	-609(4)	6542(2)	8773(2)	96(1)
C(30)	-3673(3)	8359(1)	7114(2)	77(1)
C(40)	-2810(3)	3658(2)	2873(1)	78(1)

Table 3. Bond lengths [Å] and angles [°] for ol01.

O(1)-C(1)	1.3402(19)	C(19)-H(10B)	0.9600
O(1)-C(12)	1.4155(19)	C(19)-H(10C)	0.9600
O(2)-C(2)	1.3406(19)	C(18)-H(11A)	0.9600
O(2)-C(4)	1.414(2)	C(18)-H(11B)	0.9600
O(3)-C(3)	1.3236(19)	C(18)-H(11C)	0.9600
O(3)-C(20)	1.442(2)	C(4)-C(9)	1.370(3)
O(4)-C(21)	1.3433(19)	C(4)-C(5)	1.370(3)
O(4)-C(24)	1.4131(19)	C(9)-C(8)	1.390(3)
O(5)-C(22)	1.3426(19)	C(9)-H(13)	0.9300
O(5)-C(32)	1.4170(19)	C(8)-C(7)	1.380(3)
O(6)-C(23)	1.3242(19)	C(8)-C(11)	1.510(3)
O(6)-C(40)	1.442(2)	C(7)-C(6)	1.387(3)
N(1)-C(2)	1.317(2)	C(7)-H(15)	0.9300
N(1)-C(1)	1.336(2)	C(6)-C(5)	1.383(3)
N(2)-C(3)	1.325(2)	C(6)-C(10)	1.508(3)
N(2)-C(2)	1.330(2)	C(5)-H(17)	0.9300
N(3)-C(1)	1.315(2)	C(11)-H(18A)	0.9600
N(3)-C(3)	1.335(2)	C(11)-H(18B)	0.9600
N(4)-C(21)	1.319(2)	C(11)-H(18C)	0.9600
N(4)-C(22)	1.334(2)	C(10)-H(19A)	0.9600
N(5)-C(23)	1.320(2)	C(10)-H(19B)	0.9600
N(5)-C(21)	1.331(2)	C(10)-H(19C)	0.9600
N(6)-C(22)	1.314(2)	C(20)-H(20A)	0.9600
N(6)-C(23)	1.337(2)	C(20)-H(20B)	0.9600
C(12)-C(13)	1.366(2)	C(20)-H(20C)	0.9600
C(12)-C(17)	1.375(2)	C(32)-C(33)	1.365(2)
C(17)-C(16)	1.386(2)	C(32)-C(37)	1.367(2)
C(17)-H(5)	0.9300	C(33)-C(34)	1.388(3)
C(16)-C(15)	1.383(3)	C(33)-H(25)	0.9300
C(16)-C(19)	1.506(3)	C(34)-C(35)	1.381(3)
C(15)-C(14)	1.390(3)	C(34)-C(38)	1.517(3)
C(15)-H(7)	0.9300	C(35)-C(36)	1.387(3)
C(14)-C(13)	1.389(2)	C(35)-H(27)	0.9300
C(14)-C(18)	1.499(3)	C(36)-C(37)	1.384(2)
C(13)-H(9)	0.9300	C(36)-C(39)	1.506(3)
C(19)-H(10A)	0.9600	C(37)-H(29)	0.9300
		C(38)-H(30A)	0.9600
		C(38)-H(30B)	0.9600

C(38)-H(30C)	0.9600	N(1)-C(1)-O(1)	111.58(14)
C(39)-H(31A)	0.9600	N(1)-C(2)-N(2)	127.84(15)
C(39)-H(31B)	0.9600	N(1)-C(2)-O(2)	119.38(15)
C(39)-H(31C)	0.9600	N(2)-C(2)-O(2)	112.77(14)
C(24)-C(29)	1.365(2)	O(3)-C(3)-N(2)	119.21(15)
C(24)-C(25)	1.373(2)	O(3)-C(3)-N(3)	113.79(14)
C(29)-C(28)	1.384(3)	N(2)-C(3)-N(3)	127.01(15)
C(29)-H(33)	0.9300	C(13)-C(12)-C(17)	123.07(16)
C(28)-C(27)	1.379(3)	C(13)-C(12)-O(1)	115.42(15)
C(28)-C(31)	1.516(3)	C(17)-C(12)-O(1)	121.22(15)
C(27)-C(26)	1.385(3)	C(12)-C(17)-C(16)	118.84(17)
C(27)-H(35)	0.9300	C(12)-C(17)-H(5)	120.6
C(26)-C(25)	1.384(2)	C(16)-C(17)-H(5)	120.6
C(26)-C(30)	1.503(3)	C(15)-C(16)-C(17)	118.34(17)
C(25)-H(37)	0.9300	C(15)-C(16)-C(19)	120.46(18)
C(31)-H(38A)	0.9600	C(17)-C(16)-C(19)	121.21(18)
C(31)-H(38B)	0.9600	C(16)-C(15)-C(14)	122.67(17)
C(31)-H(38C)	0.9600	C(16)-C(15)-H(7)	118.7
C(30)-H(39A)	0.9600	C(14)-C(15)-H(7)	118.7
C(30)-H(39B)	0.9600	C(13)-C(14)-C(15)	118.01(17)
C(30)-H(39C)	0.9600	C(13)-C(14)-C(18)	120.79(18)
C(40)-H(40A)	0.9600	C(15)-C(14)-C(18)	121.16(17)
C(40)-H(40B)	0.9600	C(12)-C(13)-C(14)	119.07(17)
C(40)-H(40C)	0.9600	C(12)-C(13)-H(9)	120.5
		C(14)-C(13)-H(9)	120.5
C(1)-O(1)-C(12)	121.63(13)	C(16)-C(19)-H(10A)	109.5
C(2)-O(2)-C(4)	118.20(13)	C(16)-C(19)-H(10B)	109.5
C(3)-O(3)-C(20)	117.24(14)	H(10A)-C(19)-H(10B)	109.5
C(21)-O(4)-C(24)	118.28(13)	C(16)-C(19)-H(10C)	109.5
C(22)-O(5)-C(32)	120.04(13)	H(10A)-C(19)-H(10C)	109.5
C(23)-O(6)-C(40)	117.62(14)	H(10B)-C(19)-H(10C)	109.5
C(2)-N(1)-C(1)	112.12(14)	C(14)-C(18)-H(11A)	109.5
C(3)-N(2)-C(2)	112.60(14)	C(14)-C(18)-H(11B)	109.5
C(1)-N(3)-C(3)	112.60(14)	H(11A)-C(18)-H(11B)	109.5
C(21)-N(4)-C(22)	112.26(14)	C(14)-C(18)-H(11C)	109.5
C(23)-N(5)-C(21)	112.48(14)	H(11A)-C(18)-H(11C)	109.5
C(22)-N(6)-C(23)	112.64(14)	H(11B)-C(18)-H(11C)	109.5
N(3)-C(1)-N(1)	127.83(15)	C(9)-C(4)-C(5)	122.50(17)
N(3)-C(1)-O(1)	120.59(14)	C(9)-C(4)-O(2)	118.48(17)

C(5)-C(4)-O(2)	118.92(16)	N(5)-C(21)-O(4)	112.73(14)
C(4)-C(9)-C(8)	119.27(18)	N(5)-C(23)-O(6)	119.90(15)
C(4)-C(9)-H(13)	120.4	N(5)-C(23)-N(6)	127.17(15)
C(8)-C(9)-H(13)	120.4	O(6)-C(23)-N(6)	112.93(14)
C(7)-C(8)-C(9)	118.10(18)	C(33)-C(32)-C(37)	122.34(16)
C(7)-C(8)-C(11)	121.38(19)	C(33)-C(32)-O(5)	116.29(15)
C(9)-C(8)-C(11)	120.5(2)	C(37)-C(32)-O(5)	121.18(15)
C(8)-C(7)-C(6)	122.58(18)	C(32)-C(33)-C(34)	119.83(17)
C(8)-C(7)-H(15)	118.7	C(32)-C(33)-H(25)	120.1
C(6)-C(7)-H(15)	118.7	C(34)-C(33)-H(25)	120.1
C(5)-C(6)-C(7)	118.29(19)	C(35)-C(34)-C(33)	118.02(16)
C(5)-C(6)-C(10)	120.3(2)	C(35)-C(34)-C(38)	120.81(18)
C(7)-C(6)-C(10)	121.4(2)	C(33)-C(34)-C(38)	121.17(18)
C(4)-C(5)-C(6)	119.25(18)	C(34)-C(35)-C(36)	121.90(17)
C(4)-C(5)-H(17)	120.4	C(34)-C(35)-H(27)	119.1
C(6)-C(5)-H(17)	120.4	C(36)-C(35)-H(27)	119.1
C(8)-C(11)-H(18A)	109.5	C(37)-C(36)-C(35)	119.00(17)
C(8)-C(11)-H(18B)	109.5	C(37)-C(36)-C(39)	120.55(18)
H(18A)-C(11)-H(18B)	109.5	C(35)-C(36)-C(39)	120.45(18)
C(8)-C(11)-H(18C)	109.5	C(32)-C(37)-C(36)	118.88(16)
H(18A)-C(11)-H(18C)	109.5	C(32)-C(37)-H(29)	120.6
H(18B)-C(11)-H(18C)	109.5	C(36)-C(37)-H(29)	120.6
C(6)-C(10)-H(19A)	109.5	C(34)-C(38)-H(30A)	109.5
C(6)-C(10)-H(19B)	109.5	C(34)-C(38)-H(30B)	109.5
H(19A)-C(10)-H(19B)	109.5	H(30A)-C(38)-H(30B)	109.5
C(6)-C(10)-H(19C)	109.5	C(34)-C(38)-H(30C)	109.5
H(19A)-C(10)-H(19C)	109.5	H(30A)-C(38)-H(30C)	109.5
H(19B)-C(10)-H(19C)	109.5	H(30B)-C(38)-H(30C)	109.5
O(3)-C(20)-H(20A)	109.5	C(36)-C(39)-H(31A)	109.5
O(3)-C(20)-H(20B)	109.5	C(36)-C(39)-H(31B)	109.5
H(20A)-C(20)-H(20B)	109.5	H(31A)-C(39)-H(31B)	109.5
O(3)-C(20)-H(20C)	109.5	C(36)-C(39)-H(31C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(31A)-C(39)-H(31C)	109.5
H(20B)-C(20)-H(20C)	109.5	H(31B)-C(39)-H(31C)	109.5
N(6)-C(22)-N(4)	127.57(15)	C(29)-C(24)-C(25)	122.36(16)
N(6)-C(22)-O(5)	119.95(14)	C(29)-C(24)-O(4)	118.72(15)
N(4)-C(22)-O(5)	112.46(14)	C(25)-C(24)-O(4)	118.83(16)
N(4)-C(21)-N(5)	127.67(15)	C(24)-C(29)-C(28)	119.42(17)
N(4)-C(21)-O(4)	119.60(14)	C(24)-C(29)-H(33)	120.3

C(28)-C(29)-H(33)	120.3
C(27)-C(28)-C(29)	118.43(17)
C(27)-C(28)-C(31)	121.20(19)
C(29)-C(28)-C(31)	120.32(19)
C(28)-C(27)-C(26)	122.24(17)
C(28)-C(27)-H(35)	118.9
C(26)-C(27)-H(35)	118.9
C(25)-C(26)-C(27)	118.42(16)
C(25)-C(26)-C(30)	120.46(18)
C(27)-C(26)-C(30)	121.13(17)
C(24)-C(25)-C(26)	119.11(17)
C(24)-C(25)-H(37)	120.4
C(26)-C(25)-H(37)	120.4
C(28)-C(31)-H(38A)	109.5
C(28)-C(31)-H(38B)	109.5
H(38A)-C(31)-H(38B)	109.5
C(28)-C(31)-H(38C)	109.5
H(38A)-C(31)-H(38C)	109.5
H(38B)-C(31)-H(38C)	109.5
C(26)-C(30)-H(39A)	109.5
C(26)-C(30)-H(39B)	109.5
H(39A)-C(30)-H(39B)	109.5
C(26)-C(30)-H(39C)	109.5
H(39A)-C(30)-H(39C)	109.5
H(39B)-C(30)-H(39C)	109.5
O(6)-C(40)-H(40A)	109.5
O(6)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
O(6)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for ol01. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	46(1)	56(1)	66(1)	28(1)	1(1)	11(1)
O(2)	51(1)	57(1)	74(1)	30(1)	-1(1)	12(1)
O(3)	49(1)	51(1)	72(1)	19(1)	17(1)	9(1)
O(4)	62(1)	43(1)	64(1)	7(1)	32(1)	11(1)
O(5)	62(1)	50(1)	60(1)	7(1)	27(1)	5(1)
O(6)	56(1)	66(1)	48(1)	-1(1)	13(1)	11(1)
N(1)	45(1)	45(1)	48(1)	15(1)	5(1)	13(1)
N(2)	44(1)	49(1)	51(1)	12(1)	8(1)	12(1)
N(3)	45(1)	46(1)	52(1)	15(1)	13(1)	15(1)
N(4)	53(1)	43(1)	52(1)	12(1)	21(1)	14(1)
N(5)	50(1)	45(1)	52(1)	9(1)	17(1)	17(1)
N(6)	49(1)	54(1)	47(1)	11(1)	15(1)	14(1)
C(1)	42(1)	46(1)	43(1)	11(1)	9(1)	15(1)
C(2)	48(1)	46(1)	43(1)	11(1)	7(1)	17(1)
C(3)	47(1)	42(1)	47(1)	10(1)	17(1)	14(1)
C(12)	39(1)	53(1)	54(1)	23(1)	9(1)	15(1)
C(17)	51(1)	59(1)	50(1)	14(1)	10(1)	18(1)
C(16)	55(1)	58(1)	60(1)	21(1)	20(1)	25(1)
C(15)	59(1)	70(1)	62(1)	34(1)	19(1)	29(1)
C(14)	55(1)	62(1)	50(1)	21(1)	13(1)	17(1)
C(13)	47(1)	51(1)	56(1)	17(1)	13(1)	16(1)
C(19)	105(2)	70(1)	88(2)	24(1)	31(1)	45(1)
C(18)	94(2)	85(2)	53(1)	21(1)	5(1)	24(1)
C(4)	51(1)	50(1)	56(1)	21(1)	1(1)	17(1)
C(9)	58(1)	63(1)	55(1)	19(1)	9(1)	23(1)
C(8)	62(1)	53(1)	62(1)	14(1)	2(1)	22(1)
C(7)	61(1)	55(1)	67(1)	22(1)	5(1)	11(1)
C(6)	57(1)	70(1)	60(1)	20(1)	10(1)	19(1)
C(5)	59(1)	53(1)	61(1)	11(1)	3(1)	21(1)
C(11)	95(2)	61(1)	91(2)	3(1)	9(1)	27(1)
C(10)	85(2)	113(2)	90(2)	14(2)	33(1)	15(2)
C(20)	50(1)	77(1)	85(2)	23(1)	9(1)	-2(1)
C(22)	47(1)	43(1)	52(1)	13(1)	16(1)	15(1)
C(21)	49(1)	42(1)	51(1)	14(1)	18(1)	20(1)

C(23)	45(1)	51(1)	46(1)	10(1)	11(1)	19(1)
C(32)	45(1)	48(1)	49(1)	13(1)	14(1)	9(1)
C(33)	56(1)	50(1)	73(1)	19(1)	21(1)	22(1)
C(34)	58(1)	55(1)	72(1)	30(1)	18(1)	17(1)
C(35)	51(1)	69(1)	62(1)	25(1)	21(1)	19(1)
C(36)	47(1)	58(1)	64(1)	15(1)	13(1)	21(1)
C(37)	53(1)	46(1)	60(1)	19(1)	12(1)	15(1)
C(38)	107(2)	79(2)	138(2)	66(2)	56(2)	38(2)
C(39)	85(2)	88(2)	126(2)	30(2)	47(2)	49(1)
C(24)	51(1)	41(1)	55(1)	12(1)	27(1)	12(1)
C(29)	59(1)	50(1)	69(1)	22(1)	26(1)	21(1)
C(28)	60(1)	60(1)	58(1)	20(1)	19(1)	15(1)
C(27)	60(1)	51(1)	54(1)	7(1)	23(1)	10(1)
C(26)	54(1)	42(1)	66(1)	13(1)	29(1)	16(1)
C(25)	55(1)	51(1)	54(1)	19(1)	23(1)	19(1)
C(31)	120(2)	100(2)	70(2)	30(1)	10(1)	38(2)
C(30)	93(2)	61(1)	92(2)	18(1)	41(1)	39(1)
C(40)	72(1)	70(1)	62(1)	-9(1)	12(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ol01.

	x	y	z	U(eq)
H(5)	2172	10563	8597	64
H(7)	-401	10571	6255	70
H(9)	702	8235	6628	61
H(10A)	-107	11759	7928	123
H(10B)	1200	12100	7379	123
H(10C)	1857	12040	8336	123
H(11A)	-1964	8290	5370	119
H(11B)	-260	8548	5065	119
H(11C)	-1360	9235	5071	119
H(13)	5269	6402	8997	70
H(15)	1813	5065	10144	76
H(17)	4216	7861	11047	71
H(18A)	2789	4126	9075	129
H(18B)	4216	4639	8657	129
H(18C)	2319	4587	8306	129
H(19A)	2182	7135	11748	149
H(19B)	2128	6095	11781	149
H(19C)	668	6266	11139	149
H(20A)	9185	11054	10240	114
H(20B)	9919	11660	9620	114
H(20C)	9756	10578	9445	114
H(25)	2619	8781	4465	69
H(27)	5990	8202	3172	70
H(29)	3598	6328	4374	64
H(30A)	5842	9823	3481	147
H(30B)	4512	10055	3982	147
H(30C)	3916	9526	2990	147
H(31A)	7095	6818	3621	137
H(31B)	5597	6319	2785	137
H(31C)	5577	5941	3630	137
H(33)	-1443	5465	7149	67
H(35)	-2030	7842	8415	67
H(37)	-3788	6936	5826	61

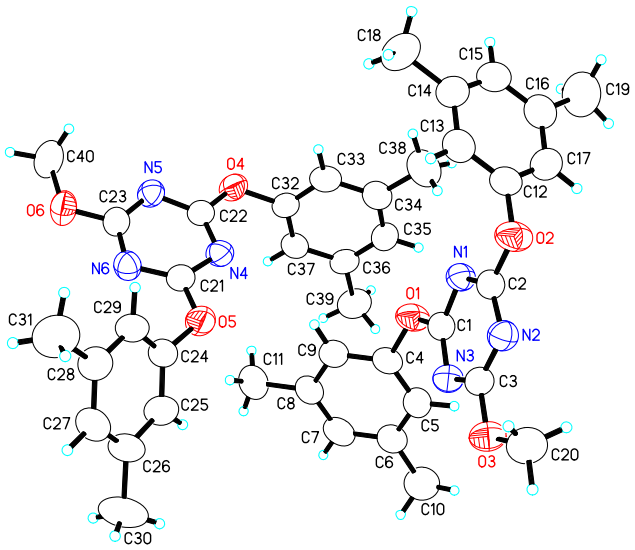
H(38A)	525	6988	8935	144
H(38B)	-551	5906	8700	144
H(38C)	-1188	6667	9222	144
H(39A)	-4075	8378	6522	115
H(39B)	-2771	8939	7415	115
H(39C)	-4594	8289	7399	115
H(40A)	-2568	3339	3322	116
H(40B)	-2829	3279	2321	116
H(40C)	-3901	3749	2853	116

Table 6. Torsion angles [°] for ol01.

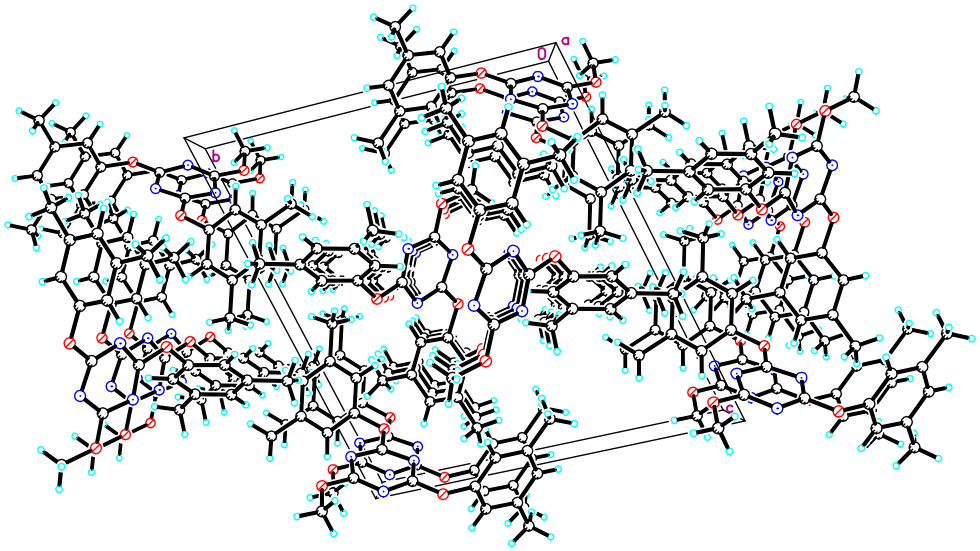
C(3)-N(3)-C(1)-N(1)	0.0(2)
C(3)-N(3)-C(1)-O(1)	-179.24(14)
C(2)-N(1)-C(1)-N(3)	-0.4(2)
C(2)-N(1)-C(1)-O(1)	178.89(14)
C(12)-O(1)-C(1)-N(3)	2.4(2)
C(12)-O(1)-C(1)-N(1)	-176.90(14)
C(1)-N(1)-C(2)-N(2)	0.7(2)
C(1)-N(1)-C(2)-O(2)	-178.71(14)
C(3)-N(2)-C(2)-N(1)	-0.6(2)
C(3)-N(2)-C(2)-O(2)	178.90(14)
C(4)-O(2)-C(2)-N(1)	-3.3(2)
C(4)-O(2)-C(2)-N(2)	177.18(15)
C(20)-O(3)-C(3)-N(2)	-3.9(2)
C(20)-O(3)-C(3)-N(3)	176.22(15)
C(2)-N(2)-C(3)-O(3)	-179.81(14)
C(2)-N(2)-C(3)-N(3)	0.0(2)
C(1)-N(3)-C(3)-O(3)	-179.93(13)
C(1)-N(3)-C(3)-N(2)	0.2(2)
C(1)-O(1)-C(12)-C(13)	125.25(17)
C(1)-O(1)-C(12)-C(17)	-60.8(2)
C(13)-C(12)-C(17)-C(16)	-0.7(3)
O(1)-C(12)-C(17)-C(16)	-174.17(15)
C(12)-C(17)-C(16)-C(15)	0.8(3)
C(12)-C(17)-C(16)-C(19)	-179.91(18)
C(17)-C(16)-C(15)-C(14)	0.0(3)
C(19)-C(16)-C(15)-C(14)	-179.32(18)
C(16)-C(15)-C(14)-C(13)	-0.9(3)
C(16)-C(15)-C(14)-C(18)	176.94(18)
C(17)-C(12)-C(13)-C(14)	-0.3(3)
O(1)-C(12)-C(13)-C(14)	173.59(14)
C(15)-C(14)-C(13)-C(12)	1.0(3)
C(18)-C(14)-C(13)-C(12)	-176.83(18)
C(2)-O(2)-C(4)-C(9)	95.17(19)
C(2)-O(2)-C(4)-C(5)	-88.4(2)
C(5)-C(4)-C(9)-C(8)	1.0(3)
O(2)-C(4)-C(9)-C(8)	177.30(15)
C(4)-C(9)-C(8)-C(7)	-0.6(3)
C(4)-C(9)-C(8)-C(11)	179.08(18)
C(9)-C(8)-C(7)-C(6)	-0.2(3)
C(11)-C(8)-C(7)-C(6)	-179.88(18)
C(8)-C(7)-C(6)-C(5)	0.6(3)
C(8)-C(7)-C(6)-C(10)	179.5(2)
C(9)-C(4)-C(5)-C(6)	-0.6(3)
O(2)-C(4)-C(5)-C(6)	-176.89(15)
C(7)-C(6)-C(5)-C(4)	-0.2(3)
C(10)-C(6)-C(5)-C(4)	-179.06(19)
C(23)-N(6)-C(22)-N(4)	-4.4(2)
C(23)-N(6)-C(22)-O(5)	176.96(14)
C(21)-N(4)-C(22)-N(6)	2.4(2)
C(21)-N(4)-C(22)-O(5)	-178.86(14)
C(32)-O(5)-C(22)-N(6)	-2.6(2)
C(32)-O(5)-C(22)-N(4)	178.55(14)
C(22)-N(4)-C(21)-N(5)	2.5(2)
C(22)-N(4)-C(21)-O(4)	-177.58(14)
C(23)-N(5)-C(21)-N(4)	-4.5(2)
C(23)-N(5)-C(21)-O(4)	175.61(13)
C(24)-O(4)-C(21)-N(4)	2.6(2)
C(24)-O(4)-C(21)-N(5)	-177.50(14)
C(21)-N(5)-C(23)-O(6)	-178.11(14)
C(21)-N(5)-C(23)-N(6)	2.0(2)
C(40)-O(6)-C(23)-N(5)	-6.5(2)
C(40)-O(6)-C(23)-N(6)	173.42(16)
C(22)-N(6)-C(23)-N(5)	2.0(2)
C(22)-N(6)-C(23)-O(6)	-177.95(14)
C(22)-O(5)-C(32)-C(33)	125.09(17)
C(22)-O(5)-C(32)-C(37)	-59.7(2)
C(37)-C(32)-C(33)-C(34)	1.7(3)
O(5)-C(32)-C(33)-C(34)	176.84(16)
C(32)-C(33)-C(34)-C(35)	-0.5(3)
C(32)-C(33)-C(34)-C(38)	179.2(2)
C(33)-C(34)-C(35)-C(36)	-0.4(3)
C(38)-C(34)-C(35)-C(36)	179.9(2)
C(34)-C(35)-C(36)-C(37)	0.1(3)
C(34)-C(35)-C(36)-C(39)	179.9(2)

C(33)-C(32)-C(37)-C(36)	-2.1(3)	C(31)-C(28)-C(27)-C(26)	177.44(19)
O(5)-C(32)-C(37)-C(36)	-176.95(15)	C(28)-C(27)-C(26)-C(25)	-0.3(3)
C(35)-C(36)-C(37)-C(32)	1.1(3)	C(28)-C(27)-C(26)-C(30)	179.56(17)
C(39)-C(36)-C(37)-C(32)	-178.69(19)	C(29)-C(24)-C(25)-C(26)	1.6(3)
C(21)-O(4)-C(24)-C(29)	-99.82(18)	O(4)-C(24)-C(25)-C(26)	177.98(14)
C(21)-O(4)-C(24)-C(25)	83.64(19)	C(27)-C(26)-C(25)-C(24)	-0.4(2)
C(25)-C(24)-C(29)-C(28)	-2.1(3)	C(30)-C(26)-C(25)-C(24)	179.79(16)
O(4)-C(24)-C(29)-C(28)	-178.47(15)		
C(24)-C(29)-C(28)-C(27)	1.3(3)		
C(24)-C(29)-C(28)-C(31)	-176.34(18)		
C(29)-C(28)-C(27)-C(26)	-0.2(3)		

Symmetry transformations used to generate equivalent atoms:



a



b

Figure S3. ORTEP plots of the crystal structure of compound **2**. Displacement ellipsoids for non-H atoms are shown at the 50% probability level and H atoms are represented by circles of arbitrary size. a) Both symmetry-independent molecules of **2**. b) Unit cell packing along the *a* axis.

