Supporting Information

A New Paradigm for the Supramolecular Structure of Laterally Offset Diarenes: Crystal Structures and Stabilities of Polymorphs II of Para-Substituted Acetophenone Azines, Y_p−Ph−(Me)C=N−N=C(Me)−Ph−Y_p (Y = Cl, Br, CH_3)

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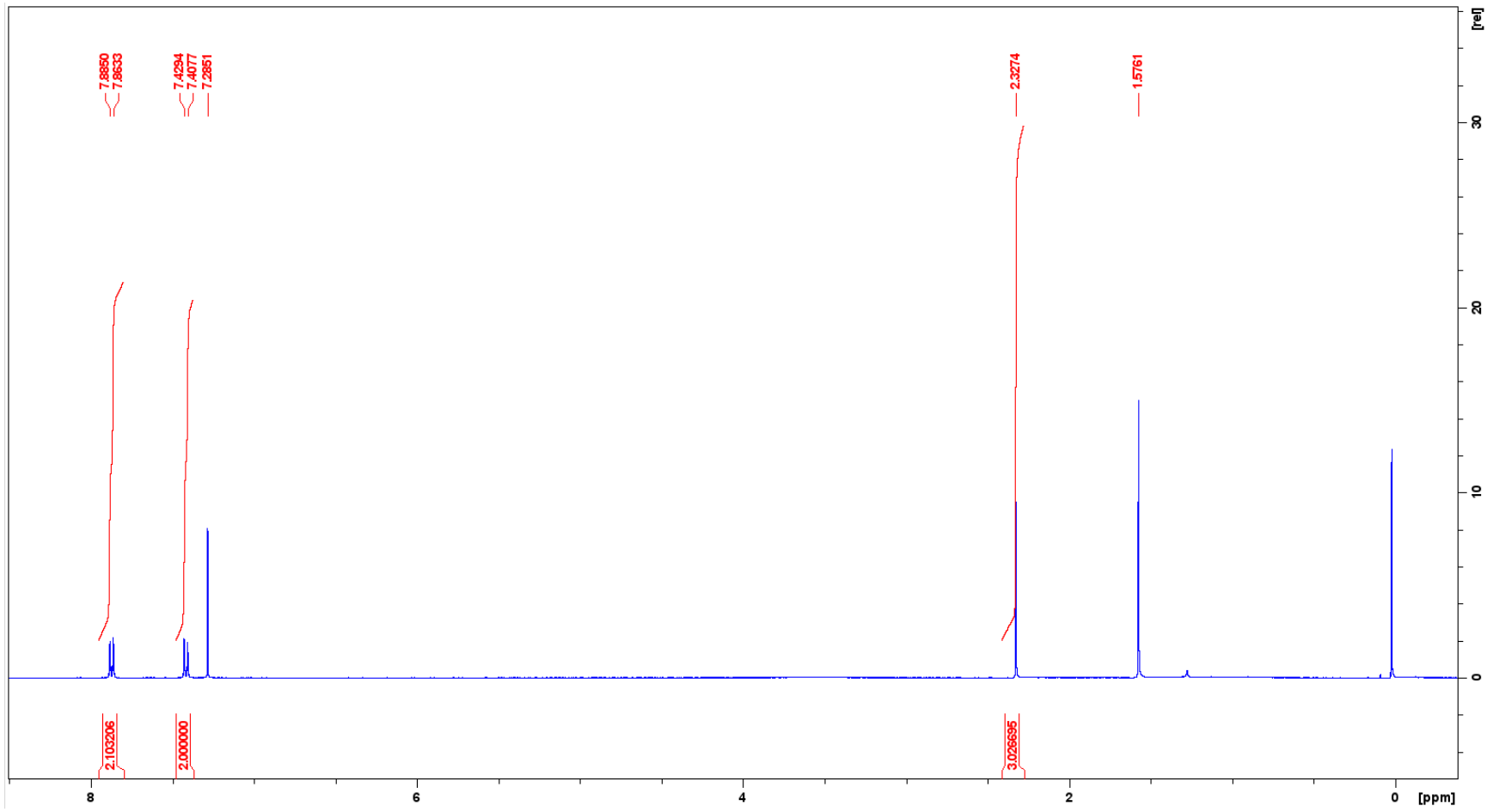

