Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Understanding Polymorphism-Dependent Emission Properties of Molecular Crystals with a Refined QM/MM Approach

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Contents

1. Crystal structures and emission spectra of two polymorphs

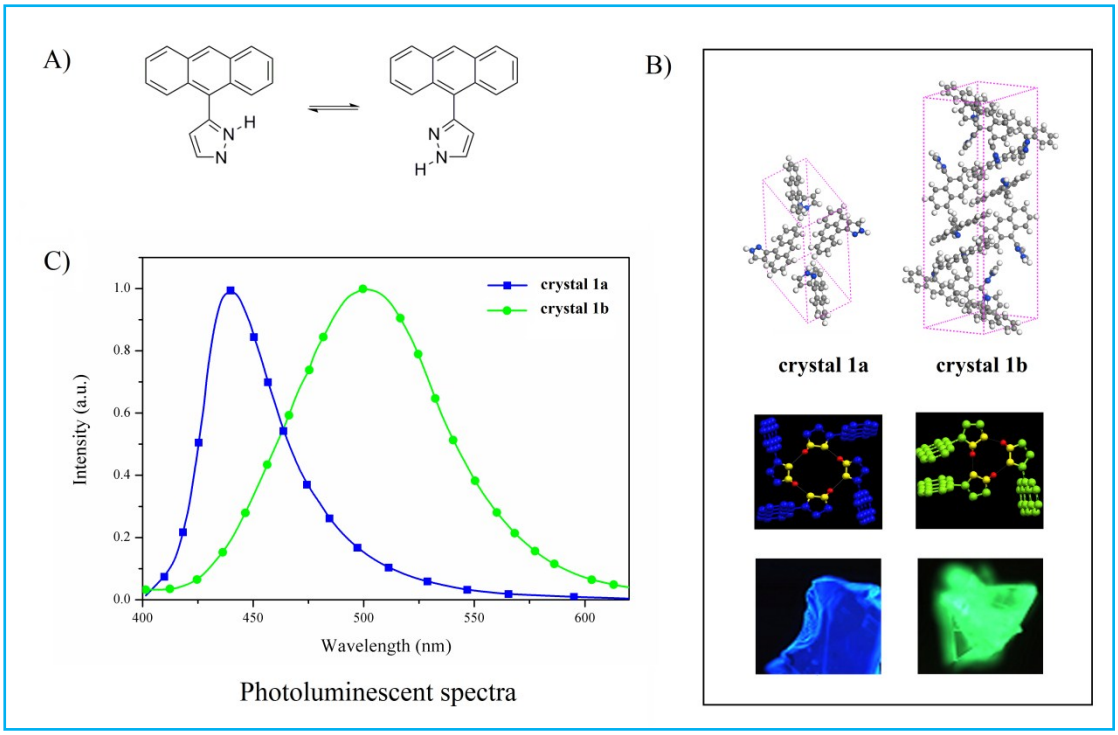


Fig. S1 A) Structure of 3(5)-(9-anthryl)pyrazole (ANP) molecule; B) two-color structure-dependent luminescence polymorphs (denoted as crystals 1a and 1b) comprised of ANP and its isomeride; and C) fluorescence spectra of crystal 1a and crystal 1b. Reprinted with permission from ref 1. Copyright 2006 Wiley-VCH Verlag GmbH & Co.KGaA.

2. Computational details of the PBC-GEBF approach.

The methodology of the PBC-GEBF method was described in our previous work.[2-4] Here, we only give a brief introduction on how to construct molecular clusters (subsystems) in PBC-GEBF calculations. With the PBC-GEBF approach, for a certain periodic molecular crystal, each molecule is usually chosen as a fragment. For each fragment in a unit cell, one should first construct a primitive subsystem including this fragment and some spatially neighboring fragments within a given distance threshold ζ. Obviously, a larger ζ will lead to larger subsystems, which leads to the higher accuracy of the PBC-GEBF method. However, its computational cost will also increase noticeably. To control the size of primitive subsystems, another parameter γ_{max} (the maximum number of fragments in a subsystem) is introduced. With this parameter, a subsystem at most contains γ_{max} fragments (those nearest-neighboring fragments). Once all primitive subsystems are available, the corresponding derivative subsystems can be generated automatically. In general, the accuracy of the PBC-GEBF method mainly depends on the values of two parameters (ζ, γ_{max}). On the basis of our previous work, we find that ζ=4.0 Å and γ_{max}=4 can give satisfactory descriptions for most of molecular crystals. In this work, PBC-GEBF calculations with the same two parameters at the M06-2X/6-31G** level will be performed for ANP-based crystals.

The PBC-GEBF method can also be used to generate all possible dimers with γ_{max}=2 or all possible trimers with γ_{max}=3 (ζ=4.0 Å is always used). We can generate 28 dimers and 23 trimers for crystal 1a, 88 dimers and 68 trimers for crystal 1b. Since many of these structures are structurally analogous to each other, we divide them into several groups (within a group the root-mean-squared deviation between any two structures is less than 0.2 Å). For each group, only one structure will be considered. Thus, for crystal 1a there are 27 dimers, and 22 trimers. For crystal 1b, there are 44 dimers and 41 trimers. Then, for all molecular clusters the binding energies were then calculated with the correction of basis set superposition error (BSSE) at the M06-2X/6-31G** level with the Gaussian 09 package.[5] Finally, all selected structures are ranked by the values of the binding energies.

3. Optimized structural parameters of both crystals

Table S1. Comparison of optimized lattice parameters of crystals 1a and 1b calculated at the PBC-GEBF-M06-2X/6-31G** level with those of experimental crystal parameters.[a]

System	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ (deg)	volume (Å^3)
crystal 1a	7.93	13.62	13.60	67.82	75.46	75.68	1298.5
X-ray	7.87	13.57	13.64	68.00	75.13	75.32	1285.7
crystal 1b	12.89	33.15	9.42	89.71	99.71	90.02	3970.2
X-ray	12.79	33.08	9.35	90.00	100.07	90.00	3893.1

[a]The experimental values are from ref 1.

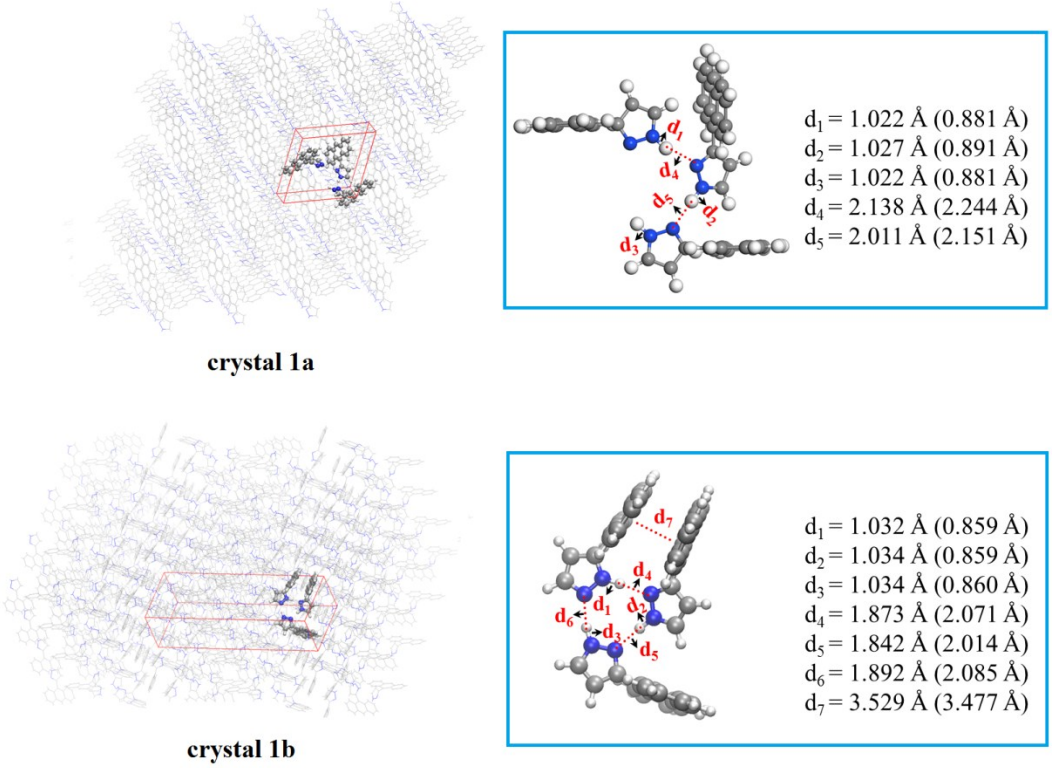
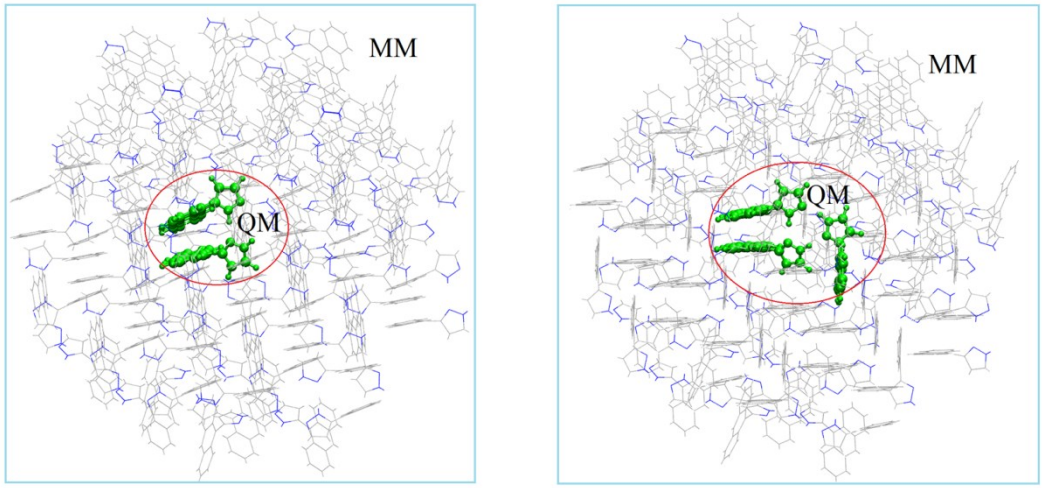


Fig. S2 Comparison of optimized structural parameters of crystals 1a and 1b calculated at the PBC-GEBF-M06-2X/6-31G** level with the corresponding X-ray structural parameters.

4. An illustrative picture for constructing the QM/MM model



dimer A model trimer A model

Fig. S3 An illustrative picture for constructing the QM/MM model of crystal 1b. The left picture corresponds to the dimer **A** model as the QM region, and the right picture denotes the trimer **A** model as the QM region.

5. Optimized S1 structures of the selected clusters

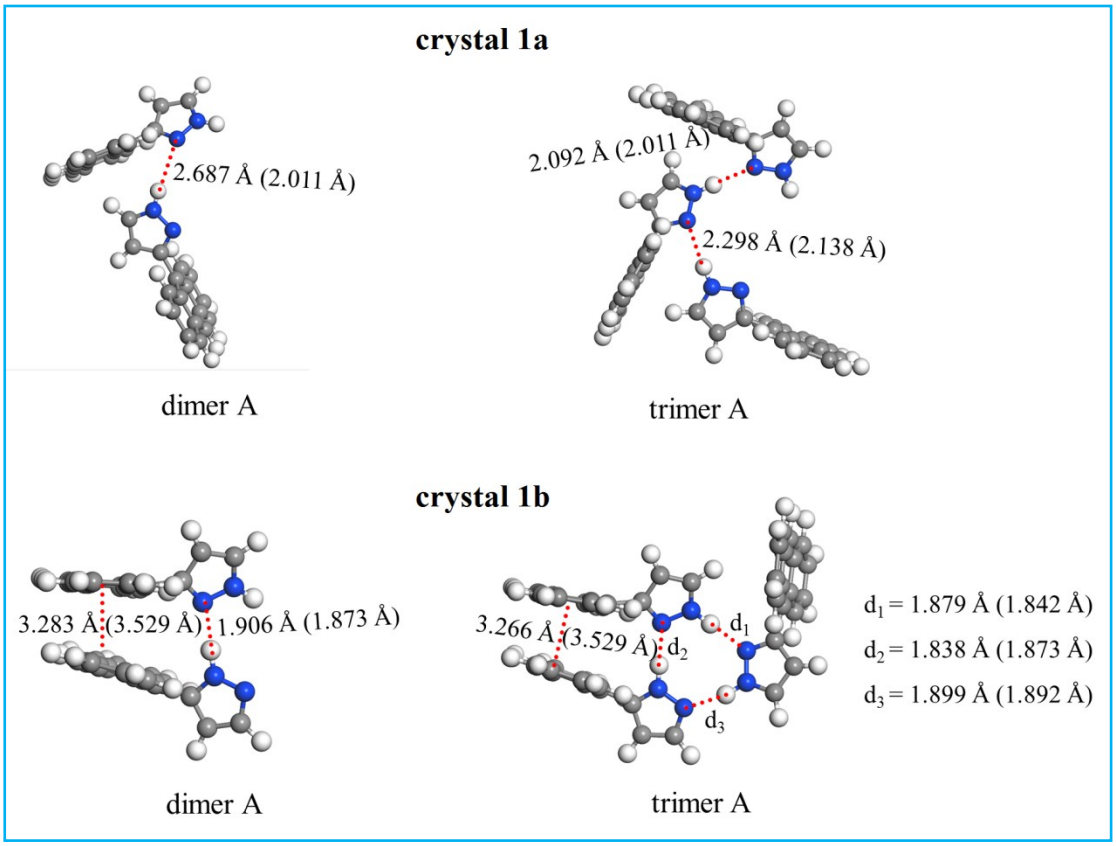


Fig. S4 Optimized S_1 structures of dimer **A** and trimer **A** models for crystals 1a and 1b. For comparison, the corresponding bond distances at the S_0 state are shown in parentheses.