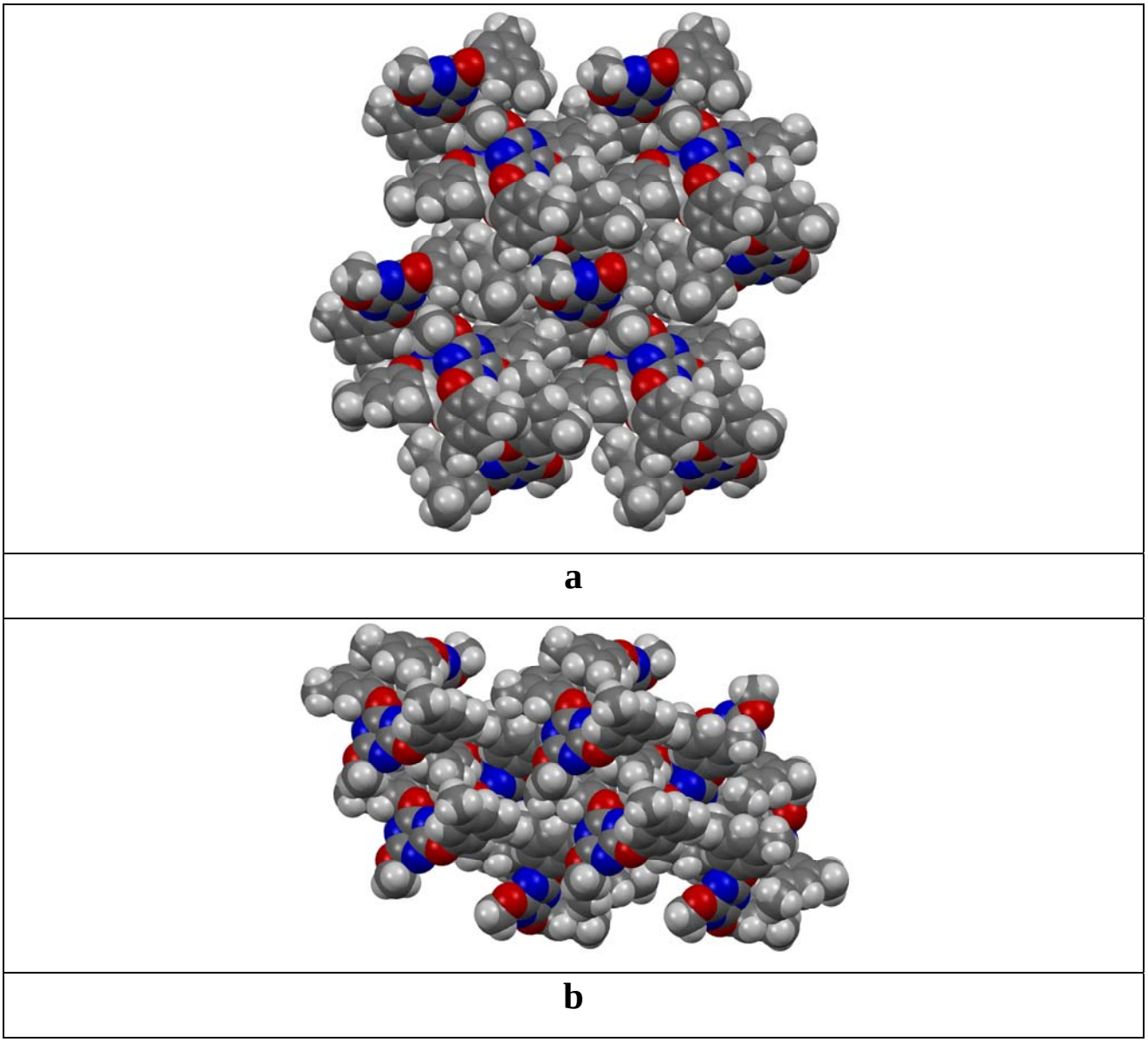


Figure S4. a) View along the *a* axis, and b) view along the *c* axis of a 2 x 2 x 2 array of unit cells in the crystal structure of compound **2**. Carbon atoms are shown in grey, hydrogen atoms in white, nitrogen atoms in blue and oxygen atoms in red.

Additional Crystal Structure Data for Compound 3

Table 1. Crystal data and structure refinement for ol04

Identification code	ol04	
Empirical formula	C20 H20 Cl N5.5	
Formula weight	372.87	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/m	
Unit cell dimensions	a = 5.9733(7) Å	α= 90°.
	b = 30.794(4) Å	β= 96.178(2)°.
	c = 10.4696(12) Å	γ = 90°.
Volume	1914.6(4) $Å^3$	
Z	4	
Density (calculated)	1.088 Mg/m^3	
Absorption coefficient	0.199 mm^{-1}	
F(000)	644	
Crystal size	0.35 x 0.15 x 0.08 mm^3	
Theta range for data collection	1.32 to 26.00°.	
Index ranges	-7<=h<=7, -37<=k<=37, -12<=l<=12	
Reflections collected	19889	
Independent reflections	3830 [R(int) = 0.0420]	
Completeness to theta = 26.00°	99.9 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9842 and 0.9336	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3830 / 2 / 455	
Goodness-of-fit on F^2	1.100	
Final R indices [I>2sigma(I)]	R1 = 0.0808, wR2 = 0.2254	
R indices (all data)	R1 = 0.0998, wR2 = 0.2403	
Largest diff. peak and hole	0.505 and -0.309 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ol04. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	492(2)	1792(1)	1804(2)	33(1)
Cl(2)	573(2)	8195(1)	4788(2)	31(1)
N(1)	-1614(6)	2500	2560(3)	28(1)
N(2)	315(8)	3132(2)	3119(5)	27(1)
N(3)	2391(5)	2500	2609(3)	26(1)
N(4)	-3567(8)	3081(2)	3015(5)	27(1)
N(5)	4189(8)	3151(2)	3167(5)	29(1)
N(6)	-1475(5)	7500	3877(3)	24(1)
N(7)	470(8)	6892(2)	3130(5)	26(1)
N(8)	2522(5)	7500	3932(3)	26(1)
N(9)	-3429(8)	6911(2)	3080(5)	28(1)
N(10)	4373(8)	6948(2)	3139(5)	28(1)
N(11)	610(13)	7349(2)	816(7)	67(2)
C(1)	401(9)	2316(2)	2395(5)	23(1)
C(2)	-1555(9)	2897(2)	2909(6)	24(1)
C(3)	2229(9)	2928(2)	2973(6)	25(1)
C(4)	-3886(9)	3536(2)	3239(6)	26(1)
C(5)	-5474(13)	3655(3)	4083(8)	28(2)
C(6)	-5934(13)	4094(3)	4281(6)	29(1)
C(7)	-4750(20)	4412(4)	3655(13)	24(3)
C(8)	-3144(19)	4280(5)	2850(16)	29(3)
C(9)	-2736(12)	3847(2)	2625(6)	28(1)
C(10)	-7708(14)	4232(3)	5154(9)	47(2)
C(11)	-1808(19)	4600(4)	2152(12)	47(2)
C(12)	4357(11)	3607(2)	3440(9)	23(2)
C(13)	3011(10)	3804(2)	4268(6)	29(1)
C(14)	3137(14)	4253(3)	4484(8)	33(2)
C(15)	4720(30)	4501(6)	3892(18)	40(4)
C(16)	6090(20)	4305(5)	3042(17)	33(3)
C(17)	5875(12)	3847(2)	2816(7)	31(1)
C(18)	1693(13)	4472(3)	5384(8)	43(2)
C(19)	7724(19)	4597(4)	2366(12)	43(2)
C(20)	553(9)	7679(2)	4127(5)	23(1)
C(21)	-1412(9)	7100(2)	3353(6)	24(1)

C(22)	2369(9)	7116(2)	3400(6)	24(1)
C(23)	-3893(14)	6510(2)	2418(9)	27(1)
C(24)	-5681(15)	6261(3)	2751(8)	27(2)
C(25)	-6210(50)	5865(11)	2173(18)	31(4)
C(26)	-5050(30)	5733(6)	1140(19)	31(3)
C(27)	-3280(20)	5983(4)	784(9)	29(2)
C(28)	-2684(13)	6372(4)	1395(9)	27(2)
C(29)	-8073(13)	5583(3)	2566(9)	47(2)
C(30)	-1963(12)	5852(2)	-346(7)	39(2)
C(31)	4667(13)	6557(2)	2415(6)	26(1)
C(32)	3383(15)	6188(3)	2500(10)	32(2)
C(33)	3830(50)	5830(10)	1790(18)	29(4)
C(34)	5540(20)	5835(5)	1009(17)	30(3)
C(35)	6854(17)	6203(5)	895(10)	33(2)
C(36)	6435(14)	6566(3)	1649(10)	31(1)
C(37)	2454(14)	5410(2)	1918(10)	50(2)
C(38)	8657(13)	6225(3)	-2(7)	47(2)
C(39)	2392(14)	7363(2)	525(6)	45(2)
C(40A)	4700(50)	7500	230(120)	52(6)
C(40B)	4730(30)	7360(30)	112(18)	52(6)

Table 3. Bond lengths [Å] and angles [°] for ol04.

Cl(1)-C(1)	1.731(6)	C(15)-C(16)	1.406(13)
Cl(2)-C(20)	1.732(6)	C(16)-C(17)	1.433(17)
N(1)-C(2)	1.275(6)	C(16)-C(19)	1.552(16)
N(1)-C(1)	1.357(6)	C(23)-C(24)	1.390(12)
N(2)-C(3)	1.329(7)	C(23)-C(28)	1.421(11)
N(2)-C(2)	1.330(7)	C(24)-C(25)	1.38(3)
N(3)-C(1)	1.314(6)	C(25)-C(26)	1.41(3)
N(3)-C(3)	1.378(6)	C(25)-C(29)	1.50(3)
N(4)-C(2)	1.344(7)	C(26)-C(27)	1.392(13)
N(4)-C(4)	1.437(8)	C(27)-C(28)	1.386(12)
N(5)-C(3)	1.353(7)	C(27)-C(30)	1.544(12)
N(5)-C(12)	1.434(9)	C(31)-C(32)	1.380(11)
N(6)-C(20)	1.331(6)	C(31)-C(36)	1.393(11)
N(6)-C(21)	1.350(6)	C(32)-C(33)	1.37(3)
N(7)-C(22)	1.331(7)	C(33)-C(34)	1.37(3)
N(7)-C(21)	1.336(7)	C(33)-C(37)	1.54(3)
N(8)-C(22)	1.307(6)	C(34)-C(35)	1.391(14)
N(8)-C(20)	1.334(6)	C(35)-C(36)	1.408(13)
N(9)-C(21)	1.342(7)	C(35)-C(38)	1.505(12)
N(9)-C(23)	1.427(8)	C(39)-C(40A)	1.50(3)
N(10)-C(22)	1.358(7)	C(39)-C(40B)	1.505(17)
N(10)-C(31)	1.442(8)		
N(11)-C(39)	1.139(10)	C(2)-N(1)-C(1)	116.0(4)
C(4)-C(9)	1.378(9)	C(3)-N(2)-C(2)	116.1(5)
C(4)-C(5)	1.413(10)	C(1)-N(3)-C(3)	111.7(4)
C(5)-C(6)	1.398(12)	C(2)-N(4)-C(4)	124.0(5)
C(6)-C(7)	1.410(16)	C(3)-N(5)-C(12)	124.6(5)
C(6)-C(10)	1.533(10)	C(20)-N(6)-C(21)	113.2(4)
C(7)-C(8)	1.403(11)	C(22)-N(7)-C(21)	115.4(5)
C(8)-C(9)	1.380(18)	C(22)-N(8)-C(20)	114.7(4)
C(8)-C(11)	1.507(15)	C(21)-N(9)-C(23)	127.1(6)
C(12)-C(13)	1.385(10)	C(22)-N(10)-C(31)	125.6(6)
C(12)-C(17)	1.388(10)	N(3)-C(1)-N(1)	126.7(4)
C(13)-C(14)	1.401(10)	N(3)-C(1)-Cl(1)	113.5(4)
C(14)-C(15)	1.41(2)	N(1)-C(1)-Cl(1)	119.7(4)
C(14)-C(18)	1.503(11)	N(1)-C(2)-N(2)	124.6(5)
		N(1)-C(2)-N(4)	115.5(5)
		N(2)-C(2)-N(4)	119.9(5)

N(2)-C(3)-N(5)	118.9(5)	N(8)-C(22)-N(7)	125.3(5)
N(2)-C(3)-N(3)	124.9(5)	N(8)-C(22)-N(10)	114.1(5)
N(5)-C(3)-N(3)	116.2(5)	N(7)-C(22)-N(10)	120.7(5)
C(9)-C(4)-C(5)	120.8(6)	C(24)-C(23)-C(28)	119.3(7)
C(9)-C(4)-N(4)	121.4(5)	C(24)-C(23)-N(9)	118.1(8)
C(5)-C(4)-N(4)	117.8(6)	C(28)-C(23)-N(9)	122.5(8)
C(6)-C(5)-C(4)	120.0(7)	C(25)-C(24)-C(23)	121.6(13)
C(5)-C(6)-C(7)	119.0(8)	C(24)-C(25)-C(26)	119(2)
C(5)-C(6)-C(10)	121.1(7)	C(24)-C(25)-C(29)	122.2(17)
C(7)-C(6)-C(10)	119.9(8)	C(26)-C(25)-C(29)	119(2)
C(8)-C(7)-C(6)	119.1(10)	C(27)-C(26)-C(25)	120(2)
C(9)-C(8)-C(7)	121.9(11)	C(28)-C(27)-C(26)	121.3(15)
C(9)-C(8)-C(11)	116.0(10)	C(28)-C(27)-C(30)	117.0(11)
C(7)-C(8)-C(11)	122.2(12)	C(26)-C(27)-C(30)	121.6(15)
C(4)-C(9)-C(8)	119.1(8)	C(27)-C(28)-C(23)	118.8(8)
C(13)-C(12)-C(17)	120.8(6)	C(32)-C(31)-C(36)	120.9(7)
C(13)-C(12)-N(5)	121.5(6)	C(32)-C(31)-N(10)	123.6(7)
C(17)-C(12)-N(5)	117.7(7)	C(36)-C(31)-N(10)	115.4(7)
C(12)-C(13)-C(14)	120.6(7)	C(33)-C(32)-C(31)	119.1(14)
C(13)-C(14)-C(15)	119.3(10)	C(32)-C(33)-C(34)	121(3)
C(13)-C(14)-C(18)	121.2(7)	C(32)-C(33)-C(37)	119.2(17)
C(15)-C(14)-C(18)	119.5(8)	C(34)-C(33)-C(37)	120(2)
C(16)-C(15)-C(14)	120.7(15)	C(33)-C(34)-C(35)	122(2)
C(15)-C(16)-C(17)	118.5(13)	C(34)-C(35)-C(36)	117.5(11)
C(15)-C(16)-C(19)	118.6(14)	C(34)-C(35)-C(38)	122.8(13)
C(17)-C(16)-C(19)	122.9(12)	C(36)-C(35)-C(38)	119.7(12)
C(12)-C(17)-C(16)	120.0(9)	C(31)-C(36)-C(35)	120.0(7)
N(6)-C(20)-N(8)	126.6(4)	N(11)-C(39)-C(40A)	165.4(15)
N(6)-C(20)-Cl(2)	115.2(4)	N(11)-C(39)-C(40B)	177(3)
N(8)-C(20)-Cl(2)	118.2(4)	C(40A)-C(39)-C(40B)	17.1(18)
N(7)-C(21)-N(9)	120.5(5)		
N(7)-C(21)-N(6)	124.7(5)		
N(9)-C(21)-N(6)	114.8(5)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for ol04. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	26(1)	23(1)	49(1)	-9(1)	9(1)	-1(1)
Cl(2)	26(1)	25(1)	43(1)	-5(1)	12(1)	-1(1)
N(1)	19(2)	34(2)	33(2)	0	6(1)	0
N(2)	18(2)	24(2)	38(3)	-2(2)	2(2)	0(2)
N(3)	19(2)	23(2)	37(2)	0	5(1)	0
N(4)	22(2)	23(2)	38(3)	-1(2)	8(2)	2(2)
N(5)	20(2)	25(3)	42(3)	-2(2)	2(2)	-1(2)
N(6)	18(2)	26(2)	31(2)	0	8(1)	0
N(7)	16(2)	26(3)	38(3)	0(2)	6(2)	4(2)
N(8)	17(2)	33(2)	30(2)	0	5(1)	0
N(9)	21(2)	30(3)	33(3)	-2(2)	4(2)	-5(2)
N(10)	19(2)	26(3)	39(3)	-2(2)	9(2)	4(2)
N(11)	69(5)	78(6)	56(4)	-5(3)	19(4)	-15(4)
C(1)	19(3)	21(2)	29(3)	-2(2)	3(2)	2(2)
C(2)	16(3)	25(3)	31(3)	0(2)	1(2)	1(2)
C(3)	18(3)	19(3)	36(3)	-2(2)	-1(2)	-1(2)
C(4)	19(3)	26(3)	33(3)	0(3)	3(2)	1(2)
C(5)	27(4)	31(4)	28(4)	-5(4)	9(4)	0(3)
C(6)	29(4)	28(4)	30(3)	-1(3)	2(3)	0(3)
C(7)	28(8)	16(5)	28(7)	-4(4)	8(5)	-2(4)
C(8)	32(7)	28(4)	28(5)	-5(3)	5(5)	9(6)
C(9)	22(3)	26(3)	37(4)	6(3)	7(3)	4(2)
C(10)	40(4)	55(4)	50(4)	-1(3)	25(3)	6(3)
C(11)	40(4)	55(4)	50(4)	-1(3)	25(3)	6(3)
C(12)	18(3)	16(3)	35(4)	0(3)	3(3)	2(2)
C(13)	22(3)	37(4)	28(3)	-2(3)	3(2)	2(3)
C(14)	24(4)	29(4)	43(4)	-9(3)	-3(3)	4(3)
C(15)	31(7)	56(9)	37(6)	-10(5)	13(4)	6(5)
C(16)	33(8)	24(5)	44(8)	0(5)	8(6)	7(6)
C(17)	23(4)	30(4)	42(4)	-4(3)	9(3)	1(3)
C(18)	40(3)	42(3)	51(4)	-13(3)	23(3)	8(3)
C(19)	40(3)	42(3)	51(4)	-13(3)	23(3)	8(3)
C(20)	19(3)	24(2)	25(3)	-1(2)	3(2)	-1(2)
C(21)	16(3)	26(3)	31(3)	2(2)	6(2)	0(2)

C(22)	13(2)	29(3)	31(3)	3(2)	3(2)	2(2)
C(23)	21(4)	28(3)	35(4)	-5(3)	11(3)	-3(3)
C(24)	23(4)	28(5)	32(4)	-4(3)	5(4)	-3(4)
C(25)	23(5)	39(8)	30(10)	5(8)	3(8)	-3(5)
C(26)	14(7)	30(7)	48(6)	0(5)	-3(6)	-14(4)
C(27)	26(5)	32(5)	26(4)	-5(4)	-4(3)	4(6)
C(28)	22(4)	31(5)	29(4)	-1(3)	8(3)	5(4)
C(29)	36(4)	45(5)	63(5)	3(4)	15(4)	-17(3)
C(30)	40(4)	41(4)	37(4)	-12(3)	12(3)	1(3)
C(31)	18(4)	27(4)	35(4)	-3(3)	6(3)	1(3)
C(32)	28(5)	22(5)	46(5)	0(3)	1(4)	0(4)
C(33)	25(5)	29(6)	32(10)	3(8)	5(9)	6(4)
C(34)	9(7)	32(9)	49(6)	-14(6)	5(6)	-7(5)
C(35)	29(5)	41(7)	30(5)	-10(5)	7(3)	2(6)
C(36)	17(4)	35(4)	41(5)	-3(4)	7(3)	0(3)
C(37)	48(5)	26(4)	76(6)	-7(4)	12(4)	3(3)
C(38)	40(4)	59(5)	45(4)	-5(4)	15(3)	5(3)
C(39)	57(4)	52(5)	26(3)	-1(3)	2(3)	-6(3)
C(40A)	48(4)	70(20)	43(6)	0	12(3)	0
C(40B)	48(4)	70(20)	43(6)	0	12(3)	0

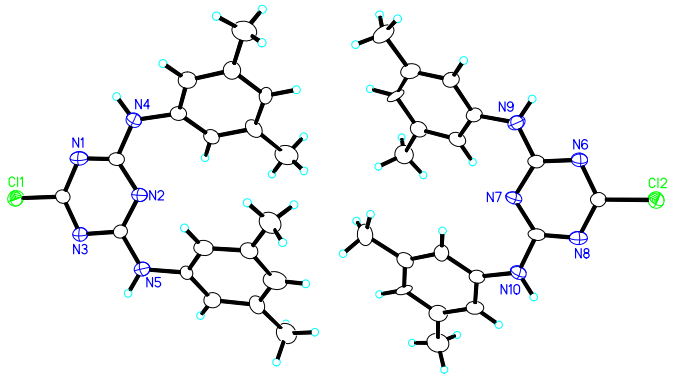
Table 5. Torsion angles [°] for ol04.

C(3)-N(3)-C(1)-N(1)	-3.3(8)
C(3)-N(3)-C(1)-Cl(1)	174.8(4)
C(2)-N(1)-C(1)-N(3)	2.9(8)
C(2)-N(1)-C(1)-Cl(1)	-175.1(4)
C(2)#1-N(1)-C(1)-Cl(1)	40.9(5)
C(1)#1-N(1)-C(1)-Cl(1)	-156.8(3)
C(1)-N(1)-C(2)-N(2)	-0.2(8)
C(1)-N(1)-C(2)-N(4)	177.3(5)
C(3)-N(2)-C(2)-N(1)	-1.5(9)
C(3)-N(2)-C(2)-N(4)	-178.9(5)
C(4)-N(4)-C(2)-N(1)	-171.9(5)
C(4)-N(4)-C(2)-N(2)	5.7(9)
C(2)-N(2)-C(3)-N(5)	179.6(5)
C(2)-N(2)-C(3)-N(3)	1.0(9)
C(12)-N(5)-C(3)-N(2)	-4.3(10)
C(1)-N(3)-C(3)-N(2)	1.2(8)
C(1)-N(3)-C(3)-N(5)	-177.5(5)
C(2)-N(4)-C(4)-C(9)	41.2(9)
C(2)-N(4)-C(4)-C(5)	-140.7(7)
C(9)-C(4)-C(5)-C(6)	1.5(11)
N(4)-C(4)-C(5)-C(6)	-176.6(6)
C(4)-C(5)-C(6)-C(7)	-1.7(13)
C(4)-C(5)-C(6)-C(10)	177.8(7)
C(5)-C(6)-C(7)-C(8)	0.1(16)
C(10)-C(6)-C(7)-C(8)	-179.4(11)
C(6)-C(7)-C(8)-C(9)	2(2)
C(6)-C(7)-C(8)-C(11)	-179.8(13)
C(5)-C(4)-C(9)-C(8)	0.4(12)
N(4)-C(4)-C(9)-C(8)	178.4(9)
C(7)-C(8)-C(9)-C(4)	-2.0(17)
C(11)-C(8)-C(9)-C(4)	179.5(10)
C(3)-N(5)-C(12)-C(17)	-137.2(7)
C(17)-C(12)-C(13)-C(14)	0.6(11)
N(5)-C(12)-C(13)-C(14)	-177.4(6)
C(12)-C(13)-C(14)-C(15)	-2.8(13)
C(12)-C(13)-C(14)-C(18)	-179.7(7)
C(13)-C(14)-C(15)-C(16)	3(2)
C(18)-C(14)-C(15)-C(16)	-179.8(13)
C(14)-C(15)-C(16)-C(17)	-1(2)
C(14)-C(15)-C(16)-C(19)	177.0(14)
C(13)-C(12)-C(17)-C(16)	1.1(13)
N(5)-C(12)-C(17)-C(16)	179.2(9)
C(15)-C(16)-C(17)-C(12)	-0.7(19)
C(19)-C(16)-C(17)-C(12)	-179.1(11)
C(21)-N(6)-C(20)-N(8)	-1.3(7)
C(21)-N(6)-C(20)-Cl(2)	179.5(4)
C(22)-N(8)-C(20)-N(6)	2.6(8)
C(22)-N(8)-C(20)-Cl(2)	-178.3(4)
C(22)-N(7)-C(21)-N(9)	178.0(5)
C(22)-N(7)-C(21)-N(6)	-3.4(8)
C(23)-N(9)-C(21)-N(7)	-7.6(10)
C(23)-N(9)-C(21)-N(6)	173.7(6)
C(20)-N(6)-C(21)-N(7)	1.8(8)
C(20)-N(6)-C(21)-N(9)	-179.6(5)
C(20)-N(8)-C(22)-N(7)	-4.4(8)
C(20)-N(8)-C(22)-N(10)	176.4(5)
C(21)-N(7)-C(22)-N(8)	4.8(9)
C(21)-N(7)-C(22)-N(10)	-176.0(5)
C(31)-N(10)-C(22)-N(8)	-171.9(5)
C(31)-N(10)-C(22)-N(7)	8.9(9)
C(21)-N(9)-C(23)-C(24)	148.4(7)
C(21)-N(9)-C(23)-C(28)	-35.1(11)
C(28)-C(23)-C(24)-C(25)	4.7(19)
N(9)-C(23)-C(24)-C(25)	-178.7(16)
C(23)-C(24)-C(25)-C(26)	-6(3)
C(23)-C(24)-C(25)-C(29)	177.1(15)
C(24)-C(25)-C(26)-C(27)	5(3)
C(29)-C(25)-C(26)-C(27)	-178.1(17)
C(25)-C(26)-C(27)-C(28)	-3(2)
C(25)-C(26)-C(27)-C(30)	-179.8(17)
C(26)-C(27)-C(28)-C(23)	1.2(15)
C(30)-C(27)-C(28)-C(23)	178.4(7)
C(24)-C(23)-C(28)-C(27)	-2.1(12)
N(9)-C(23)-C(28)-C(27)	-178.5(7)

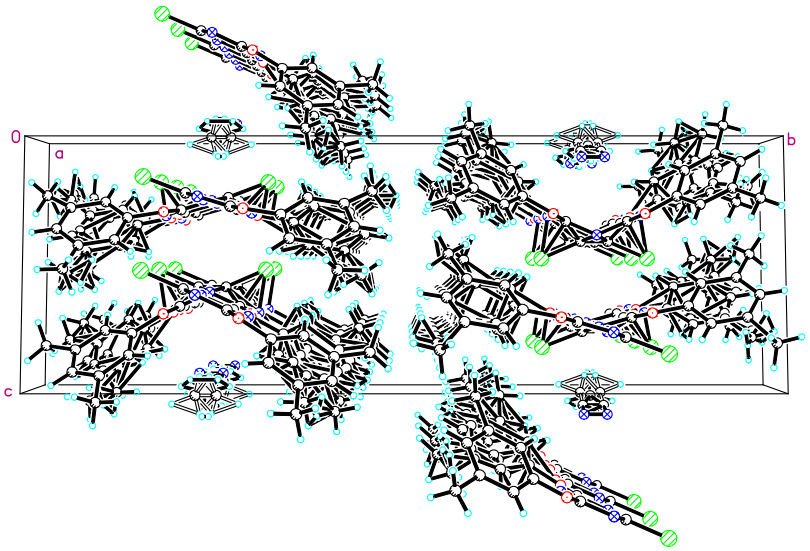
C(22)-N(10)-C(31)-C(32)	-38.5(10)	C(33)-C(34)-C(35)-C(38)	-176.8(16)
C(22)-N(10)-C(31)-C(36)	144.4(7)	C(32)-C(31)-C(36)-C(35)	3.4(12)
C(36)-C(31)-C(32)-C(33)	-1.7(17)	N(10)-C(31)-C(36)-C(35)	-179.4(7)
N(10)-C(31)-C(32)-C(33)	-178.6(14)	C(34)-C(35)-C(36)-C(31)	-3.8(14)
C(31)-C(32)-C(33)-C(34)	0(3)	C(38)-C(35)-C(36)-C(31)	175.6(7)
C(31)-C(32)-C(33)-C(37)	177.9(13)		
C(32)-C(33)-C(34)-C(35)	-1(3)		
C(37)-C(33)-C(34)-C(35)	-178.3(15)		
C(33)-C(34)-C(35)-C(36)	3(2)		

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z



a



b

Figure S5. ORTEP plots of the crystal structure of compound **3**. Displacement ellipsoids for non-H atoms are shown at the 50% probability level and H atoms are represented by circles of arbitrary size. a) Both symmetry-independent molecules of **2**. b) Unit cell packing along the *a* axis.