Figure S1. ^{1}H NMR spectra of 1M

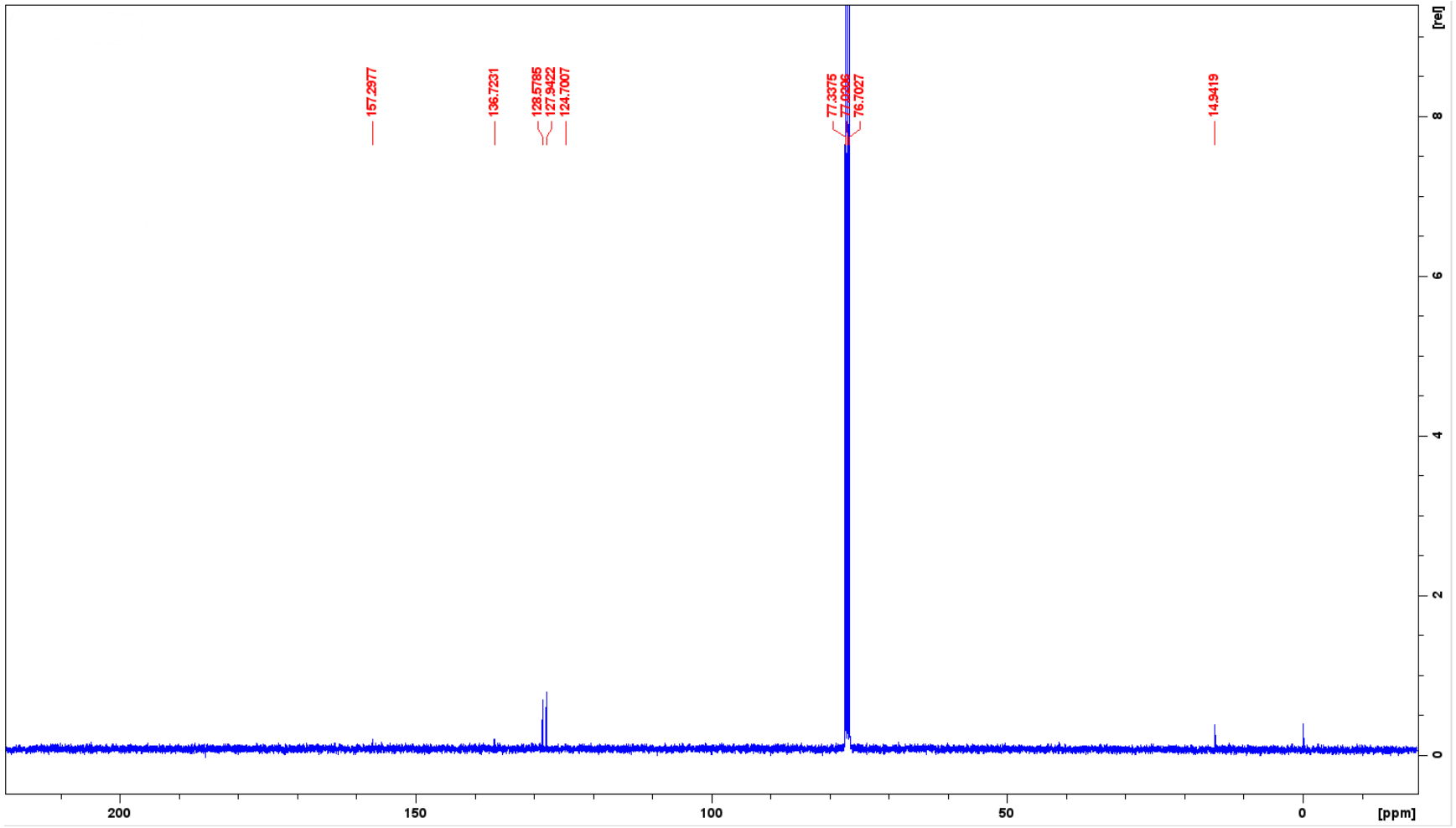

Figure S2. ^{13}C NMR spectra of 1M

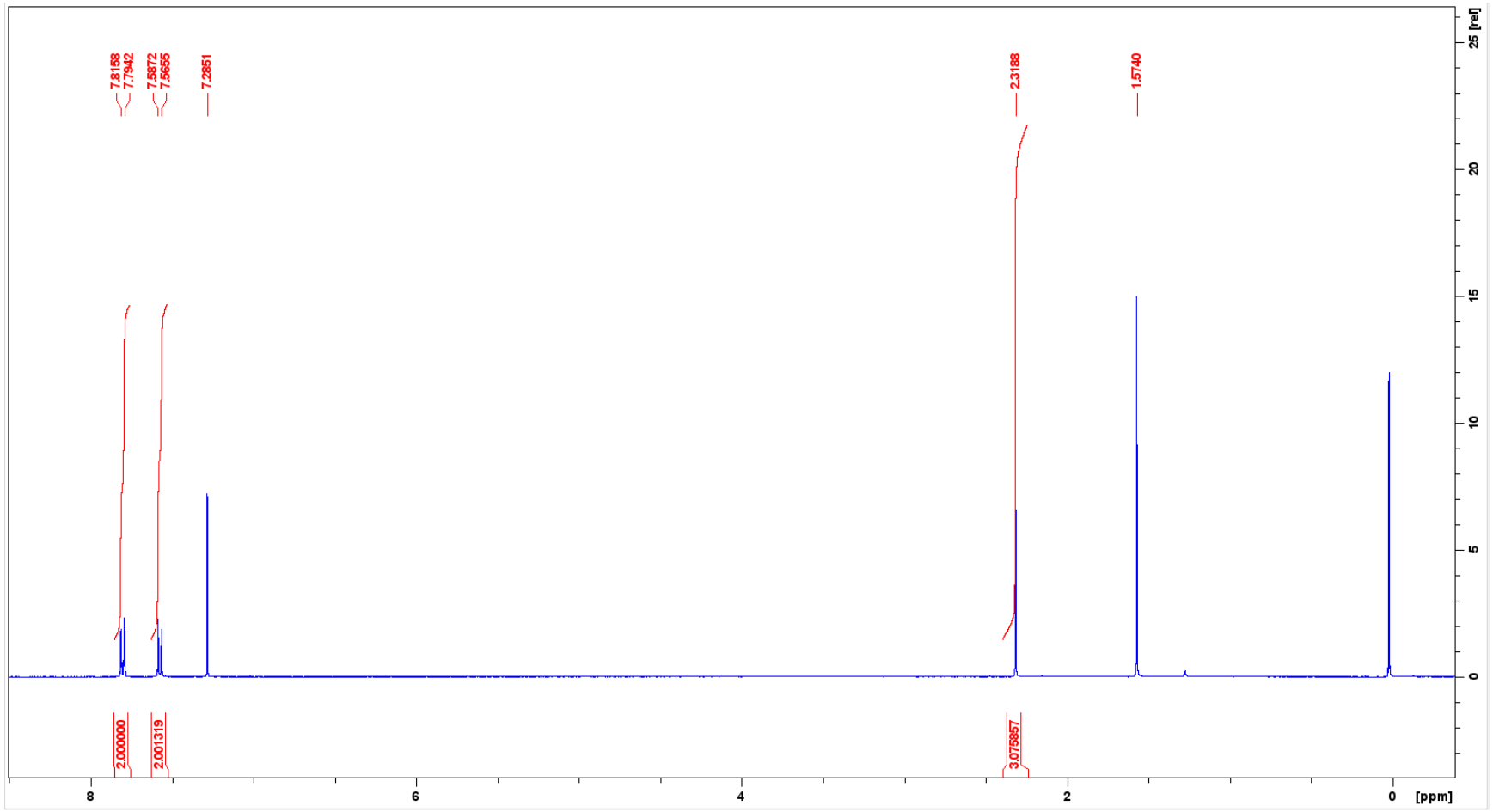

Figure S3. ^{1}H NMR spectra of 2M

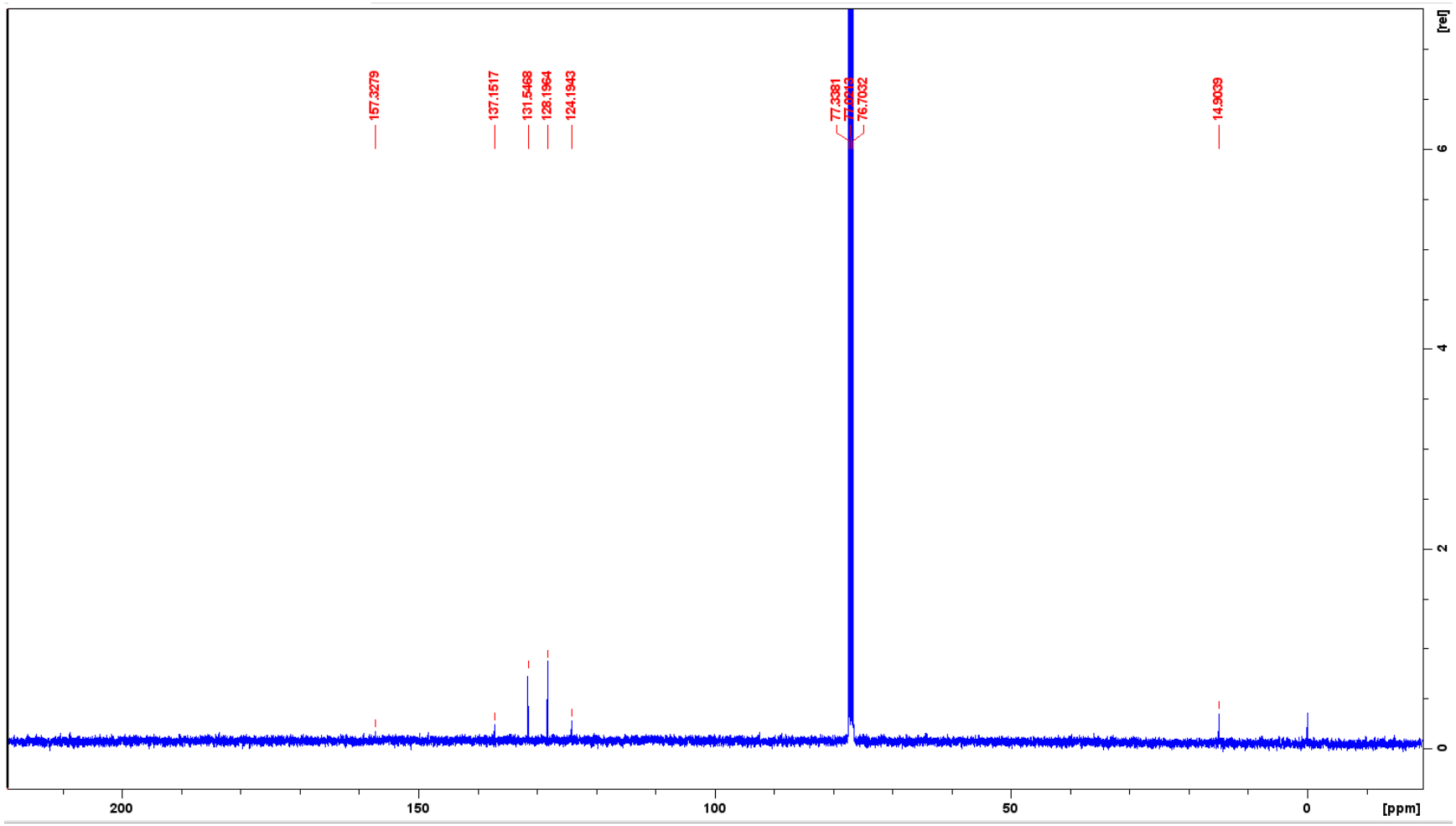

Figure S4. ^{13}C NMR spectra of 2M

Table S1. Selected Structural Parameters (Å, °) of Azine 1M

Parameter	SCXRD		APFD/6-311G*		MP2(full)/6-311G*		
	1M-Ia	**1M-II**	C_2-**1M** M	C_{2h}-**1M** TS	C_2-**1M** M	C_{2h}-**1M** SOSP	C_i-**1M** "TS"
N1–N2	1.40	1.41	1.35	1.37	1.37	1.38	1.39
N1–C1	1.29	1.29	1.29	1.29	1.30	1.30	1.30
N2–C9	1.28	1.29	1.29	1.29	1.30	1.30	1.30
C1–C2	1.48	1.49	1.48	1.48	1.48	1.48	1.48
C1–C8/C1–H	1.49	1.50	1.50	1.50	1.50	1.50	1.50
C9–C10	1.48	1.49	1.48	1.48	1.48	1.48	1.48
C9–C16/C9–H	1.50	1.50	1.50	1.50	1.50	1.50	1.50
C5–Cl1	1.74	1.74	1.74	1.73	1.73	1.73	1.73
C13–Cl2	1.74	1.74	1.74	1.73	1.73	1.73	1.73
N2–N1–C1	115.26	113.77	117.72	115.42	115.79	114.25	113.78
N1–N2–C9	115.75	113.77	117.72	115.42	115.79	114.25	113.78
N1–C1–C2	115.71	115.48	116.76	116.34	116.21	115.87	115.64
N1–C1–C8/N1–C1–H	124.45	126.32	123.55	124.86	123.60	125.20	125.40