6. Calculated emission energies with different basis sets and methods.

Table S2. Deviations of the calculated emission energies (in eV) of crystals 1a and 1b relative to the experimental values.[a]

Cluster Model		Deviations (eV)			
		6-31G**	6-31+G**	6-311G**	6-311++G**
Crystal 1a	Monomer	0.19	0.13	0.12	0.09
	Dimer **A**	0.17	0.11	0.10	0.07
	Trimer **A**	0.18	0.13	0.13	0.10
Crystal 1b	Monomer	0.54	0.48	0.46	0.44
	Dimer **A**	0.19	0.15	0.15	0.13
	Trimer **A**	0.10	0.05	0.05	0.02

[a]Calculations are done at the TD-M06-2X/Y:UFF (Y=6-31G**, 6-31+G**, 6-311G** and 6-311++G**) level.

Table S3. The deviations of the calculated emission energies (in eV) of crystals 1a and 1b relative to the experimental values.[a]

Cluster Model		Crystal 1a		Crystal 1b	
		M06-2X	CAM-B3LYP	M06-2X	CAM-B3LYP
Monomer		0.09	0.08	0.44	0.42
Dimer	**A**	0.07	0.06	0.13	0.16
	B	0.10	0.09	0.40	0.39
	C	0.07	0.06	0.46	0.44
Trimer	**A**	0.10	0.08	0.02	0.05
	B	0.09	0.07	0.14	0.17
	C	0.10	0.08	0.42	0.40

[a]QM/MM calculations are done at the TD-Y/6-311++G**:UFF (Y=M06-2X, CAM-B3LYP) level.

7. Calculated emission properties from selected clusters

Table S4. The calculated emission energies, the frontier molecular orbitals in the transition, and the energy gap between frontier molecular orbitals in the transition at the optimized geometries of the S_1 state for ANP in chloroform, crystals 1a and 1b.[a]

Systems		Emission energies (eV)[b]	Frontier molecular orbitals in the transition	Energy gap (eV)
ANP in chloroform		2.85 (2.93)	HOMO→LUMO (100%)	4.69
Crystal 1a	Monomer	2.91 (2.82)	HOMO→LUMO (100%)	4.69
Crystal 1b	Trimer A	2.50 (2.48)	HOMO→LUMO (100%)	4.36

[a]For ANP in chloroform, the S_1 optimization was calculated with the linear-response polarizable continuum model (PCM) at the TD-M06-2X/6-31G** level, and single point TDDFT calculation was done at the TD-M06-2X/6-311++G** level with the linear-response PCM method. For crystals 1a and 1b, QM/MM calculations were done at the TD-M06-2X/6-311++G**:UFF level.

[b]The corresponding experiment values are presented in the parentheses.

Table S5. The calculated emission energies, the frontier molecular orbitals in the transition, and the energy gap between frontier molecular orbitals in the transition at the optimized geometries of the S_1 state for different cluster models of crystal 1a.[a]

Cluster model		Emission energies (eV)	Frontier molecular orbitals in the transition	Energy gap (eV)
Monomer		2.91	HOMO→LUMO (100%)	4.69
Dimer	**A**	2.89	HOMO→LUMO (100%)	4.68
	B	2.92	HOMO→LUMO+1 (100%)	4.71
	C	2.89	HOMO→LUMO (90.1%)	4.67
Trimer	**A**	2.91	HOMO→LUMO (100%)	4.72
	B	2.90	HOMO→LUMO (92%)	4.70
	C	2.91	HOMO→LUMO+1 (58%)	4.72

[a]QM/MM calculations are done at the TD-M06-2X/6-311++G**:UFF level.

Table S6. The calculated emission energies, the frontier molecular orbitals in the transition, and the energy gap between frontier molecular orbitals in the transition at the optimized geometries of the S_1 state for different cluster models of crystal 1b.[a]

Cluster model		Emission energies (eV)	Frontier molecular orbitals in the transition	Energy gap (eV)
Monomer		2.92	HOMO→LUMO (100%)	4.70
Dimer	**A**	2.61	HOMO→LUMO (100%)	4.38
	B	2.88	HOMO→LUMO+1 (100%)	4.69
	C	2.94	HOMO→LUMO+1 (100%)	4.72
Trimer	**A**	2.50	HOMO→LUMO (100%)	4.36
	B	2.62	HOMO→LUMO (100%)	4.38
	C	2.90	HOMO→LUMO+2 (79%)	4.69

[a]QM/MM calculations are done at the TD-M06-2X/6-311++G**:UFF level.

8. Calculated emission properties of AA organic polymorphs.

First, the ground-state (S_0) structures of crystals 2a and 2b were optimized with the PBC-GEBF method at the M06-2X/6-31G** level (with their X-ray crystal structures[6] as the initial structures). The optimized structures and lattice parameters are presents in Fig. S5 and Table S7. As shown in Table S7, the optimized lattice parameters of crystals 2a and 2b are in good agreement with the experimental results.

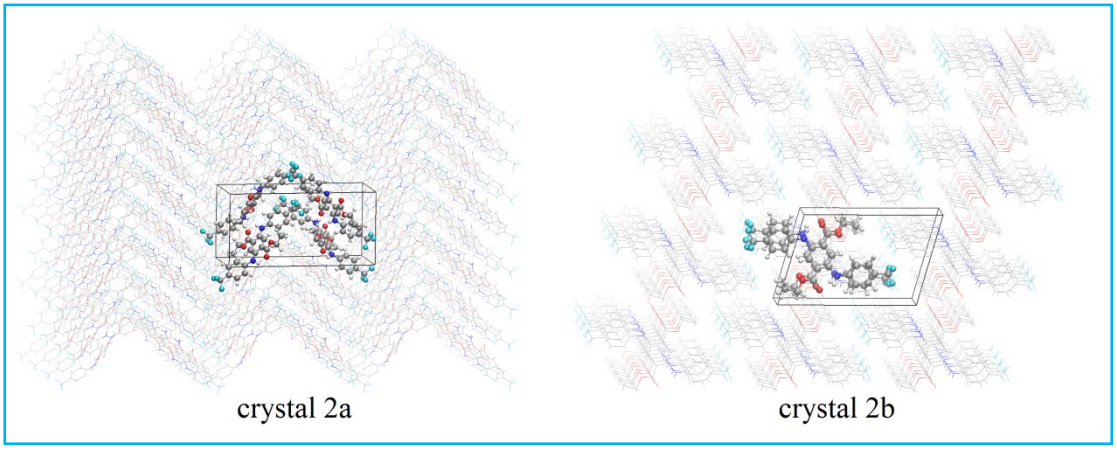


Fig. S5 Optimized structures of crystal 2a and crystal 2b calculated at the PBC-GEBF-M06-2X/6-31G** level.

Table S7. Comparison of optimized lattice parameters of crystals 2a and 2b calculated at the PBC-GEBF-M06-2X/6-31G** level with those of experimental crystal parameters.[a]

System	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ (deg)	volume (Å^3)
crystal 2a	10.36	10.93	22.12	90.10	90.32	89.91	2504.6
X-ray	10.32	10.83	22.15	90.00	90.00	90.00	2476.1
crystal 2b	7.99	10.46	15.65	105.86	103.08	96.01	1206.9
X-ray	8.09	10.41	15.74	105.83	103.84	96.21	1217.1

[a]The experimental values are from ref 6.

Then, based on the optimized crystal structures, three dimer models are automatically selected for crystals 2a and 2b, whose binding energies are the highest values among all possible dimers. As shown in Fig. S6, there exist a clear strong π···π stacking interaction (3.576 Å) in dimer **A** of crystal 2b (with the binding energies of -13.6 kcal/mol).

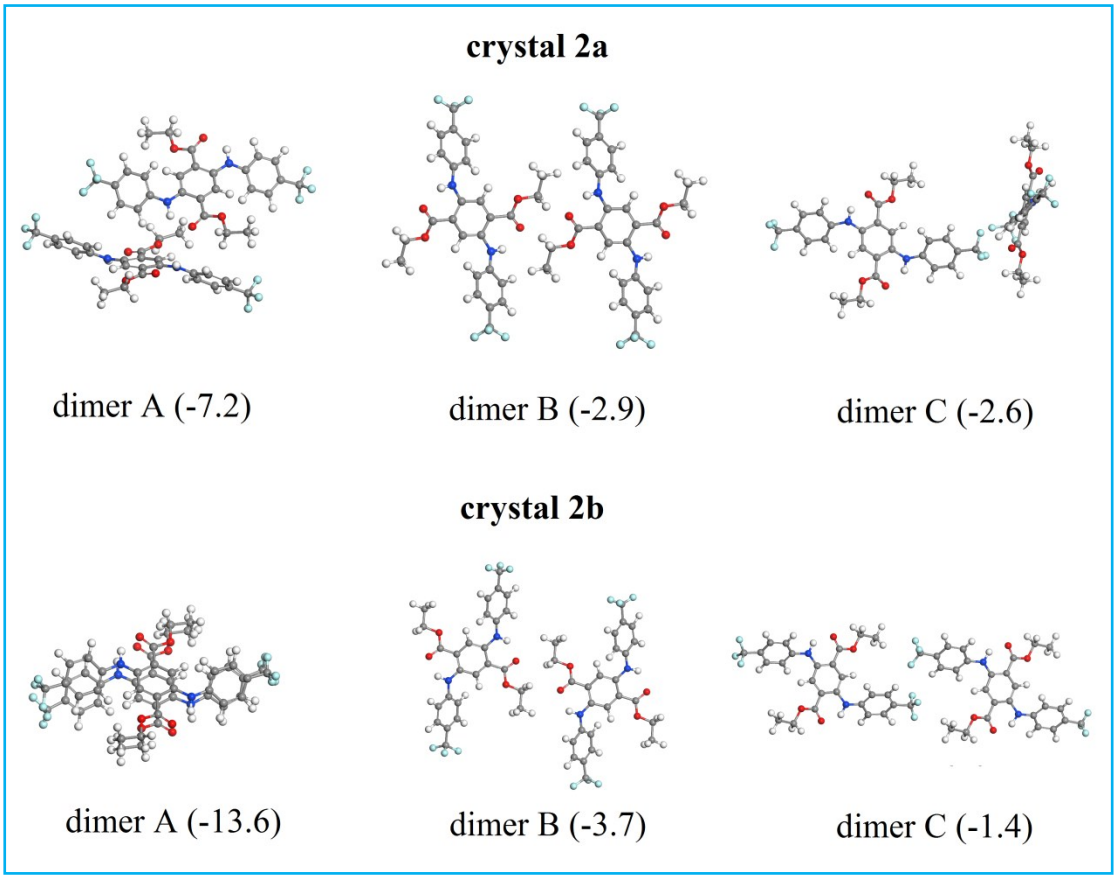


Fig. S6 Three dimer models taken from the optimized crystal structures of crystal 2a and crystal 2b. The corresponding binding energies (in kcal/mol) are shown in parentheses.

With the refined QM/MM approach, the monomer model is chosen for crystal 2a, while the most stable dimer A model is selected for crystal 2b, due to the notable intermolecular π···π stacking interactions. Then, the corresponding two-layer QM/MM calculations was then performed to investigate the emission spectra at the TD-M06-2X/6-31G**:UFF level. The corresponding deviations of the calculated emission energies (in eV) of crystals 2a and 2b relative to the experimental values are shown in Table S8. One can see from Table S8 that for the crystal 2a (without the intermolecular π···π stacking interaction), the calculated emission energy from the monomer model

differs from the emission maximum of the experimental data (2.28 eV) by only 0.04 eV at the 6-31G** level. While for the crystal 2b (with notable intermolecular π···π stacking interaction), the calculated emission energy from the dimer A model differs from the emission maximum of the experimental data (2.13 eV) by only -0.02 eV. Our results again demonstrate that for crystals constructed with notable intermolecular π···π stacking interaction, the most stable dimer model can provide satisfactory descriptions for the emission properties. Further studies demonstrated that the calculated emission energies at a larger 6-311++G** basis set are in better agreement with the experimental values.

Table S8. The deviations of the calculated emission energies (in eV) of crystals 2a and 2b relative to the experimental values.[a]

Cluster Model	Deviations (eV)	
	6-31G**	6-311++G**[b]
Monomer model for crystal 2a	0.04	-0.01 (0.166)
Dimer A model for crystal 2b	-0.02	-0.07 (0.025)

[a]Two-layer QM/MM calculations at the TD-M06-2X/Y:UFF (Y=6-31G**, 6-311++G**) level.

[b]The calculated oscillator strengths (f) are presented in the parentheses.

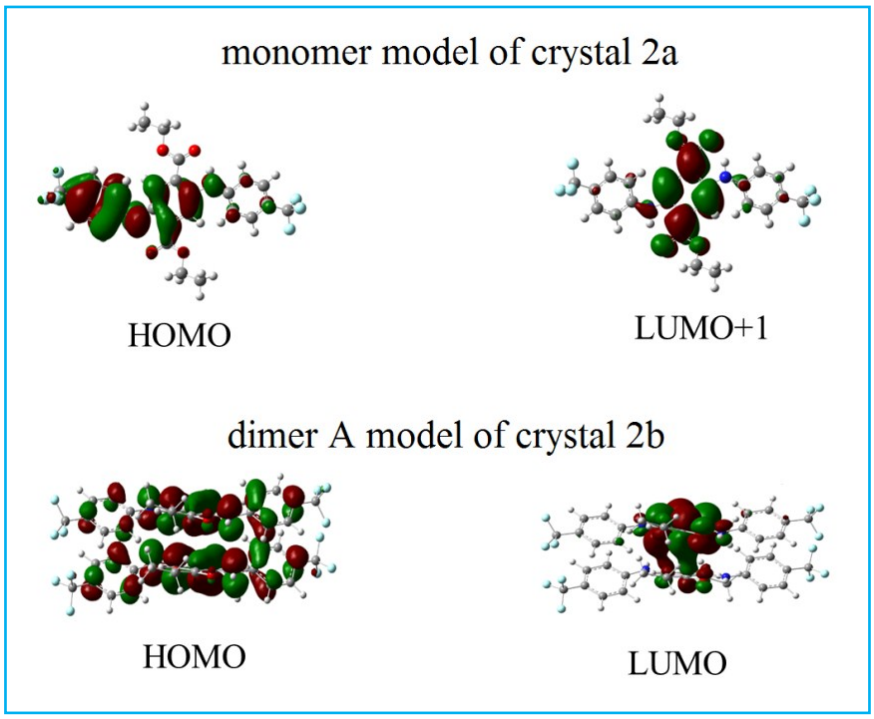


Fig. S7 Frontier molecular orbitals involved in the transition from S_0 to S_1 (calculated at the optimized geometries of the S_1 state) for various cluster models of crystal 2a (monomer model) and crystal 2b (dimer A model) obtained at the TD-M06-2X/6-311++G**:UFF level.