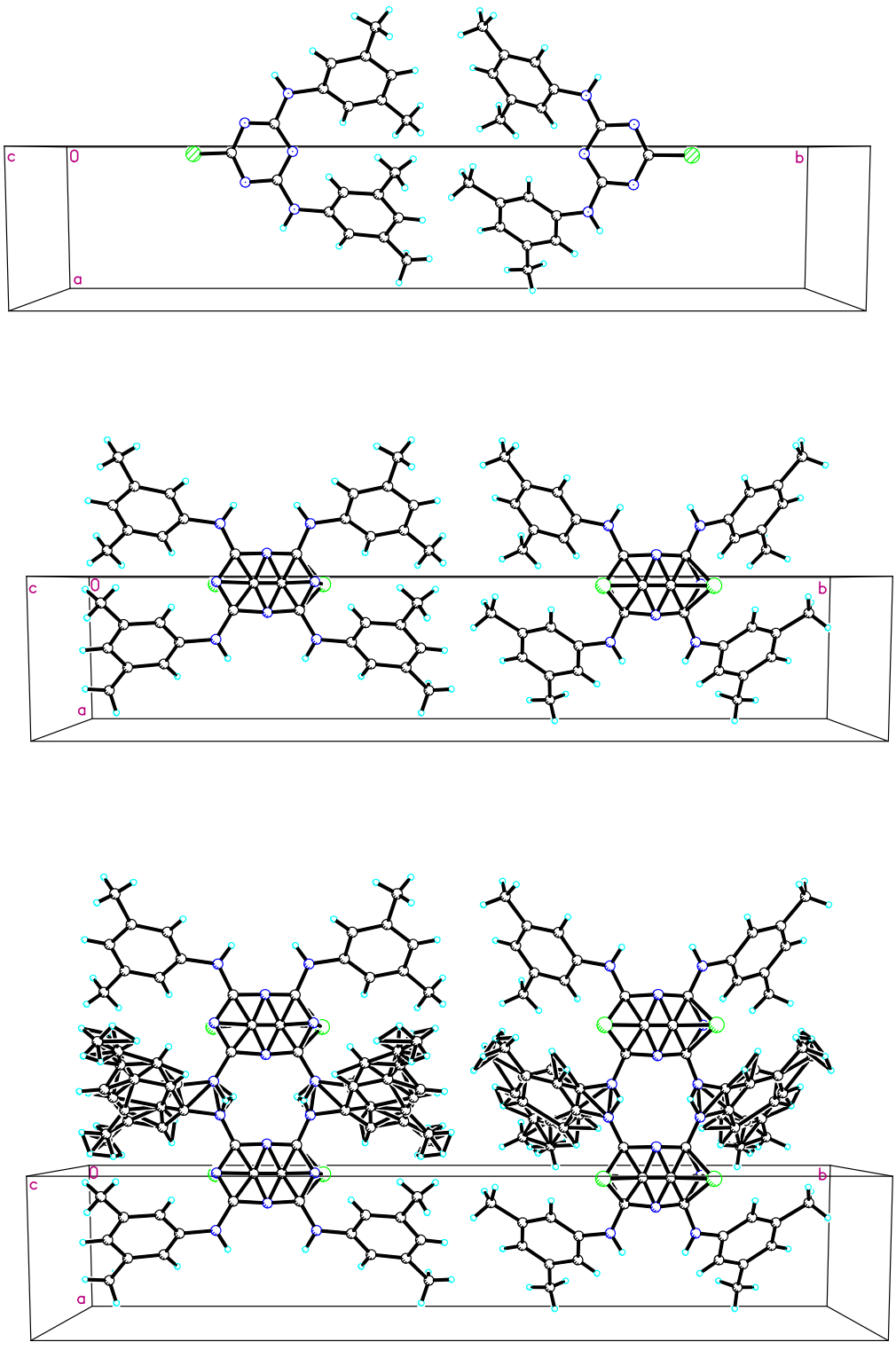
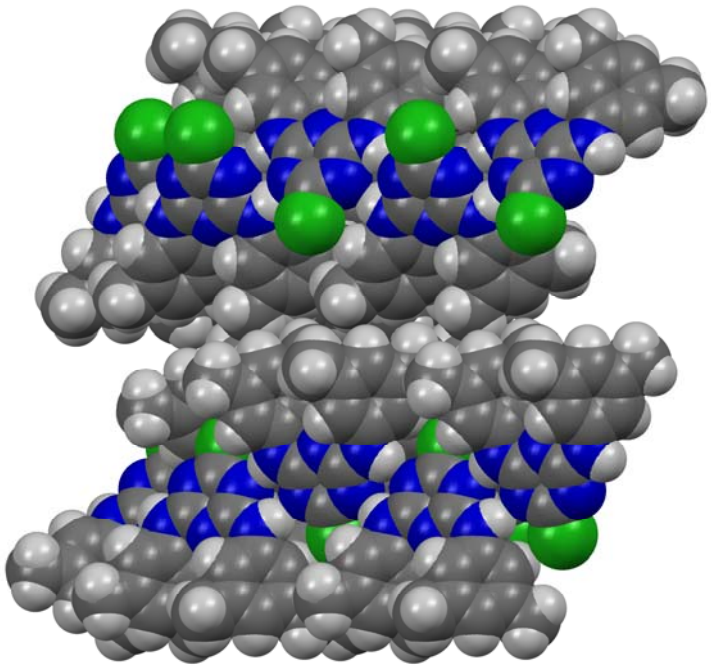
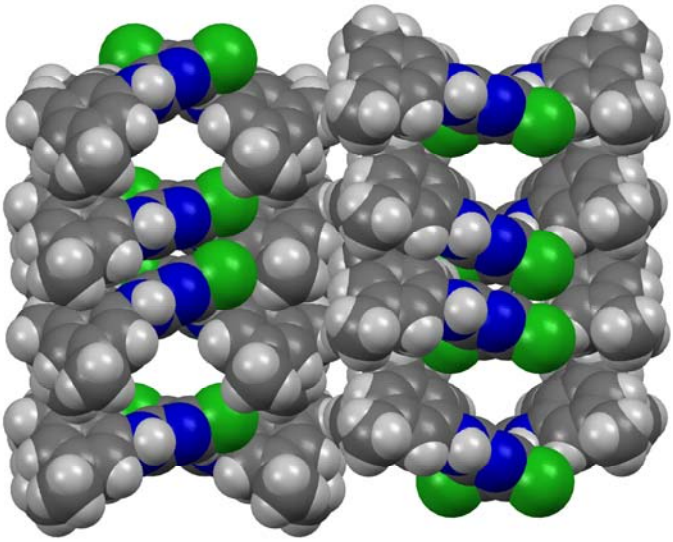


Figure S6. ORTEP plots of the crystal structure of compound **3**. Detail about the disorder present in the structure of **3**. Each molecule is disordered over two positions with an occupancy of 0.5 for each.



a



b

Figure S7. a) View along the *a* axis, and b) view along the *c* axis of a 2 x 2 x 2 array of unit cells in the crystal structure of compound **3**. Molecules of **3** form V-shaped hydrogen-bonded ribbons which stack in pairs. Carbon atoms are shown in grey, hydrogen atoms in white, nitrogen atoms in blue and oxygen atoms in red. For clarity purposes, solvent molecules are omitted, only one of two disordered positions is shown and the hydrogen atoms were simulated.

Modified .CIF Files of Compounds 3-4 Used for Hirshfeld Surface Calculations

Compound 3

```
##################################################################################
#
#                Cambridge Crystallographic Data Centre
#                                CCDC
#
##################################################################################
#
# If this CIF has been generated directly or indirectly from an entry in the
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# for validating and visualising CIF files, please visit www.ccdc.cam.ac.uk
#
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_symmetry_Int_Tables_number 14

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3 -x,-y,-z

4 x,1/2-y,1/2+z

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_cell_length_b 30.8935(18)

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N3 N 0.110633 0.751518 0.432616

N4 N 0.1922 0.691927 0.178007

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N5 N 0.186451 0.694152 0.563502

H5B H 0.157846 0.707724 0.608933

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C3 C 0.16012 0.712105 0.450094

C4 C 0.256315 0.651452 0.187585
C5 C 0.220412 0.627757 0.08075
H5A H 0.155762 0.637832 0.008925
C6 C 0.280246 0.588837 0.079579
C7 C 0.375853 0.575193 0.187146
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C8 C 0.41755 0.60077 0.296242
C9 C 0.355319 0.637849 0.294999
H9A H 0.37895 0.654221 0.366213
C10 C 0.237017 0.562116 -0.035622
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H10B H 0.233025 0.579996 -0.102533
H10C H 0.155114 0.550436 -0.053838
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C13 C 0.242707 0.619228 0.543406
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C15 C 0.399295 0.58328 0.724083
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C28 C 0.778675 0.616135 -0.152498
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C34 C 0.864027 0.560768 0.414347
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C35 C 0.783264 0.571386 0.296193
C36 C 0.762764 0.61606 0.268434
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C37 C 1.00792 0.57776 0.628863
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H37B H 0.962971 0.578864 0.6797
H37C H 1.07874 0.597021 0.661095
C38 C 0.720723 0.53763 0.202065
H38A H 0.64327 0.548851 0.140957
H38B H 0.703417 0.512754 0.240353
H38C H 0.775054 0.529466 0.164038
N11 N 0.423033 0.765052 0.489638
C39 C 0.448829 0.763941 0.589095
C40 C 0.482332 0.761338 0.721315
H40A H 0.534536 0.736432 0.755057
H40B H 0.40709 0.758884 0.734253
H40C H 0.527264 0.786995 0.761035

#END

Compound 4

```
##################################################################################
#
#                Cambridge Crystallographic Data Centre
#                              CCDC
#
##################################################################################
#
# If this CIF has been generated directly or indirectly from an entry in the
# Cambridge Structural Database, then it will include bibliographic, chemical,
# crystal, experimental, refinement or atomic coordinate data resulting from
# the CCDC's data processing and validation procedures. Files generated from
# CSD entries are Copyright 2008 Cambridge Crystallographic Data Centre. They
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2 -x,y,1/2-z
3 1/2+x,1/2+y,z
4 1/2-x,1/2+y,1/2-z
5 -x,-y,-z
6 x,-y,1/2+z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z
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H1B H 0.35255 0.073574 0.309337

H1C H 0.291435 0.095741 0.238283

C2 C 0.332561 0.210513 0.167025

C3 C 0.370744 0.236901 0.124893

C4 C 0.459494 0.269229 0.124663

C5 C 0.376011 0.276913 0.015224

C6 C 0.371393 0.308407 -0.115027

C7 C 0.422099 0.365076 -0.098581

H7 H 0.442767 0.392114 -0.049325

C8 C 0.442577 0.382149 -0.154713

C9 C 0.410304 0.341368 -0.22725

H9 H 0.424269 0.350883 -0.265303

C10 C 0.358291 0.287239 -0.245108

C11 C 0.340051 0.269784 -0.187641

H11 H 0.305807 0.231062 -0.197965

C12 C 0.497601 0.44363 -0.137185

H12A H 0.529991 0.400156 -0.133902

H12B H 0.508407 0.478001 -0.088776

H12C H 0.489939 0.492437 -0.177559

C13 C 0.322461 0.242486 -0.324989

H13A H 0.285276 0.215423 -0.327587

H13B H 0.345351 0.18946 -0.334381

H13C H 0.314145 0.294331 -0.363411

C14 C 0.560545 0.300461 0.133374
C15 C 0.607635 0.362709 0.17662
H15 H 0.60967 0.389368 0.222871
C16 C 0.651555 0.38605 0.152676
C17 C 0.64819 0.343713 0.08466
H17 H 0.678282 0.357752 0.068355
C18 C 0.60178 0.281765 0.040775
C19 C 0.557575 0.261126 0.065458
H19 H 0.525338 0.219986 0.035629
C20 C 0.702213 0.454758 0.199291
H20A H 0.734766 0.415637 0.235814
H20B H 0.688699 0.502592 0.2265
H20C H 0.715752 0.490233 0.165537
C21 C 0.599348 0.235723 -0.031466
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H21B H 0.622052 0.276442 -0.051476
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O1 O 0.361862 0.152635 0.227228
O2 O 0.282701 0.240772 0.147603
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H22 H 0.252838 0.372712 0.030572
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CL2 Cl 0.200871 0.470375 0.078562
CL3 Cl 0.321372 0.492706 0.092938
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#END

Additional Views of the Hirshfeld Surfaces of Compounds 1-4

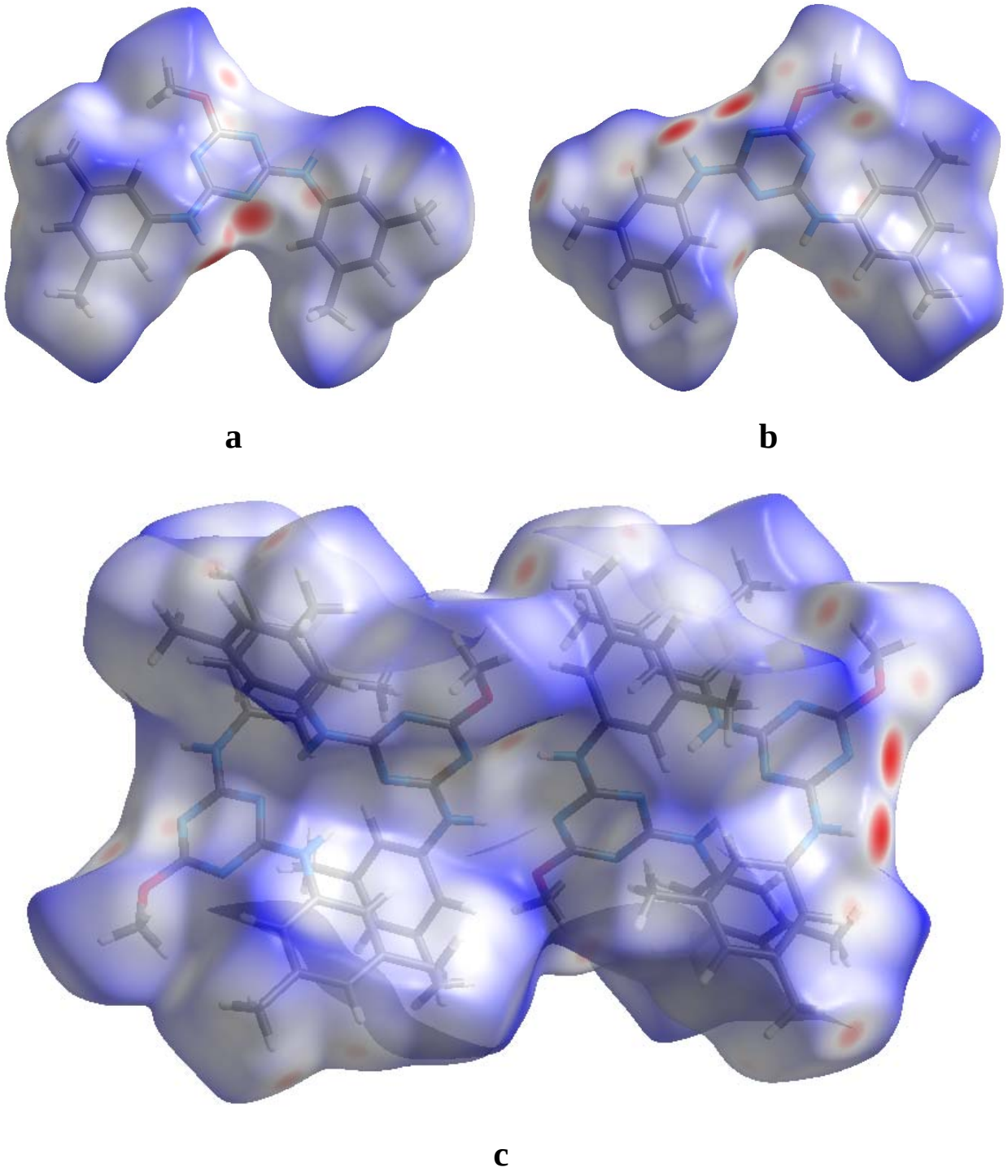


Figure S8. Hirshfeld surfaces of compound **1** mapped with d_{norm}. a) and b) single molecule, c) hydrogen-bonded aggregate.

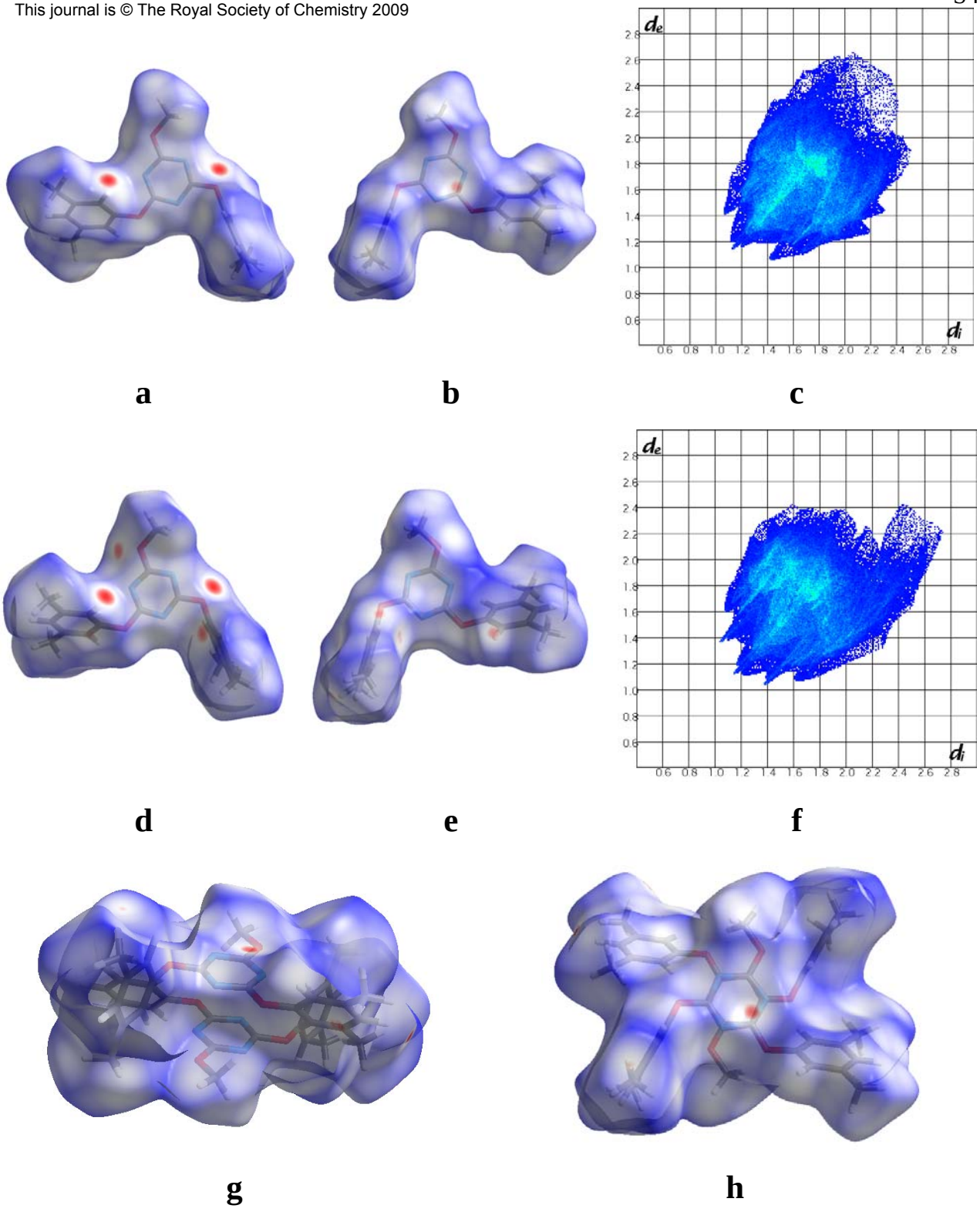
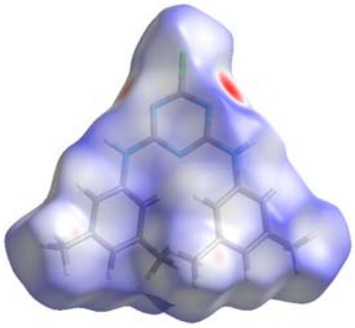


Figure S9. Hirshfeld surfaces of compound **2** mapped with d_{norm}. a) and b) single molecule, and c) fingerprint plot of one of two symmetry-independent molecules. d) and e) single molecule, and f) fingerprint plot of the other symmetry-independent molecule. g) and h) π-stacked dimer of the molecule shown in a) and b).



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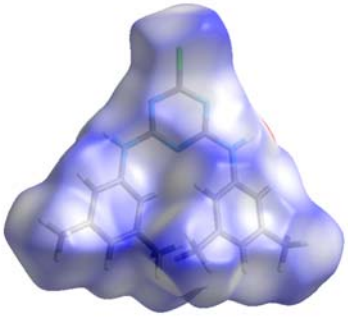
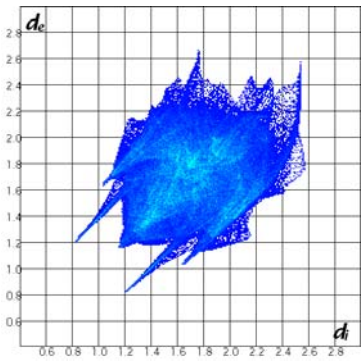
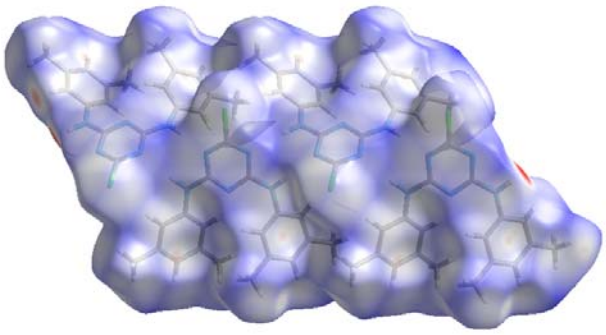


b



c



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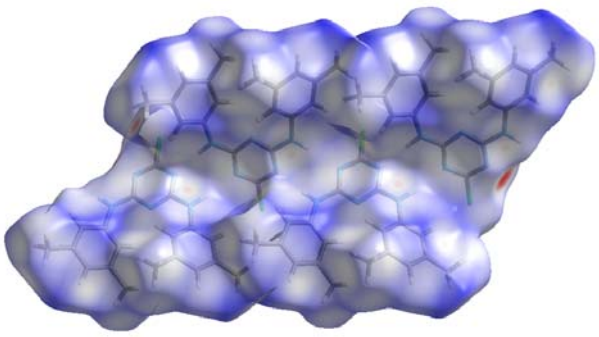

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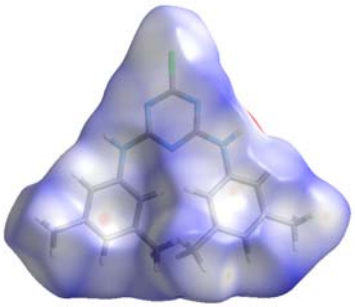

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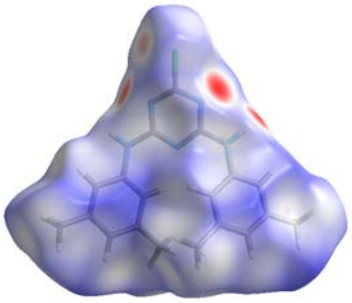
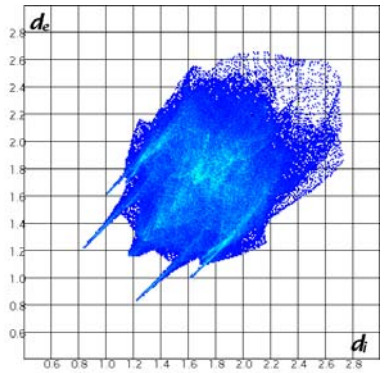


g



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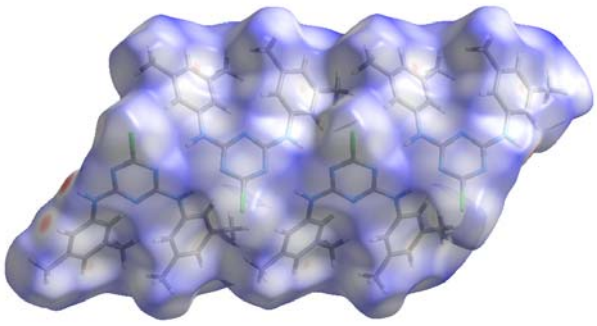

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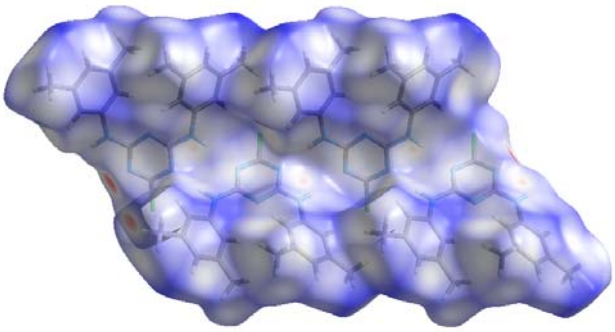

j

Figure S10. Hirshfeld surfaces of compound **3** mapped with d_{norm}, generated with the modified .cif file found in page 39 (*vide infra*). a) and b) single molecule, and c) fingerprint plot of one of two symmetry-independent molecules. d) and e) hydrogen-bonded ribbon of the molecule shown in a) and b). f) and g) single molecule, and h) fingerprint plot of the other symmetry-independent molecule. i) and j) π-stacked dimer of the molecule shown in a) and b).