C2–C1–C8/ C2–C1–H	119.84	118.19	119.69	118.80	120.19	118.93	118.96
C1–C2–C3	121.22	120.53	121.20	121.35	120.94	121.06	120.96
C10–C9–C16/ C10–C9–H	119.67	118.19	119.69	118.80	120.19	118.93	118.96
C9–C10–C11	121.33	120.53	121.20	121.35	120.94	121.06	120.96
N2–C9–C10	116.33	115.48	116.76	116.34	116.21	115.87	115.64
N2–C9–C16/ N2–C9–H	124.00	126.32	123.55	124.86	123.60	125.20	125.40
C1–N1–N2–C9 = τ	134.70	180.00	134.71	180.00	126.69	180.00	180.00
C7−C2−C1=N1 = ϕ_1	29.31	26.39	-15.60	-0.19	-21.91	0.00	-19.44
C15−C10−C9=N2 = ϕ_2	30.53	-26.39	-15.58	-0.19	-21.91	0.00	19.44
N1–N2–C9–C16/N1–N2–C9–H	-4.5	0.84	-6.03	-0.00	-5.25	0.00	0.47
N2–N1–C1–C8/N2–N1–C1–H	-4.4	-0.84	-6.03	0.00	-5.25	0.00	-0.47
N2–N1–C1–C2	176.20	-179.67	174.70	179.98	175.14	180.00	179.83
N1–N2–C9–C10	176.00	179.67	174.70	180.00	175.14	180.00	-179.83

Selected structural parameters (Å, °) of azines **1**(Me, Cl, Cl) in crystal **I** and **II**. Data from crystal structure determinations and computations of the free azines **1**(Me, Cl, Cl) at the APFD and MP2 levels.