As shown in Fig. S7, we have analyzed the transition nature from the S_0 state to the S_1 state for various cluster models. For the dimer A model of crystal 2b, one can see that two molecular orbitals (HOMO and LUMO) involved in the transition are mainly distributed over two molecules involved in the π···π stacking interaction. One should also mention that the energy gap between two involved orbitals in the transition is 3.93 eV for dimer A of crystal 2b, being about 0.20 eV lower than those from the monomer model for crystal 2a (see Tables S9), which is in agreement with our previous studies. Thus, one can see that in cluster models with the π···π stacking structure of crystal 2b, the intermolecular π···π interaction can significantly reduce the energy gap between frontier molecular orbitals and thus result in red-shift of the emission maximum.

Table S9. The calculated the frontier molecular orbitals in the transition, and the energy gap between frontier molecular orbitals in the transition at the optimized geometries of the S_1 state for different cluster models of crystals 2a and 2b.[a]

Cluster model	Emission energies (eV)	Frontier molecular orbitals in the transition	Energy gap (eV)
Monomer model for crystal 2a	2.27	HOMO→LUMO+1 (86.8%)	4.10
Dimer A model for crystal 2b	2.06	HOMO→LUMO (100%)	3.93

[a]QM/MM calculations are done at the TD-M06-2X/6-311++G**:UFF level.

9. Cartesian coordinates of the selected clusters.

Dimer **A** of crystal 1a

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	3.40248661	5.95687906	1.98673462
N	4.39743312	5.06775954	2.13996597
C	3.87410134	4.07411711	2.86489726
C	2.52116218	4.33635672	3.17095934
C	2.26010759	5.55755392	2.58338246
H	3.57067576	6.81174737	1.44423947
H	1.35694091	6.14652820	2.53954553
H	1.84227461	3.72206087	3.74531925
C	4.69291729	2.91045218	3.28129177
C	4.38512263	1.62032064	2.79894864
C	3.30679462	1.36237316	1.88878855
C	3.08073599	0.10912969	1.39981778
C	3.89826195	-0.98823940	1.80093354
C	4.92340133	-0.78954982	2.67722555
C	5.20821499	0.51196787	3.19235614
C	6.27786338	0.71550649	4.06407251
C	6.56532363	1.97713917	4.58074085
C	7.62800879	2.15695283	5.52468468
C	7.89134329	3.38875490	6.04781695
C	7.10651414	4.51305060	5.64513891
C	6.08534748	4.37726197	4.74919841
C	5.76683834	3.10176298	4.17827731
H	5.48557542	5.23380241	4.46183510
H	7.31155560	5.49019283	6.07401175
H	8.67816024	3.50690333	6.78801381
H	8.19531507	1.27324430	5.82579990
H	6.88961093	-0.13483221	4.36062108
H	5.55812600	-1.60601564	3.00609370
H	3.70045767	-1.97968266	1.40733513
H	2.28134875	-0.05255944	0.68252692
H	2.67025361	2.18628005	1.58577232

N	3.93962774	8.57838620	0.55550683
N	4.45601015	9.03972822	-0.59428611
C	4.11272037	10.32102847	-0.83873769
C	3.31501799	10.72608060	0.21411921
C	3.24419535	9.60010397	1.05809080
C	2.55919560	9.49281460	2.36792424
C	3.18907142	10.02351110	3.51389092
C	4.47324552	10.65478710	3.46709049
C	5.04119297	11.16112152	4.60303288
C	4.37559465	11.07861962	5.86664930
C	3.15372452	10.48007850	5.94928333
C	2.52459196	9.93992327	4.78326874
C	1.27472876	9.32704104	4.85111993
C	0.63683884	8.81871617	3.72257964
C	-0.65410857	8.21741170	3.80856856
C	-1.29860414	7.77818614	2.69271838
C	-0.68295112	7.91764136	1.40975956
C	0.56212432	8.46634812	1.28081107
C	1.27692161	8.91914181	2.44180782
H	1.02049263	8.59176610	0.30201679
H	-1.22396523	7.59438124	0.52706208
H	-2.28793713	7.33913266	2.77430285
H	-1.10937715	8.14794198	4.79280940
H	0.78197955	9.23980044	5.81569035
H	2.63679796	10.38318115	6.90391418
H	4.83820889	11.48896550	6.76428644
H	6.02942968	11.60965806	4.54178086
H	4.98926957	10.72319708	2.51265584
H	2.86272245	11.69164360	0.37973405
H	4.44471209	10.83922552	-1.72755823
H	5.11199933	8.46710295	-1.12979777

Dimer **B** of crystal 1a

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	3.40248661	5.95687906	1.98673462
N	4.39743312	5.06775954	2.13996597
C	3.87410134	4.07411711	2.86489726
C	2.52116218	4.33635672	3.17095934
C	2.26010759	5.55755392	2.58338246
H	3.57067576	6.81174737	1.44423947
H	1.35694091	6.14652820	2.53954553
H	1.84227461	3.72206087	3.74531925
C	4.69291729	2.91045218	3.28129177
C	4.38512263	1.62032064	2.79894864
C	3.30679462	1.36237316	1.88878855
C	3.08073599	0.10912969	1.39981778
C	3.89826195	-0.98823940	1.80093354
C	4.92340133	-0.78954982	2.67722555
C	5.20821499	0.51196787	3.19235614
C	6.27786338	0.71550649	4.06407251
C	6.56532363	1.97713917	4.58074085
C	7.62800879	2.15695283	5.52468468
C	7.89134329	3.38875490	6.04781695
C	7.10651414	4.51305060	5.64513891
C	6.08534748	4.37726197	4.74919841
C	5.76683834	3.10176298	4.17827731
H	5.48557542	5.23380241	4.46183510
H	7.31155560	5.49019283	6.07401175
H	8.67816024	3.50690333	6.78801381
H	8.19531507	1.27324430	5.82579990
H	6.88961093	-0.13483221	4.36062108
H	5.55812600	-1.60601564	3.00609370
H	3.70045767	-1.97968266	1.40733513
H	2.28134875	-0.05255944	0.68252692
H	2.67025361	2.18628005	1.58577232
N	7.42736394	4.52265716	-0.51321438
N	6.91074465	4.06300754	0.63565322

C	7.25538786	2.78201395	0.88048802
C	8.05301678	2.37851711	-0.17213345
C	8.12409771	3.50469173	-1.01809128
C	8.80768613	3.61180684	-2.32836816
C	8.17615275	3.08189340	-3.47350525
C	6.89373546	2.44961608	-3.42546611
C	6.32713526	1.94396227	-4.56251709
C	6.99203804	2.02535403	-5.82680829
C	8.21351129	2.62467402	-5.90961640
C	8.84086981	3.16530436	-4.74292834
C	10.09209971	3.77651609	-4.80980194
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C	12.04905250	5.18876858	-1.37096701
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H	10.35058598	4.50830475	-0.26002846
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H	12.47914595	4.95622356	-4.74859347
H	10.58657972	3.86470716	-5.77215248
H	8.73372384	2.72310318	-6.86073290
H	6.52953306	1.61188556	-6.72130743
H	5.34080582	1.49326678	-4.49546571
H	6.38003033	2.38045427	-2.46895268
H	8.50573085	1.41136198	-0.33196451
H	6.92692797	2.26342688	1.77067809
H	6.25416420	4.63206501	1.17351714

Dimer **C** of crystal 1a

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	-1.13918737	19.16799988	2.02993265
N	-0.14424086	18.27888036	2.18316400
C	-0.66757264	17.28523793	2.90809529
C	-2.02051180	17.54747754	3.21415737
C	-2.28156639	18.76867474	2.62658049
H	-0.97099822	20.02286819	1.48743750
H	-3.18473307	19.35764902	2.58274356
H	-2.69939937	16.93318169	3.78851728
C	0.15124331	16.12157300	3.32448980
C	-0.15655135	14.83144146	2.84214667
C	-1.23487936	14.57349398	1.93198658
C	-1.46093799	13.32025051	1.44301581
C	-0.64341203	12.22288142	1.84413157
C	0.38172735	12.42157100	2.72042358
C	0.66654101	13.72308869	3.23555417
C	1.73618940	13.92662731	4.10727054
C	2.02364965	15.18825999	4.62393888
C	3.08633481	15.36807365	5.56788271
C	3.34966931	16.59987572	6.09101498
C	2.56484016	17.72417142	5.68833694
C	1.54367350	17.58838279	4.79239644
C	1.22516436	16.31288380	4.22147534
H	0.94390144	18.44492323	4.50503313
H	2.76988162	18.70131365	6.11720978
H	4.13648626	16.71802415	6.83121184
H	3.65364109	14.48436512	5.86899793
H	2.34793695	13.07628861	4.40381911
H	1.01645202	11.60510518	3.04929173
H	-0.84121631	11.23143816	1.45053316
H	-2.26032523	13.15856138	0.72572495
H	-1.87142037	15.39740087	1.62897035
N	3.93962774	8.57838620	0.55550683
N	4.45601015	9.03972822	-0.59428611

C	4.11272037	10.32102847	-0.83873769
C	3.31501799	10.72608060	0.21411921
C	3.24419535	9.60010397	1.05809080
C	2.55919560	9.49281460	2.36792424
C	3.18907142	10.02351110	3.51389092
C	4.47324552	10.65478710	3.46709049
C	5.04119297	11.16112152	4.60303288
C	4.37559465	11.07861962	5.86664930
C	3.15372452	10.48007850	5.94928333
C	2.52459196	9.93992327	4.78326874
C	1.27472876	9.32704104	4.85111993
C	0.63683884	8.81871617	3.72257964
C	-0.65410857	8.21741170	3.80856856
C	-1.29860414	7.77818614	2.69271838
C	-0.68295112	7.91764136	1.40975956
C	0.56212432	8.46634812	1.28081107
C	1.27692161	8.91914181	2.44180782
H	1.02049263	8.59176610	0.30201679
H	-1.22396523	7.59438124	0.52706208
H	-2.28793713	7.33913266	2.77430285
H	-1.10937715	8.14794198	4.79280940
H	0.78197955	9.23980044	5.81569035
H	2.63679796	10.38318115	6.90391418
H	4.83820889	11.48896550	6.76428644
H	6.02942968	11.60965806	4.54178086
H	4.98926957	10.72319708	2.51265584
H	2.86272245	11.69164360	0.37973405
H	4.44471209	10.83922552	-1.72755823
H	5.11199933	8.46710295	-1.12979777

Trimer **A** of crystal 1a

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	3.40248661	5.95687906	1.98673462
N	4.39743312	5.06775954	2.13996597
C	3.87410134	4.07411711	2.86489726
C	2.52116218	4.33635672	3.17095934
C	2.26010759	5.55755392	2.58338246
H	3.57067576	6.81174737	1.44423947
H	1.35694091	6.14652820	2.53954553
H	1.84227461	3.72206087	3.74531925
C	4.69291729	2.91045218	3.28129177
C	4.38512263	1.62032064	2.79894864
C	3.30679462	1.36237316	1.88878855
C	3.08073599	0.10912969	1.39981778
C	3.89826195	-0.98823940	1.80093354
C	4.92340133	-0.78954982	2.67722555
C	5.20821499	0.51196787	3.19235614
C	6.27786338	0.71550649	4.06407251
C	6.56532363	1.97713917	4.58074085
C	7.62800879	2.15695283	5.52468468
C	7.89134329	3.38875490	6.04781695
C	7.10651414	4.51305060	5.64513891
C	6.08534748	4.37726197	4.74919841
C	5.76683834	3.10176298	4.17827731
H	5.48557542	5.23380241	4.46183510
H	7.31155560	5.49019283	6.07401175
H	8.67816024	3.50690333	6.78801381
H	8.19531507	1.27324430	5.82579990
H	6.88961093	-0.13483221	4.36062108
H	5.55812600	-1.60601564	3.00609370
H	3.70045767	-1.97968266	1.40733513
H	2.28134875	-0.05255944	0.68252692
H	2.67025361	2.18628005	1.58577232
N	7.42736394	4.52265716	-0.51321438
N	6.91074465	4.06300754	0.63565322

C	7.25538786	2.78201395	0.88048802
C	8.05301678	2.37851711	-0.17213345
C	8.12409771	3.50469173	-1.01809128
C	8.80768613	3.61180684	-2.32836816
C	8.17615275	3.08189340	-3.47350525
C	6.89373546	2.44961608	-3.42546611
C	6.32713526	1.94396227	-4.56251709
C	6.99203804	2.02535403	-5.82680829
C	8.21351129	2.62467402	-5.90961640
C	8.84086981	3.16530436	-4.74292834
C	10.09209971	3.77651609	-4.80980194
C	10.72888591	4.28688314	-3.68120216
C	12.02137855	4.88639491	-3.76751844
C	12.66581296	5.32883090	-2.65258413
C	12.04905250	5.18876858	-1.37096701
C	10.80451490	4.63902061	-1.24126593
C	10.08805793	4.18709312	-2.40126455
H	10.35058598	4.50830475	-0.26002846
H	12.59102535	5.50784896	-0.48553216
H	13.65683429	5.76539586	-2.72981904
H	12.47914595	4.95622356	-4.74859347
H	10.58657972	3.86470716	-5.77215248
H	8.73372384	2.72310318	-6.86073290
H	6.52953306	1.61188556	-6.72130743
H	5.34080582	1.49326678	-4.49546571
H	6.38003033	2.38045427	-2.46895268
H	8.50573085	1.41136198	-0.33196451
H	6.92692797	2.26342688	1.77067809
H	6.25416420	4.63206501	1.17351714
N	3.93962774	8.57838620	0.55550683
N	4.45601015	9.03972822	-0.59428611
C	4.11272037	10.32102847	-0.83873769
C	3.31501799	10.72608060	0.21411921
C	3.24419535	9.60010397	1.05809080
C	2.55919560	9.49281460	2.36792424
C	3.18907142	10.02351110	3.51389092
C	4.47324552	10.65478710	3.46709049
C	5.04119297	11.16112152	4.60303288
C	4.37559465	11.07861962	5.86664930