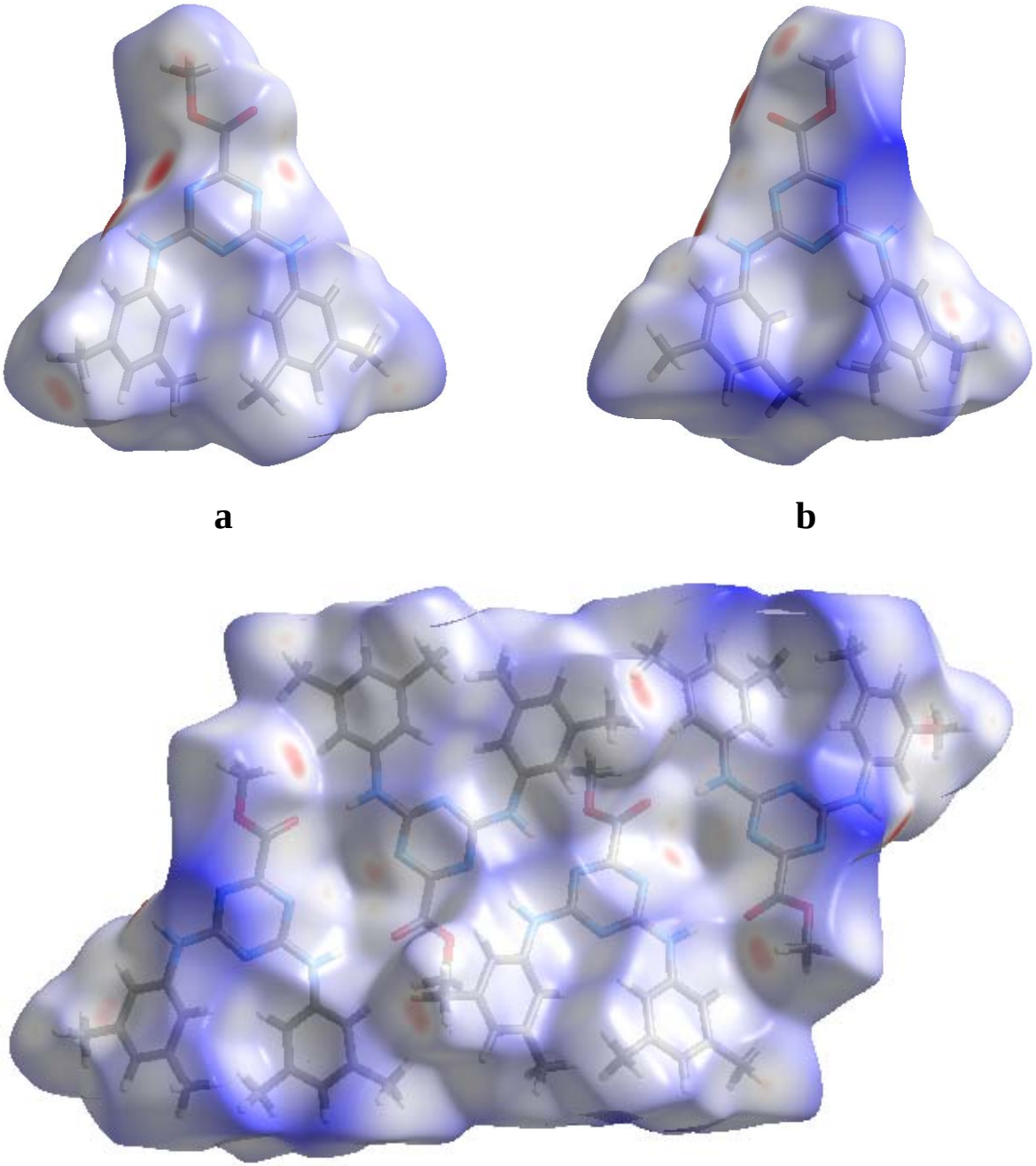

Figure S11. Hirshfeld surfaces of compound **4** mapped with d_{norm}, generated with the modified .cif file found in page 43 (*vide infra*). a) and b) single molecule, c) hydrogen-bonded aggregate.

DFT Calculations on Compounds 1-4

Files corresponding to the molecules in the crystal structures were used as input files for geometry optimization and as both input and output files for energy calculations on crystal structures. Output files for optimized structures are included as well. Files can be saved in .mol2 format and imported in simulation softwares such as Spartan or Gaussian.

Crystal structure files

Compound 1 - Monomer

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#          File Created by: Spartan `06 Export
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49 51
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NO_CHARGES


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   7  N7        1.330732740    0.728374911   -0.169062600    N.3   1  ol03a
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   9  C9        0.538764142   -2.606052207    0.475371608    C.ar  1  ol03a
  10  C10      -1.356039909   -1.407110847    0.414261967    C.ar  1  ol03a
  11  C11       0.651300154   -0.418550494    0.033878114    C.ar  1  ol03a
  12  C12       2.422242940   -4.010137499    0.258817358    C.3   1  ol03a
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  14  H14       2.546560255   -3.652030357   -0.644562094    H     1  ol03a
  15  H15       3.002184691   -3.528051437    0.883083436    H     1  ol03a
  16  C16      -3.610908401   -0.344004575    0.222273158    C.ar  1  ol03a
  17  C17      -4.802909197   -0.646654811   -0.484238435    C.ar  1  ol03a
  18  H18      -4.957080756   -1.530621567   -0.796305939    H     1  ol03a
  19  C19      -5.747006145    0.342352943   -0.719477745    C.ar  1  ol03a
  20  C20      -5.507120731    1.625363739   -0.262648200    C.ar  1  ol03a
  21  H21      -6.161127065    2.297714541   -0.415265542    H     1  ol03a
  22  C22      -4.336424410    1.960217475    0.410978902    C.ar  1  ol03a
  23  C23      -3.406301141    0.948326862    0.667831831    C.ar  1  ol03a
  24  H24      -2.619097321    1.152946069    1.157451198    H     1  ol03a
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  27  H27      -6.813534575   -0.353133723   -2.353762506    H     1  ol03a
  28  H28      -7.520094161   -0.699756969   -0.960885433    H     1  ol03a
  29  C29      -4.062732129    3.375741773    0.879457738    C.3   1  ol03a
  30  H30      -3.615165104    3.351346239    1.750503933    H     1  ol03a
  31  H31      -3.486249194    3.829450199    0.228243454    H     1  ol03a
  32  H32      -4.908453240    3.862219308    0.959599313    H     1  ol03a
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35	H35	2.605144776	2.863952856	0.379292264	H	1	ol03a
36	C36	4.591752398	2.486947434	0.066428137	C.ar	1	ol03a
37	C37	5.453849407	1.492417197	-0.303162892	C.ar	1	ol03a
38	H38	6.386174269	1.676653533	-0.324468213	H	1	ol03a
39	C39	5.012583201	0.226121223	-0.643849160	C.ar	1	ol03a
40	C40	3.641151563	-0.039609665	-0.622790917	C.ar	1	ol03a
41	H41	3.324563359	-0.899526528	-0.878012680	H	1	ol03a
42	C42	5.081917542	3.869181825	0.453478137	C.3	1	ol03a
43	H43	6.044850028	3.935245511	0.278173190	H	1	ol03a
44	H44	4.606910402	4.544803191	-0.075202516	H	1	ol03a
45	H45	4.911878412	4.021250420	1.407088964	H	1	ol03a
46	C46	6.010571319	-0.890363746	-0.970652879	C.3	1	ol03a
47	H47	6.853431579	-0.724712572	-0.498943091	H	1	ol03a
48	H48	5.640320013	-1.752103027	-0.686994942	H	1	ol03a
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Compound 1 – Dimer 1 (N-H---Northo)

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98 102
SMALL
NO_CHARGES


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4	N4	4.092755424	-0.693830686	0.348821536	N.ar	1	ol03a
5	N5	0.926056626	1.818683564	0.151765798	N.3	1	ol03a
6	H6	0.149535411	1.408088681	0.105606934	H	1	ol03a
7	N7	5.504271267	1.160998649	0.199078088	N.3	1	ol03a
8	H8	5.548079276	2.038327189	0.172286876	H	1	ol03a
9	C9	2.829455070	-1.075291221	0.271820691	C.ar	1	ol03a
10	C10	2.026264003	1.015938490	0.157260269	C.ar	1	ol03a
11	C11	4.262223323	0.639266293	0.257091241	C.ar	1	ol03a
12	C12	3.545554959	-3.282025475	0.700042573	C.3	1	ol03a
13	H13	3.172562827	-4.170705463	0.876269684	H	1	ol03a
14	H14	3.989356726	-2.948288701	1.507167483	H	1	ol03a
15	H15	4.196027344	-3.339474764	-0.029363775	H	1	ol03a
16	C16	0.876098100	3.235329335	0.211253355	C.ar	1	ol03a
17	C17	-0.145744763	3.813619802	1.006892032	C.ar	1	ol03a
18	H18	-0.737850410	3.255056450	1.496760419	H	1	ol03a
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20	C20	0.585040128	5.992800207	0.355573469	C.ar	1	ol03a
21	H21	0.478437994	6.936384275	0.392423443	H	1	ol03a
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27	H27	-1.298367699	5.516552980	2.849546484	H	1	ol03a
28	H28	-2.273581840	5.473326809	1.582040310	H	1	ol03a
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30	H30	2.800051539	5.929194876	-2.032099447	H	1	ol03a
31	H31	3.410446482	6.441470250	-0.643764479	H	1	ol03a
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34	C34	7.821959290	1.136219515	-0.437361948	C.ar	1	ol03a
35	H35	7.685374460	1.996750054	-0.815725678	H	1	ol03a

36	C36	9.097666254	0.549195389	-0.504842759	C.ar	1	ol03a
37	C37	9.260675433	-0.699563551	0.027068954	C.ar	1	ol03a
38	H38	10.115419533	-1.112523306	-0.022972515	H	1	ol03a
39	C39	8.220616366	-1.382066669	0.632673541	C.ar	1	ol03a
40	C40	6.967927551	-0.769016658	0.715277351	C.ar	1	ol03a
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42	C42	10.237454507	1.286943410	-1.181048537	C.3	1	ol03a
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44	H44	10.332051525	2.178252901	-0.783281095	H	1	ol03a
45	H45	10.047381189	1.374851507	-2.138940478	H	1	ol03a
46	C46	8.414471525	-2.814484980	1.142496891	C.3	1	ol03a
47	H47	9.112975830	-3.257501857	0.616956609	H	1	ol03a
48	H48	7.573487348	-3.309274852	1.052653184	H	1	ol03a
49	H49	8.679482024	-2.791314514	2.085406998	H	1	ol03a
50	O50	-2.549716009	2.436289955	-0.351128214	O.3	1	ol03a
51	N51	-1.743154427	0.312819196	-0.110974576	N.ar	1	ol03a
52	N52	-3.250471454	-1.551810892	-0.231643135	N.ar	1	ol03a
53	N53	-4.092755424	0.693830686	-0.348821536	N.ar	1	ol03a
54	N54	-0.926056626	-1.818683564	-0.151765798	N.3	1	ol03a
55	H55	-0.149535411	-1.408088681	-0.105606934	H	1	ol03a
56	N56	-5.504271267	-1.160998649	-0.199078088	N.3	1	ol03a
57	H57	-5.548079276	-2.038327189	-0.172286876	H	1	ol03a
58	C58	-2.829455070	1.075291221	-0.271820691	C.ar	1	ol03a
59	C59	-2.026264003	-1.015938490	-0.157260269	C.ar	1	ol03a
60	C60	-4.262223323	-0.639266293	-0.257091241	C.ar	1	ol03a
61	C61	-3.545554959	3.282025475	-0.700042573	C.3	1	ol03a
62	H62	-3.172562827	4.170705463	-0.876269684	H	1	ol03a
63	H63	-3.989356726	2.948288701	-1.507167483	H	1	ol03a
64	H64	-4.196027344	3.339474764	0.029363775	H	1	ol03a
65	C65	-0.876098100	-3.235329335	-0.211253355	C.ar	1	ol03a
66	C66	0.145744763	-3.813619802	-1.006892032	C.ar	1	ol03a
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70	H70	-0.478437994	-6.936384275	-0.392423443	H	1	ol03a
71	C71	-1.613612174	-5.457269478	0.413633015	C.ar	1	ol03a
72	C72	-1.726751588	-4.065934831	0.493723353	C.ar	1	ol03a
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74	C74	1.408999724	-5.791662210	-1.915399984	C.3	1	ol03a
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79	H79	-2.800051539	-5.929194876	2.032099447	H	1	ol03a
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85	C85	-9.097666254	-0.549195389	0.504842759	C.ar	1	ol03a
86	C86	-9.260675433	0.699563551	-0.027068954	C.ar	1	ol03a
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88	C88	-8.220616366	1.382066669	-0.632673541	C.ar	1	ol03a
89	C89	-6.967927551	0.769016658	-0.715277351	C.ar	1	ol03a
90	H90	-6.251713309	1.218952253	-1.150500498	H	1	ol03a
91	C91	-10.237454507	-1.286943410	1.181048537	C.3	1	ol03a
92	H92	-11.070769100	-0.784275791	1.057565359	H	1	ol03a
93	H93	-10.332051525	-2.178252901	0.783281095	H	1	ol03a
94	H94	-10.047381189	-1.374851507	2.138940478	H	1	ol03a
95	C95	-8.414471525	2.814484980	-1.142496891	C.3	1	ol03a
96	H96	-9.112975830	3.257501857	-0.616956609	H	1	ol03a

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97   H97      -7.573487348    3.309274852    -1.052653184    H   1  ol03a
98   H98      -8.679482024    2.791314514    -2.085406998    H   1  ol03a


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Compound 1 – Dimer 2 (N-H---Npara)

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98 102
SMALL
NO_CHARGES

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3 N3 -0.072272128 1.780788357 0.398521995 N.ar 1 ol03a
4 N4 1.604277817 2.993040027 -0.820373044 N.ar 1 ol03a
5 N5 -1.626896382 3.038103880 1.616227545 N.3 1 ol03a
6 H6 -1.864909101 3.844311739 1.875231030 H 1 ol03a
7 N7 1.568352599 0.659257391 -0.734583065 N.3 1 ol03a
8 H8 1.136111254 -0.048928603 -0.444786023 H 1 ol03a
9 C9 1.063097847 4.082674337 -0.303468336 C.ar 1 ol03a
10 C10 -0.506900168 2.965429807 0.844727054 C.ar 1 ol03a
11 C11 1.040556885 1.849829201 -0.384977874 C.ar 1 ol03a
12 C12 2.464934226 5.357652699 -1.708862887 C.3 1 ol03a
13 H13 2.613331459 6.288778935 -1.975158879 H 1 ol03a
14 H14 2.108921966 4.853292500 -2.469564539 H 1 ol03a
15 H15 3.312821034 4.960557718 -1.422765137 H 1 ol03a
16 C16 -2.458103258 1.975130659 2.054523185 C.ar 1 ol03a
17 C17 -3.857480625 2.206142759 2.054524853 C.ar 1 ol03a
18 H18 -4.200998692 3.033261441 1.737628749 H 1 ol03a
19 C19 -4.727658744 1.230145467 2.518220905 C.ar 1 ol03a
20 C20 -4.213378119 0.029638835 2.972815278 C.ar 1 ol03a
21 H21 -4.811364366 -0.632202689 3.300612588 H 1 ol03a
22 C22 -2.847768314 -0.237612430 2.961913483 C.ar 1 ol03a
23 C23 -1.979136091 0.765000735 2.520017575 C.ar 1 ol03a
24 H24 -1.042479575 0.611490259 2.539916428 H 1 ol03a
25 C25 -6.228750618 1.510390937 2.530822803 C.3 1 ol03a
26 H26 -6.703756852 0.730669748 2.884019567 H 1 ol03a
27 H27 -6.535219080 1.693229355 1.618024155 H 1 ol03a
28 H28 -6.410528304 2.288559255 3.097725979 H 1 ol03a
29 C29 -2.291628076 -1.568224641 3.429107300 C.3 1 ol03a
30 H30 -1.451541498 -1.420721486 3.910907308 H 1 ol03a
31 H31 -2.126257204 -2.143846279 2.652205129 H 1 ol03a
32 H32 -2.937874117 -2.001516175 4.023205471 H 1 ol03a
33 C33 2.737765340 0.393282821 -1.511484395 C.ar 1 ol03a
34 C34 3.390029509 -0.811680564 -1.277889981 C.ar 1 ol03a
35 H35 3.051381729 -1.407896727 -0.620492716 H 1 ol03a
36 C36 4.544144813 -1.165293291 -1.998691721 C.ar 1 ol03a
37 C37 5.023172301 -0.278603199 -2.922387720 C.ar 1 ol03a
38 H38 5.809788593 -0.500522009 -3.407788827 H 1 ol03a
39 C39 4.401305160 0.932190227 -3.170482103 C.ar 1 ol03a
40 C40 3.239024428 1.251759463 -2.464180537 C.ar 1 ol03a
41 H41 2.789724426 2.070787233 -2.643476740 H 1 ol03a
42 C42 5.238196990 -2.484821023 -1.719797885 C.3 1 ol03a
43 H43 5.962493194 -2.616379968 -2.368198479 H 1 ol03a
44 H44 4.591768341 -3.217881462 -1.799500644 H 1 ol03a
45 H45 5.609561882 -2.473550282 -0.812398424 H 1 ol03a
46 C46 5.011421681 1.940694378 -4.150277655 C.3 1 ol03a
47 H47 5.983517921 1.820507224 -4.181078595 H 1 ol03a
48 H48 4.803143786 2.850942874 -3.853273802 H 1 ol03a
49 H49 4.635277529 1.795463166 -5.043177657 H 1 ol03a
50 O50 -1.579828629 -5.316592610 -0.687307195 O.3 1 ol03a
51 N51 -0.060802799 -4.171190470 0.576796371 N.ar 1 ol03a
52 N52 0.072227717 -1.780752073 0.398506659 N.ar 1 ol03a
53 N53 -1.604323368 -2.992993327 -0.820397146 N.ar 1 ol03a
54 N54 1.626932586 -3.038138805 1.616199924 N.3 1 ol03a
55 H55 1.864884786 -3.844428319 1.875196268 H 1 ol03a
56 N56 -1.568318631 -0.659272196 -0.734587196 N.3 1 ol03a
57 H57 -1.136156483 0.048972116 -0.444784502 H 1 ol03a
58 C58 -1.063063503 -4.082692805 -0.303502303 C.ar 1 ol03a
59 C59 0.506935667 -2.965458151 0.844701142 C.ar 1 ol03a
60 C60 -1.040602056 -1.849786201 -0.384992722 C.ar 1 ol03a

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62	H62	-2.613298736	-6.288783073	-1.975210255	H	1	ol03a
63	H63	-2.108889754	-4.853292443	-2.469604099	H	1	ol03a
64	H64	-3.312787776	-4.960566592	-1.422804449	H	1	ol03a
65	C65	2.458060453	-1.975108571	2.054503871	C.ar	1	ol03a
66	C66	3.857437819	-2.206120671	2.054502203	C.ar	1	ol03a
67	H67	4.200955621	-3.033236669	1.737598675	H	1	ol03a
68	C68	4.727555618	-1.230206789	2.518205777	C.ar	1	ol03a
69	C69	4.213415607	-0.029685431	2.972810939	C.ar	1	ol03a
70	H70	4.811402213	0.632153250	3.300613343	H	1	ol03a
71	C71	2.847805791	0.237565927	2.961912759	C.ar	1	ol03a
72	C72	1.979093737	-0.764982638	2.520009099	C.ar	1	ol03a
73	H73	1.042516675	-0.611533102	2.539910176	H	1	ol03a
74	C74	6.228787709	-1.510433702	2.530803817	C.3	1	ol03a
75	H75	6.703794285	-0.730715541	2.884006805	H	1	ol03a
76	H76	6.535255286	-1.693264296	1.618003305	H	1	ol03a
77	H77	6.410565954	-2.288606954	3.097700146	H	1	ol03a
78	C78	2.291666038	1.568174176	3.429118521	C.3	1	ol03a
79	H79	1.451500501	1.420727586	3.910918080	H	1	ol03a
80	H80	2.126294412	2.143802473	2.652221445	H	1	ol03a
81	H81	2.937912655	2.001460617	4.023219780	H	1	ol03a
82	C82	-2.737732168	-0.393290935	-1.511485113	C.ar	1	ol03a
83	C83	-3.389996110	0.811670448	-1.277879737	C.ar	1	ol03a
84	H84	-3.051427127	1.407941746	-0.620477689	H	1	ol03a
85	C85	-4.544112103	1.165289280	-1.998677327	C.ar	1	ol03a
86	C86	-5.023219931	0.278667950	-2.922380462	C.ar	1	ol03a
87	H87	-5.809897463	0.500511486	-3.407778904	H	1	ol03a
88	C88	-4.401273586	-0.932184194	-3.170485827	C.ar	1	ol03a
89	C89	-3.239071614	-1.251698640	-2.464188127	C.ar	1	ol03a
90	H90	-2.789692308	-2.070785675	-2.643491787	H	1	ol03a
91	C91	-5.238243487	2.484875423	-1.719771507	C.3	1	ol03a
92	H92	-5.962460852	2.616379198	-2.368170271	H	1	ol03a
93	H93	-4.591735406	3.217875785	-1.799468609	H	1	ol03a
94	H94	-5.609528032	2.473536176	-0.812371783	H	1	ol03a
95	C95	-5.011470459	-1.940619133	-4.150289433	C.3	1	ol03a
96	H96	-5.983487336	-1.820492453	-4.181088401	H	1	ol03a
97	H97	-4.803192276	-2.850870176	-3.853293585	H	1	ol03a
98	H98	-4.635327173	-1.795380268	-5.043188554	H	1	ol03a

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Compound 2 – Monomer

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47 49
SMALL
NO_CHARGES


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   3  O3        1.318359491   -3.685950326    0.586693088   O.3   1  ol01
   4  N4       -0.727379317   -0.319053154    0.047215816   N.ar  1  ol01
   5  N5       -0.719839976   -2.662400957    0.449385929   N.ar  1  ol01
   6  N6        1.339271946   -1.490344978    0.214421744   N.ar  1  ol01
   7  C7        0.605568878   -0.412435336    0.042465707   C.ar  1  ol01
   8  C8       -1.305394747   -1.483134388    0.263015447   C.ar  1  ol01
   9  C9        0.602826261   -2.586117400    0.412013667   C.ar  1  ol01
  10  C10       2.589400723    0.937935577   -0.133363036   C.ar  1  ol01
  11  C11       3.393802911    0.272491041   -1.028298509   C.ar  1  ol01
  12  H12       3.033931952   -0.355579691   -1.611144102   H     1  ol01
  13  C13       4.750746109    0.553974695   -1.044829883   C.ar  1  ol01
  14  C14       5.234227096    1.508171855   -0.168050807   C.ar  1  ol01
  15  H15       6.144122389    1.701004135   -0.174752387   H     1  ol01
  16  C16       4.415117117    2.191057486    0.724335266   C.ar  1  ol01
  17  C17       3.061850989    1.879041644    0.737083075   C.ar  1  ol01
  18  H18       2.485749703    2.304038205    1.329640934   H     1  ol01
  19  C19       5.680774653   -0.144678298   -2.001102224   C.3   1  ol01
  20  H20       5.872578115    0.434310920   -2.742405453   H     1  ol01
  21  H21       6.498168962   -0.365285220   -1.549570511   H     1  ol01
  22  H22       5.265546490   -0.948573362   -2.320923934   H     1  ol01
  23  C23       4.963127455    3.267100737    1.612419004   C.3   1  ol01
  24  H24       4.580330398    4.111968509    1.364479969   H     1  ol01
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25	H25	4.741267489	3.071256436	2.526173797	H	1	ol01
26	H26	5.916760947	3.306747012	1.515200780	H	1	ol01
27	C27	-3.384068255	-0.373424100	0.080455724	C.ar	1	ol01
28	C28	-3.779959384	0.381602292	1.152362020	C.ar	1	ol01
29	H29	-3.530861415	0.140148114	2.015111784	H	1	ol01
30	C30	-4.557907078	1.513678919	0.936297878	C.ar	1	ol01
31	C31	-4.910537513	1.822225142	-0.361522614	C.ar	1	ol01
32	H32	-5.428994011	2.578894537	-0.515106285	H	1	ol01
33	C33	-4.523184658	1.046974023	-1.444809378	C.ar	1	ol01
34	C34	-3.742585437	-0.069423023	-1.206593121	C.ar	1	ol01
35	H35	-3.463702336	-0.608018100	-1.911611605	H	1	ol01
36	C36	-4.992585556	2.377625201	2.096175553	C.3	1	ol01
37	H37	-5.810099266	2.826891474	1.870835990	H	1	ol01
38	H38	-5.132507853	1.827959330	2.870379139	H	1	ol01
39	H39	-4.310883756	3.028125871	2.283693121	H	1	ol01
40	C40	-4.914845531	1.415843767	-2.853414139	C.3	1	ol01
41	H41	-4.529793296	0.786058762	-3.467604266	H	1	ol01
42	H42	-5.870727086	1.399090808	-2.935709070	H	1	ol01
43	H43	-4.592214283	2.297264841	-3.055476398	H	1	ol01
44	C44	0.597869542	-4.926999695	0.722937204	C.3	1	ol01
45	H45	0.025536466	-5.049605230	-0.036928254	H	1	ol01
46	H46	1.220679012	-5.654977030	0.773506074	H	1	ol01
47	H47	0.068166956	-4.903254310	1.523457085	H	1	ol01

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49   44   47   1
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Compound 2 – Dimer

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#          File Created by: Spartan `06 Export
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@<TRIPOS>MOLECULE
ol01
94 98
SMALL
NO_CHARGES