Table S2. Selected Structural Parameters (Å, °) of Azine 2M

Parameter	SCXRD		APFD/6-311G*		MP2(full)/6-311G*		
	2M-Ic	**2M-II**	C_2-**2M** M	C_{2h}-**2M** TS	C_2-**2M** M	C_{2h}-**2M** SOSP	C_i-**2M** "TS"
N1–N2	1.39	1.47	1.35	1.37	1.37	1.38	1.39
N1–C1	1.28	1.29	1.29	1.29	1.30	1.30	1.30
N2–C9	1.28	1.29	1.29	1.29	1.30	1.30	1.30
C1–C2	1.48	1.49	1.48	1.48	1.48	1.48	1.48
C1–C8/C1–H	1.50	1.50	1.50	1.50	1.50	1.50	1.50
C9–C10	1.48	1.49	1.48	1.48	1.48	1.48	1.48
C9–C16/C9–H	1.50	1.50	1.50	1.50	1.50	1.50	1.50
C5–Br1	1.90	1.90	1.90	1.90	1.89	1.89	1.89
C13–Br2	1.90	1.90	1.90	1.90	1.89	1.89	1.89
N2–N1–C1	115.21	113.76	117.92	115.43	115.80	114.24	113.80
N1–N2–C9	116.18	113.76	117.92	115.43	115.80	114.24	113.80
N1–C1–C2	116.00	115.52	116.77	116.31	116.19	115.85	115.62
N1–C1–C8/N1–C1–H	125.03	126.07	123.49	124.87	123.60	125.21	125.43
C2–C1–C8/ C2–C1–H	118.98	118.39	119.73	118.81	120.20	118.95	118.96
C1–C2–C3	121.42	120.85	121.18	121.35	116.19	121.05	120.95
C10–C9–C16/ C10–C9–H	119.35	118.39	119.73	118.81	120.20	118.95	118.96
C9–C10–C11	121.43	120.85	121.18	121.35	116.19	121.05	120.95
N2–C9–C10	115.78	115.52	116.77	116.31	116.19	115.85	115.62
N2–C9–C16/ N2–C9–H	124.86	126.07	123.49	124.87	123.60	125.21	125.43
C1–N1–N2–C9 = τ	131.85	180.00	132.06	180.00	126.40	180.00	180.00
C7−C2−C1=N1 = ϕ_1	29.19	26.33	-15.74	0.00	22.51	0.00	19.84
C15−C10−C9=N2 = ϕ_2	29.70	-26.33	-15.74	0.00	-22.51	0.00	-19.84
N1–N2–C9–C16/N1–N2–C9–H	4.72	-1.07	-5.97	0.00	-5.25	0.00	-0.44
N2–N1–C1–C8/N2–N1–C1–H	4.99	1.07	-5.97	0.00	-5.25	0.00	0.44
N2–N1–C1–C2	-174.72	179.62	174.72	180.00	175.14	180.00	179.86
N1–N2–C9–C10	-176.10	-179.62	174.72	180.00	175.14	180.00	-179.86

Selected structural parameters (Å, °) of azines **2**(Me,Br, Br) in crystal **Ic** and **II**. Data from crystal structure determinations and computations of the free azines **2**(Me, Br, Br) at the APFD and MP2 levels.

Table S3. Selected Structural Parameters (Å, °) of Azine 8M

Parameter	SCXRD		APFD/6-311G*		MP2(full)/6-311G*		
	8M-I	**8M-II**	C_2-**8M** M	C_{2h}-**8M** TS	C_2-**8M** M	C_{2h}-**8M** FOSP	C_i-**8M** M
N1–N2	1.41	1.40	1.35	1.37	1.38	1.38	1.39
N1–C1	1.28	1.28	1.29	1.29	1.30	1.30	1.30
N2–C9	1.28	1.28	1.29	1.29	1.30	1.30	1.30
C1–C2	1.48	1.48	1.48	1.48	1.48	1.48	1.48
C1–C8/C1–H	1.50	1.49	1.50	1.50	1.50	1.50	1.50
C9–C10	1.48	1.48	1.48	1.48	1.48	1.48	1.48
C9–C16/C9–H	1.50	1.49	1.50	1.50	1.50	1.50	1.50
C5–C17	1.52	1.51	1.50	1.50	1.51	1.50	1.50
C13–Cl8	1.52	1.51	1.50	1.50	1.51	1.50	1.50
N2–N1–C1	114.16	114.09	117.76	115.45	115.74	114.32	113.80
N1–N2–C9	114.16	114.09	117.76	115.45	115.74	114.32	113.80
N1–C1–C2	116.55	116.02	117.00	116.56	116.40	116.03	115.80
N1–C1–C8/N1–C1–H	123.51	124.88	123.34	124.69	123.43	125.07	125.25
C2–C1–C8/ C2–C1–H	119.94	119.10	119.65	118.76	120.17	118.90	118.93
C1–C2–C3	121.19	121.27	121.33	121.49	121.01	116.03	121.04
C10–C9–C16/ C10–C9–H	119.94	119.10	119.65	118.76	120.17	125.07	118.93
C9–C10–C11	121.19	121.27	121.33	121.49	121.01	116.03	121.04
N2–C9–C10	116.55	116.02	117.00	116.56	116.40	116.03	115.80
N2–C9–C16/ N2–C9–H	123.51	124.88	123.34	124.69	123.43	125.07	125.25
C1–N1–N2–C9 = τ	142.76	180.00	133.46	180.00	126.34	180.00	180.00
C7−C2−C1=N1 = ϕ_1	-19.89	-23.75	-15.47	0.00	-22.66	0.00	20.26
C15−C10−C9=N2 = ϕ_2	0.45	23.75	-15.47	0.00	-22.66	0.00	-20.26
N1–N2–C9–C16/N1–N2–C9–H	-2.52	0.57	-5.90	0.00	-5.18	0.00	0.49
N2–N1–C1–C8/N2–N1–C1–H	-3.62	-0.57	-5.90	0.00	-5.18	0.00	-0.49
N2–N1–C1–C2	176.74	-179.83	174.80	180.00	175.22	180.00	179.83
N1–N2–C9–C10	178.21	179.83	174.80	180.00	175.22	180.00	-179.83

Selected structural parameters (Å, °) of azine **8**(Me, Me, Me) in crystal I and II. Data from crystal structure determinations and computations of the free azines **8**(Me, Me, Me) at the APFD and MP2 levels.