C	3.15372452	10.48007850	5.94928333
C	2.52459196	9.93992327	4.78326874
C	1.27472876	9.32704104	4.85111993
C	0.63683884	8.81871617	3.72257964
C	-0.65410857	8.21741170	3.80856856
C	-1.29860414	7.77818614	2.69271838
C	-0.68295112	7.91764136	1.40975956
C	0.56212432	8.46634812	1.28081107
C	1.27692161	8.91914181	2.44180782
H	1.02049263	8.59176610	0.30201679
H	-1.22396523	7.59438124	0.52706208
H	-2.28793713	7.33913266	2.77430285
H	-1.10937715	8.14794198	4.79280940
H	0.78197955	9.23980044	5.81569035
H	2.63679796	10.38318115	6.90391418
H	4.83820889	11.48896550	6.76428644
H	6.02942968	11.60965806	4.54178086
H	4.98926957	10.72319708	2.51265584
H	2.86272245	11.69164360	0.37973405
H	4.44471209	10.83922552	-1.72755823
H	5.11199933	8.46710295	-1.12979777

Trimer **B** of crystal 1a

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	10.87264283	8.91032119	11.88509860
N	10.35602354	8.45067157	13.03396620
C	10.70066675	7.16967798	13.27880100
C	11.49829567	6.76618114	12.22617953
C	11.56937660	7.89235576	11.38022170
C	12.25296502	7.99947087	10.06994482
C	11.62143164	7.46955743	8.92480773
C	10.33901435	6.83728011	8.97284687
C	9.77241415	6.33162630	7.83579589
C	10.43731693	6.41301806	6.57150469
C	11.65879018	7.01233805	6.48869658
C	12.28614870	7.55296839	7.65538464
C	13.53737860	8.16418012	7.58851104
C	14.17416480	8.67454717	8.71711082
C	15.46665744	9.27405894	8.63079454
C	16.11109185	9.71649493	9.74572885
C	15.49433139	9.57643261	11.02734597
C	14.24979379	9.02668464	11.15704705
C	13.53333682	8.57475715	9.99704843
H	13.79586487	8.89596878	12.13828452
H	16.03630424	9.89551299	11.91278082
H	17.10211318	10.15305989	9.66849394
H	15.92442484	9.34388759	7.64971951
H	14.03185861	8.25237119	6.62616050
H	12.17900273	7.11076721	5.53758008
H	9.97481195	5.99954959	5.67700555
H	8.78608471	5.88093081	7.90284727
H	9.82530922	6.76811830	9.92936030
H	11.95100974	5.79902601	12.06634847
H	10.37220686	6.65109091	14.16899107
H	9.69944309	9.01972904	13.57183012
N	11.41161384	11.53826589	10.45677817
N	10.41595331	12.42905373	10.30520547

C	10.93784522	13.42071130	9.57703562
C	12.29145108	13.15731602	9.26958023
C	12.55370466	11.93755070	9.85704079
H	11.24207400	10.68183096	10.99271947
H	13.45475213	11.34488482	9.90196133
H	12.96947218	13.76897329	8.69291553
C	10.11879805	14.58341231	9.15907917
C	10.42848107	15.87282185	9.64007311
C	11.50586814	16.13107090	10.55053990
C	11.73274899	17.38490889	11.03796166
C	10.91569442	18.48266690	10.63739688
C	9.88959214	18.28304008	9.76217949
C	9.60583528	16.98126116	9.24656837
C	8.53527149	16.77697824	8.37572210
C	8.24870026	15.51554786	7.85704393
C	7.18517951	15.33677768	6.91346958
C	6.92201397	14.10492968	6.39040359
C	7.70712044	12.98141322	6.79392530
C	8.72814244	13.11515523	7.69058888
C	9.04691658	14.39072168	8.26024188
H	9.32499189	12.25657280	7.97996063
H	7.49812020	12.00295821	6.36921554
H	6.13230322	13.98269234	5.65482530
H	6.61461361	16.21869669	6.61667046
H	7.92181192	17.62702382	8.08389308
H	9.25197065	19.09994246	9.44084340
H	11.10980959	19.47286033	11.03612405
H	12.52901336	17.54676080	11.76001102
H	12.13888935	15.30547682	10.85806698
N	7.38490663	12.96605023	12.95381981
N	7.90128904	13.42739225	11.80402687
C	7.55799926	14.70869250	11.55957529
C	6.76029688	15.11374463	12.61243219
C	6.68947424	13.98776800	13.45640378
C	6.00447449	13.88047863	14.76623722
C	6.63435031	14.41117513	15.91220390
C	7.91852441	15.04245113	15.86540347
C	8.48647186	15.54878555	17.00134586
C	7.82087354	15.46628365	18.26496228

C	6.59900341	14.86774253	18.34759631
C	5.96987085	14.32758730	17.18158172
C	4.72000765	13.71470507	17.24943291
C	4.08211773	13.20638020	16.12089262
C	2.79117032	12.60507573	16.20688154
C	2.14667475	12.16585017	15.09103136
C	2.76232777	12.30530539	13.80807254
C	4.00740321	12.85401215	13.67912405
C	4.72220050	13.30680584	14.84012080
H	4.46577152	12.97943013	12.70032977
H	2.22131366	11.98204527	12.92537506
H	1.15734176	11.72679669	15.17261583
H	2.33590174	12.53560601	17.19112238
H	4.22725844	13.62746447	18.21400333
H	6.08207685	14.77084518	19.30222716
H	8.28348778	15.87662953	19.16259942
H	9.47470857	15.99732209	16.94009384
H	8.43454846	15.11086111	14.91096882
H	6.30800134	16.07930763	12.77804703
H	7.88999098	15.22688955	10.67075475
H	8.55727822	12.85476698	11.26851521

Trimer **C** of crystal 1a

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	3.40248661	5.95687906	1.98673462
N	4.39743312	5.06775954	2.13996597
C	3.87410134	4.07411711	2.86489726
C	2.52116218	4.33635672	3.17095934
C	2.26010759	5.55755392	2.58338246
H	3.57067576	6.81174737	1.44423947
H	1.35694091	6.14652820	2.53954553
H	1.84227461	3.72206087	3.74531925
C	4.69291729	2.91045218	3.28129177
C	4.38512263	1.62032064	2.79894864
C	3.30679462	1.36237316	1.88878855
C	3.08073599	0.10912969	1.39981778
C	3.89826195	-0.98823940	1.80093354
C	4.92340133	-0.78954982	2.67722555
C	5.20821499	0.51196787	3.19235614
C	6.27786338	0.71550649	4.06407251
C	6.56532363	1.97713917	4.58074085
C	7.62800879	2.15695283	5.52468468
C	7.89134329	3.38875490	6.04781695
C	7.10651414	4.51305060	5.64513891
C	6.08534748	4.37726197	4.74919841
C	5.76683834	3.10176298	4.17827731
H	5.48557542	5.23380241	4.46183510
H	7.31155560	5.49019283	6.07401175
H	8.67816024	3.50690333	6.78801381
H	8.19531507	1.27324430	5.82579990
H	6.88961093	-0.13483221	4.36062108
H	5.55812600	-1.60601564	3.00609370
H	3.70045767	-1.97968266	1.40733513
H	2.28134875	-0.05255944	0.68252692
H	2.67025361	2.18628005	1.58577232
N	-0.50794397	4.53676980	-0.49742806
N	-1.02456326	4.07712018	0.65143954

C	-0.67992005	2.79612659	0.89627434
C	0.11770887	2.39262975	-0.15634713
C	0.18878980	3.51880437	-1.00230496
C	0.87237822	3.62591948	-2.31258184
C	0.24084484	3.09600604	-3.45771893
C	-1.04157245	2.46372872	-3.40967979
C	-1.60817265	1.95807491	-4.54673077
C	-0.94326987	2.03946667	-5.81102197
C	0.27820338	2.63878666	-5.89383008
C	0.90556190	3.17941700	-4.72714202
C	2.15679180	3.79062873	-4.79401562
C	2.79357800	4.30099578	-3.66541584
C	4.08607064	4.90050755	-3.75173212
C	4.73050505	5.34294354	-2.63679781
C	4.11374459	5.20288122	-1.35518069
C	2.86920699	4.65313325	-1.22547961
C	2.15275002	4.20120576	-2.38547823
H	2.41527807	4.52241739	-0.24424214
H	4.65571744	5.52196160	-0.46974584
H	5.72152638	5.77950850	-2.71403272
H	4.54383804	4.97033620	-4.73280715
H	2.65127181	3.87881980	-5.75636616
H	0.79841593	2.73721582	-6.84494658
H	-1.40577485	1.62599820	-6.70552111
H	-2.59450209	1.50737942	-4.47967939
H	-1.55527758	2.39456691	-2.45316636
H	0.57042294	1.42547462	-0.31617819
H	-1.00837994	2.27753952	1.78646441
H	-1.68114371	4.64617765	1.18930346
N	7.42736394	4.52265716	-0.51321438
N	6.91074465	4.06300754	0.63565322
C	7.25538786	2.78201395	0.88048802
C	8.05301678	2.37851711	-0.17213345
C	8.12409771	3.50469173	-1.01809128
C	8.80768613	3.61180684	-2.32836816
C	8.17615275	3.08189340	-3.47350525
C	6.89373546	2.44961608	-3.42546611
C	6.32713526	1.94396227	-4.56251709
C	6.99203804	2.02535403	-5.82680829

C	8.21351129	2.62467402	-5.90961640
C	8.84086981	3.16530436	-4.74292834
C	10.09209971	3.77651609	-4.80980194
C	10.72888591	4.28688314	-3.68120216
C	12.02137855	4.88639491	-3.76751844
C	12.66581296	5.32883090	-2.65258413
C	12.04905250	5.18876858	-1.37096701
C	10.80451490	4.63902061	-1.24126593
C	10.08805793	4.18709312	-2.40126455
H	10.35058598	4.50830475	-0.26002846
H	12.59102535	5.50784896	-0.48553216
H	13.65683429	5.76539586	-2.72981904
H	12.47914595	4.95622356	-4.74859347
H	10.58657972	3.86470716	-5.77215248
H	8.73372384	2.72310318	-6.86073290
H	6.52953306	1.61188556	-6.72130743
H	5.34080582	1.49326678	-4.49546571
H	6.38003033	2.38045427	-2.46895268
H	8.50573085	1.41136198	-0.33196451
H	6.92692797	2.26342688	1.77067809
H	6.25416420	4.63206501	1.17351714

Dimer **A** of crystal 1b

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	4.66577601	3.98984659	2.69896538
N	5.46806140	3.81106520	3.75612365
C	5.54079165	2.52391191	4.13608019
C	4.73086101	1.81005391	3.27469220
C	4.20452302	2.77516153	2.38820296
C	3.21579904	2.48317153	1.31091527
C	3.61999394	1.76115867	0.16316273
C	4.97020523	1.57434480	-0.04177151
C	5.33105051	0.87115570	-1.15941219
C	4.33431040	0.34596868	-2.03452673
C	3.01357883	0.55594746	-1.77910414
C	2.59724205	1.30940443	-0.63454008
C	1.24559671	1.52860238	-0.37725673
C	0.86525120	2.22581271	0.60716087
C	-0.51225392	2.47341255	0.84480457
C	-0.90964713	3.24074139	1.89785459
C	0.04637753	3.78660726	2.80905825
C	1.37694843	3.53670521	2.62883346
C	1.84435343	2.76390549	1.51520503
H	2.10190909	3.93404956	3.32520968
H	-0.28458464	4.38824510	3.64605483
H	-1.97012985	3.43441196	2.03693957
H	-1.24034358	2.05006465	0.15384526
H	0.50533727	1.09112895	-1.05518010
H	2.24411166	0.14702502	-2.43854740
H	4.63938606	-0.24186721	-2.90382149
H	6.37470688	0.67110998	-1.38757353
H	5.76163449	1.88390831	0.52104350
H	4.52811881	0.74620875	3.29328116
H	6.14495538	2.20135024	4.97334310
H	6.01454805	4.59804303	4.14369411
N	4.73393401	6.70836399	1.67650224
N	5.66314506	7.58699721	2.08623941

C	5.40470750	8.70613132	1.41005253
C	4.29641295	8.54749746	0.56372371
C	3.89394363	7.23669388	0.75758184
H	4.69099267	5.74332433	2.03889198
C	2.80633425	6.44879808	0.12205211
C	3.07768030	5.63669608	-0.83618297
C	4.41875933	5.39036532	-1.28662807
C	4.66725103	4.51613903	-2.30702666
C	3.59898008	3.83932853	-2.96604576
C	2.30819809	4.05775276	-2.58341462
C	2.00649801	4.95208429	-1.50941477
C	0.69004337	5.16260148	-1.09332861
C	0.38904419	5.99994750	-0.01681552
C	-0.91932240	6.10363034	0.32196354
C	-1.20279082	6.90050059	1.39510187
C	-0.15949811	7.58905216	2.08899630
C	1.13353674	7.46091209	1.67479783
C	1.47769830	6.62442729	0.55743350
H	1.92461661	7.99842493	2.18588210
H	-0.39570706	8.21078933	2.94602267
H	-2.23386732	7.01326094	1.72091597
H	-1.73609873	5.62737131	-0.09299225
H	-0.10921622	4.62603003	-1.61231173
H	1.48981307	3.51923876	-3.06500911
H	3.81205234	3.11876938	-3.75422398
H	5.68791132	4.30932260	-2.61779488
H	5.24401407	5.90136792	-0.80498575
H	3.86090948	9.27525583	-0.10506917
H	6.02008890	9.58785893	1.52924757