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   1  O1        0.858785982   -3.137396269   -0.025072264   O.3   1  ol01
   2  O2       -2.825570418   -0.962234477    1.388685660   O.3   1  ol01
   3  O3        1.250917212    0.564785872    2.556069614   O.3   1  ol01
   4  N4       -0.983750947   -2.093888773    0.619630022   N.ar  1  ol01
   5  N5       -0.841997003   -0.153010404    1.985638414   N.ar  1  ol01
   6  N6        1.145930195   -1.257616145    1.280412842   N.ar  1  ol01
   7  C7        0.351934842   -2.103475432    0.660837522   C.ar  1  ol01
   8  C8       -1.494007331   -1.094778095    1.310339124   C.ar  1  ol01
   9  C9        0.473784106   -0.301020869    1.924640999   C.ar  1  ol01
  10  C10       2.251340330   -3.388650004   -0.067583189   C.ar  1  ol01
  11  C11       3.126502439   -2.464921891   -0.588589310   C.ar  1  ol01
  12  H12       2.827395823   -1.624119482   -0.848110427   H     1  ol01
  13  C13       4.462757833   -2.809102490   -0.718255408   C.ar  1  ol01
  14  C14       4.854382092   -4.078149353   -0.331974074   C.ar  1  ol01
  15  H15       5.750044118   -4.314495825   -0.416763326   H     1  ol01
  16  C16       3.963567197   -5.015494952    0.179117828   C.ar  1  ol01
  17  C17       2.633121605   -4.642379140    0.318447101   C.ar  1  ol01
  18  H18       2.011202790   -5.236826298    0.669941489   H     1  ol01
  19  C19       5.467484198   -1.838212412   -1.279882784   C.3   1  ol01
  20  H20       5.647747506   -2.057942180   -2.196819208   H     1  ol01
  21  H21       6.281056429   -1.890641365   -0.774017753   H     1  ol01
  22  H22       5.115077370   -0.947204633   -1.226777866   H     1  ol01
  23  C23       4.411545714   -6.403807952    0.523764785   C.3   1  ol01
  24  H24       3.984892678   -7.032358745   -0.063347467   H     1  ol01
  25  H25       4.171064317   -6.600979989    1.432537271   H     1  ol01
  26  H26       5.363468348   -6.466689494    0.422860023   H     1  ol01
  27  C27      -3.631211213   -1.868188080    0.662019998   C.ar  1  ol01
  28  C28      -4.110651119   -2.977546962    1.306259174   C.ar  1  ol01
  29  H29      -3.876755923   -3.145690298    2.190384566   H     1  ol01
  30  C30      -4.950679428   -3.850258323    0.623461227   C.ar  1  ol01
  31  C31      -5.277166852   -3.549701225   -0.683045643   C.ar  1  ol01
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32	H32	-5.836805431	-4.129212641	-1.147702146	H	1	ol01
33	C33	-4.804541541	-2.416675502	-1.329042562	C.ar	1	ol01
34	C34	-3.963654116	-1.567703061	-0.632830671	C.ar	1	ol01
35	H35	-3.627158737	-0.801476834	-1.038516057	H	1	ol01
36	C36	-5.478851088	-5.092533666	1.300406350	C.3	1	ol01
37	H37	-6.314823650	-5.342854724	0.901210062	H	1	ol01
38	H38	-5.610307473	-4.917076220	2.234796921	H	1	ol01
39	H39	-4.846525339	-5.808151022	1.194470533	H	1	ol01
40	C40	-5.169901245	-2.120372281	-2.761556301	C.3	1	ol01
41	H41	-4.724961787	-1.318340869	-3.045702800	H	1	ol01
42	H42	-6.119490948	-2.001535376	-2.832723396	H	1	ol01
43	H43	-4.896929266	-2.852197314	-3.319935219	H	1	ol01
44	C44	0.606114575	1.677533919	3.207162757	C.3	1	ol01
45	H45	0.069202227	2.153238291	2.570433518	H	1	ol01
46	H46	1.271525048	2.267677786	3.566816943	H	1	ol01
47	H47	0.048613935	1.352774835	3.918376889	H	1	ol01
48	O48	-0.858829408	3.137361908	0.025085432	O.3	1	ol01
49	O49	2.825527033	0.962200057	-1.388672514	O.3	1	ol01
50	O50	-1.250960613	-0.564820273	-2.556056421	O.3	1	ol01
51	N51	0.983660212	2.093928963	-0.619663719	N.ar	1	ol01
52	N52	0.841906225	0.153050564	-1.985672114	N.ar	1	ol01
53	N53	-1.145891221	1.257638103	-1.280393262	N.ar	1	ol01
54	C54	-0.351895894	2.103497341	-0.660817992	C.ar	1	ol01
55	C55	1.494046287	1.094799983	-1.310319523	C.ar	1	ol01
56	C56	-0.473796346	0.300950910	-1.924715940	C.ar	1	ol01
57	C57	-2.251301374	3.388671893	0.067602790	C.ar	1	ol01
58	C58	-3.126514671	2.464851911	0.588514441	C.ar	1	ol01
59	H59	-2.827356875	1.624141391	0.848129957	H	1	ol01
60	C60	-4.462718877	2.809124379	0.718275009	C.ar	1	ol01
61	C61	-4.854425493	4.078114952	0.331987266	C.ar	1	ol01
62	H62	-5.750005118	4.314517744	0.416782930	H	1	ol01
63	C63	-3.963528197	5.015516871	-0.179098223	C.ar	1	ol01
64	C64	-2.633051463	4.642365431	-0.318515609	C.ar	1	ol01
65	H65	-2.011163790	5.236848217	-0.669921885	H	1	ol01
66	C66	-5.467445242	1.838234301	1.279902385	C.3	1	ol01
67	H67	-5.647708506	2.057964098	2.196838812	H	1	ol01
68	H68	-6.281099814	1.890606945	0.774030899	H	1	ol01
69	H69	-5.115120771	0.947170232	1.226791059	H	1	ol01
70	C70	-4.411506758	6.403829841	-0.523745184	C.3	1	ol01
71	H71	-3.984853722	7.032380634	0.063367068	H	1	ol01
72	H72	-4.171107743	6.600945627	-1.432524103	H	1	ol01
73	H73	-5.363511749	6.466655093	-0.422846830	H	1	ol01
74	C74	3.631167812	1.868153679	-0.662006805	C.ar	1	ol01
75	C75	4.110690075	2.977568850	-1.306239573	C.ar	1	ol01
76	H76	3.876712454	3.145655906	-2.190371401	H	1	ol01
77	C77	4.950718384	3.850280211	-0.623441625	C.ar	1	ol01
78	C78	5.277205852	3.549723144	0.683065247	C.ar	1	ol01
79	H79	5.836844387	4.129234530	1.147721747	H	1	ol01
80	C80	4.804529326	2.416605504	1.328967646	C.ar	1	ol01
81	C81	3.963610731	1.567668641	0.632843817	C.ar	1	ol01
82	H82	3.627115311	0.801442472	1.038529225	H	1	ol01
83	C83	5.478842711	5.092630146	-1.300433639	C.3	1	ol01
84	H84	6.314862606	5.342876613	-0.901190461	H	1	ol01
85	H85	5.610346404	4.917098149	-2.234777344	H	1	ol01
86	H86	4.846481913	5.808116660	-1.194457365	H	1	ol01
87	C87	5.169940202	2.120394170	2.761575902	C.3	1	ol01
88	H88	4.724918342	1.318306438	3.045715989	H	1	ol01
89	H89	6.119447504	2.001500945	2.832736585	H	1	ol01
90	H90	4.896885865	2.852162913	3.319948412	H	1	ol01
91	C91	-0.606075602	-1.677512049	-3.207143203	C.3	1	ol01
92	H92	-0.069163271	-2.153216403	-2.570413917	H	1	ol01

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93   H93      -1.271533425    -2.267581307    -3.566844232     H   1  ol01
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Compound 3 – Monomer

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ol02a in P2(1)/c
45 47
SMALL
NO_CHARGES


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   2  N2        3.397747782    0.935857190    0.267200679    N.ar   1  ol02a in P2(1)/c
   3  N3        1.260005386   -0.083336374    0.150223646    N.ar   1  ol02a in P2(1)/c
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4	N4	3.213686087	-1.417987335	-0.085111511	N.ar	1	ol02a in P2(1)/c
5	N5	1.488680984	2.162005775	0.514576726	N.3	1	ol02a in P2(1)/c
6	H6	2.013162084	2.825157109	0.671753195	H	1	ol02a in P2(1)/c
7	N7	1.144561119	-2.375515644	-0.205173392	N.3	1	ol02a in P2(1)/c
8	H8	1.560308637	-3.127425047	-0.242332212	H	1	ol02a in P2(1)/c
9	C9	3.885106730	-0.284595379	0.005602969	C.ar	1	ol02a in P2(1)/c
10	C10	2.052231209	0.952249733	0.305797238	C.ar	1	ol02a in P2(1)/c
11	C11	1.898262401	-1.262382536	-0.061280729	C.ar	1	ol02a in P2(1)/c
12	C12	0.083505686	2.418507540	0.492887649	C.ar	1	ol02a in P2(1)/c
13	C13	-0.811708400	1.550719309	1.110854998	C.ar	1	ol02a in P2(1)/c
14	H14	-0.511425319	0.804685232	1.578100718	H	1	ol02a in P2(1)/c
15	C15	-2.160238604	1.832060219	1.008685300	C.ar	1	ol02a in P2(1)/c
16	C16	-2.588876133	2.971576779	0.372902057	C.ar	1	ol02a in P2(1)/c
17	H17	-3.500453347	3.153576751	0.343347622	H	1	ol02a in P2(1)/c
18	C18	-1.699742054	3.869137433	-0.232504614	C.ar	1	ol02a in P2(1)/c
19	C19	-0.360333712	3.553087641	-0.170764936	C.ar	1	ol02a in P2(1)/c
20	H20	0.259020333	4.111687242	-0.582276570	H	1	ol02a in P2(1)/c
21	C21	-3.136337588	0.845092377	1.670822485	C.3	1	ol02a in P2(1)/c
22	H22	-4.010190321	0.954472628	1.288753738	H	1	ol02a in P2(1)/c
23	H23	-2.832444875	-0.053423464	1.522652194	H	1	ol02a in P2(1)/c
24	H24	-3.175545178	1.018183223	2.614218797	H	1	ol02a in P2(1)/c
25	C25	-2.188169545	5.090044271	-0.998903024	C.3	1	ol02a in P2(1)/c
26	H26	-2.192212474	4.897196886	-1.939330252	H	1	ol02a in P2(1)/c
27	H27	-3.077658799	5.311977314	-0.713975628	H	1	ol02a in P2(1)/c
28	H28	-1.602877447	5.831194996	-0.826760464	H	1	ol02a in P2(1)/c
29	C29	-0.289866291	-2.415405483	-0.301510985	C.ar	1	ol02a in P2(1)/c
30	C30	-0.953314032	-3.461400499	0.320092094	C.ar	1	ol02a in P2(1)/c
31	H31	-0.478986104	-4.099175875	0.802960798	H	1	ol02a in P2(1)/c
32	C32	-2.355419509	-3.546575817	0.211293049	C.ar	1	ol02a in P2(1)/c
33	C33	-3.007338947	-2.565289199	-0.506405950	C.ar	1	ol02a in P2(1)/c
34	H34	-3.933843686	-2.613183556	-0.570466184	H	1	ol02a in P2(1)/c
35	C35	-2.369793172	-1.521586141	-1.131908208	C.ar	1	ol02a in P2(1)/c
36	C36	-0.958381660	-1.477433219	-1.021878492	C.ar	1	ol02a in P2(1)/c
37	H37	-0.484488731	-0.799623893	-1.447158359	H	1	ol02a in P2(1)/c
38	C38	-3.077218707	-4.638503871	0.834745431	C.3	1	ol02a in P2(1)/c
39	H39	-3.993265841	-4.382992455	0.965844505	H	1	ol02a in P2(1)/c
40	H40	-3.038832416	-5.412439141	0.268012091	H	1	ol02a in P2(1)/c
41	H41	-2.677567130	-4.843090497	1.683279451	H	1	ol02a in P2(1)/c
42	C42	-3.125229826	-0.487819358	-1.884461131	C.3	1	ol02a in P2(1)/c
43	H43	-2.560281536	-0.108232472	-2.561551772	H	1	ol02a in P2(1)/c
44	H44	-3.893368644	-0.889591165	-2.296873242	H	1	ol02a in P2(1)/c
45	H45	-3.410203160	0.202642014	-1.281443452	H	1	ol02a in P2(1)/c

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Compound 3 – Dimer

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ol02a in P2(1)/c
90 94
SMALL
NO_CHARGES


@<TRIPOS>ATOM
   1  Cl1      -0.584517486   -4.061952512   -1.038945491     Cl   1  ol02a in P2(1)/c
   2  N2       -2.918061655   -3.313179201   -0.217391113   N.ar   1  ol02a in P2(1)/c
   3  N3       -3.516642598   -1.033706330    0.043510823   N.ar   1  ol02a in P2(1)/c
   4  N4       -1.269291382   -1.607089155   -0.479586787   N.ar   1  ol02a in P2(1)/c
   5  N5       -5.053243523   -2.705049294    0.312766587    N.3   1  ol02a in P2(1)/c
   6  H6       -5.210433234   -3.548919464    0.365850553      H   1  ol02a in P2(1)/c
   7  N7       -1.871219115    0.581533736   -0.234529491    N.3   1  ol02a in P2(1)/c
   8  H8       -1.034492095    0.759562231   -0.322208915      H   1  ol02a in P2(1)/c
   9  C9       -1.697565661   -2.855205822   -0.527175358   C.ar   1  ol02a in P2(1)/c
  10  C10      -3.787415519   -2.318682238    0.042164768   C.ar   1  ol02a in P2(1)/c
  11  C11      -2.226938990   -0.722793084   -0.242946914   C.ar   1  ol02a in P2(1)/c
  12  C12      -6.149344811   -1.811962931    0.517097115   C.ar   1  ol02a in P2(1)/c
  13  C13      -6.003834633   -0.666922012    1.294231024   C.ar   1  ol02a in P2(1)/c
  14  H14      -5.200655080   -0.477053868    1.722780791      H   1  ol02a in P2(1)/c
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15	C15	-7.089907253	0.178857487	1.409253714	C.ar	1	ol02a in P2(1)/c
16	C16	-8.290936929	-0.144688739	0.826440378	C.ar	1	ol02a in P2(1)/c
17	H17	-9.015313728	0.426775466	0.943248282	H	1	ol02a in P2(1)/c
18	C18	-8.461721743	-1.306172851	0.061951072	C.ar	1	ol02a in P2(1)/c
19	C19	-7.358648378	-2.117114760	-0.090565275	C.ar	1	ol02a in P2(1)/c
20	H20	-7.425945727	-2.884527727	-0.611415142	H	1	ol02a in P2(1)/c
21	C21	-6.901286069	1.455297295	2.246011268	C.3	1	ol02a in P2(1)/c
22	H22	-7.577363960	2.094953184	2.010824146	H	1	ol02a in P2(1)/c
23	H23	-6.033874692	1.827466771	2.070728253	H	1	ol02a in P2(1)/c
24	H24	-6.974740063	1.240264768	3.178674501	H	1	ol02a in P2(1)/c
25	C25	-9.774772816	-1.618940611	-0.641598311	C.3	1	ol02a in P2(1)/c
26	H26	-9.713478528	-1.359092047	-1.563704887	H	1	ol02a in P2(1)/c
27	H27	-10.487554087	-1.134054701	-0.219141173	H	1	ol02a in P2(1)/c
28	H28	-9.951334093	-2.560903194	-0.585598345	H	1	ol02a in P2(1)/c
29	C29	-2.766461435	1.698200911	-0.092155571	C.ar	1	ol02a in P2(1)/c
30	C30	-2.336359421	2.783737123	0.654532279	C.ar	1	ol02a in P2(1)/c
31	H31	-1.503066171	2.770722605	1.067284196	H	1	ol02a in P2(1)/c
32	C32	-3.177219244	3.907054581	0.780294496	C.ar	1	ol02a in P2(1)/c
33	C33	-4.407300649	3.864790919	0.157335279	C.ar	1	ol02a in P2(1)/c
34	H34	-4.968764488	4.600676717	0.247927012	H	1	ol02a in P2(1)/c
35	C35	-4.852571648	2.800874466	-0.588845116	C.ar	1	ol02a in P2(1)/c
36	C36	-3.974192682	1.696832829	-0.714155876	C.ar	1	ol02a in P2(1)/c
37	H37	-4.226771110	0.963560282	-1.227311368	H	1	ol02a in P2(1)/c
38	C38	-2.749333821	5.065756678	1.539549988	C.3	1	ol02a in P2(1)/c
39	H39	-3.518530074	5.570447287	1.813854838	H	1	ol02a in P2(1)/c
40	H40	-2.184064754	5.615851859	0.992382603	H	1	ol02a in P2(1)/c
41	H41	-2.262106813	4.778001871	2.315123247	H	1	ol02a in P2(1)/c
42	C42	-6.191911570	2.807374674	-1.230416866	C.3	1	ol02a in P2(1)/c
43	H43	-6.180914596	2.233613829	-2.000035995	H	1	ol02a in P2(1)/c
44	H44	-6.412738266	3.701531595	-1.501085236	H	1	ol02a in P2(1)/c
45	H45	-6.847899531	2.491148708	-0.604909964	H	1	ol02a in P2(1)/c
46	Cl46	0.102825882	3.291848668	-1.795445561	Cl	1	ol02a in P2(1)/c
47	N47	1.077308380	1.139130479	-0.747785223	N.ar	1	ol02a in P2(1)/c
48	N48	3.387580617	0.867424109	-0.288215030	N.ar	1	ol02a in P2(1)/c
49	N49	2.574424584	2.978399620	-1.020409657	N.ar	1	ol02a in P2(1)/c
50	N50	1.909979832	-0.855540108	-0.014898109	N.3	1	ol02a in P2(1)/c
51	H51	1.091542808	-1.119460008	-0.006997645	H	1	ol02a in P2(1)/c
52	N52	4.796495802	2.690094963	-0.582416125	N.3	1	ol02a in P2(1)/c
53	H53	4.872566975	3.535260481	-0.722071707	H	1	ol02a in P2(1)/c
54	C54	1.398497997	2.385890041	-1.119115481	C.ar	1	ol02a in P2(1)/c
55	C55	2.151614174	0.429101198	-0.355483799	C.ar	1	ol02a in P2(1)/c
56	C56	3.552665620	2.164769902	-0.651393348	C.ar	1	ol02a in P2(1)/c
57	C57	2.917015050	-1.807145340	0.333111593	C.ar	1	ol02a in P2(1)/c
58	C58	3.970942473	-1.458836252	1.172318318	C.ar	1	ol02a in P2(1)/c
59	H59	4.023287618	-0.610319844	1.549592682	H	1	ol02a in P2(1)/c
60	C60	4.936861238	-2.412766056	1.427554998	C.ar	1	ol02a in P2(1)/c
61	C61	4.814895862	-3.682585876	0.918504600	C.ar	1	ol02a in P2(1)/c
62	H62	5.463292594	-4.315164594	1.129210864	H	1	ol02a in P2(1)/c
63	C63	3.747019589	-4.057441629	0.092782504	C.ar	1	ol02a in P2(1)/c
64	C64	2.816358140	-3.084516025	-0.198766512	C.ar	1	ol02a in P2(1)/c
65	H65	2.106072771	-3.288118310	-0.763581861	H	1	ol02a in P2(1)/c
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67	H67	6.847373738	-2.599821293	2.192980435	H	1	ol02a in P2(1)/c
68	H68	6.381579047	-1.104929934	2.115618328	H	1	ol02a in P2(1)/c
69	H69	5.835494877	-2.038376767	3.250540259	H	1	ol02a in P2(1)/c
70	C70	3.659318505	-5.444738579	-0.527104016	C.3	1	ol02a in P2(1)/c
71	H71	3.979509924	-5.412082247	-1.431549564	H	1	ol02a in P2(1)/c
72	H72	4.197042430	-6.056739724	-0.019228561	H	1	ol02a in P2(1)/c
73	H73	2.746127631	-5.740636439	-0.521438411	H	1	ol02a in P2(1)/c
74	C74	6.003835701	1.962806982	-0.296341622	C.ar	1	ol02a in P2(1)/c
75	C75	6.964857005	2.582572654	0.486594689	C.ar	1	ol02a in P2(1)/c

76	H76	6.814111093	3.432739822	0.832136105	H	1	ol02a in P2(1)/c
77	C77	8.173184540	1.908595076	0.752475058	C.ar	1	ol02a in P2(1)/c
78	C78	8.336200702	0.644553230	0.224611434	C.ar	1	ol02a in P2(1)/c
79	H79	9.128364485	0.193188119	0.407793273	H	1	ol02a in P2(1)/c
80	C80	7.398316609	0.012685494	-0.555229583	C.ar	1	ol02a in P2(1)/c
81	C81	6.204255995	0.726242333	-0.822055810	C.ar	1	ol02a in P2(1)/c
82	H82	5.550915716	0.344504994	-1.362691410	H	1	ol02a in P2(1)/c
83	C83	9.205881503	2.536889109	1.552962028	C.3	1	ol02a in P2(1)/c
84	H84	9.781915265	1.861864173	1.919217058	H	1	ol02a in P2(1)/c
85	H85	9.720005369	3.131966651	1.002329454	H	1	ol02a in P2(1)/c
86	H86	8.799557499	3.032827761	2.267478323	H	1	ol02a in P2(1)/c
87	C87	7.624962196	-1.354269695	-1.089796356	C.3	1	ol02a in P2(1)/c
88	H88	7.115415564	-1.471485162	-1.894984601	H	1	ol02a in P2(1)/c
89	H89	8.558146020	-1.472243484	-1.281610360	H	1	ol02a in P2(1)/c
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Compound 4 – Monomer

#
File Created by: Spartan `06 Export
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jw1027

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51 53
SMALL
NO_CHARGES


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      1 C1          -6.909327137   -0.349721492    0.639146560 C.3  1 jw1027
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      3 H3          -7.242252012   -0.939829851    1.332636597 H    1 jw1027
      4 H4          -7.186958958    0.559321153    0.830078631 H    1 jw1027
      5 C5          -4.850522344    0.484573300   -0.156717900 C.2  1 jw1027
      6 C6          -3.345055257    0.320221638   -0.126843577 C.ar 1 jw1027
      7 C7          -1.521922171   -0.985154528    0.018725367 C.ar 1 jw1027
      8 C8          -1.314165452    1.235534424   -0.285572612 C.ar 1 jw1027
      9 C9           0.831148799    2.505526578   -0.347113452 C.ar 1 jw1027
     10 C10          1.727321921    1.546086398   -0.805436524 C.ar 1 jw1027
     11 H11          1.406240215    0.739789396   -1.167655825 H    1 jw1027
     12 C12          3.091760683    1.773587312   -0.730033833 C.ar 1 jw1027
     13 C13          3.532032278    2.984326721   -0.203265967 C.ar 1 jw1027
     14 H14          4.455420856    3.140793120   -0.136298740 H    1 jw1027
     15 C15          2.656028943    3.962778996    0.221817782 C.ar 1 jw1027
     16 C16          1.288730451    3.697451540    0.164030478 C.ar 1 jw1027
     17 H17          0.674244756    4.338439169    0.475362943 H    1 jw1027
     18 C18          4.062413850    0.723818547   -1.216299949 C.3  1 jw1027
     19 H19          4.598801288    0.410308692   -0.472086520 H    1 jw1027
     20 H20          3.571342745   -0.020813675   -1.595510098 H    1 jw1027
     21 H21          4.641215738    1.108320879   -1.893184573 H    1 jw1027
     22 C22          3.135982158    5.295297842    0.785606423 C.3  1 jw1027
     23 H23          2.398870860    5.924902723    0.799704703 H    1 jw1027
     24 H24          3.467076411    5.163759207    1.687903483 H    1 jw1027
     25 H25          3.849010990    5.643533697    0.227542943 H    1 jw1027
     26 C26          0.383797337   -2.544315356    0.239868514 C.ar 1 jw1027
     27 C27          0.767606293   -3.721754815   -0.389132077 C.ar 1 jw1027
     28 H28          0.130656211   -4.230971244   -0.858010871 H    1 jw1027
     29 C29          2.086785189   -4.148335945   -0.327073799 C.ar 1 jw1027
     30 C30          3.006868155   -3.381968878    0.373549410 C.ar 1 jw1027
     31 H31          3.901841798   -3.666451137    0.415871858 H    1 jw1027
     32 C32          2.640009318   -2.208472066    1.012764262 C.ar 1 jw1027
     33 C33          1.312596416   -1.788028983    0.928680336 C.ar 1 jw1027
     34 H34          1.048617369   -0.986063963    1.343067189 H    1 jw1027
     35 C35          2.513241323   -5.414529209   -1.033562276 C.3  1 jw1027
     36 H36          2.252428715   -6.184601721   -0.504832078 H    1 jw1027
     37 H37          2.084937621   -5.458512514   -1.903179296 H    1 jw1027
     38 H38          3.477757703   -5.412750763   -1.146162360 H    1 jw1027
     39 C39          3.637812890   -1.407699964    1.797638897 C.3  1 jw1027
     40 H40          3.712049956   -1.772778130    2.693319764 H    1 jw1027
     41 H41          4.503044241   -1.448058713    1.359721382 H    1 jw1027
     42 H42          3.343119588   -0.484066489    1.848377793 H    1 jw1027
     43 N43         -2.882952537   -0.918029354    0.010995216 N.ar 1 jw1027
     44 N44         -2.662422410    1.433415370   -0.281859288 N.ar 1 jw1027
     45 N45         -0.707087999    0.063627292   -0.146067928 N.ar 1 jw1027
     46 N46         -0.995064224   -2.199074116    0.194153016 N.3  1 jw1027
     47 H47         -1.560604854   -2.853349419    0.292107296 H    1 jw1027
     48 N48         -0.577091361    2.357517131   -0.430236613 N.3  1 jw1027
     49 H49         -1.023145534    3.084933717   -0.595599812 H    1 jw1027
     50 O50         -5.455282313   -0.415400063    0.601951701 O.3  1 jw1027
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Compound 4 – Dimer 1 (N-H---O)

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#          File Created by: Spartan `06 Export
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jw1027
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SMALL
NO_CHARGES

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3	H3	0.141717867	5.574779059	-1.893290685	H	1	jw1027
4	H4	1.064530842	4.343666555	-1.524704049	H	1	jw1027
5	C5	-0.712345743	2.936498916	-0.384140350	C.2	1	jw1027
6	C6	-1.999096655	2.141769102	-0.300391266	C.ar	1	jw1027
7	C7	-4.242530856	2.054799756	-0.208436869	C.ar	1	jw1027
8	C8	-3.021517523	0.167287298	-0.091614820	C.ar	1	jw1027
9	C9	-3.928362684	-2.154125290	-0.003740763	C.ar	1	jw1027
10	C10	-5.167986318	-1.962603877	0.596564476	C.ar	1	jw1027
11	H11	-5.367713526	-1.140784069	1.007822534	H	1	jw1027
12	C12	-6.110192540	-2.978157865	0.590669563	C.ar	1	jw1027
13	C13	-5.775537458	-4.187001961	-0.012585899	C.ar	1	jw1027
14	H14	-6.413356489	-4.875767797	-0.032639505	H	1	jw1027
15	C15	-4.536646336	-4.406923317	-0.580240841	C.ar	1	jw1027
16	C16	-3.617100273	-3.359254797	-0.588646408	C.ar	1	jw1027
17	H17	-2.777080418	-3.477361185	-0.995836788	H	1	jw1027
18	C18	-7.460370821	-2.762060427	1.231730677	C.3	1	jw1027
19	H19	-8.152383902	-2.821786022	0.555413347	H	1	jw1027
20	H20	-7.487109114	-1.884901064	1.643198504	H	1	jw1027
21	H21	-7.609030082	-3.441585432	1.907876792	H	1	jw1027
22	C22	-4.163007901	-5.735016695	-1.228610944	C.3	1	jw1027
23	H23	-3.201769079	-5.777889311	-1.347425349	H	1	jw1027
24	H24	-4.599741397	-5.807181425	-2.091815847	H	1	jw1027
25	H25	-4.451956819	-6.464806438	-0.658497360	H	1	jw1027
26	C26	-6.713452379	2.119442441	-0.163408278	C.ar	1	jw1027
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44	N44	-1.841532742	0.840000047	-0.201445049	N.ar	1	jw1027
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Compound 4 – Dimer 2 (N-H---N)