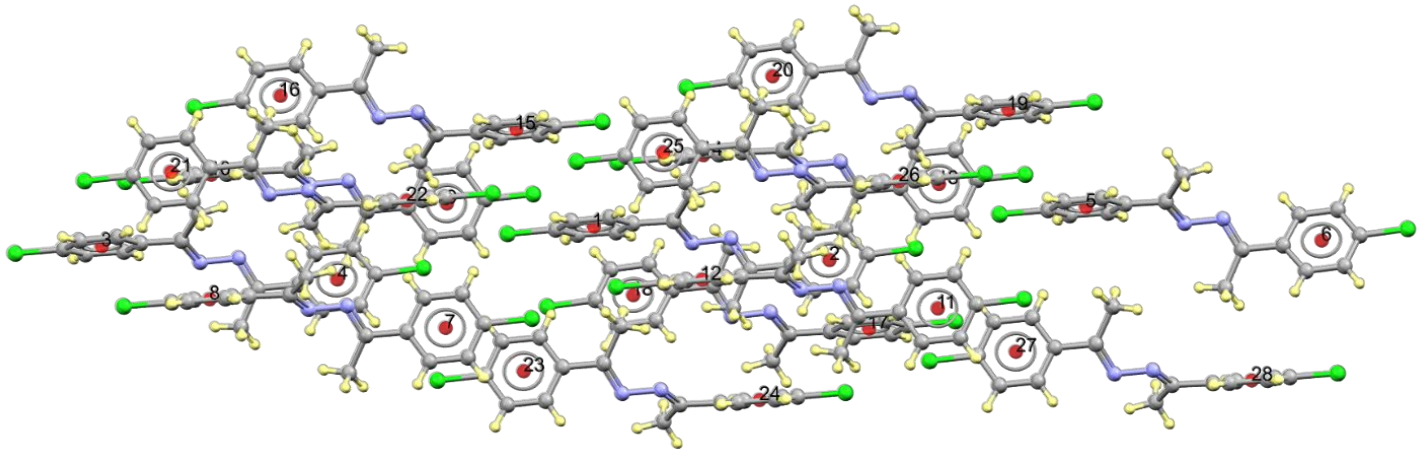

Figure S5. Centroid Numbering in 1M-I

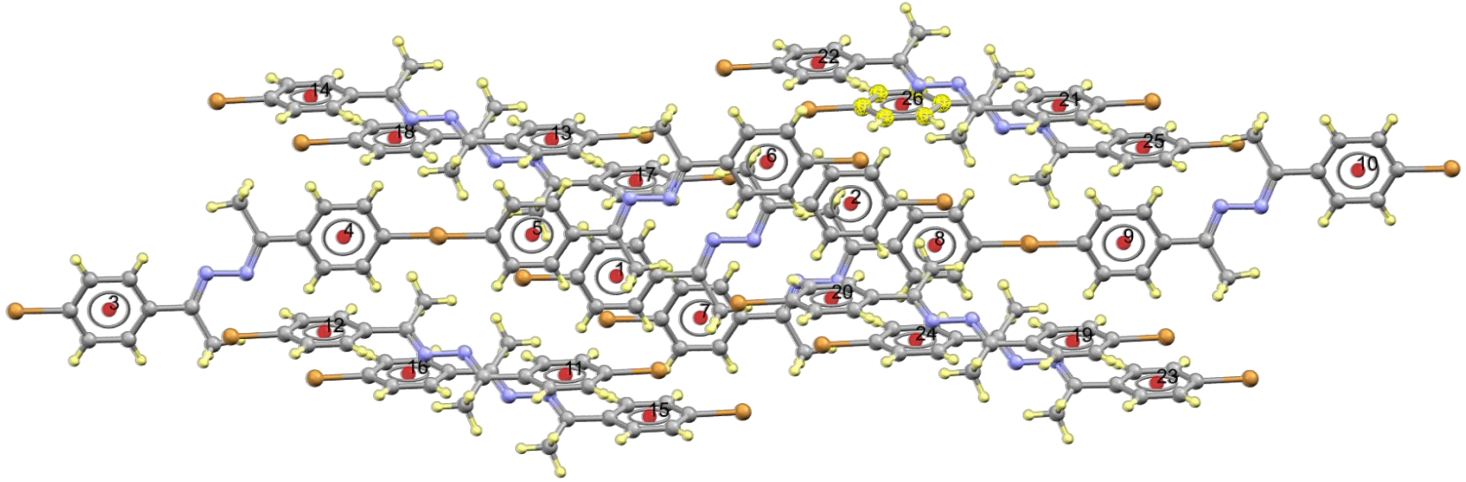

Figure S6. Centroid Numbering in 2M-I

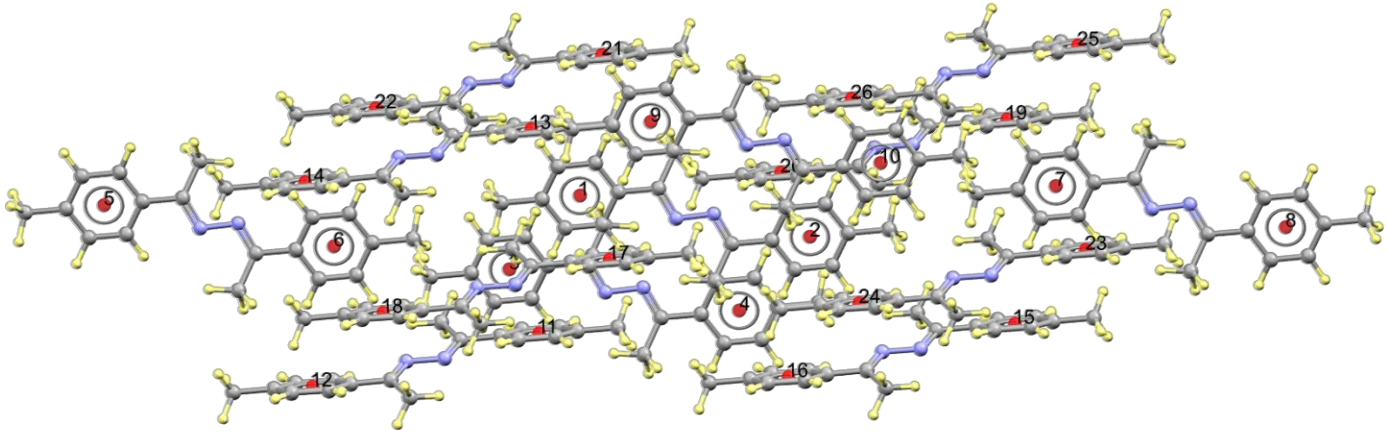

Figure S7. Centroid Numbering in 8M-I

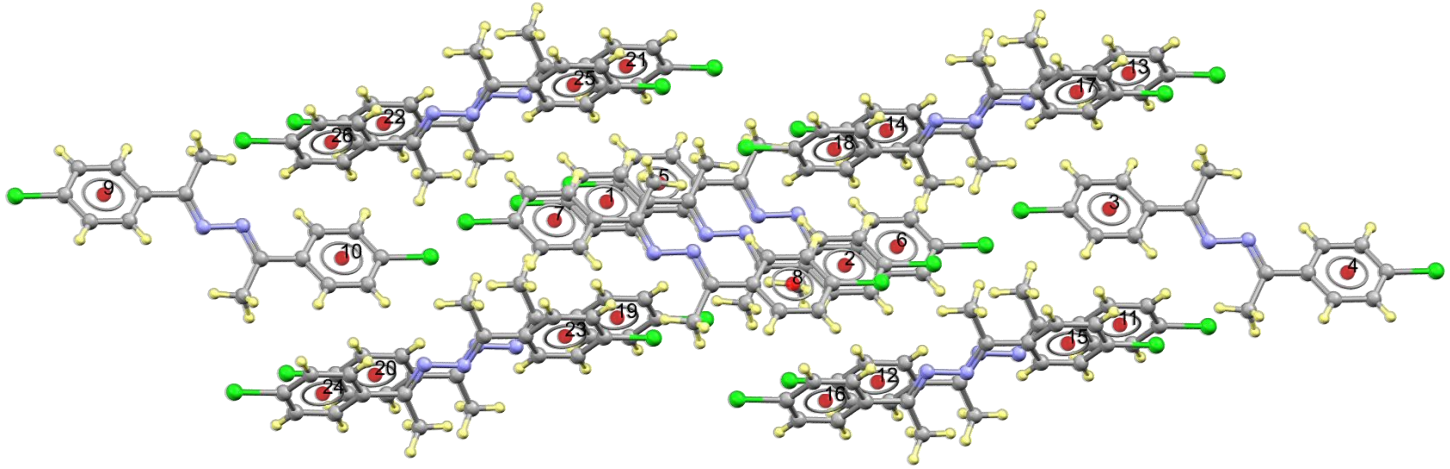

Figure S8. Centroid Numbering in 1M-II

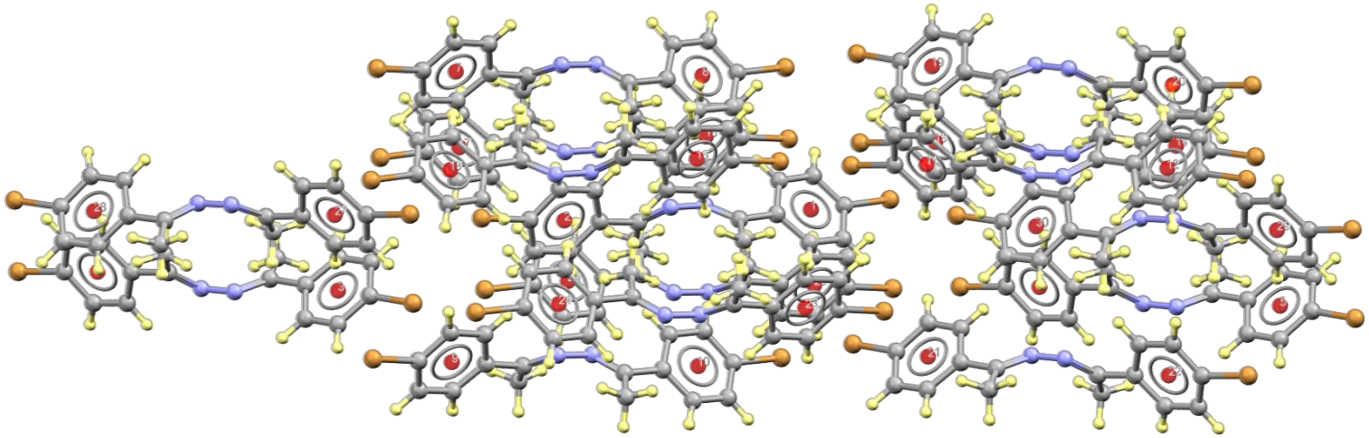

Figure S9. Centroid Numbering in 2M-II

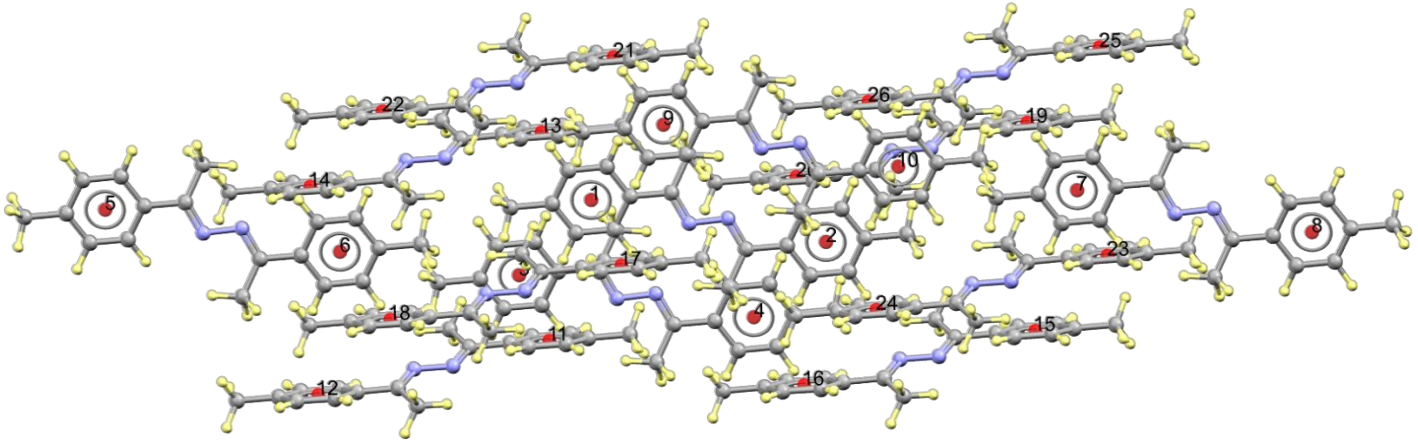

Figure S10. Centroid Numbering in 8M-II

Table S4. Scores of Favorable *Intra*layer Interactions in 1M-I

Centroid1	Centroid2	Distance (Ang.)	Relative Orientation (Degrees)	Intermolecular	Score
1	18	4.78	69.61	1	8.6
2	17	4.78	69.61	1	8.6
1	15	4.48	0	1	7.8
1	14	5.9	13.48	1	6
2	11	5.9	13.48	1	6
1	12	6.17	13.48	1	5.2
2	13	6.17	13.48	1	5.2
1	23	5.77	83.07	1	4.9
1	25	5.77	83.07	1	4.9
2	24	5.62	56.14	1	4.8