Dimer **B** of crystal 1b

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	4.66577601	3.98984659	2.69896538
N	5.46806140	3.81106520	3.75612365
C	5.54079165	2.52391191	4.13608019
C	4.73086101	1.81005391	3.27469220
C	4.20452302	2.77516153	2.38820296
C	3.21579904	2.48317153	1.31091527
C	3.61999394	1.76115867	0.16316273
C	4.97020523	1.57434480	-0.04177151
C	5.33105051	0.87115570	-1.15941219
C	4.33431040	0.34596868	-2.03452673
C	3.01357883	0.55594746	-1.77910414
C	2.59724205	1.30940443	-0.63454008
C	1.24559671	1.52860238	-0.37725673
C	0.86525120	2.22581271	0.60716087
C	-0.51225392	2.47341255	0.84480457
C	-0.90964713	3.24074139	1.89785459
C	0.04637753	3.78660726	2.80905825
C	1.37694843	3.53670521	2.62883346
C	1.84435343	2.76390549	1.51520503
H	2.10190909	3.93404956	3.32520968
H	-0.28458464	4.38824510	3.64605483
H	-1.97012985	3.43441196	2.03693957
H	-1.24034358	2.05006465	0.15384526
H	0.50533727	1.09112895	-1.05518010
H	2.24411166	0.14702502	-2.43854740
H	4.63938606	-0.24186721	-2.90382149
H	6.37470688	0.67110998	-1.38757353
H	5.76163449	1.88390831	0.52104350
H	4.52811881	0.74620875	3.29328116
H	6.14495538	2.20135024	4.97334310
H	6.01454805	4.59804303	4.14369411
N	7.73303567	6.86630320	3.99809853
N	7.33728919	5.77154387	4.66112951

C	8.32685998	5.48537657	5.51258027
C	9.37050763	6.42460693	5.39715977
C	8.94402280	7.29139172	4.40592664
H	7.09634776	7.23168837	3.27017983
H	9.41466190	8.16907670	3.98710595
H	10.30027018	6.45378151	5.94551014
C	8.19997065	4.32332024	6.42567665
C	7.47938160	4.46296583	7.62771289
C	6.95724651	5.73194928	8.05921980
C	6.35791305	5.79872506	9.15711773
C	6.17181970	4.66509068	10.01034395
C	6.62324671	3.43377663	9.62248445
C	7.28355211	3.32273358	8.48228534
C	7.78640393	2.07708445	8.08454599
C	8.57321770	1.95319414	6.93329883
C	9.18650335	0.70795805	6.58475373
C	10.00393229	0.60639981	5.49775238
C	10.24235942	1.74174626	4.66880205
C	9.64461229	2.93862300	4.94097570
C	8.80116046	3.09611313	6.09206988
H	9.81367857	3.78749873	4.28754229
H	10.89671634	1.64122232	3.80555587
H	10.46994760	-0.34668110	5.25439422
H	9.00347671	-0.15994762	7.21113102
H	7.59679393	1.18305233	8.68588689
H	6.49099032	2.55926709	10.25932029
H	5.66560064	4.78063203	10.96108959
H	5.98196176	6.77261573	9.47357017
H	7.09663138	6.58472671	7.39680372

Dimer **C** of crystal 1b

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	3.42199013	26.22274750	5.20831385
N	3.81345455	27.31123460	4.53939541
C	2.82449279	27.59380353	3.68909065
C	1.78150286	26.65704661	3.80976279
C	2.21477764	25.79183079	4.80270183
H	4.07105619	25.85581435	5.93831307
H	1.74740197	24.91052750	5.21335024
H	0.85527716	26.61060555	3.25350319
C	2.95022863	28.76069392	2.78187888
C	3.67683590	28.62741931	1.58441044
C	4.19443443	27.35477611	1.15197884
C	4.79401101	27.28584162	0.05572952
C	4.97565976	28.42189862	-0.78877069
C	4.52687457	29.65581271	-0.40957794
C	3.87215512	29.77107506	0.73475061
C	3.36353056	31.01576830	1.12128609
C	2.58184711	31.14101427	2.27636434
C	1.96735171	32.38645389	2.61897791
C	1.15155941	32.48248867	3.70728326
C	0.91596161	31.34360979	4.53432865
C	1.51188021	30.14562705	4.26352247
C	2.35548145	29.99397961	3.11419574
H	1.34313678	29.28167938	4.90134143
H	0.25382524	31.41742044	5.39140729
H	0.66737140	33.41788108	3.95113926
H	2.14582700	33.22916237	1.96552921
H	3.55361139	31.88251264	0.48788532
H	4.66187360	30.50115482	-1.08237549
H	5.47566598	28.28929270	-1.75191815
H	5.16590473	26.31289690	-0.28171769
H	4.05574986	26.48652993	1.79239928
N	6.42704727	26.36736768	7.51699330
N	5.49405622	25.48933367	7.10418987
C	5.75227787	24.37229285	7.78812699

C	6.85809502	24.53218665	8.63467025
C	7.26205330	25.84564868	8.44377597
H	6.44161792	27.33158343	7.16323041
C	8.34978781	26.63610470	9.07912295
C	8.07566917	27.45257470	10.03258682
C	6.73699065	27.69849171	10.48441269
C	6.49102200	28.57572559	11.50334587
C	7.55613123	29.25628261	12.16427573
C	8.84662196	29.03461952	11.78085673
C	9.14610084	28.13997795	10.70521683
C	10.46351383	27.92297403	10.29216082
C	10.76559995	27.08396978	9.21603012
C	12.07562861	26.98119512	8.87801755
C	12.36052676	26.18377232	7.80535555
C	11.31571286	25.49616288	7.11400562
C	10.02192757	25.62179799	7.52667462
C	9.67710923	26.45765765	8.64291078
H	9.22809177	25.08717103	7.01184370
H	11.54581862	24.87659521	6.25243238
H	13.39092997	26.06414013	7.48247757
H	12.90060411	27.44044324	9.29258905
H	11.26832125	28.43479520	10.81793242
H	9.66924466	29.53871815	12.27985167
H	7.33311761	29.93978974	12.97640002
H	5.46497187	28.74678126	11.82154135
H	5.91093626	27.17018184	10.01093535
H	7.28124156	23.81099604	9.31538797
H	5.12551070	23.49917839	7.66819051

Trimer **A** of crystal 1b

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	4.66577601	3.98984659	2.69896538
N	5.46806140	3.81106520	3.75612365
C	5.54079165	2.52391191	4.13608019
C	4.73086101	1.81005391	3.27469220
C	4.20452302	2.77516153	2.38820296
C	3.21579904	2.48317153	1.31091527
C	3.61999394	1.76115867	0.16316273
C	4.97020523	1.57434480	-0.04177151
C	5.33105051	0.87115570	-1.15941219
C	4.33431040	0.34596868	-2.03452673
C	3.01357883	0.55594746	-1.77910414
C	2.59724205	1.30940443	-0.63454008
C	1.24559671	1.52860238	-0.37725673
C	0.86525120	2.22581271	0.60716087
C	-0.51225392	2.47341255	0.84480457
C	-0.90964713	3.24074139	1.89785459
C	0.04637753	3.78660726	2.80905825
C	1.37694843	3.53670521	2.62883346
C	1.84435343	2.76390549	1.51520503
H	2.10190909	3.93404956	3.32520968
H	-0.28458464	4.38824510	3.64605483
H	-1.97012985	3.43441196	2.03693957
H	-1.24034358	2.05006465	0.15384526
H	0.50533727	1.09112895	-1.05518010
H	2.24411166	0.14702502	-2.43854740
H	4.63938606	-0.24186721	-2.90382149
H	6.37470688	0.67110998	-1.38757353
H	5.76163449	1.88390831	0.52104350
H	4.52811881	0.74620875	3.29328116
H	6.14495538	2.20135024	4.97334310
H	6.01454805	4.59804303	4.14369411
N	7.73303567	6.86630320	3.99809853
N	7.33728919	5.77154387	4.66112951

C	8.32685998	5.48537657	5.51258027
C	9.37050763	6.42460693	5.39715977
C	8.94402280	7.29139172	4.40592664
H	7.09634776	7.23168837	3.27017983
H	9.41466190	8.16907670	3.98710595
H	10.30027018	6.45378151	5.94551014
C	8.19997065	4.32332024	6.42567665
C	7.47938160	4.46296583	7.62771289
C	6.95724651	5.73194928	8.05921980
C	6.35791305	5.79872506	9.15711773
C	6.17181970	4.66509068	10.01034395
C	6.62324671	3.43377663	9.62248445
C	7.28355211	3.32273358	8.48228534
C	7.78640393	2.07708445	8.08454599
C	8.57321770	1.95319414	6.93329883
C	9.18650335	0.70795805	6.58475373
C	10.00393229	0.60639981	5.49775238
C	10.24235942	1.74174626	4.66880205
C	9.64461229	2.93862300	4.94097570
C	8.80116046	3.09611313	6.09206988
H	9.81367857	3.78749873	4.28754229
H	10.89671634	1.64122232	3.80555587
H	10.46994760	-0.34668110	5.25439422
H	9.00347671	-0.15994762	7.21113102
H	7.59679393	1.18305233	8.68588689
H	6.49099032	2.55926709	10.25932029
H	5.66560064	4.78063203	10.96108959
H	5.98196176	6.77261573	9.47357017
H	7.09663138	6.58472671	7.39680372
N	4.73393401	6.70836399	1.67650224
N	5.66314506	7.58699721	2.08623941
C	5.40470750	8.70613132	1.41005253
C	4.29641295	8.54749746	0.56372371
C	3.89394363	7.23669388	0.75758184
H	4.69099267	5.74332433	2.03889198
C	2.80633425	6.44879808	0.12205211
C	3.07768030	5.63669608	-0.83618297
C	4.41875933	5.39036532	-1.28662807
C	4.66725103	4.51613903	-2.30702666

C	3.59898008	3.83932853	-2.96604576
C	2.30819809	4.05775276	-2.58341462
C	2.00649801	4.95208429	-1.50941477
C	0.69004337	5.16260148	-1.09332861
C	0.38904419	5.99994750	-0.01681552
C	-0.91932240	6.10363034	0.32196354
C	-1.20279082	6.90050059	1.39510187
C	-0.15949811	7.58905216	2.08899630
C	1.13353674	7.46091209	1.67479783
C	1.47769830	6.62442729	0.55743350
H	1.92461661	7.99842493	2.18588210
H	-0.39570706	8.21078933	2.94602267
H	-2.23386732	7.01326094	1.72091597
H	-1.73609873	5.62737131	-0.09299225
H	-0.10921622	4.62603003	-1.61231173
H	1.48981307	3.51923876	-3.06500911
H	3.81205234	3.11876938	-3.75422398
H	5.68791132	4.30932260	-2.61779488
H	5.24401407	5.90136792	-0.80498575
H	3.86090948	9.27525583	-0.10506917
H	6.02008890	9.58785893	1.52924757

Trimer **B** of crystal 1b

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	4.66577601	3.98984659	2.69896538
N	5.46806140	3.81106520	3.75612365
C	5.54079165	2.52391191	4.13608019
C	4.73086101	1.81005391	3.27469220
C	4.20452302	2.77516153	2.38820296
C	3.21579904	2.48317153	1.31091527
C	3.61999394	1.76115867	0.16316273
C	4.97020523	1.57434480	-0.04177151
C	5.33105051	0.87115570	-1.15941219
C	4.33431040	0.34596868	-2.03452673
C	3.01357883	0.55594746	-1.77910414
C	2.59724205	1.30940443	-0.63454008
C	1.24559671	1.52860238	-0.37725673
C	0.86525120	2.22581271	0.60716087
C	-0.51225392	2.47341255	0.84480457
C	-0.90964713	3.24074139	1.89785459
C	0.04637753	3.78660726	2.80905825
C	1.37694843	3.53670521	2.62883346
C	1.84435343	2.76390549	1.51520503
H	2.10190909	3.93404956	3.32520968
H	-0.28458464	4.38824510	3.64605483
H	-1.97012985	3.43441196	2.03693957
H	-1.24034358	2.05006465	0.15384526
H	0.50533727	1.09112895	-1.05518010
H	2.24411166	0.14702502	-2.43854740
H	4.63938606	-0.24186721	-2.90382149
H	6.37470688	0.67110998	-1.38757353
H	5.76163449	1.88390831	0.52104350
H	4.52811881	0.74620875	3.29328116
H	6.14495538	2.20135024	4.97334310
H	6.01454805	4.59804303	4.14369411
N	4.73393401	6.70836399	1.67650224
N	5.66314506	7.58699721	2.08623941

C	5.40470750	8.70613132	1.41005253
C	4.29641295	8.54749746	0.56372371
C	3.89394363	7.23669388	0.75758184
H	4.69099267	5.74332433	2.03889198
C	2.80633425	6.44879808	0.12205211
C	3.07768030	5.63669608	-0.83618297
C	4.41875933	5.39036532	-1.28662807
C	4.66725103	4.51613903	-2.30702666
C	3.59898008	3.83932853	-2.96604576
C	2.30819809	4.05775276	-2.58341462
C	2.00649801	4.95208429	-1.50941477
C	0.69004337	5.16260148	-1.09332861
C	0.38904419	5.99994750	-0.01681552
C	-0.91932240	6.10363034	0.32196354
C	-1.20279082	6.90050059	1.39510187
C	-0.15949811	7.58905216	2.08899630
C	1.13353674	7.46091209	1.67479783
C	1.47769830	6.62442729	0.55743350
H	1.92461661	7.99842493	2.18588210
H	-0.39570706	8.21078933	2.94602267
H	-2.23386732	7.01326094	1.72091597
H	-1.73609873	5.62737131	-0.09299225
H	-0.10921622	4.62603003	-1.61231173
H	1.48981307	3.51923876	-3.06500911
H	3.81205234	3.11876938	-3.75422398
H	5.68791132	4.30932260	-2.61779488
H	5.24401407	5.90136792	-0.80498575
H	3.86090948	9.27525583	-0.10506917
H	6.02008890	9.58785893	1.52924757
N	3.92147306	9.81906367	6.29586098
N	4.86701964	8.94964064	6.69286610
C	4.60673372	7.82870854	6.01658155
C	3.48890564	7.98081541	5.18237841
C	3.07285805	9.28376162	5.39138303
H	3.87806339	10.78533127	6.65018501
C	1.98096128	10.06554985	4.76947586
C	2.28825474	10.94840598	3.71632050
C	3.63246501	11.18322330	3.28062912
C	3.88808214	12.05924565	2.26548610