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jw1027
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SMALL
NO_CHARGES


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   5  C5        0.537501369    3.719872862   -1.051362428    C.2   1  jw1027
   6  C6        1.572809781    2.669750388   -0.705361710   C.ar   1  jw1027
   7  C7        2.124626533    0.536154567   -0.266860406   C.ar   1  jw1027
   8  C8        3.681358613    2.159540718   -0.175061273   C.ar   1  jw1027
   9  C9        6.115965542    1.824305161    0.248439112   C.ar   1  jw1027
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16	C16	7.287191157	2.323783481	-0.271260798	C.ar	1	jw1027
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40	H40	5.866726272	-3.890355543	-1.520256190	H	1	jw1027
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Optimized files

Compound 1 – Monomer

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#          File Created by: Spartan `06 Export
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ol03a
49 51
SMALL
NO_CHARGES


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   3  N3       -0.611026817   -0.313251723   -0.129133740    N.ar  1  ol03a
   4  N4        1.322497144   -1.724642613   -0.189857595    N.ar  1  ol03a
   5  N5       -2.709087361   -1.369925268   -0.257801805    N.3   1  ol03a
   6  H6       -3.112623559   -2.295226443   -0.333076281    H     1  ol03a
   7  N7        1.460957788    0.614985008   -0.006264080    N.3   1  ol03a
   8  H8        0.871915100    1.436580033    0.035447186    H     1  ol03a
   9  C9        0.465595431   -2.749051760   -0.291391474    C.ar  1  ol03a
  10  C10      -1.344248013   -1.427045110   -0.230909612    C.ar  1  ol03a
  11  C11       0.720564657   -0.527889989   -0.112163457    C.ar  1  ol03a
  12  C12       2.379921063   -4.150429404   -0.360900672    C.3   1  ol03a
  13  H13       2.545825037   -5.224417833   -0.458928700    H     1  ol03a
  14  H14       2.846293590   -3.617289450   -1.194328676    H     1  ol03a
  15  H15       2.804207508   -3.787004082    0.579688215    H     1  ol03a
  16  C16      -3.626758120   -0.306439839   -0.187772161    C.ar  1  ol03a
  17  C17      -4.988694086   -0.660030777   -0.207727320    C.ar  1  ol03a
  18  H18      -5.265986220   -1.710937405   -0.273816447    H     1  ol03a
  19  C19      -5.985727796    0.309254002   -0.146202133    C.ar  1  ol03a
  20  C20      -5.609018808    1.657485447   -0.058442837    C.ar  1  ol03a
  21  H21      -6.378217689    2.425494950   -0.006377535    H     1  ol03a
  22  C22      -4.264071435    2.028646332   -0.037043395    C.ar  1  ol03a
  23  C23      -3.269598571    1.043011042   -0.104677614    C.ar  1  ol03a
  24  H24      -2.223574342    1.315610488   -0.089678250    H     1  ol03a
  25  C25      -7.445914150   -0.079848470   -0.190547853    C.3   1  ol03a
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26	H26	-8.016474484	0.419488609	0.601177722	H	1	ol03a
27	H27	-7.904316107	0.205468528	-1.146308774	H	1	ol03a
28	H28	-7.577357430	-1.159849302	-0.069790138	H	1	ol03a
29	C29	-3.863527785	3.482650100	0.076149523	C.3	1	ol03a
30	H30	-3.431297441	3.700949953	1.061473869	H	1	ol03a
31	H31	-3.107649454	3.748415383	-0.672421562	H	1	ol03a
32	H32	-4.722709723	4.146655896	-0.061589112	H	1	ol03a
33	C33	2.846402654	0.861389822	0.036626086	C.ar	1	ol03a
34	C34	3.232622169	2.213155059	0.099930261	C.ar	1	ol03a
35	H35	2.466819123	2.987265443	0.110405637	H	1	ol03a
36	C36	4.575263918	2.575889541	0.150575357	C.ar	1	ol03a
37	C37	5.546520676	1.563806037	0.133470293	C.ar	1	ol03a
38	H38	6.599781929	1.834931884	0.170703292	H	1	ol03a
39	C39	5.184175562	0.218006372	0.070839496	C.ar	1	ol03a
40	C40	3.827811513	-0.134180766	0.024657637	C.ar	1	ol03a
41	H41	3.529060298	-1.172027623	-0.022626921	H	1	ol03a
42	C42	4.982641888	4.028984341	0.236670868	C.3	1	ol03a
43	H43	5.735221595	4.277829984	-0.520979731	H	1	ol03a
44	H44	4.126951461	4.696167527	0.092559831	H	1	ol03a
45	H45	5.422691141	4.261117622	1.215106970	H	1	ol03a
46	C46	6.236497526	-0.867806411	0.038941818	C.3	1	ol03a
47	H47	7.231968735	-0.466517098	0.253414028	H	1	ol03a
48	H48	6.022708431	-1.652183411	0.774558121	H	1	ol03a
49	H49	6.278682564	-1.352300340	-0.945201299	H	1	ol03a

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Compound 1 – Dimer 1 (-NHAr/-OMe)

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#          File Created by: Spartan `06 Export
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ol03a
98 102
SMALL
NO_CHARGES


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   3  N3        3.307834520    1.437004327   -0.061997742    N.ar  1  ol03a
   4  N4        4.117399075   -0.810208458    0.076970171    N.ar  1  ol03a
   5  N5        1.002790521    1.779885781   -0.085830340    N.3   1  ol03a
   6  H6        0.082211404    1.333017871   -0.001259124    H     1  ol03a
   7  N7        5.543639995    1.061723111    0.003494156    N.3   1  ol03a
   8  H8        5.507382692    2.072627185   -0.034712635    H     1  ol03a
   9  C9        2.834476486   -1.175929086    0.064602299    C.ar  1  ol03a
  10  C10       2.063109355    0.937467906   -0.059373024    C.ar  1  ol03a
  11  C11       4.287619070    0.523550420    0.005613192    C.ar  1  ol03a
  12  C12       3.617973465   -3.412598178    0.258438458    C.3   1  ol03a
  13  H13       3.138201276   -4.388195404    0.348575822    H     1  ol03a
  14  H14       4.220738982   -3.201752735    1.145985341    H     1  ol03a
  15  H15       4.260196219   -3.383183027   -0.626755704    H     1  ol03a
  16  C16       1.051890156    3.198353461   -0.068983831    C.ar  1  ol03a
  17  C17       0.195295947    3.881399521    0.798329122    C.ar  1  ol03a
  18  H18      -0.457771073    3.312338927    1.453141421    H     1  ol03a
  19  C19       0.170086378    5.280576371    0.823872179    C.ar  1  ol03a
  20  C20       1.024396871    5.983432967   -0.029861776    C.ar  1  ol03a
  21  H21       1.014698220    7.071812258   -0.016053907    H     1  ol03a
  22  C22       1.892928519    5.316407105   -0.904327985    C.ar  1  ol03a
  23  C23       1.893703075    3.920696682   -0.924309391    C.ar  1  ol03a
  24  H24       2.550537147    3.386714649   -1.601181861    H     1  ol03a
  25  C25      -0.756512127    6.007795694    1.772595204    C.3   1  ol03a
  26  H26      -0.659659454    7.093462424    1.670947287    H     1  ol03a
  27  H27      -0.541904077    5.750326212    2.817307814    H     1  ol03a
  28  H28      -1.806910427    5.747431085    1.590206307    H     1  ol03a
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29	C29	2.826570793	6.095239177	-1.803562377	C.3	1	ol03a
30	H30	3.073640042	5.530910642	-2.709101437	H	1	ol03a
31	H31	3.772554374	6.323938522	-1.293993819	H	1	ol03a
32	H32	2.385865784	7.050484149	-2.109350587	H	1	ol03a
33	C33	6.831657765	0.500023792	0.064419150	C.ar	1	ol03a
34	C34	7.903891178	1.411492756	0.088207615	C.ar	1	ol03a
35	H35	7.695914721	2.480063630	0.064245580	H	1	ol03a
36	C36	9.222754411	0.970549883	0.139859364	C.ar	1	ol03a
37	C37	9.469661679	-0.410121647	0.171312111	C.ar	1	ol03a
38	H38	10.496323374	-0.768917941	0.212616122	H	1	ol03a
39	C39	8.420499378	-1.329848471	0.149936588	C.ar	1	ol03a
40	C40	7.096489634	-0.872710189	0.094349402	C.ar	1	ol03a
41	H41	6.271763205	-1.571347338	0.076514655	H	1	ol03a
42	C42	10.369310787	1.955618425	0.148821136	C.3	1	ol03a
43	H43	11.063234028	1.752011912	0.973055695	H	1	ol03a
44	H44	10.013895775	2.985411154	0.255545394	H	1	ol03a
45	H45	10.949524157	1.898836727	-0.781108274	H	1	ol03a
46	C46	8.693384050	-2.816611470	0.197492508	C.3	1	ol03a
47	H47	9.762616183	-3.030294360	0.102020087	H	1	ol03a
48	H48	8.171294847	-3.345414289	-0.609087119	H	1	ol03a
49	H49	8.350728607	-3.254824902	1.143879904	H	1	ol03a
50	O50	-2.538053862	2.481275657	-0.139331457	O.3	1	ol03a
51	N51	-1.765679919	0.388679289	0.013509836	N.ar	1	ol03a
52	N52	-3.307834520	-1.437004327	0.061997742	N.ar	1	ol03a
53	N53	-4.117399075	0.810208458	-0.076970171	N.ar	1	ol03a
54	N54	-1.002790521	-1.779885781	0.085830340	N.3	1	ol03a
55	H55	-0.082211404	-1.333017871	0.001259124	H	1	ol03a
56	N56	-5.543639995	-1.061723111	-0.003494156	N.3	1	ol03a
57	H57	-5.507382692	-2.072627185	0.034712635	H	1	ol03a
58	C58	-2.834476486	1.175929086	-0.064602299	C.ar	1	ol03a
59	C59	-2.063109355	-0.937467906	0.059373024	C.ar	1	ol03a
60	C60	-4.287619070	-0.523550420	-0.005613192	C.ar	1	ol03a
61	C61	-3.617973465	3.412598178	-0.258438458	C.3	1	ol03a
62	H62	-3.138201276	4.388195404	-0.348575822	H	1	ol03a
63	H63	-4.220738982	3.201752735	-1.145985341	H	1	ol03a
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65	C65	-1.051890156	-3.198353461	0.068983831	C.ar	1	ol03a
66	C66	-0.195295947	-3.881399521	-0.798329122	C.ar	1	ol03a
67	H67	0.457771073	-3.312338927	-1.453141421	H	1	ol03a
68	C68	-0.170086378	-5.280576371	-0.823872179	C.ar	1	ol03a
69	C69	-1.024396871	-5.983432967	0.029861776	C.ar	1	ol03a
70	H70	-1.014698220	-7.071812258	0.016053907	H	1	ol03a
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73	H73	-2.550537147	-3.386714649	1.601181861	H	1	ol03a
74	C74	0.756512127	-6.007795694	-1.772595204	C.3	1	ol03a
75	H75	0.659659454	-7.093462424	-1.670947287	H	1	ol03a
76	H76	0.541904077	-5.750326212	-2.817307814	H	1	ol03a
77	H77	1.806910427	-5.747431085	-1.590206307	H	1	ol03a
78	C78	-2.826570793	-6.095239177	1.803562377	C.3	1	ol03a
79	H79	-3.073640042	-5.530910642	2.709101437	H	1	ol03a
80	H80	-3.772554374	-6.323938522	1.293993819	H	1	ol03a
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83	C83	-7.903891178	-1.411492756	-0.088207615	C.ar	1	ol03a
84	H84	-7.695914721	-2.480063630	-0.064245580	H	1	ol03a
85	C85	-9.222754411	-0.970549883	-0.139859364	C.ar	1	ol03a
86	C86	-9.469661679	0.410121647	-0.171312111	C.ar	1	ol03a
87	H87	-10.496323374	0.768917941	-0.212616122	H	1	ol03a
88	C88	-8.420499378	1.329848471	-0.149936588	C.ar	1	ol03a
89	C89	-7.096489634	0.872710189	-0.094349402	C.ar	1	ol03a

90	H90	-6.271763205	1.571347338	-0.076514655	H	1	ol03a
91	C91	-10.369310787	-1.955618425	-0.148821136	C.3	1	ol03a
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93	H93	-10.013895775	-2.985411154	-0.255545394	H	1	ol03a
94	H94	-10.949524157	-1.898836727	0.781108274	H	1	ol03a
95	C95	-8.693384050	2.816611470	-0.197492508	C.3	1	ol03a
96	H96	-9.762616183	3.030294360	-0.102020087	H	1	ol03a
97	H97	-8.171294847	3.345414289	0.609087119	H	1	ol03a
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Compound 1 – Dimer 2 (-NHAr/-NHAr)

#
File Created by: Spartan `06 Export
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ol03a
98 102
SMALL
NO_CHARGES


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   3  N3       -0.161528316    1.804283963    0.167707251    N.ar  1  ol03a
   4  N4        1.342007371    3.106042184   -1.169400470    N.ar  1  ol03a
   5  N5       -1.807626721    2.992648814    1.369115839    N.3   1  ol03a
   6  H6       -2.150377204    3.938958845    1.479593127    H     1  ol03a
   7  N7        1.540644965    0.780288314   -0.968637437    N.3   1  ol03a
   8  H8        1.182229573   -0.031283939   -0.461947285    H     1  ol03a
   9  C9        0.648330356    4.172258855   -0.763213360    C.ar  1  ol03a
  10  C10      -0.741024439    2.962556317    0.512581057    C.ar  1  ol03a
  11  C11       0.904846737    1.940428981   -0.664449934    C.ar  1  ol03a
  12  C12       2.113416360    5.456475388   -2.116054360    C.3   1  ol03a
  13  H13       2.264204923    6.522968818   -2.289936578    H     1  ol03a
  14  H14       1.882478226    4.950459936   -3.058459012    H     1  ol03a
  15  H15       3.009685032    5.007609676   -1.680339173    H     1  ol03a
  16  C16      -2.426331367    2.025882600    2.185974888    C.ar  1  ol03a
  17  C17      -3.584139369    2.445136783    2.866612982    C.ar  1  ol03a
  18  H18      -3.949820308    3.460042229    2.719674234    H     1  ol03a
  19  C19      -4.265277958    1.586234940    3.724204266    C.ar  1  ol03a
  20  C20      -3.776693861    0.283163406    3.898723983    C.ar  1  ol03a
  21  H21      -4.299880049   -0.397769651    4.566988913    H     1  ol03a
  22  C22      -2.631751264   -0.154211544    3.232050023    C.ar  1  ol03a
  23  C23      -1.952938990    0.723284362    2.373138813    C.ar  1  ol03a
  24  H24      -1.063608780    0.391086357    1.857416244    H     1  ol03a
  25  C25      -5.503156949    2.046270890    4.459159521    C.3   1  ol03a
  26  H26      -5.349802989    2.030132314    5.545511747    H     1  ol03a
  27  H27      -6.358117006    1.393008339    4.246245049    H     1  ol03a
  28  H28      -5.783565407    3.066228389    4.177575655    H     1  ol03a
  29  C29      -2.126723733   -1.568009184    3.408977019    C.3   1  ol03a
  30  H30      -1.033661596   -1.599743082    3.472995212    H     1  ol03a
  31  H31      -2.419404123   -2.199025398    2.559752764    H     1  ol03a
  32  H32      -2.535097561   -2.026261490    4.315385517    H     1  ol03a
  33  C33       2.652920937    0.526098724   -1.802619966    C.ar  1  ol03a
  34  C34       3.319274480   -0.693516251   -1.592863252    C.ar  1  ol03a
  35  H35       2.985844762   -1.351749732   -0.795597828    H     1  ol03a
  36  C36       4.408121987   -1.061563617   -2.379437924    C.ar  1  ol03a
  37  C37       4.834860215   -0.187704056   -3.389091500    C.ar  1  ol03a
  38  H38       5.691109612   -0.458726766   -4.003833034    H     1  ol03a
  39  C39       4.182297395    1.024799310   -3.618101737    C.ar  1  ol03a
  40  C40       3.085410420    1.380516375   -2.821534986    C.ar  1  ol03a
  41  H41       2.576116822    2.320168142   -2.985500426    H     1  ol03a
  42  C42       5.106760089   -2.383285941   -2.154884786    C.3   1  ol03a
  43  H43       6.195415505   -2.275599903   -2.222126144    H     1  ol03a
  44  H44       4.808307648   -3.124560575   -2.908048229    H     1  ol03a
  45  H45       4.867317816   -2.799884820   -1.171290479    H     1  ol03a
  46  C46       4.638016108    1.953444671   -4.721707779    C.3   1  ol03a
  47  H47       5.554135691    1.589044869   -5.197242636    H     1  ol03a
  48  H48       4.835862529    2.962749414   -4.340674145    H     1  ol03a
  49  H49       3.873460014    2.049107490   -5.503389416    H     1  ol03a
  50  O50      -1.006028555   -5.381007763   -1.211329069    O.3   1  ol03a
  51  N51       0.384339456   -4.187183816    0.073385049    N.ar  1  ol03a
  52  N52       0.161528316   -1.804283963    0.167707251    N.ar  1  ol03a
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54	N54	1.807626721	-2.992648814	1.369115839	N.3	1	ol03a
55	H55	2.150377204	-3.938958845	1.479593127	H	1	ol03a
56	N56	-1.540644965	-0.780288314	-0.968637437	N.3	1	ol03a
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58	C58	-0.648330356	-4.172258855	-0.763213360	C.ar	1	ol03a
59	C59	0.741024439	-2.962556317	0.512581057	C.ar	1	ol03a
60	C60	-0.904846737	-1.940428981	-0.664449934	C.ar	1	ol03a
61	C61	-2.113416360	-5.456475388	-2.116054360	C.3	1	ol03a
62	H62	-2.264204923	-6.522968818	-2.289936578	H	1	ol03a
63	H63	-1.882478226	-4.950459936	-3.058459012	H	1	ol03a
64	H64	-3.009685032	-5.007609676	-1.680339173	H	1	ol03a
65	C65	2.426331367	-2.025882600	2.185974888	C.ar	1	ol03a
66	C66	3.584139369	-2.445136783	2.866612982	C.ar	1	ol03a
67	H67	3.949820308	-3.460042229	2.719674234	H	1	ol03a
68	C68	4.265277958	-1.586234940	3.724204266	C.ar	1	ol03a
69	C69	3.776693861	-0.283163406	3.898723983	C.ar	1	ol03a
70	H70	4.299880049	0.397769651	4.566988913	H	1	ol03a
71	C71	2.631751264	0.154211544	3.232050023	C.ar	1	ol03a
72	C72	1.952938990	-0.723284362	2.373138813	C.ar	1	ol03a
73	H73	1.063608780	-0.391086357	1.857416244	H	1	ol03a
74	C74	5.503156949	-2.046270890	4.459159521	C.3	1	ol03a
75	H75	5.349802989	-2.030132314	5.545511747	H	1	ol03a
76	H76	6.358117006	-1.393008339	4.246245049	H	1	ol03a
77	H77	5.783565407	-3.066228389	4.177575655	H	1	ol03a
78	C78	2.126723733	1.568009184	3.408977019	C.3	1	ol03a
79	H79	1.033661596	1.599743082	3.472995212	H	1	ol03a
80	H80	2.419404123	2.199025398	2.559752764	H	1	ol03a
81	H81	2.535097561	2.026261490	4.315385517	H	1	ol03a
82	C82	-2.652920937	-0.526098724	-1.802619966	C.ar	1	ol03a
83	C83	-3.319274480	0.693516251	-1.592863252	C.ar	1	ol03a
84	H84	-2.985844762	1.351749732	-0.795597828	H	1	ol03a
85	C85	-4.408121987	1.061563617	-2.379437924	C.ar	1	ol03a
86	C86	-4.834860215	0.187704056	-3.389091500	C.ar	1	ol03a
87	H87	-5.691109612	0.458726766	-4.003833034	H	1	ol03a
88	C88	-4.182297395	-1.024799310	-3.618101737	C.ar	1	ol03a
89	C89	-3.085410420	-1.380516375	-2.821534986	C.ar	1	ol03a
90	H90	-2.576116822	-2.320168142	-2.985500426	H	1	ol03a
91	C91	-5.106760089	2.383285941	-2.154884786	C.3	1	ol03a
92	H92	-6.195415505	2.275599903	-2.222126144	H	1	ol03a
93	H93	-4.808307648	3.124560575	-2.908048229	H	1	ol03a
94	H94	-4.867317816	2.799884820	-1.171290479	H	1	ol03a
95	C95	-4.638016108	-1.953444671	-4.721707779	C.3	1	ol03a
96	H96	-5.554135691	-1.589044869	-5.197242636	H	1	ol03a
97	H97	-4.835862529	-2.962749414	-4.340674145	H	1	ol03a
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Compound 2 – Monomer

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ol01
47 49
SMALL
NO_CHARGES


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   1  O1        1.217690570    0.889571197   -0.187789942    O.3   1  ol01
   2  O2       -2.618345676   -1.511561291    0.258863599    O.3   1  ol01
   3  O3        1.401959739   -3.537970634    0.849396396    O.3   1  ol01
   4  N4       -0.704409201   -0.245324288    0.010346892    N.ar  1  ol01
   5  N5       -0.661160041   -2.565674096    0.561518129    N.ar  1  ol01
   6  N6        1.384335552   -1.352678966    0.340208952    N.ar  1  ol01
   7  C7        0.633677657   -0.293802563    0.064955842    C.ar  1  ol01
   8  C8       -1.278118456   -1.413235125    0.272154408    C.ar  1  ol01
   9  C9        0.666967229   -2.460373747    0.576716780    C.ar  1  ol01
  10  C10       2.614770927    1.007260691   -0.181395843    C.ar  1  ol01
  11  C11       3.367561299    0.503066772   -1.236985422    C.ar  1  ol01
  12  H12       2.877434916   -0.056881342   -2.027291110      H  1  ol01
  13  C13       4.748545467    0.715693636   -1.254704226    C.ar  1  ol01
  14  C14       5.332784022    1.436655546   -0.203685519    C.ar  1  ol01
  15  H15       6.408824969    1.598391246   -0.210652558      H  1  ol01
  16  C16       4.574681030    1.953081868    0.851384726    C.ar  1  ol01
  17  C17       3.191999421    1.727799947    0.854797018    C.ar  1  ol01
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18	H18	2.561051894	2.107034644	1.653426607	H	1	ol01
19	C19	5.591896122	0.200187394	-2.398100145	C.3	1	ol01
20	H20	5.658694505	0.939466185	-3.207534629	H	1	ol01
21	H21	6.614178454	-0.018442930	-2.072188656	H	1	ol01
22	H22	5.170122367	-0.714631895	-2.827454148	H	1	ol01
23	C23	5.220345763	2.747579008	1.962837246	C.3	1	ol01
24	H24	5.001286752	3.818908745	1.864731005	H	1	ol01
25	H25	4.853860315	2.431445016	2.946219194	H	1	ol01
26	H26	6.308796334	2.632963979	1.955110997	H	1	ol01
27	C27	-3.394309291	-0.369865301	0.004621514	C.ar	1	ol01
28	C28	-3.789814488	0.426198097	1.070371927	C.ar	1	ol01
29	H29	-3.434984640	0.196210841	2.070752576	H	1	ol01
30	C30	-4.645161426	1.510649361	0.838389038	C.ar	1	ol01
31	C31	-5.075361478	1.755695513	-0.470029564	C.ar	1	ol01
32	H32	-5.741549811	2.594933457	-0.659130912	H	1	ol01
33	C33	-4.677652365	0.950099626	-1.545436028	C.ar	1	ol01
34	C34	-3.828227446	-0.131597853	-1.294278199	C.ar	1	ol01
35	H35	-3.503023626	-0.787883327	-2.095921716	H	1	ol01
36	C36	-5.106488463	2.376510623	1.988008978	C.3	1	ol01
37	H37	-5.552600919	3.309894077	1.630796088	H	1	ol01
38	H38	-5.861424171	1.861287703	2.596328050	H	1	ol01
39	H39	-4.274269469	2.631820428	2.653605057	H	1	ol01
40	C40	-5.134422023	1.258417461	-2.952934080	C.3	1	ol01
41	H41	-5.157951825	0.355693041	-3.572280512	H	1	ol01
42	H42	-6.135093984	1.703347683	-2.960060877	H	1	ol01
43	H43	-4.456751342	1.971608989	-3.440843106	H	1	ol01
44	C44	0.704630185	-4.763168109	1.118309807	C.3	1	ol01
45	H45	0.096441450	-5.061344584	0.260381437	H	1	ol01
46	H46	1.489013218	-5.497031990	1.307183450	H	1	ol01
47	H47	0.057309710	-4.658699997	1.992895134	H	1	ol01

@<TRIPOS>BOND

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28	23	25	1

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Compound 2 – Dimer

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#          File Created by: Spartan `06 Export
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ol01
94 98
SMALL
NO_CHARGES