2	26	5.62	56.14	1	4.8
2	12	6.68	56.14	1	3.1
2	14	6.68	56.14	1	3.1
1	7	7.18	83.07	1	1.6
1	9	7.18	83.07	1	1.6
2	20	6.97	0	1	1.4
1	22	7.52	13.48	1	1.2
2	27	7.52	13.48	1	1.2
2	18	7.93	0	1	0.9
1	20	8.41	69.61	1	0.5
2	19	8.41	69.61	1	0.5
1	24	8.64	13.48	1	0.4
2	25	8.64	13.48	1	0.4
1	4	9.45	69.61	1	0.1
2	5	9.45	69.61	1	0.1
1	3	17.69	0	1	0
1	5	17.69	0	1	0
1	6	26.14	69.61	1	0
1	8	14.56	13.48	1	0
1	10	14.45	13.48	1	0
1	11	13.21	83.07	1	0
1	13	13.21	83.07	1	0
1	16	12.19	69.61	1	0
1	17	11.37	0	1	0
1	19	15.46	0	1	0
1	21	15.82	83.07	1	0
1	26	11.69	13.48	1	0
1	27	15.82	83.07	1	0
1	28	24.26	13.48	1	0
2	3	26.14	69.61	1	0
2	4	17.69	0	1	0
2	6	17.69	0	1	0
2	7	14.45	13.48	1	0
2	8	22.71	56.14	1	0
2	9	14.56	13.48	1	0
2	10	22.71	56.14	1	0
2	15	12.19	69.61	1	0
2	16	20.58	0	1	0
2	21	24.26	13.48	1	0
2	22	15.76	56.14	1	0
2	23	11.69	13.48	1	0
2	28	15.76	56.14	1	0