C	2.82439131	12.74259328	1.60158105
C	1.53073776	12.52963075	1.97653715
C	1.22035619	11.63521622	3.04523742
C	-0.09811229	11.42337040	3.45027863
C	-0.40275090	10.58446432	4.52098928
C	-1.74066397	10.39710041	4.95724645
C	-2.02387112	9.60093912	6.02717729
C	-0.98355301	8.92600520	6.72291608
C	0.31202910	9.05230347	6.31191678
C	0.65422362	9.88964069	5.20051943
H	1.10426724	8.50881364	6.81750494
H	-1.22059098	8.29609871	7.57514006
H	-3.05640525	9.48083335	6.34617659
H	-2.53259429	10.93210733	4.43562971
H	-0.90098079	11.93166537	2.92720040
H	0.70669397	13.04796309	1.48864238
H	3.04459164	13.44113429	0.80112197
H	4.91327232	12.24414724	1.95561530
H	4.44665442	10.65174179	3.76547074
H	3.05032824	7.25271042	4.51525010
H	5.21835590	6.94323295	6.13614869

Trimer **C** of crystal 1b

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
N	5.83529085	23.36845687	-8.62591496
N	6.19687865	22.35054787	-9.19614630
C	5.21207721	22.06948995	-10.05215772
C	4.17382627	23.01287506	-9.92722904
C	4.62924512	23.80442498	-9.03356428
H	6.47695420	23.75166013	-7.89247175
H	4.16372039	24.69012834	-8.60826470
H	3.24795458	23.07341174	-10.48347468
C	5.33078258	20.89778261	-10.96145398
C	6.06204837	21.02299774	-12.15365280
C	6.58331922	22.28638049	-12.58609520
C	7.23214135	22.39784240	-13.78095323
C	7.42033183	21.25710490	-14.61622025
C	6.95571817	20.03289070	-14.24045611
C	6.25972687	19.87598733	-12.99713476
C	5.74094959	18.63931941	-12.61907976
C	4.95476927	18.51944020	-11.47032156
C	4.34220053	17.27068699	-11.13946125
C	3.53098251	17.16747514	-10.04723305
C	3.30820978	18.30750110	-9.21008679
C	3.90448337	19.51086379	-9.47519752
C	4.73604666	19.66590973	-10.63020688
H	3.77054608	20.31051499	-8.94019090
H	2.67963868	18.18790336	-8.45048030
H	3.05054606	16.22688489	-9.81725359
H	4.53367900	16.43330209	-11.79812584
H	5.93132576	17.78090454	-13.25635793
H	7.08482380	19.18559069	-14.90445810
H	7.92876537	21.39083132	-15.57567112
H	7.60136599	23.37000412	-14.11883163
H	6.43089750	23.16895370	-11.96508271
N	4.23428376	23.35397287	0.56055562
N	4.59587156	22.33606387	-0.00967572

C	3.61107012	22.05500595	-0.86568714
C	2.57281918	22.99839106	-0.74075846
C	3.02823803	23.78994098	0.15290630
H	4.87594711	23.73717613	1.29399883
H	2.56271330	24.67564434	0.57820588
H	1.64694749	23.05892774	-1.29700410
C	3.72977549	20.88329861	-1.77498340
C	4.46104128	21.00851374	-2.96718222
C	4.98231213	22.27189649	-3.39962462
C	5.63113426	22.38335840	-4.59448265
C	5.81932474	21.24262090	-5.42974967
C	5.35471108	20.01840670	-5.05398553
C	4.65871978	19.86150333	-3.81066418
C	4.13994250	18.62483541	-3.43260918
C	3.35376218	18.50495620	-2.28385098
C	2.74119344	17.25620299	-1.95299067
C	1.92997542	17.15299114	-0.86076247
C	1.70720269	18.29301710	-0.02361621
C	2.30347628	19.49637979	-0.28872694
C	3.13503957	19.65142573	-1.44373630
H	2.16953899	20.29603099	0.24627968
H	1.07863159	18.17341936	0.73599028
H	1.44953897	16.21240089	-0.63078301
H	2.93267191	16.41881809	-2.61165526
H	4.33031867	17.76642054	-4.06988735
H	5.48381671	19.17110669	-5.71798752
H	6.32775828	21.37634732	-6.38920054
H	6.00035890	23.35552012	-4.93236105
H	4.82989041	23.15446970	-2.77861213
N	8.83609097	23.27378680	-6.28327613
N	7.88950346	24.14435283	-6.68224375
C	8.15200809	25.26478909	-6.00038601
C	9.26635685	25.11152046	-5.16558469
C	9.68306295	23.80581455	-5.37636640
H	8.85626905	22.31447714	-6.65106633
C	10.77564436	23.02265353	-4.75391529
C	10.46579758	22.13696782	-3.70585996
C	9.12342727	21.90212670	-3.27048206
C	8.86987077	21.02620114	-2.25573780

C	9.93178017	20.34217691	-1.59010658
C	11.22485459	20.55765204	-1.96491940
C	11.53355922	21.45010492	-3.03593758
C	12.85280508	21.66826828	-3.43643124
C	13.15870668	22.50702913	-4.50644483
C	14.49921696	22.69298013	-4.93906438
C	14.78402407	23.48896791	-6.00771908
C	13.74071449	24.16104432	-6.69935864
C	12.44410354	24.03796623	-6.29311849
C	12.10068655	23.20182696	-5.18373920
H	11.65241565	24.57832064	-6.81047675
H	13.97156042	24.78763464	-7.56008697
H	15.81350180	23.61691246	-6.33489530
H	15.30073629	22.17515094	-4.42111835
H	13.66069386	21.18476190	-2.90660410
H	12.05291591	20.07240383	-1.46097608
H	9.70227631	19.67802919	-0.76826134
H	7.84046517	20.87567385	-1.93824709
H	8.30783745	22.44750409	-3.74806305
H	9.69610335	25.84148522	-4.49789167
H	7.53315092	26.14478215	-6.12801492

Dimer **A** of crystal 2a

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
C	4.51474888	-8.01665761	25.40946727
C	4.41377101	-8.72149972	26.60090826
C	3.51819971	-9.79076418	26.72761432
C	2.73743018	-10.15888648	25.63361244
C	2.83767157	-9.46781999	24.44304056
C	3.72166157	-8.37769363	24.29249337
H	5.19266366	-7.18018116	25.37245497
N	3.70973074	-7.75717085	23.07405467
C	4.42840811	-6.62696315	22.62324887
C	3.84528825	-5.72786669	21.70895419
C	4.57848734	-4.64237944	21.23202730
C	5.90111104	-4.39316347	21.63550677
C	6.46877214	-5.30369198	22.56567129
C	5.73521573	-6.39664399	23.02342699
H	6.21650051	-7.10772997	23.68575363
C	7.88694007	-5.14206664	23.03605242
O	8.36393694	-6.25239123	23.57250797
C	9.71988868	-6.15809050	24.10681772
C	10.00098773	-7.46857033	24.77440533
H	9.95740830	-8.30568161	24.05627973
H	9.28258608	-7.67358892	25.57608300
H	10.99403518	-7.44978646	25.20101319
H	9.76768933	-5.33619753	24.81784443
H	10.37724936	-5.98397146	23.26668241
O	8.51897655	-4.11967610	22.89750977
N	6.61325797	-3.30543292	21.20569841
C	6.58279425	-2.65149387	19.96724069
C	5.80342631	-3.02782024	18.87129993
C	5.88539178	-2.31232947	17.67419768
C	6.74444217	-1.23304979	17.55283591
C	7.56047837	-0.87409610	18.63691166
C	7.47892207	-1.57743370	19.82501786
H	8.11247113	-1.34022211	20.67084138
H	8.26187173	-0.06031032	18.55361891

C	6.85122411	-0.49945698	16.24668660
F	5.74213758	-0.61283272	15.48941343
F	7.05455769	0.81194384	16.43663861
F	7.89245592	-0.93194887	15.51189910
H	5.25347768	-2.63095394	16.84272674
H	5.12527740	-3.87762436	18.92106531
H	7.32336468	-3.03017131	21.87451573
H	4.07183585	-3.94661930	20.58639227
C	2.44191409	-5.89981957	21.24328906
O	1.95929497	-4.78944219	20.68470181
C	0.61825074	-4.87202071	20.18062032
C	0.31741421	-3.55557550	19.50501343
H	-0.68620287	-3.63991368	19.08791391
H	0.34253453	-2.75394868	20.23708096
H	1.02960439	-3.40222248	18.69547897
H	-0.05417986	-5.08759033	21.01090509
H	0.54521157	-5.72196509	19.48022869
O	1.77068344	-6.91866768	21.33058460
H	2.97601732	-8.06774657	22.45094959
H	2.18788517	-9.73871558	23.61455185
H	2.03711017	-10.98995597	25.72364027
C	3.43262062	-10.57955003	27.98689438
F	3.40291273	-9.82977896	29.09259839
F	2.32068642	-11.36167012	28.02990460
F	4.49041890	-11.42043106	28.13865257
H	5.04685051	-8.43805676	27.43747025
C	9.67641451	2.48129077	18.87068519
C	9.56841591	3.17895018	17.66970107
C	8.66701368	4.23300325	17.55054563
C	7.89079960	4.61260024	18.64659494
C	7.99946411	3.92214722	19.84272485
C	8.90023154	2.85387726	19.97624291
H	10.33508349	1.62199484	18.92910507
N	8.89640770	2.18794403	21.21066738
C	9.59710423	1.08146904	21.62881598
C	9.04577104	0.16647718	22.55364626
C	9.78945388	-0.95069997	22.98526613
C	11.07296617	-1.18791265	22.56861428
C	11.63930516	-0.27172771	21.64746741

C	10.90356996	0.81466612	21.19608615
H	11.39073816	1.53163650	20.56211391
C	13.05375640	-0.43056910	21.15107267
O	13.51694984	0.67572992	20.60288706
C	14.88563516	0.61315716	20.07825344
C	15.17458672	1.93716158	19.41017300
H	15.14475947	2.72248190	20.16095833
H	16.16815653	1.86136675	18.97007220
H	14.42332063	2.11281478	18.63325992
H	14.91329414	-0.25542240	19.40179810
H	15.54905254	0.40620644	20.92326650
O	13.71717626	-1.45034802	21.25184848
N	11.80655364	-2.31723396	22.99946325
C	11.81028551	-2.95180377	24.21438120
C	11.01939662	-2.59745954	25.33122411
C	11.13151030	-3.29604355	26.52556655
C	12.03015522	-4.35758089	26.65192775
C	12.80657998	-4.73222803	25.55374621
C	12.69918496	-4.04441536	24.36146637
H	13.35057495	-4.32825974	23.54178234
H	13.49956117	-5.56662918	25.64809232
C	12.12323204	-5.13855374	27.91400892
F	12.13812308	-4.38885727	29.02422408
F	13.22062264	-5.91507340	27.95305603
F	11.05159429	-5.98697344	28.06641393
H	10.49467502	-3.01889036	27.36516266
H	10.33464057	-1.76437099	25.29758070
H	12.53047230	-2.62502210	22.36323284
H	9.31168665	-1.65926330	23.65233732
C	7.66206007	0.33129299	23.04388244
O	7.15798760	-0.80656243	23.58592390
C	5.83431510	-0.71574767	24.11464007
C	5.53730492	-2.03385556	24.78857664
H	5.54016025	-2.86631322	24.06636818
H	4.53374168	-2.00889837	25.23720034
H	6.25478257	-2.27164225	25.57949759
H	5.11052291	-0.55936413	23.30374457
H	5.75437068	0.10885861	24.82397021
O	6.98119860	1.32698433	22.90835762

H	8.16559080	2.45388780	21.86405185
H	7.34304203	4.16547947	20.67572841
H	7.17407614	5.42148435	18.56345017
C	8.57452777	5.02058333	16.27939705
F	8.56468049	4.26113513	15.16629991
F	7.47709763	5.79104809	16.24907835
F	9.62945986	5.83997943	16.16475592
H	10.18270665	2.86183534	16.83078638

Dimer **B** of crystal 2a

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
C	-0.68554075	2.48364104	18.94080407
C	-0.79353935	3.18130045	17.73981995
C	-1.69494158	4.23535352	17.62066451
C	-2.47115566	4.61495051	18.71671382
C	-2.36249115	3.92449749	19.91284373
C	-1.46172372	2.85622753	20.04636179
H	-0.02687177	1.62434511	18.99922395
N	-1.46554756	2.19029430	21.28078626
C	-0.76485103	1.08381931	21.69893486
C	-1.31618422	0.16882745	22.62376514
C	-0.57250138	-0.94834970	23.05538501
C	0.71101091	-1.18556238	22.63873316
C	1.27734990	-0.26937744	21.71758629
C	0.54161470	0.81701639	21.26620503
H	1.02878290	1.53398677	20.63223279
C	2.69180114	-0.42821883	21.22119155
O	3.15499458	0.67808019	20.67300594
C	4.52367990	0.61550743	20.14837232
C	4.81263146	1.93951185	19.48029188
H	4.78280421	2.72483217	20.23107721
H	5.80620127	1.86371702	19.04019108
H	4.06136537	2.11516505	18.70337880
H	4.55133888	-0.25307213	19.47191698
H	5.18709728	0.40855671	20.99338538
O	3.35522100	-1.44799775	21.32196736
N	1.44459838	-2.31488369	23.06958213
C	1.44833025	-2.94945350	24.28450008
C	0.65744136	-2.59510927	25.40134299
C	0.76955504	-3.29369328	26.59568543
C	1.66819996	-4.35523062	26.72204663
C	2.44462472	-4.72987776	25.62386509
C	2.33722970	-4.04206509	24.43158525
H	2.98861969	-4.32590947	23.61190122