@<TRIPOS>ATOM
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   3  O3        1.350557072    0.476039797    2.816026253   O.3   1  ol01
   4  N4       -0.940689483   -2.031277612    0.706309528   N.ar  1  ol01
   5  N5       -0.766946810   -0.193774404    2.216753833   N.ar  1  ol01
   6  N6        1.207649013   -1.271448339    1.416394841   N.ar  1  ol01
   7  C7        0.398277078   -2.070274306    0.728427275   C.ar  1  ol01
   8  C8       -1.450309636   -1.077657160    1.475838933   C.ar  1  ol01
   9  C9        0.554523626   -0.346663218    2.136329195   C.ar  1  ol01
  10  C10       2.309315092   -3.185000261   -0.147178253   C.ar  1  ol01
  11  C11       2.978762469   -2.504513353   -1.156073624   C.ar  1  ol01
  12  H12       2.433985172   -1.812114618   -1.790812069   H     1  ol01
  13  C13       4.353608183   -2.708731383   -1.318114342   C.ar  1  ol01
  14  C14       5.006950639   -3.601818855   -0.459335108   C.ar  1  ol01
  15  H15       6.077162702   -3.759594300   -0.577384707   H     1  ol01
  16  C16       4.325959267   -4.295929107    0.547464140   C.ar  1  ol01
  17  C17       2.951187055   -4.077471348    0.700558644   C.ar  1  ol01
  18  H18       2.382486830   -4.591243899    1.470344065   H     1  ol01
  19  C19       5.102471427   -1.984697971   -2.412926838   C.3   1  ol01
  20  H20       4.980430405   -2.492569458   -3.379123922   H     1  ol01
  21  H21       6.175628571   -1.938187916   -2.200775175   H     1  ol01
  22  H22       4.729523565   -0.962598734   -2.532917352   H     1  ol01
  23  C23       5.048955016   -5.270656578    1.448666753   C.3   1  ol01
  24  H24       4.762219295   -6.306906907    1.227086637   H     1  ol01
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26	H26	6.134088230	-5.195636319	1.326882223	H	1	ol01
27	C27	-3.617481489	-1.667357086	0.701898097	C.ar	1	ol01
28	C28	-4.246847306	-2.805775566	1.182796586	C.ar	1	ol01
29	H29	-4.030268706	-3.155685972	2.188045610	H	1	ol01
30	C30	-5.147615782	-3.488297635	0.354436087	C.ar	1	ol01
31	C31	-5.383774300	-2.989666319	-0.931248860	C.ar	1	ol01
32	H32	-6.081196883	-3.515312650	-1.580890040	H	1	ol01
33	C33	-4.750927663	-1.833342712	-1.408142643	C.ar	1	ol01
34	C34	-3.854610253	-1.162375752	-0.570834131	C.ar	1	ol01
35	H35	-3.343809719	-0.262374159	-0.898249276	H	1	ol01
36	C36	-5.821824851	-4.751207015	0.838461959	C.3	1	ol01
37	H37	-6.689067054	-5.004053395	0.220048783	H	1	ol01
38	H38	-6.163409769	-4.651697450	1.875196591	H	1	ol01
39	H39	-5.133567826	-5.606118494	0.806171790	H	1	ol01
40	C40	-5.041155582	-1.297524171	-2.791276539	C.3	1	ol01
41	H41	-4.190623890	-0.725559083	-3.175127829	H	1	ol01
42	H42	-5.911276190	-0.627337640	-2.783544575	H	1	ol01
43	H43	-5.262661666	-2.106677079	-3.496240847	H	1	ol01
44	C44	0.741441378	1.592126426	3.488257206	C.3	1	ol01
45	H45	0.247688333	2.244976483	2.764296556	H	1	ol01
46	H46	1.568855656	2.114825664	3.968566139	H	1	ol01
47	H47	0.017018861	1.250167486	4.231167844	H	1	ol01
48	O48	-0.913982502	3.037326117	0.044970149	O.3	1	ol01
49	O49	2.781130681	0.940304666	-1.570947175	O.3	1	ol01
50	O50	-1.350557072	-0.476039797	-2.816026253	O.3	1	ol01
51	N51	0.940689483	2.031277612	-0.706309528	N.ar	1	ol01
52	N52	0.766946810	0.193774404	-2.216753833	N.ar	1	ol01
53	N53	-1.207649013	1.271448339	-1.416394841	N.ar	1	ol01
54	C54	-0.398277078	2.070274306	-0.728427275	C.ar	1	ol01
55	C55	1.450309636	1.077657160	-1.475838933	C.ar	1	ol01
56	C56	-0.554523626	0.346663218	-2.136329195	C.ar	1	ol01
57	C57	-2.309315092	3.185000261	0.147178253	C.ar	1	ol01
58	C58	-2.978762469	2.504513353	1.156073624	C.ar	1	ol01
59	H59	-2.433985172	1.812114618	1.790812069	H	1	ol01
60	C60	-4.353608183	2.708731383	1.318114342	C.ar	1	ol01
61	C61	-5.006950639	3.601818855	0.459335108	C.ar	1	ol01
62	H62	-6.077162702	3.759594300	0.577384707	H	1	ol01
63	C63	-4.325959267	4.295929107	-0.547464140	C.ar	1	ol01
64	C64	-2.951187055	4.077471348	-0.700558644	C.ar	1	ol01
65	H65	-2.382486830	4.591243899	-1.470344065	H	1	ol01
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69	H69	-4.729523565	0.962598734	2.532917352	H	1	ol01
70	C70	-5.048955016	5.270656578	-1.448666753	C.3	1	ol01
71	H71	-4.762219295	6.306906907	-1.227086637	H	1	ol01
72	H72	-4.814581094	5.090569496	-2.504409476	H	1	ol01
73	H73	-6.134088230	5.195636319	-1.326882223	H	1	ol01
74	C74	3.617481489	1.667357086	-0.701898097	C.ar	1	ol01
75	C75	4.246847306	2.805775566	-1.182796586	C.ar	1	ol01
76	H76	4.030268706	3.155685972	-2.188045610	H	1	ol01
77	C77	5.147615782	3.488297635	-0.354436087	C.ar	1	ol01
78	C78	5.383774300	2.989666319	0.931248860	C.ar	1	ol01
79	H79	6.081196883	3.515312650	1.580890040	H	1	ol01
80	C80	4.750927663	1.833342712	1.408142643	C.ar	1	ol01
81	C81	3.854610253	1.162375752	0.570834131	C.ar	1	ol01
82	H82	3.343809719	0.262374159	0.898249276	H	1	ol01
83	C83	5.821824851	4.751207015	-0.838461959	C.3	1	ol01
84	H84	6.689067054	5.004053395	-0.220048783	H	1	ol01
85	H85	6.163409769	4.651697450	-1.875196591	H	1	ol01

86	H86	5.133567826	5.606118494	-0.806171790	H	1	ol01
87	C87	5.041155582	1.297524171	2.791276539	C.3	1	ol01
88	H88	4.190623890	0.725559083	3.175127829	H	1	ol01
89	H89	5.911276190	0.627337640	2.783544575	H	1	ol01
90	H90	5.262661666	2.106677079	3.496240847	H	1	ol01
91	C91	-0.741441378	-1.592126426	-3.488257206	C.3	1	ol01
92	H92	-0.247688333	-2.244976483	-2.764296556	H	1	ol01
93	H93	-1.568855656	-2.114825664	-3.968566139	H	1	ol01
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Compound 3 – Monomer

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SMALL

NO_CHARGES

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3	N3	0.008017402	-1.124058098	0.027880008	N.ar	1	ol02a in P2(1)/c
4	N4	1.198196801	-3.206840931	0.031433643	N.ar	1	ol02a in P2(1)/c
5	N5	-2.336209349	-1.249318580	-0.000218868	N.3	1	ol02a in P2(1)/c
6	H6	-3.087826642	-1.922050029	0.070925064	H	1	ol02a in P2(1)/c
7	N7	2.351208818	-1.244514658	0.047425213	N.3	1	ol02a in P2(1)/c
8	H8	3.106041444	-1.913238491	-0.026123881	H	1	ol02a in P2(1)/c
9	C9	0.009439142	-3.779721336	0.043948309	C.ar	1	ol02a in P2(1)/c
10	C10	-1.116875949	-1.850956951	0.022259936	C.ar	1	ol02a in P2(1)/c
11	C11	1.133704148	-1.850072061	0.039008441	C.ar	1	ol02a in P2(1)/c
12	C12	-2.720453924	0.103801826	-0.110780030	C.ar	1	ol02a in P2(1)/c
13	C13	-1.877365529	1.112816897	-0.597275201	C.ar	1	ol02a in P2(1)/c
14	H14	-0.860722213	0.874190932	-0.876857613	H	1	ol02a in P2(1)/c
15	C15	-2.358196812	2.418830601	-0.728142631	C.ar	1	ol02a in P2(1)/c
16	C16	-3.679474204	2.707887928	-0.364564217	C.ar	1	ol02a in P2(1)/c
17	H17	-4.051172997	3.724942468	-0.466506674	H	1	ol02a in P2(1)/c
18	C18	-4.532904199	1.712463392	0.119675548	C.ar	1	ol02a in P2(1)/c
19	C19	-4.041814766	0.410349246	0.239215521	C.ar	1	ol02a in P2(1)/c
20	H20	-4.691921094	-0.376844881	0.615614782	H	1	ol02a in P2(1)/c
21	C21	-1.472414894	3.500232799	-1.303734751	C.3	1	ol02a in P2(1)/c
22	H22	-1.591257570	4.444740929	-0.762962848	H	1	ol02a in P2(1)/c
23	H23	-0.417758518	3.216320449	-1.267082734	H	1	ol02a in P2(1)/c
24	H24	-1.725130196	3.696287057	-2.352992198	H	1	ol02a in P2(1)/c
25	C25	-5.949929607	2.034349802	0.533782692	C.3	1	ol02a in P2(1)/c
26	H26	-6.029001880	2.150538497	1.621751448	H	1	ol02a in P2(1)/c
27	H27	-6.295116526	2.966833073	0.078767150	H	1	ol02a in P2(1)/c
28	H28	-6.643086017	1.238578298	0.243168050	H	1	ol02a in P2(1)/c
29	C29	2.724143240	0.113943820	0.134478481	C.ar	1	ol02a in P2(1)/c
30	C30	4.017589996	0.440251821	-0.297669206	C.ar	1	ol02a in P2(1)/c
31	H31	4.650798273	-0.337330070	-0.719206260	H	1	ol02a in P2(1)/c
32	C32	4.495263257	1.748104151	-0.207216082	C.ar	1	ol02a in P2(1)/c
33	C33	3.654283897	2.733069556	0.323737418	C.ar	1	ol02a in P2(1)/c
34	H34	4.011935528	3.757910618	0.394931092	H	1	ol02a in P2(1)/c
35	C35	2.364304044	2.424827552	0.768144073	C.ar	1	ol02a in P2(1)/c
36	C36	1.897553737	1.109033863	0.669953746	C.ar	1	ol02a in P2(1)/c
37	H37	0.901110695	0.856719941	1.005410370	H	1	ol02a in P2(1)/c
38	C38	5.895338596	2.091000846	-0.659529382	C.3	1	ol02a in P2(1)/c
39	H39	5.914180314	3.036776037	-1.210229968	H	1	ol02a in P2(1)/c
40	H40	6.572276949	2.202115739	0.196273231	H	1	ol02a in P2(1)/c
41	H41	6.309997989	1.314346443	-1.308093952	H	1	ol02a in P2(1)/c
42	C42	1.494351714	3.493449703	1.389990390	C.3	1	ol02a in P2(1)/c
43	H43	1.770446692	3.662167893	2.438191018	H	1	ol02a in P2(1)/c
44	H44	1.604025764	4.450613048	0.870443406	H	1	ol02a in P2(1)/c
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Compound 3 – Dimer

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   2  N2       -3.052156771   -3.026386660   -1.429922194   N.ar   1  ol02a in P2(1)/c
   3  N3       -3.480496383   -0.841024265   -0.543583937   N.ar   1  ol02a in P2(1)/c
   4  N4       -1.285448966   -1.433256858   -1.310249037   N.ar   1  ol02a in P2(1)/c
   5  N5       -5.108724663   -2.528376983   -0.612122366    N.3   1  ol02a in P2(1)/c
   6  H6       -5.244395396   -3.469504141   -0.952414519      H   1  ol02a in P2(1)/c
   7  N7       -1.730153214    0.699589296   -0.567028026    N.3   1  ol02a in P2(1)/c
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8	H8	-0.746119670	0.856429812	-0.806074186	H	1	ol02a in P2(1)/c
9	C9	-1.819876323	-2.607021279	-1.603922190	C.ar	1	ol02a in P2(1)/c
10	C10	-3.848815659	-2.083847282	-0.853644034	C.ar	1	ol02a in P2(1)/c
11	C11	-2.196206086	-0.543206306	-0.807533983	C.ar	1	ol02a in P2(1)/c
12	C12	-6.242852485	-1.903601739	-0.056282317	C.ar	1	ol02a in P2(1)/c
13	C13	-6.197798715	-0.701263826	0.659422339	C.ar	1	ol02a in P2(1)/c
14	H14	-5.263398144	-0.173006132	0.775512992	H	1	ol02a in P2(1)/c
15	C15	-7.377606753	-0.180368385	1.204028036	C.ar	1	ol02a in P2(1)/c
16	C16	-8.583452368	-0.867296763	1.034245656	C.ar	1	ol02a in P2(1)/c
17	H17	-9.491897739	-0.452586541	1.462097189	H	1	ol02a in P2(1)/c
18	C18	-8.642793101	-2.067627902	0.315836751	C.ar	1	ol02a in P2(1)/c
19	C19	-7.462380937	-2.578593653	-0.222002238	C.ar	1	ol02a in P2(1)/c
20	H20	-7.475486383	-3.505327845	-0.789466246	H	1	ol02a in P2(1)/c
21	C21	-7.323079456	1.092608057	2.017129472	C.3	1	ol02a in P2(1)/c
22	H22	-8.215811498	1.708852624	1.878660117	H	1	ol02a in P2(1)/c
23	H23	-6.455651183	1.696941152	1.741992254	H	1	ol02a in P2(1)/c
24	H24	-7.264260823	0.871713814	3.088802415	H	1	ol02a in P2(1)/c
25	C25	-9.962478516	-2.775421491	0.106236882	C.3	1	ol02a in P2(1)/c
26	H26	-10.496711678	-2.365404647	-0.758161194	H	1	ol02a in P2(1)/c
27	H27	-10.614952868	-2.658902237	0.975501382	H	1	ol02a in P2(1)/c
28	H28	-9.828283570	-3.845082335	-0.071043068	H	1	ol02a in P2(1)/c
29	C29	-2.454134556	1.832569404	-0.099511230	C.ar	1	ol02a in P2(1)/c
30	C30	-1.809403941	2.694044253	0.792689743	C.ar	1	ol02a in P2(1)/c
31	H31	-0.809772600	2.445747327	1.134182115	H	1	ol02a in P2(1)/c
32	C32	-2.440413040	3.856273217	1.246446414	C.ar	1	ol02a in P2(1)/c
33	C33	-3.730426810	4.138373625	0.786551223	C.ar	1	ol02a in P2(1)/c
34	H34	-4.243116827	5.029717795	1.136001985	H	1	ol02a in P2(1)/c
35	C35	-4.387966213	3.292180475	-0.115993968	C.ar	1	ol02a in P2(1)/c
36	C36	-3.740512567	2.135802797	-0.557631228	C.ar	1	ol02a in P2(1)/c
37	H37	-4.227185119	1.464426887	-1.251673665	H	1	ol02a in P2(1)/c
38	C38	-1.727434079	4.776363237	2.207272605	C.3	1	ol02a in P2(1)/c
39	H39	-2.408254128	5.500030446	2.660709407	H	1	ol02a in P2(1)/c
40	H40	-0.948426625	5.347074681	1.690133635	H	1	ol02a in P2(1)/c
41	H41	-1.253948543	4.218005663	3.020446267	H	1	ol02a in P2(1)/c
42	C42	-5.752202154	3.656092658	-0.656214740	C.3	1	ol02a in P2(1)/c
43	H43	-5.678617453	4.114020889	-1.649064941	H	1	ol02a in P2(1)/c
44	H44	-6.261299049	4.369758464	-0.004076045	H	1	ol02a in P2(1)/c
45	H45	-6.381022619	2.769353133	-0.769218407	H	1	ol02a in P2(1)/c
46	Cl46	0.396626356	3.580296053	-2.246512157	Cl	1	ol02a in P2(1)/c
47	N47	1.160683225	1.286898038	-1.245431036	N.ar	1	ol02a in P2(1)/c
48	N48	3.415758198	0.825011651	-0.585481987	N.ar	1	ol02a in P2(1)/c
49	N49	2.821257533	2.975677012	-1.475621383	N.ar	1	ol02a in P2(1)/c
50	N50	1.745468545	-0.792138747	-0.427761162	N.3	1	ol02a in P2(1)/c
51	H51	0.826727168	-1.064970670	-0.781122704	H	1	ol02a in P2(1)/c
52	N52	4.957575136	2.578112165	-0.846897417	N.3	1	ol02a in P2(1)/c
53	H53	5.008543193	3.545975095	-1.132045284	H	1	ol02a in P2(1)/c
54	C54	1.605020521	2.491568260	-1.580553176	C.ar	1	ol02a in P2(1)/c
55	C55	2.134032133	0.464207607	-0.754340624	C.ar	1	ol02a in P2(1)/c
56	C56	3.701912619	2.075820670	-0.956824025	C.ar	1	ol02a in P2(1)/c
57	C57	2.554647128	-1.800936046	0.168437596	C.ar	1	ol02a in P2(1)/c
58	C58	3.375271444	-1.515072648	1.267275273	C.ar	1	ol02a in P2(1)/c
59	H59	3.421074901	-0.502783196	1.647240114	H	1	ol02a in P2(1)/c
60	C60	4.132162428	-2.527383718	1.862280578	C.ar	1	ol02a in P2(1)/c
61	C61	4.040564996	-3.829093757	1.351171818	C.ar	1	ol02a in P2(1)/c
62	H62	4.594418471	-4.632877632	1.827737593	H	1	ol02a in P2(1)/c
63	C63	3.210805954	-4.134098911	0.267556921	C.ar	1	ol02a in P2(1)/c
64	C64	2.473064788	-3.104695512	-0.325787148	C.ar	1	ol02a in P2(1)/c
65	H65	1.812346011	-3.320374144	-1.157124680	H	1	ol02a in P2(1)/c
66	C66	4.984564913	-2.228744433	3.075202749	C.3	1	ol02a in P2(1)/c
67	H67	5.773435922	-2.975318609	3.191965448	H	1	ol02a in P2(1)/c
68	H68	5.457565075	-1.245825412	3.004269270	H	1	ol02a in P2(1)/c

69	H69	4.384253219	-2.225187373	3.992020648	H	1	ol02a in P2(1)/c
70	C70	3.121691052	-5.541473911	-0.275012433	C.3	1	ol02a in P2(1)/c
71	H71	3.539338014	-5.591996381	-1.285833252	H	1	ol02a in P2(1)/c
72	H72	3.659567947	-6.248720370	0.360227024	H	1	ol02a in P2(1)/c
73	H73	2.086222815	-5.890328265	-0.337099931	H	1	ol02a in P2(1)/c
74	C74	6.176287781	1.998531481	-0.446189705	C.ar	1	ol02a in P2(1)/c
75	C75	7.256108997	2.879532623	-0.288643358	C.ar	1	ol02a in P2(1)/c
76	H76	7.118870351	3.942092750	-0.471935670	H	1	ol02a in P2(1)/c
77	C77	8.517755223	2.408006430	0.079102993	C.ar	1	ol02a in P2(1)/c
78	C78	8.683293407	1.036079192	0.292894960	C.ar	1	ol02a in P2(1)/c
79	H79	9.661535846	0.648062756	0.562317419	H	1	ol02a in P2(1)/c
80	C80	7.614913152	0.145569835	0.141922379	C.ar	1	ol02a in P2(1)/c
81	C81	6.353645853	0.627821723	-0.222280576	C.ar	1	ol02a in P2(1)/c
82	H82	5.526151358	-0.054931124	-0.343001131	H	1	ol02a in P2(1)/c
83	C83	9.682600636	3.359363714	0.208107533	C.3	1	ol02a in P2(1)/c
84	H84	10.442117842	2.968877695	0.889486934	H	1	ol02a in P2(1)/c
85	H85	10.162651677	3.532115539	-0.762058301	H	1	ol02a in P2(1)/c
86	H86	9.368819338	4.334900201	0.588338653	H	1	ol02a in P2(1)/c
87	C87	7.829084160	-1.339910828	0.324464889	C.3	1	ol02a in P2(1)/c
88	H88	8.215230745	-1.800814063	-0.591806058	H	1	ol02a in P2(1)/c
89	H89	8.553637954	-1.545552382	1.117261677	H	1	ol02a in P2(1)/c
90	H90	6.894743331	-1.849712616	0.568111985	H	1	ol02a in P2(1)/c

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Compound 4 – Monomer

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jw1027
51 53
SMALL
NO_CHARGES


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   3  H3      -7.208639703   -1.557889891   -0.336924773     H   1  jw1027
   4  H4      -7.220663345   -0.224696703    0.866434202     H   1  jw1027
   5  C5      -4.784595068    0.514713534    0.138668928   C.2   1  jw1027
   6  C6      -3.272909261    0.344434112    0.125310384   C.ar  1  jw1027
   7  C7      -1.427063790   -0.940658844    0.106915080   C.ar  1  jw1027
   8  C8      -1.239211035    1.301980635    0.125744944   C.ar  1  jw1027
   9  C9       0.846786548    2.731997867   -0.021852629   C.ar  1  jw1027
  10  C10      1.764630402    1.812017832   -0.544125456   C.ar  1  jw1027
  11  H11      1.429858797    0.823541073   -0.827766022     H   1  jw1027
  12  C12      3.106005777    2.176423878   -0.707325495   C.ar  1  jw1027
  13  C13      3.519828753    3.459926710   -0.337347427   C.ar  1  jw1027
  14  H14      4.563551379    3.742689688   -0.462337659     H   1  jw1027
  15  C15      2.615640100    4.391715224    0.186939872   C.ar  1  jw1027
  16  C16      1.280273477    4.017298208    0.337816860   C.ar  1  jw1027
  17  H17      0.564429872    4.728729058    0.745583352     H   1  jw1027
  18  C18      4.085513409    1.200988951   -1.320940464   C.3   1  jw1027
  19  H19      5.063687357    1.252371826   -0.829565700     H   1  jw1027
  20  H20      3.721646489    0.171268189   -1.251652515     H   1  jw1027
  21  H21      4.247236886    1.421130657   -2.384572317     H   1  jw1027
  22  C22      3.084150502    5.766822723    0.604706804   C.3   1  jw1027
  23  H23      2.243129443    6.451228610    0.755538336     H   1  jw1027
  24  H24      3.647549538    5.724747225    1.546062468     H   1  jw1027
  25  H25      3.747540548    6.208158299   -0.147734682     H   1  jw1027
  26  C26      0.396776544   -2.696297523    0.191781735   C.ar  1  jw1027
  27  C27      0.609144905   -4.016398078   -0.227901188   C.ar  1  jw1027
  28  H28     -0.222508345   -4.585643990   -0.639788857     H   1  jw1027
  29  C29      1.873155714   -4.604392149   -0.138852341   C.ar  1  jw1027
  30  C30      2.929542340   -3.846881729    0.376319937   C.ar  1  jw1027
  31  H31      3.920914174   -4.290426143    0.443453924     H   1  jw1027
  32  C32      2.735287020   -2.529929248    0.810370757   C.ar  1  jw1027
  33  C33      1.465275290   -1.953407682    0.713324246   C.ar  1  jw1027
  34  H34      1.303073703   -0.934316128    1.037512099     H   1  jw1027
  35  C35      2.084026293   -6.035948175   -0.575928253   C.3   1  jw1027
  36  H36      1.779586637   -6.740637151    0.209386025     H   1  jw1027
  37  H37      1.497398663   -6.275003302   -1.470023331     H   1  jw1027
  38  H38      3.137229813   -6.232758309   -0.800659988     H   1  jw1027
  39  C39      3.878508786   -1.746750887    1.416375473   C.3   1  jw1027
  40  H40      4.041390631   -2.035556802    2.463302107     H   1  jw1027
  41  H41      4.818026619   -1.929577942    0.882610455     H   1  jw1027
  42  H42      3.680913301   -0.670531184    1.400114975     H   1  jw1027
  43  N43     -2.781292768   -0.891365636    0.089202732   N.ar  1  jw1027
  44  N44     -2.580970328    1.479192698    0.157339774   N.ar  1  jw1027
  45  N45     -0.607863027    0.119072075    0.112916900   N.ar  1  jw1027
  46  N46     -0.923005711   -2.207059839    0.105158794   N.3   1  jw1027
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48	N48	-0.530843696	2.466026416	0.118724882	N.3	1	jw1027
49	H49	-1.135415400	3.273286458	0.207931953	H	1	jw1027
50	O50	-5.421188067	-0.642960956	-0.106754580	O.3	1	jw1027
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Compound 4 – Dimer 1 (N-H---O)

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jw1027
102 106
SMALL
NO_CHARGES