Table S5. Scores of Favorable *Intra*layer Interactions in 2M-I

Centroid1	Centroid2	Distance (Ang.)	Relative Orientation (Degrees)	Intermolecular	Score
1	18	4.83	67.8	1	7.9
2	17	4.83	67.8	1	7.9
1	8	6.19	5.73	1	5.1
2	9	6.19	5.73	1	5.1
1	19	6.03	57.46	1	4.8
1	21	6.03	57.46	1	4.8
2	24	5.67	62.21	1	4.8
2	26	5.67	62.21	1	4.8
1	23	5.88	73.35	1	4.6
1	25	5.88	73.35	1	4.6
1	10	6.54	5.73	1	3.7
2	7	6.54	5.73	1	3.7
2	8	6.43	62.21	1	3.5
2	10	6.43	62.21	1	3.5
1	11	6.7	79.88	1	2.2
1	13	6.7	79.88	1	2.2
2	16	6.59	0	1	2.2
2	18	7.76	0	1	1
1	30	7.75	58.64	1	0.9
2	27	7.75	58.64	1	0.9
1	6	8.17	84.45	1	0.6
2	3	8.17	84.45	1	0.6
1	26	8.43	5.73	1	0.5
2	23	8.43	5.73	1	0.5
1	16	8.74	67.8	1	0.4
2	15	8.74	67.8	1	0.4
1	3	15.41	57.46	1	0
1	4	23.25	84.45	1	0
1	5	15.41	57.46	1	0
1	7	13.6	73.35	1	0
1	9	13.6	73.35	1	0
1	12	14.61	58.64	1	0
1	14	11.98	58.64	1	0
1	15	15.96	0	1	0
1	17	11.49	0	1	0
1	20	12.92	84.45	1	0
1	22	13.09	84.45	1	0
1	24	11.87	5.73	1	0
1	27	16.26	79.88	1	0
1	28	23.11	58.64	1	0
1	29	16.26	79.88	1	0
2	4	16.44	59.16	1	0
2	5	23.25	84.45	1	0
2	6	16.44	59.16	1	0
2	11	11.98	58.64	1	0
2	12	20.29	88.78	1	0
2	13	14.61	58.64	1	0
2	14	20.29	88.78	1	0
2	19	13.09	84.45	1	0
2	20	20.03	59.16	1	0
2	21	12.92	84.45	1	0
2	22	20.03	59.16	1	0
2	25	11.87	5.73	1	0
2	28	15.16	88.78	1	0
2	29	23.11	58.64	1	0
2	30	15.16	88.78	1	0

Table S6. Scores of Favorable *Intra*layer Interactions in 8M-I

Centroid1	Centroid2	Distance (Ang.)	Relative Orientation (Degrees)	Intermolecular	Score
1	20	4.8	58.89	1	8.6
2	19	4.8	58.89	1	8.6
1	16	4.82	58.89	1	8.3
2	15	4.82	58.89	1	8.3
1	9	4.81	59.87	1	8.2
1	13	4.81	59.87	1	8.2
2	8	4.89	59.56	1	8.2
2	12	4.89	59.56	1	8.2
1	28	5.71	9.04	1	6.4
2	21	5.71	9.04	1	6.4
1	24	5.75	9.04	1	6.1
2	25	5.75	9.04	1	6.1
2	20	8.59	0	1	0.6
1	17	9.17	0	1	0.4
1	10	9.12	9.04	1	0.3
2	13	9.12	9.04	1	0.3
2	16	9.48	0	1	0.3
1	6	9.24	58.89	1	0.2
2	3	9.24	58.89	1	0.2
1	8	10.35	9.04	1	0.1
1	14	9.95	9.04	1	0.1
1	15	10.24	0	1	0.1
2	9	9.95	9.04	1	0.1
2	11	10.35	9.04	1	0.1
1	3	17.73	0	1	0
1	4	26.29	58.89	1	0
1	5	17.73	0	1	0
1	7	18.71	59.87	1	0
1	11	18.71	59.87	1	0
1	12	11.09	9.04	1	0
1	18	17.47	58.89	1	0
1	19	10.98	0	1	0
1	21	10.41	59.87	1	0
1	22	18.11	9.04	1	0
1	23	10.79	59.87	1	0
1	25	10.79	59.87	1	0
1	26	18.54	9.04	1	0
1	27	10.41	59.87	1	0
2	4	17.73	0	1	0
2	5	26.29	58.89	1	0
2	6	17.73	0	1	0
2	7	11.09	9.04	1	0
2	10	17.4	59.56	1	0
2	14	17.4	59.56	1	0
2	17	17.47	58.89	1	0
2	18	25.98	0	1	0
2	22	10.41	59.56	1	0
2	23	18.54	9.04	1	0
2	24	10.79	59.56	1	0
2	26	10.79	59.56	1	0
2	27	18.11	9.04	1	0
2	28	10.41	59.56	1	0

Table S7. Scores of Favorable *Intra*layer Interactions in 1M-II

Centroid1	Centroid2	Distance (Ang.)	Relative Orientation (Degrees)	Intermolecular	Score
1	5	5.38	0	1	7.2
1	7	5.38	0	1	7.2
2	6	5.38	0	1	7.2
2	8	5.38	0	1	7.2
1	19	5.07	82.26	1	7.1
1	21	5.07	82.26	1	7.1
2	16	5.07	82.26	1	7.1
2	18	5.07	82.26	1	7.1
1	23	5.19	82.26	1	5.8
1	25	5.19	82.26	1	5.8
2	12	5.19	82.26	1	5.8
2	14	5.19	82.26	1	5.8
1	8	7.79	0	1	1
2	5	7.79	0	1	1
1	18	8.17	82.26	1	0.6
1	22	8.17	82.26	1	0.6
2	15	8.17	82.26	1	0.6
2	19	8.17	82.26	1	0.6
1	10	9.34	0	1	0.3
2	3	9.34	0	1	0.3
1	3	17.45	0	1	0
1	4	25.89	0	1	0
1	6	12.05	0	1	0
1	9	17.45	0	1	0
1	11	18.99	82.26	1	0
1	12	12.11	82.26	1	0
1	13	18.99	82.26	1	0
1	14	10.5	82.26	1	0
1	15	16.58	82.26	1	0
1	16	10.15	82.26	1	0
1	17	16.58	82.26	1	0
1	20	10.15	82.26	1	0
1	24	12.11	82.26	1	0
1	26	10.5	82.26	1	0
2	4	17.45	0	1	0
2	7	12.05	0	1	0
2	9	25.89	0	1	0
2	10	17.45	0	1	0
2	11	10.5	82.26	1	0
2	13	12.11	82.26	1	0
2	17	10.15	82.26	1	0
2	20	16.58	82.26	1	0
2	21	10.15	82.26	1	0
2	22	16.58	82.26	1	0
2	23	10.5	82.26	1	0
2	24	18.99	82.26	1	0
2	25	12.11	82.26	1	0
2	26	18.99	82.26	1	0