H	3.13760591	-5.56427891	25.71821120
C	1.76127678	-5.13620347	27.98412780
F	1.77616782	-4.38650700	29.09434296
F	2.85866738	-5.91272313	28.02317491
F	0.68963903	-5.98462317	28.13653281
H	0.13271976	-3.01654009	27.43528154
H	-0.02731469	-1.76202072	25.36769958
H	2.16851704	-2.62267183	22.43335172
H	-1.05026861	-1.65691303	23.72245620
C	-2.69989519	0.33364326	23.11400132
O	-3.20396766	-0.80421216	23.65604278
C	-4.52764016	-0.71339740	24.18475895
C	-4.82465034	-2.03150529	24.85869552
H	-4.82179501	-2.86396295	24.13648706
H	-5.82821358	-2.00654810	25.30731922
H	-4.10717269	-2.26929198	25.64961647
H	-5.25143235	-0.55701386	23.37386345
H	-4.60758458	0.11120888	24.89408909
O	-3.38075666	1.32933460	22.97847650
H	-2.19636446	2.45623807	21.93417073
H	-3.01891323	4.16782974	20.74584729
H	-3.18787912	5.42383462	18.63356905
C	-1.78742749	5.02293360	16.34951593
F	-1.79727477	4.26348540	15.23641879
F	-2.88485763	5.79339836	16.31919723
F	-0.73249540	5.84232970	16.23487480
H	-0.17924861	2.86418561	16.90090526
C	9.67641451	2.48129077	18.87068519
C	9.56841591	3.17895018	17.66970107
C	8.66701368	4.23300325	17.55054563
C	7.89079960	4.61260024	18.64659494
C	7.99946411	3.92214722	19.84272485
C	8.90023154	2.85387726	19.97624291
H	10.33508349	1.62199484	18.92910507
N	8.89640770	2.18794403	21.21066738
C	9.59710423	1.08146904	21.62881598
C	9.04577104	0.16647718	22.55364626
C	9.78945388	-0.95069997	22.98526613
C	11.07296617	-1.18791265	22.56861428

C	11.63930516	-0.27172771	21.64746741
C	10.90356996	0.81466612	21.19608615
H	11.39073816	1.53163650	20.56211391
C	13.05375640	-0.43056910	21.15107267
O	13.51694984	0.67572992	20.60288706
C	14.88563516	0.61315716	20.07825344
C	15.17458672	1.93716158	19.41017300
H	15.14475947	2.72248190	20.16095833
H	16.16815653	1.86136675	18.97007220
H	14.42332063	2.11281478	18.63325992
H	14.91329414	-0.25542240	19.40179810
H	15.54905254	0.40620644	20.92326650
O	13.71717626	-1.45034802	21.25184848
N	11.80655364	-2.31723396	22.99946325
C	11.81028551	-2.95180377	24.21438120
C	11.01939662	-2.59745954	25.33122411
C	11.13151030	-3.29604355	26.52556655
C	12.03015522	-4.35758089	26.65192775
C	12.80657998	-4.73222803	25.55374621
C	12.69918496	-4.04441536	24.36146637
H	13.35057495	-4.32825974	23.54178234
H	13.49956117	-5.56662918	25.64809232
C	12.12323204	-5.13855374	27.91400892
F	12.13812308	-4.38885727	29.02422408
F	13.22062264	-5.91507340	27.95305603
F	11.05159429	-5.98697344	28.06641393
H	10.49467502	-3.01889036	27.36516266
H	10.33464057	-1.76437099	25.29758070
H	12.53047230	-2.62502210	22.36323284
H	9.31168665	-1.65926330	23.65233732
C	7.66206007	0.33129299	23.04388244
O	7.15798760	-0.80656243	23.58592390
C	5.83431510	-0.71574767	24.11464007
C	5.53730492	-2.03385556	24.78857664
H	5.54016025	-2.86631322	24.06636818
H	4.53374168	-2.00889837	25.23720034
H	6.25478257	-2.27164225	25.57949759
H	5.11052291	-0.55936413	23.30374457
H	5.75437068	0.10885861	24.82397021

O	6.98119860	1.32698433	22.90835762
H	8.16559080	2.45388780	21.86405185
H	7.34304203	4.16547947	20.67572841
H	7.17407614	5.42148435	18.56345017
C	8.57452777	5.02058333	16.27939705
F	8.56468049	4.26113513	15.16629991
F	7.47709763	5.79104809	16.24907835
F	9.62945986	5.83997943	16.16475592
H	10.18270665	2.86183534	16.83078638

Dimer **C** of crystal 2a

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
C	4.50618008	2.94275280	3.28260179
C	4.40520221	2.23791069	4.47404278
C	3.50963091	1.16864623	4.60074884
C	2.72886138	0.80052393	3.50674696
C	2.82910277	1.49159042	2.31617508
C	3.71309277	2.58171678	2.16562789
H	5.18409486	3.77922925	3.24558949
N	3.70116194	3.20223956	0.94718919
C	4.41983931	4.33244726	0.49638339
C	3.83671945	5.23154372	-0.41791129
C	4.56991854	6.31703097	-0.89483818
C	5.89254224	6.56624694	-0.49135871
C	6.46020334	5.65571843	0.43880581
C	5.72664693	4.56276642	0.89656151
H	6.20793171	3.85168044	1.55888815
C	7.87837127	5.81734377	0.90918694
O	8.35536814	4.70701918	1.44564249
C	9.71131988	4.80131991	1.97995224
C	9.99241893	3.49084008	2.64753985
H	9.94883950	2.65372880	1.92941425
H	9.27401728	3.28582149	3.44921752
H	10.98546638	3.50962395	3.07414771
H	9.75912053	5.62321288	2.69097895
H	10.36868056	4.97543895	1.13981693
O	8.51040775	6.83973431	0.77064429
N	6.60468917	7.65397749	-0.92116707
C	6.57422545	8.30791654	-2.15962479
C	5.79485751	7.93159017	-3.25556555
C	5.87682298	8.64708094	-4.45266780
C	6.73587337	9.72636062	-4.57402957
C	7.55190957	10.08531431	-3.48995382
C	7.47035327	9.38197671	-2.30184762
H	8.10390233	9.61918830	-1.45602410

H	8.25330293	10.89910009	-3.57324657
C	6.84265531	10.45995343	-5.88017888
F	5.73356878	10.34657769	-6.63745205
F	7.04598889	11.77135425	-5.69022687
F	7.88388712	10.02746154	-6.61496638
H	5.24490888	8.32845647	-5.28413874
H	5.11670860	7.08178605	-3.20580017
H	7.31479588	7.92923910	-0.25234975
H	4.06326705	7.01279111	-1.54047321
C	2.43334529	5.05959084	-0.88357642
O	1.95072617	6.16996822	-1.44216367
C	0.60968194	6.08738970	-1.94624516
C	0.30884541	7.40383491	-2.62185205
H	-0.69477167	7.31949673	-3.03895157
H	0.33396573	8.20546173	-1.88978452
H	1.02103559	7.55718793	-3.43138651
H	-0.06274866	5.87182008	-1.11596039
H	0.53664277	5.23744532	-2.64663679
O	1.76211464	4.04074273	-0.79628088
H	2.96744852	2.89166384	0.32408411
H	2.17931637	1.22069483	1.48768637
H	2.02854137	-0.03054556	3.59677479
C	3.42405182	0.37986038	5.86002890
F	3.39434393	1.12963145	6.96573291
F	2.31211762	-0.40225971	5.90303912
F	4.48185010	-0.46102065	6.01178709
H	5.03828171	2.52135365	5.31060477
C	5.81922706	8.37668878	7.80448988
C	5.90745146	7.66236503	6.61859222
C	6.76246743	6.56744865	6.48804655
C	7.57986029	6.21304453	7.57004255
C	7.50397051	6.91505001	8.75483958
C	6.61702128	8.01694643	8.91812777
H	5.12041593	9.19642334	7.82902950
N	6.62971715	8.64269059	10.12743422
C	5.89162788	9.76501547	10.58155281
C	6.47416897	10.67227472	11.50425508
C	5.74724222	11.74989869	11.97919777
C	4.42212787	12.02575264	11.56346565

C	3.86217581	11.12285926	10.62383445
C	4.59050561	10.00177850	10.18252636
H	4.10125551	9.29142753	9.51933430
C	2.47001694	11.29119860	10.16167586
O	1.96362373	10.14925115	9.65053723
C	0.64611469	10.23886089	9.11059716
C	0.35189247	8.92392526	8.43562066
H	-0.64490916	8.94501125	7.99656405
H	0.37865190	8.07936727	9.13790914
H	1.05050082	8.71284423	7.62316853
H	-0.07228324	10.39412280	9.90431046
H	0.57012281	11.06585202	8.39072665
O	1.79833857	12.29590448	10.27909486
N	3.72837254	13.11714589	12.00867461
C	3.75466648	13.78675270	13.25494398
C	4.53264390	13.40326291	14.35044403
C	4.44321069	14.11178884	15.54848553
C	3.57232811	15.18920915	15.66651029
C	2.76344514	15.55454102	14.58736474
C	2.85614674	14.85379057	13.39385942
H	2.20989643	15.10192581	12.55135474
H	2.04603337	16.36684994	14.65784028
C	3.46178467	15.92566708	16.97216867
F	4.57878667	15.79351927	17.70198041
F	3.26489808	17.23592100	16.77538917
F	2.43627806	15.47377488	17.71196793
H	5.05864677	13.79418990	16.38291388
H	5.19371625	12.54583979	14.28881909
H	3.00125116	13.40720773	11.36083151
H	6.25127730	12.46526580	12.60430488
C	7.89445998	10.49788885	11.98027532
O	8.36223008	11.60553073	12.52122116
C	9.72461751	11.53845531	13.05303892
C	10.00586756	12.85953779	13.73011184
H	9.95395690	13.64469881	12.97115732
H	9.27000073	13.02634099	14.51578673
H	11.00524309	12.80788679	14.13325487
H	9.75254558	10.65980923	13.71472793
H	10.36785969	11.35227513	12.19779817

O	8.52656264	9.45585556	11.93824253
H	7.32974682	8.27757301	10.75953995
H	8.15847514	6.60771781	9.56373199
H	8.27326574	5.37438869	7.46934237
C	6.88555133	5.84440704	5.19475069
F	5.76547855	5.96440671	4.41725667
F	7.08517195	4.51069188	5.34214662
F	7.88996241	6.28086211	4.41160118
H	5.27673674	7.93722305	5.77488336

Dimer **A** of crystal 2b

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
C	1.82844588	1.84119776	0.48303972
C	1.65028816	2.36198267	-0.89770812
C	1.10372146	1.53228685	-1.86003546
C	1.04554317	1.96478718	-3.18095294
C	1.53111593	3.22705139	-3.52766714
C	2.04350130	4.07331463	-2.53767104
C	2.11343494	3.64398028	-1.21861396
H	2.52829306	4.32424623	-0.46482504
H	2.40413384	5.07177512	-2.76583092
N	1.45585481	3.72454158	-4.85209540
C	1.62663511	3.01823080	-6.00388214
C	1.27638561	3.52359959	-7.29431084
C	1.49296165	2.78698867	-8.45873169
C	2.11835836	1.54157052	-8.42977370
C	2.45983810	1.02862596	-7.16760917
C	2.24205623	1.75220248	-6.00917713
H	2.57847249	1.32138230	-5.08879002
C	3.08020996	-0.32690383	-7.07271280
O	3.52719474	-0.59505668	-5.85461950
C	4.08932201	-1.91887686	-5.63684434
C	4.53239250	-1.98006395	-4.19513572
H	3.67311824	-1.86819753	-3.52401524
H	4.92404240	-2.98698351	-4.01490341
H	5.29907564	-1.24423086	-3.99230815
H	3.31719309	-2.66868961	-5.86735454
H	4.91185205	-2.07023778	-6.34201685
O	3.20216469	-1.10643858	-7.99938070
N	2.35753191	0.82345169	-9.60594594
C	2.23842229	1.30832796	-10.88784734
C	2.69629475	2.59017070	-11.29521972
C	2.65690973	3.07603509	-12.59503417
C	2.11049592	2.24365959	-13.55080241
C	1.88264819	2.66534340	-15.00951510

F	2.77699928	3.42300780	-15.27083976
F	1.89224020	1.76080191	-15.74876824
F	0.83454275	3.22399428	-15.03448158
C	1.67790652	1.01188719	-13.19551253
C	1.74780322	0.46739502	-11.91516792
H	1.32012292	-0.53701956	-11.73016147
H	1.63648022	0.56928976	-14.18085182
H	3.04235252	4.07848616	-12.83967664
H	3.03582139	3.22918048	-10.50700484
H	2.40887709	-0.19490321	-9.55087588
H	1.11545980	3.16413370	-9.39159367
C	0.64743869	4.85749522	-7.41147301
O	0.23055428	5.14677398	-8.65105650
C	-0.35137525	6.45484791	-8.83991392
C	-0.79071604	6.52550037	-10.27780562
H	0.04850125	6.37024031	-10.95974678
H	-1.21864106	7.50937790	-10.47726610
H	-1.55753812	5.77422960	-10.48959570
H	0.40202685	7.21185890	-8.61495086
H	-1.20320811	6.57344881	-8.16209229
O	0.55959772	5.67239232	-6.50721682
H	1.20270642	4.69679117	-4.93780700
H	0.67305888	1.30498920	-3.97012397
H	0.72088227	0.53802094	-1.61360522
F	0.85136255	0.98266004	0.84363914
F	1.85564524	2.83656400	1.34588694
F	2.99331486	1.17049697	0.60415649
C	5.87254260	2.75381054	0.62167182
C	5.79011064	2.97914645	-0.85110224
C	5.33025257	1.99079767	-1.69096305
C	5.23167613	2.24805911	-3.05522224
C	5.61975291	3.49051329	-3.55072006
C	6.04693223	4.50264321	-2.68082493
C	6.11023642	4.25902996	-1.32071253
H	6.34172589	5.07623265	-0.63489063
H	6.27351850	5.49538882	-3.05126714
N	5.49259679	3.85768229	-4.91382178
C	5.64781633	3.08788991	-6.00915421
C	5.24164630	3.55864745	-7.28926896