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   3  H3       -0.340617423    6.375913282   -0.538397486      H   1  jw1027
   4  H4        0.844413348    5.067046202   -0.881860558      H   1  jw1027
   5  C5       -0.779757285    3.237202831    0.041276176    C.2   1  jw1027
   6  C6       -2.008276563    2.346798128    0.003410387    C.ar  1  jw1027
   7  C7       -4.235492384    2.074064430   -0.002911744    C.ar  1  jw1027
   8  C8       -2.871998575    0.273071842   -0.025184168    C.ar  1  jw1027
   9  C9       -3.631370110   -2.093740025    0.008084025    C.ar  1  jw1027
  10  C10      -4.696558536   -2.046731803    0.911414988    C.ar  1  jw1027
  11  H11      -4.809607571   -1.187436251    1.562368210      H   1  jw1027
  12  C12      -5.613891205   -3.102685879    0.981110774    C.ar  1  jw1027
  13  C13      -5.447264904   -4.201330305    0.133165487    C.ar  1  jw1027
  14  H14      -6.158990770   -5.023733805    0.183586847      H   1  jw1027
  15  C15      -4.379563839   -4.270621164   -0.772695894    C.ar  1  jw1027
  16  C16      -3.474947823   -3.209506395   -0.826258873    C.ar  1  jw1027
  17  H17      -2.636643876   -3.238041471   -1.514846951      H   1  jw1027
  18  C18      -6.739939432   -3.061061187    1.990477113    C.3   1  jw1027
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  21  H21      -6.369079331   -3.250957676    3.006387519      H   1  jw1027
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  24  H24      -5.034036352   -5.499390267   -2.434975103      H   1  jw1027
  25  H25      -4.262445591   -6.406538871   -1.134440392      H   1  jw1027
  26  C26      -6.770184649    2.185996214   -0.090533506    C.ar  1  jw1027
  27  C27      -7.803960494    3.114654434    0.101405712    C.ar  1  jw1027
  28  H28      -7.557693742    4.150646896    0.329709815      H   1  jw1027
  29  C29      -9.143043315    2.729291656    0.013414002    C.ar  1  jw1027
  30  C30      -9.438986029    1.392036294   -0.267969094    C.ar  1  jw1027
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  33  C33      -7.084196058    0.848620358   -0.374834114    C.ar  1  jw1027
  34  H34      -6.287681325    0.131371418   -0.515968319      H   1  jw1027
  35  C35     -10.245412777    3.747290882    0.197539552    C.3   1  jw1027
  36  H36     -10.432647347    4.303932698   -0.730555889      H   1  jw1027
  37  H37      -9.991186621    4.482217721    0.969581806      H   1  jw1027
  38  H38     -11.186422200    3.266985230    0.485107933      H   1  jw1027
  39  C39      -8.764191319   -0.980372625   -0.816186518    C.3   1  jw1027
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  42  H42      -7.910433975   -1.647061560   -0.661937190      H   1  jw1027
  43  N43      -3.195054836    2.946445735    0.016157679    N.ar  1  jw1027
  44  N44      -1.754925825    1.043949220   -0.020673093    N.ar  1  jw1027
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48	N48	-2.658235197	-1.063826325	-0.055466111	N.3	1	jw1027
49	H49	-1.685342965	-1.349132793	-0.168755762	H	1	jw1027
50	O50	-1.064680787	4.513622153	-0.234230780	O.3	1	jw1027
51	O51	0.339233361	2.837463796	0.296397700	O.2	1	jw1027
52	C52	-0.055549086	-5.414907953	0.210551696	C.3	1	jw1027
53	H53	-0.459647270	-5.491938555	-0.802762514	H	1	jw1027
54	H54	0.340617423	-6.375913282	0.538397486	H	1	jw1027
55	H55	-0.844413348	-5.067046202	0.881860558	H	1	jw1027
56	C56	0.779757285	-3.237202831	-0.041276176	C.2	1	jw1027
57	C57	2.008276563	-2.346798128	-0.003410387	C.ar	1	jw1027
58	C58	4.235492384	-2.074064430	0.002911744	C.ar	1	jw1027
59	C59	2.871998575	-0.273071842	0.025184168	C.ar	1	jw1027
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61	C61	4.696558536	2.046731803	-0.911414988	C.ar	1	jw1027
62	H62	4.809607571	1.187436251	-1.562368210	H	1	jw1027
63	C63	5.613891205	3.102685879	-0.981110774	C.ar	1	jw1027
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67	C67	3.474947823	3.209506395	0.826258873	C.ar	1	jw1027
68	H68	2.636643876	3.238041471	1.514846951	H	1	jw1027
69	C69	6.739939432	3.061061187	-1.990477113	C.3	1	jw1027
70	H70	7.500219193	3.817852296	-1.771390532	H	1	jw1027
71	H71	7.229062919	2.080686339	-2.003696854	H	1	jw1027
72	H72	6.369079331	3.250957676	-3.006387519	H	1	jw1027
73	C73	4.227439951	5.462148483	1.691200002	C.3	1	jw1027
74	H74	3.279198583	5.427036478	2.237496195	H	1	jw1027
75	H75	5.034036352	5.499390267	2.434975103	H	1	jw1027
76	H76	4.262445591	6.406538871	1.134440392	H	1	jw1027
77	C77	6.770184649	-2.185996214	0.090533506	C.ar	1	jw1027
78	C78	7.803960494	-3.114654434	-0.101405712	C.ar	1	jw1027
79	H79	7.557693742	-4.150646896	-0.329709815	H	1	jw1027
80	C80	9.143043315	-2.729291656	-0.013414002	C.ar	1	jw1027
81	C81	9.438986029	-1.392036294	0.267969094	C.ar	1	jw1027
82	H82	10.479057599	-1.077665627	0.331770536	H	1	jw1027
83	C83	8.421515768	-0.451549380	0.469370791	C.ar	1	jw1027
84	C84	7.084196058	-0.848620358	0.374834114	C.ar	1	jw1027
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89	H89	11.186422200	-3.266985230	-0.485107933	H	1	jw1027
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91	H91	9.064414440	1.069296904	1.868882081	H	1	jw1027
92	H92	9.601362721	1.348744059	0.211877655	H	1	jw1027
93	H93	7.910433975	1.647061560	0.661937190	H	1	jw1027
94	N94	3.195054836	-2.946445735	-0.016157679	N.ar	1	jw1027
95	N95	1.754925825	-1.043949220	0.020673093	N.ar	1	jw1027
96	N96	4.133551198	-0.744006405	0.015420906	N.ar	1	jw1027
97	N97	5.456156718	-2.685037589	0.004141180	N.3	1	jw1027
98	H98	5.367255405	-3.692079253	-0.046046866	H	1	jw1027
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101	O101	1.064680787	-4.513622153	0.234230780	O.3	1	jw1027
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Compound 4 – Dimer 2 (N-H---N)

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102 106
SMALL
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5	C5	0.723849047	3.617755550	-1.719385451	C.2	1	jw1027
6	C6	1.703805580	2.576276369	-1.202782067	C.ar	1	jw1027
7	C7	2.189448776	0.465222202	-0.546178081	C.ar	1	jw1027
8	C8	3.776550402	2.071953966	-0.500342410	C.ar	1	jw1027
9	C9	6.170456184	1.932781421	0.317289608	C.ar	1	jw1027
10	C10	6.126848401	0.757309597	1.079538278	C.ar	1	jw1027
11	H11	5.184001040	0.248032298	1.224949662	H	1	jw1027
12	C12	7.299323760	0.254936841	1.653153922	C.ar	1	jw1027
13	C13	8.509568969	0.928324839	1.450232323	C.ar	1	jw1027
14	H14	9.421074869	0.534673085	1.896264874	H	1	jw1027
15	C15	8.570155555	2.101509295	0.690718122	C.ar	1	jw1027
16	C16	7.390880218	2.597852662	0.132511742	C.ar	1	jw1027
17	H17	7.417532271	3.510210749	-0.460922269	H	1	jw1027
18	C18	7.250355731	-0.982861080	2.520695692	C.3	1	jw1027
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20	H20	6.311305532	-1.529167963	2.389483609	H	1	jw1027
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22	C22	9.887951596	2.802689776	0.452268743	C.3	1	jw1027
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26	C26	2.462099023	-1.967356735	0.001831323	C.ar	1	jw1027
27	C27	1.709025647	-2.992213936	0.587448013	C.ar	1	jw1027
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33	C33	3.830751144	-2.162897743	-0.235173667	C.ar	1	jw1027
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89	H89	-2.026950267	6.238556289	1.650680866	H	1	jw1027
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91	H91	-6.034219988	4.149631458	-1.134476535	H	1	jw1027
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101	O101	0.255236037	-3.052254306	-2.440827166	O.3	1	jw1027
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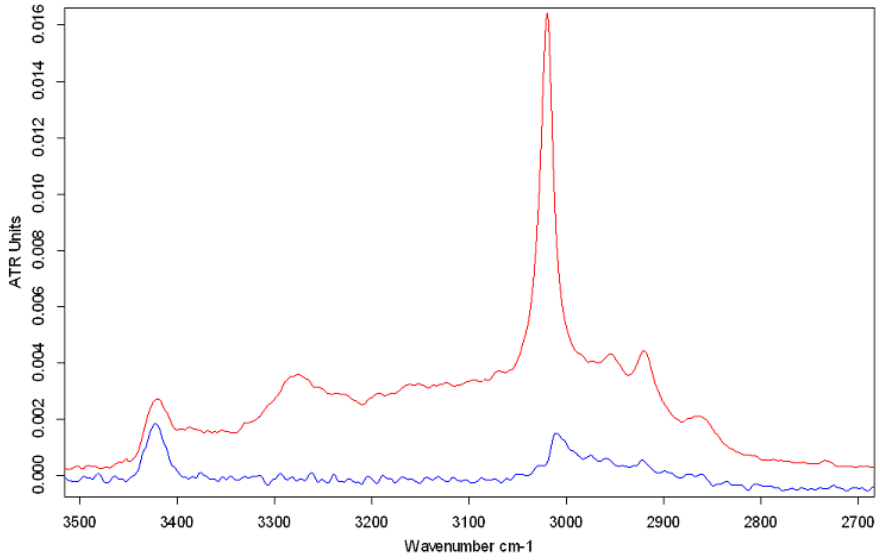
FTIR Spectra of Compound 1



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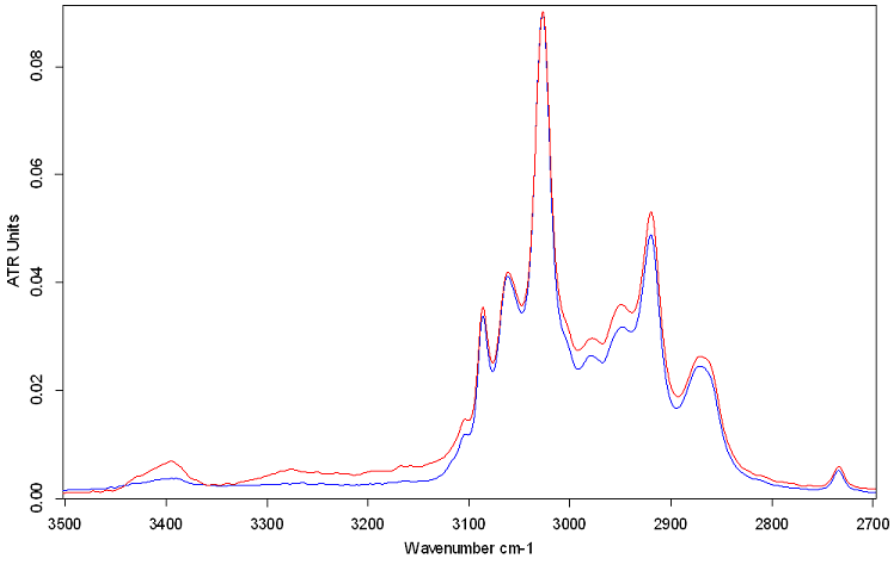
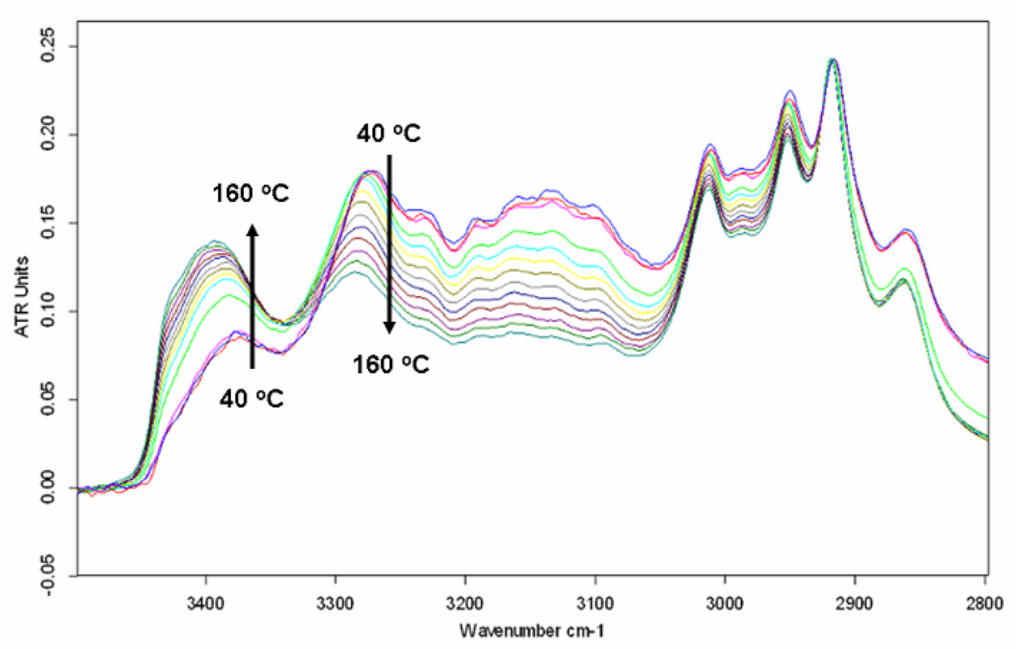


b

Figure S12. Region from 3500 to 2700 cm^{-1} from the FTIR spectra of compound **1** in a) $CHCl_3$ solution, and b) toluene solution. In both cases, the spectrum of a diluted sample is shown in blue and the spectrum of a concentrated sample is shown in red.



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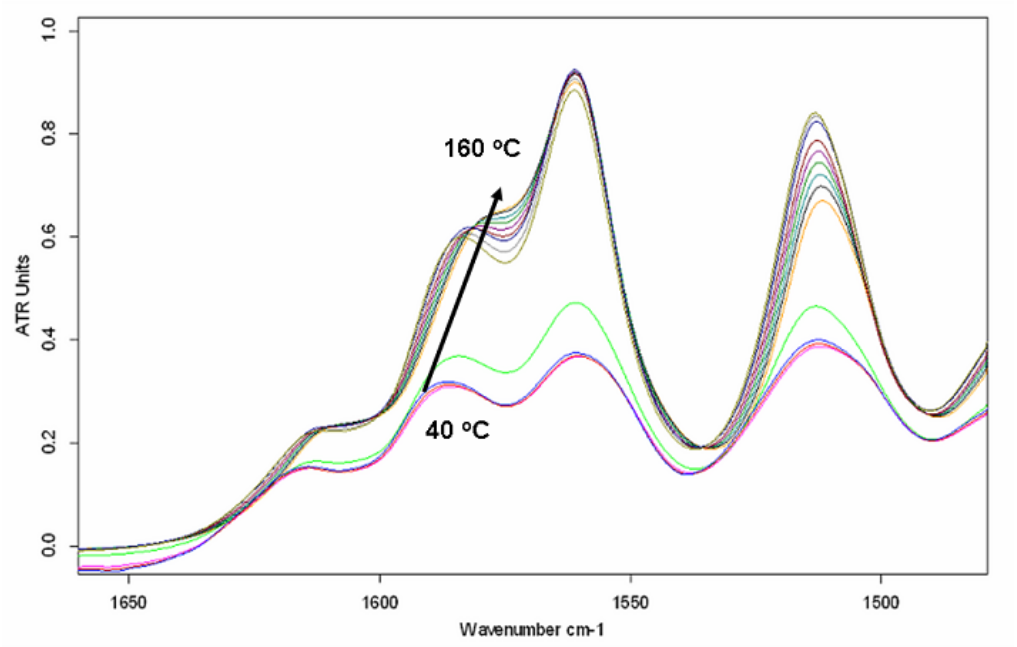
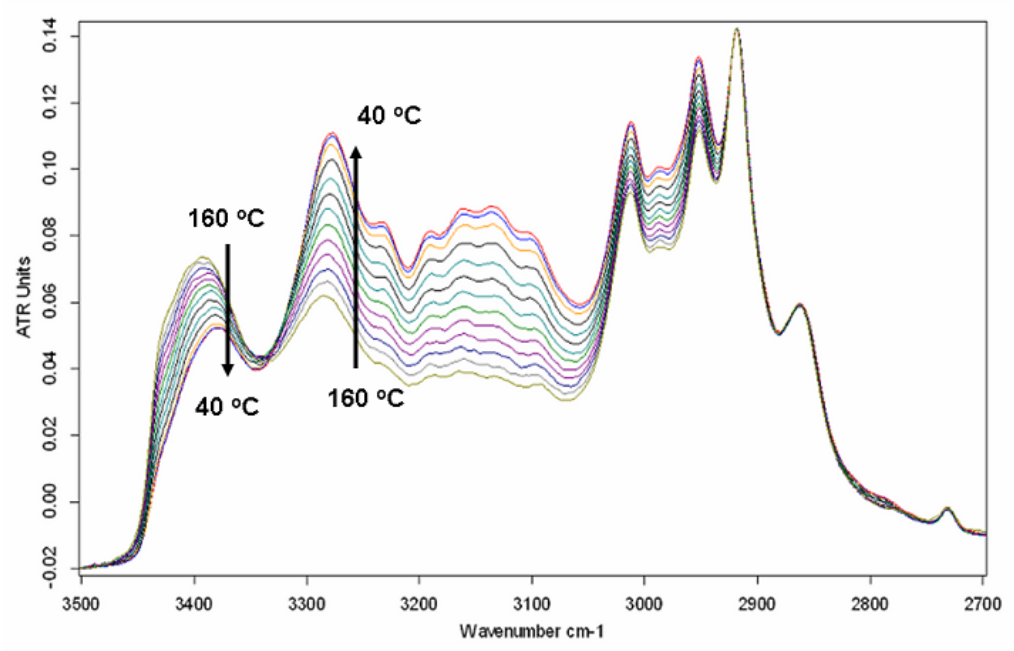


b

Figure S13. Regions from a) 3500 to 2700 cm^{-1}, and b) 1660 to 1480 cm^{-1} from the FTIR spectra of an amorphous sample of compound **1** heated at 2 ^{o}C/min from 40 to 160 ^{o}C. The directions in which the positions or intensities of major bands are shifted are shown.



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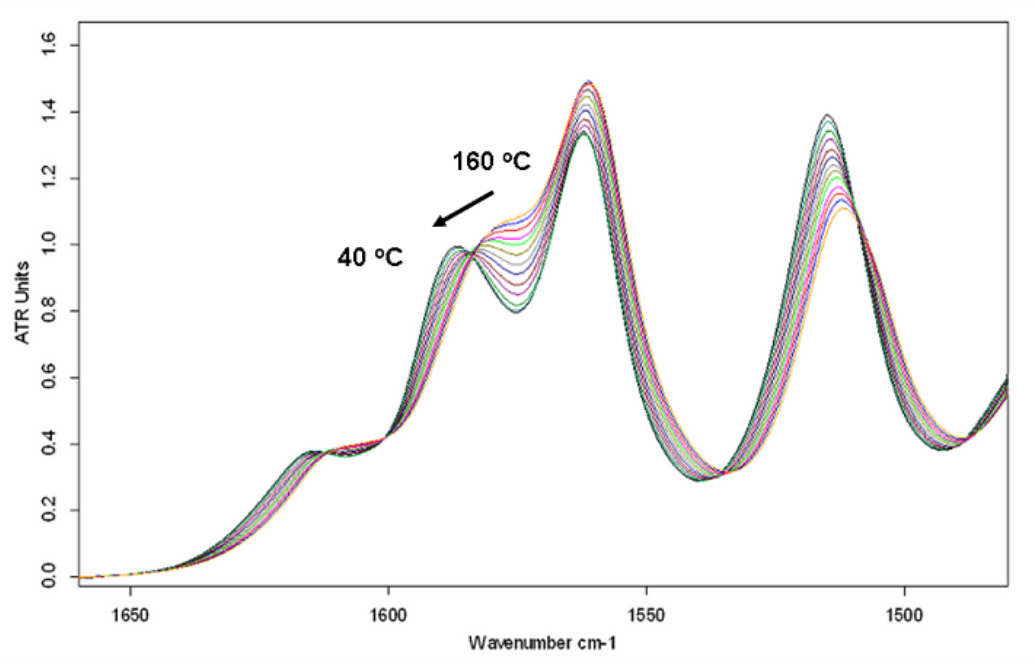
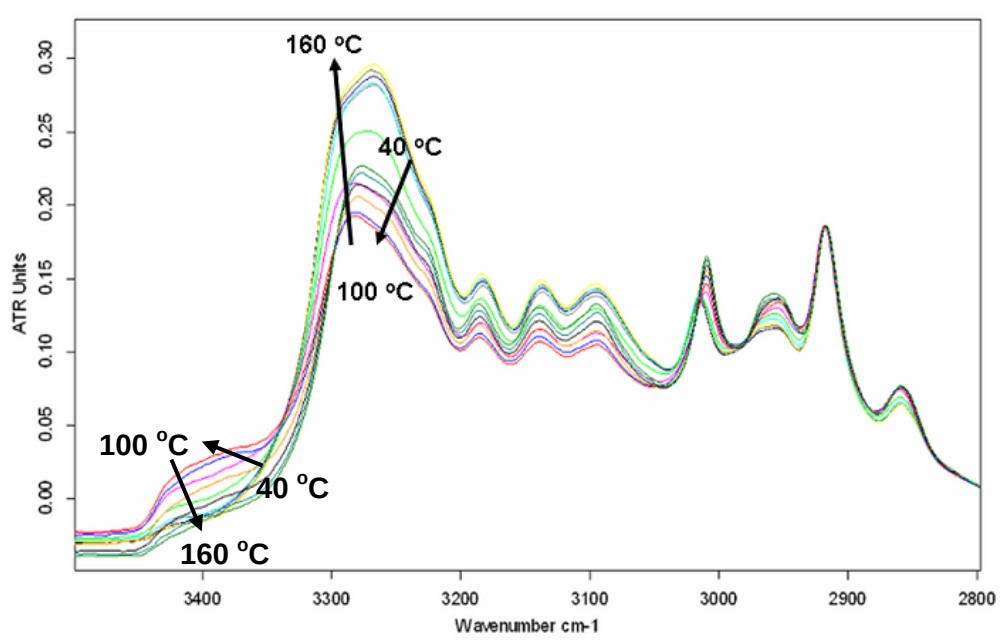


b

Figure S14. Regions from a) 3500 to 2700 cm^{-1}, and b) 1660 to 1480 cm^{-1} from the FTIR spectra of an amorphous sample of compound **1** cooled at 2 ^{o}C/min from 160 to 40 ^{o}C. The directions in which the positions or intensities of major bands are shifted are shown.



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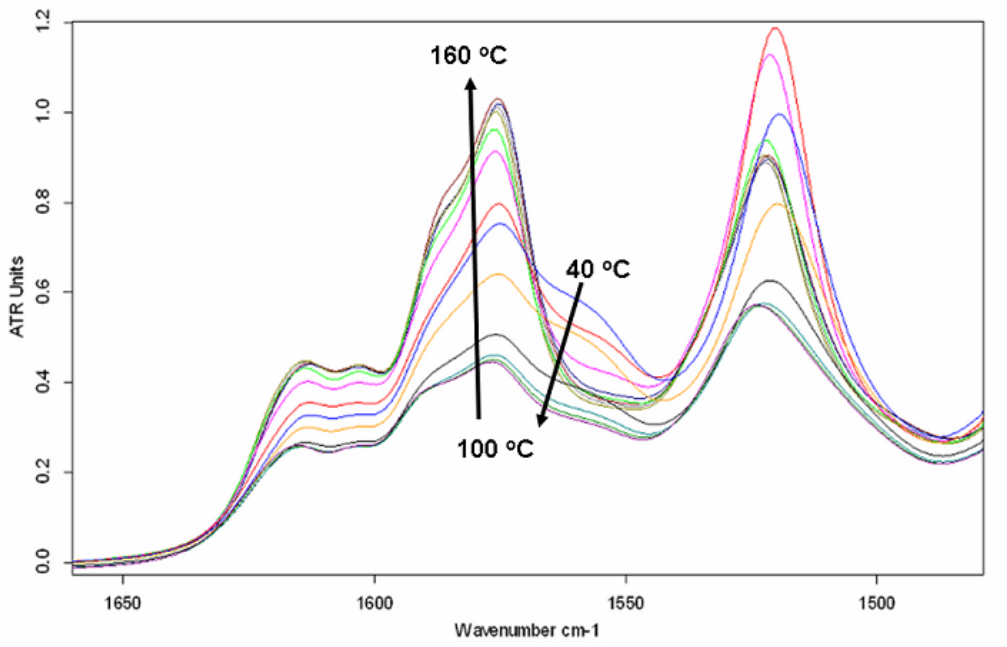

b

Figure S15. Regions from a) 3500 to 2700 cm^{-1}, and b) 1660 to 1480 cm^{-1} from the FTIR spectra of an crystalline sample of compound **1** heated at 2 ^{o}C/min from 40 to 160 ^{o}C. The directions in which the positions or intensities of major bands are shifted are shown.

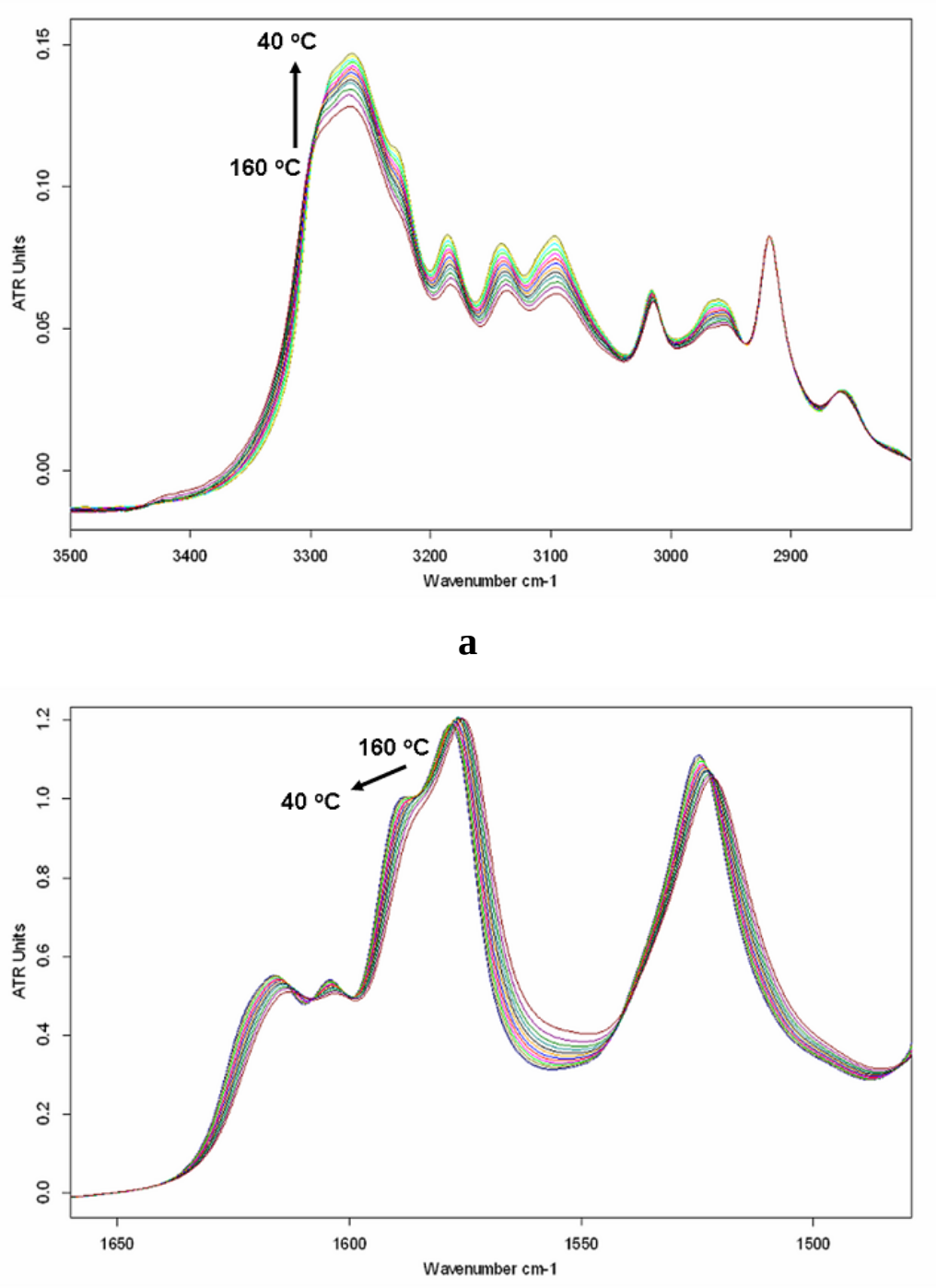

Figure S16. Regions from a) 3500 to 2700 cm^{-1}, and b) 1660 to 1480 cm^{-1} from the FTIR spectra of an crystalline sample of compound **1** cooled at 2 ^{o}C/min from 160 to 40 ^{o}C. The directions in which the positions or intensities of major bands are shifted are shown.