C	5.45943292	2.78101568	-8.42816256
C	6.08496368	1.53456074	-8.36780236
C	6.47795205	1.05364742	-7.09958296
C	6.26774589	1.81208220	-5.96136269
H	6.58976071	1.40557242	-5.02119619
C	7.11301548	-0.30513420	-6.95331326
O	7.57810290	-0.53868513	-5.73280272
C	8.15076609	-1.85776532	-5.50055333
C	8.60117657	-1.90678884	-4.06058723
H	7.74792967	-1.77264366	-3.39554532
H	8.97963255	-2.91975150	-3.88264941
H	9.38585589	-1.18166463	-3.87405820
H	7.38353550	-2.61800863	-5.71854197
H	8.96838464	-2.01573309	-6.21039363
O	7.23172115	-1.12686824	-7.84613998
N	6.28726423	0.74891162	-9.51488989
C	6.13556020	1.09021333	-10.82853366
C	6.48362867	2.34682615	-11.37649600
C	6.39606114	2.59281022	-12.73595509
C	5.97120161	1.61136345	-13.62628746
C	5.86707423	1.82249568	-15.07571254
F	6.72532609	1.40396715	-15.59630014
F	5.80309049	2.92799963	-15.24809413
F	4.86444606	1.32189352	-15.39097672
C	5.60144044	0.37654622	-13.08838436
C	5.68553522	0.10776763	-11.72642176
H	5.42159073	-0.88919337	-11.36437612
H	5.27428387	-0.47426772	-13.72395340
H	6.70173407	3.58778137	-13.07596345
H	6.87157557	3.09269161	-10.69891521
H	6.40088199	-0.24742874	-9.31657540
H	5.09697912	3.14611254	-9.37187964
C	4.60697171	4.89730243	-7.43806181
O	4.16487438	5.15322716	-8.68557326
C	3.57731833	6.45840327	-8.88455416
C	3.12355997	6.51398454	-10.31920599
H	3.96425656	6.33847362	-11.00532891
H	2.71537977	7.50460214	-10.52840499
H	2.34649532	5.77305713	-10.51181299

H	4.32636781	7.22304206	-8.66956939
H	2.73179969	6.57856207	-8.20272054
O	4.51791276	5.74893120	-6.56951252
H	5.21664922	4.81111223	-5.09168089
H	4.81720831	1.48832137	-3.71757564
H	4.99519806	1.02621034	-1.32453440
F	4.82414211	3.30404302	1.23528950
F	5.91900429	1.45240710	0.95793697
F	6.97525920	3.33048837	1.08655386

Dimer **B** of crystal 2b

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
C	1.82844588	1.84119776	0.48303972
C	1.65028816	2.36198267	-0.89770812
C	1.10372146	1.53228685	-1.86003546
C	1.04554317	1.96478718	-3.18095294
C	1.53111593	3.22705139	-3.52766714
C	2.04350130	4.07331463	-2.53767104
C	2.11343494	3.64398028	-1.21861396
H	2.52829306	4.32424623	-0.46482504
H	2.40413384	5.07177512	-2.76583092
N	1.45585481	3.72454158	-4.85209540
C	1.62663511	3.01823080	-6.00388214
C	1.27638561	3.52359959	-7.29431084
C	1.49296165	2.78698867	-8.45873169
C	2.11835836	1.54157052	-8.42977370
C	2.45983810	1.02862596	-7.16760917
C	2.24205623	1.75220248	-6.00917713
H	2.57847249	1.32138230	-5.08879002
C	3.08020996	-0.32690383	-7.07271280
O	3.52719474	-0.59505668	-5.85461950
C	4.08932201	-1.91887686	-5.63684434
C	4.53239250	-1.98006395	-4.19513572
H	3.67311824	-1.86819753	-3.52401524
H	4.92404240	-2.98698351	-4.01490341
H	5.29907564	-1.24423086	-3.99230815
H	3.31719309	-2.66868961	-5.86735454
H	4.91185205	-2.07023778	-6.34201685
O	3.20216469	-1.10643858	-7.99938070
N	2.35753191	0.82345169	-9.60594594
C	2.23842229	1.30832796	-10.88784734
C	2.69629475	2.59017070	-11.29521972
C	2.65690973	3.07603509	-12.59503417
C	2.11049592	2.24365959	-13.55080241
C	1.88264819	2.66534340	-15.00951510

F	2.77699928	3.42300780	-15.27083976
F	1.89224020	1.76080191	-15.74876824
F	0.83454275	3.22399428	-15.03448158
C	1.67790652	1.01188719	-13.19551253
C	1.74780322	0.46739502	-11.91516792
H	1.32012292	-0.53701956	-11.73016147
H	1.63648022	0.56928976	-14.18085182
H	3.04235252	4.07848616	-12.83967664
H	3.03582139	3.22918048	-10.50700484
H	2.40887709	-0.19490321	-9.55087588
H	1.11545980	3.16413370	-9.39159367
C	0.64743869	4.85749522	-7.41147301
O	0.23055428	5.14677398	-8.65105650
C	-0.35137525	6.45484791	-8.83991392
C	-0.79071604	6.52550037	-10.27780562
H	0.04850125	6.37024031	-10.95974678
H	-1.21864106	7.50937790	-10.47726610
H	-1.55753812	5.77422960	-10.48959570
H	0.40202685	7.21185890	-8.61495086
H	-1.20320811	6.57344881	-8.16209229
O	0.55959772	5.67239232	-6.50721682
H	1.20270642	4.69679117	-4.93780700
H	0.67305888	1.30498920	-3.97012397
H	0.72088227	0.53802094	-1.61360522
F	0.85136255	0.98266004	0.84363914
F	1.85564524	2.83656400	1.34588694
F	2.99331486	1.17049697	0.60415649
C	-3.29368870	13.08888596	0.50194301
C	-3.37612066	13.31422187	-0.97083105
C	-3.83597873	12.32587309	-1.81069186
C	-3.93455517	12.58313453	-3.17495105
C	-3.54647839	13.82558871	-3.67044887
C	-3.11929907	14.83771863	-2.80055374
C	-3.05599488	14.59410538	-1.44044134
H	-2.82450541	15.41130807	-0.75461944
H	-2.89271280	15.83046424	-3.17099595
N	-3.67363451	14.19275771	-5.03355059
C	-3.51841497	13.42296533	-6.12888302
C	-3.92458500	13.89372287	-7.40899777

C	-3.70679838	13.11609110	-8.54789137
C	-3.08126762	11.86963616	-8.48753117
C	-2.68827925	11.38872284	-7.21931177
C	-2.89848541	12.14715762	-6.08109150
H	-2.57647059	11.74064784	-5.14092500
C	-2.05321582	10.02994122	-7.07304207
O	-1.58812840	9.79639029	-5.85253153
C	-1.01546521	8.47731010	-5.62028214
C	-0.56505473	8.42828658	-4.18031604
H	-1.41830163	8.56243176	-3.51527413
H	-0.18659875	7.41532392	-4.00237822
H	0.21962459	9.15341079	-3.99378701
H	-1.78269580	7.71706679	-5.83827078
H	-0.19784666	8.31934233	-6.33012244
O	-1.93451015	9.20820718	-7.96586879
N	-2.87896707	11.08398704	-9.63461870
C	-3.03067110	11.42528875	-10.94826247
C	-2.68260263	12.68190157	-11.49622481
C	-2.77017016	12.92788564	-12.85568390
C	-3.19502969	11.94643887	-13.74601627
C	-3.29915707	12.15757110	-15.19544135
F	-2.44090521	11.73904257	-15.71602895
F	-3.36314081	13.26307505	-15.36782294
F	-4.30178524	11.65696894	-15.51070553
C	-3.56479086	10.71162164	-13.20811317
C	-3.48069608	10.44284305	-11.84615057
H	-3.74464057	9.44588205	-11.48410493
H	-3.89194743	9.86080770	-13.84368221
H	-2.46449723	13.92285679	-13.19569226
H	-2.29465573	13.42776703	-10.81864402
H	-2.76534931	10.08764668	-9.43630421
H	-4.06925218	13.48118796	-9.49160845
C	-4.55925959	15.23237785	-7.55779062
O	-5.00135692	15.48830258	-8.80530207
C	-5.58891297	16.79347869	-9.00428297
C	-6.04267133	16.84905996	-10.43893480
H	-5.20197474	16.67354904	-11.12505772
H	-6.45085153	17.83967756	-10.64813380
H	-6.81973598	16.10813255	-10.63154180

H	-4.83986349	17.55811748	-8.78929820
H	-6.43443161	16.91363749	-8.32244935
O	-4.64831854	16.08400662	-6.68924133
H	-3.94958208	15.14618765	-5.21140970
H	-4.34902299	11.82339679	-3.83730445
H	-4.17103324	11.36128576	-1.44426321
F	-4.34208919	13.63911844	1.11556069
F	-3.24722701	11.78748252	0.83820816
F	-2.19097210	13.66556379	0.96682505

Dimer **C** of crystal 2b

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
C	1.82844588	1.84119776	0.48303972
C	1.65028816	2.36198267	-0.89770812
C	1.10372146	1.53228685	-1.86003546
C	1.04554317	1.96478718	-3.18095294
C	1.53111593	3.22705139	-3.52766714
C	2.04350130	4.07331463	-2.53767104
C	2.11343494	3.64398028	-1.21861396
H	2.52829306	4.32424623	-0.46482504
H	2.40413384	5.07177512	-2.76583092
N	1.45585481	3.72454158	-4.85209540
C	1.62663511	3.01823080	-6.00388214
C	1.27638561	3.52359959	-7.29431084
C	1.49296165	2.78698867	-8.45873169
C	2.11835836	1.54157052	-8.42977370
C	2.45983810	1.02862596	-7.16760917
C	2.24205623	1.75220248	-6.00917713
H	2.57847249	1.32138230	-5.08879002
C	3.08020996	-0.32690383	-7.07271280
O	3.52719474	-0.59505668	-5.85461950
C	4.08932201	-1.91887686	-5.63684434
C	4.53239250	-1.98006395	-4.19513572
H	3.67311824	-1.86819753	-3.52401524
H	4.92404240	-2.98698351	-4.01490341
H	5.29907564	-1.24423086	-3.99230815
H	3.31719309	-2.66868961	-5.86735454
H	4.91185205	-2.07023778	-6.34201685
O	3.20216469	-1.10643858	-7.99938070
N	2.35753191	0.82345169	-9.60594594
C	2.23842229	1.30832796	-10.88784734
C	2.69629475	2.59017070	-11.29521972
C	2.65690973	3.07603509	-12.59503417
C	2.11049592	2.24365959	-13.55080241
C	1.88264819	2.66534340	-15.00951510

F	2.77699928	3.42300780	-15.27083976
F	1.89224020	1.76080191	-15.74876824
F	0.83454275	3.22399428	-15.03448158
C	1.67790652	1.01188719	-13.19551253
C	1.74780322	0.46739502	-11.91516792
H	1.32012292	-0.53701956	-11.73016147
H	1.63648022	0.56928976	-14.18085182
H	3.04235252	4.07848616	-12.83967664
H	3.03582139	3.22918048	-10.50700484
H	2.40887709	-0.19490321	-9.55087588
H	1.11545980	3.16413370	-9.39159367
C	0.64743869	4.85749522	-7.41147301
O	0.23055428	5.14677398	-8.65105650
C	-0.35137525	6.45484791	-8.83991392
C	-0.79071604	6.52550037	-10.27780562
H	0.04850125	6.37024031	-10.95974678
H	-1.21864106	7.50937790	-10.47726610
H	-1.55753812	5.77422960	-10.48959570
H	0.40202685	7.21185890	-8.61495086
H	-1.20320811	6.57344881	-8.16209229
O	0.55959772	5.67239232	-6.50721682
H	1.20270642	4.69679117	-4.93780700
H	0.67305888	1.30498920	-3.97012397
H	0.72088227	0.53802094	-1.61360522
F	0.85136255	0.98266004	0.84363914
F	1.85564524	2.83656400	1.34588694
F	2.99331486	1.17049697	0.60415649
C	1.55576701	7.37491716	-13.94934426
C	1.47333505	7.60025307	-15.42211832
C	1.01347698	6.61190429	-16.26197913
C	0.91490054	6.86916573	-17.62623832
C	1.30297732	8.11161991	-18.12173614
C	1.73015664	9.12374983	-17.25184101
C	1.79346083	8.88013658	-15.89172861
H	2.02495030	9.69733927	-15.20590671
H	1.95674291	10.11649544	-17.62228322
N	1.17582120	8.47878891	-19.48483786
C	1.33104074	7.70899653	-20.58017029
C	0.92487071	8.17975407	-21.86028504

C	1.14265733	7.40212230	-22.99917864
C	1.76818809	6.15566736	-22.93881844
C	2.16117646	5.67475404	-21.67059904
C	1.95097030	6.43318882	-20.53237877
H	2.27298512	6.02667904	-19.59221227
C	2.79623989	4.31597242	-21.52432934
O	3.26132731	4.08242149	-20.30381880
C	3.83399050	2.76334130	-20.07156941
C	4.28440098	2.71431778	-18.63160331
H	3.43115408	2.84846296	-17.96656140
H	4.66285696	1.70135512	-18.45366549
H	5.06908030	3.43944199	-18.44507428
H	3.06675991	2.00309799	-20.28955805
H	4.65160905	2.60537353	-20.78140971
O	2.91494556	3.49423838	-22.41715606
N	1.97048864	5.37001824	-24.08590597
C	1.81878461	5.71131995	-25.39954974
C	2.16685308	6.96793277	-25.94751208
C	2.07928555	7.21391684	-27.30697117
C	1.65442602	6.23247007	-28.19730354
C	1.55029864	6.44360230	-29.64672862
F	2.40855050	6.02507377	-30.16731622
F	1.48631490	7.54910625	-29.81911021
F	0.54767047	5.94300014	-29.96199280
C	1.28466485	4.99765284	-27.65940044
C	1.36875963	4.72887425	-26.29743784
H	1.10481514	3.73191325	-25.93539220
H	0.95750828	4.14683890	-28.29496948
H	2.38495848	8.20888799	-27.64697953
H	2.55479998	7.71379823	-25.26993129
H	2.08410640	4.37367788	-23.88759148
H	0.78020353	7.76721916	-23.94289572
C	0.29019612	9.51840905	-22.00907789
O	-0.15190121	9.77433378	-23.25658934
C	-0.73945726	11.07950989	-23.45557024
C	-1.19321562	11.13509116	-24.89022207
H	-0.35251903	10.95958024	-25.57634499
H	-1.60139582	12.12570876	-25.09942107
H	-1.97028027	10.39416375	-25.08282907

H	0.00959222	11.84414868	-23.24058547
H	-1.58497590	11.19966869	-22.77373662
O	0.20113717	10.37003782	-21.14052860
H	0.89987363	9.43221885	-19.66269697
H	0.50043272	6.10942799	-18.28859172
H	0.67842247	5.64731696	-15.89555048
F	0.50736652	7.92514964	-13.33572658
F	1.60222870	6.07351372	-13.61307911
F	2.65848361	7.95159499	-13.48446222

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