Table S8. Scores of Favorable *Intra*layer Interactions in 2M-II

Centroid1	Centroid2	Distance (Ang.)	Relative Orientation (Degrees)	Intermolecular	Score
1	15	5.11	81.77	1	7.2
1	17	5.11	81.77	1	7.2
2	20	5.11	81.77	1	7.2
2	22	5.11	81.77	1	7.2
1	5	5.57	0	1	6.7
1	7	5.57	0	1	6.7
2	6	5.57	0	1	6.7
2	8	5.57	0	1	6.7
1	11	5.32	81.77	1	5.5
1	13	5.32	81.77	1	5.5
2	24	5.32	81.77	1	5.5
2	26	5.32	81.77	1	5.5
1	6	7.64	0	1	1.3
2	7	7.64	0	1	1.3
1	16	8.2	81.77	1	0.6
1	20	8.2	81.77	1	0.6
2	17	8.2	81.77	1	0.6
2	21	8.2	81.77	1	0.6
1	4	9.68	0	1	0.2
2	9	9.68	0	1	0.2
1	3	17.76	0	1	0
1	8	12.3	0	1	0
1	9	17.76	0	1	0
1	10	26.17	0	1	0
1	12	10.77	81.77	1	0
1	14	12.39	81.77	1	0
1	18	10.24	81.77	1	0
1	19	16.59	81.77	1	0
1	21	16.59	81.77	1	0
1	22	10.24	81.77	1	0
1	23	19.25	81.77	1	0
1	24	10.77	81.77	1	0
1	25	19.25	81.77	1	0
1	26	12.39	81.77	1	0
2	3	26.17	0	1	0
2	4	17.76	0	1	0
2	5	12.3	0	1	0
2	10	17.76	0	1	0
2	11	12.39	81.77	1	0
2	12	19.25	81.77	1	0
2	13	10.77	81.77	1	0
2	14	19.25	81.77	1	0
2	15	10.24	81.77	1	0
2	16	16.59	81.77	1	0
2	18	16.59	81.77	1	0
2	19	10.24	81.77	1	0
2	23	12.39	81.77	1	0
2	25	10.77	81.77	1	0

Table S9. Scores of Favorable *Intra*layer Interactions in 8M-II

Centroid1	Centroid2	Distance (Ang.)	Relative Orientation (Degrees)	Intermolecular	Score
1	17	5.18	80.82	1	6.9
1	21	5.18	80.82	1	6.9
2	16	5.18	80.82	1	6.9
2	20	5.18	80.82	1	6.9
1	3	5.61	0	1	6.3
1	9	5.61	0	1	6.3
2	4	5.61	0	1	6.3
2	10	5.61	0	1	6.3
1	11	5.26	80.82	1	5.9
1	13	5.26	80.82	1	5.9
2	24	5.26	80.82	1	5.9
2	26	5.26	80.82	1	5.9
1	4	7.9	0	1	0.9
2	9	7.9	0	1	0.9
1	20	8.21	80.82	1	0.6
1	22	8.21	80.82	1	0.6
2	15	8.21	80.82	1	0.6
2	17	8.21	80.82	1	0.6
1	6	9.3	0	1	0.3
2	7	9.3	0	1	0.3
1	5	17.43	0	1	0
1	7	17.43	0	1	0
1	8	25.87	0	1	0
1	10	12.19	0	1	0
1	12	12.12	80.82	1	0
1	14	10.55	80.82	1	0
1	15	16.59	80.82	1	0
1	16	10.15	80.82	1	0
1	18	10.15	80.82	1	0
1	19	16.59	80.82	1	0
1	23	19.03	80.82	1	0
1	24	12.12	80.82	1	0
1	25	19.03	80.82	1	0
1	26	10.55	80.82	1	0
2	3	12.19	0	1	0
2	5	25.87	0	1	0
2	6	17.43	0	1	0
2	8	17.43	0	1	0
2	11	10.55	80.82	1	0
2	12	19.03	80.82	1	0
2	13	12.12	80.82	1	0
2	14	19.03	80.82	1	0
2	18	16.59	80.82	1	0
2	19	10.15	80.82	1	0
2	21	10.15	80.82	1	0
2	22	16.59	80.82	1	0
2	23	10.55	80.82	1	0
2	25	12.12	80.82	1	0

Partially Optimized Crystal Structures of 4-Chloroacetophenone Azine

Polymorph **1M-I** partial optimization (Hs only) at RHF/3-21G

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	11.691717	3.655944	10.366934
2	17	0	14.280652	3.769150	2.720380
3	7	0	6.008534	3.884454	6.963219
4	7	0	4.944912	3.864183	6.056586
5	6	0	7.086879	3.307499	6.558375
6	6	0	8.242848	3.397722	7.471423
7	6	0	9.201252	2.393266	7.521399
8	6	0	10.269378	2.466066	8.417699
9	6	0	10.360368	3.555785	9.248082
10	6	0	9.439734	4.579960	9.209215
11	6	0	8.383354	4.495213	8.323895
12	6	0	7.215905	2.570475	5.268527
13	6	0	3.801489	3.554192	6.546175
14	6	0	2.654691	3.618031	5.621164
15	6	0	2.645034	4.531858	4.571791
16	6	0	1.580463	4.591590	3.691424
17	6	0	0.532993	3.708633	3.854882
18	6	0	0.519899	2.800418	4.868683
19	6	0	1.567094	2.763021	5.758145
20	6	0	3.584970	3.131215	7.969598
21	1	0	9.126763	1.539216	6.881135
22	1	0	11.003554	1.690133	8.459950
23	1	0	9.548716	5.428860	9.849974
24	1	0	7.661534	5.280023	8.268332
25	1	0	8.151933	2.815809	4.789762
26	1	0	6.399202	2.825059	4.614822
27	1	0	7.194617	1.498088	5.434728
28	1	0	3.471600	5.197360	4.448747
29	1	0	1.563590	5.311402	2.902702
30	1	0	-0.307715	2.134069	4.984398
31	1	0	1.532751	2.057346	6.562022
32	1	0	2.620029	3.457091	8.330078
33	1	0	4.370040	3.536517	8.588182
34	1	0	3.627470	2.050715	8.057629
35	17	0	2.251786	8.327936	5.281276
36	17	0	2.626961	5.688067	0.065201
37	17	0	12.066891	1.016028	5.150841
38	17	0	0.413152	8.441090	2.495686
39	17	0	0.037978	5.574910	7.711760
40	17	0	13.905445	0.902879	7.936514
41	7	0	7.934957	8.556417	8.684986
42	7	0	8.310136	5.459599	3.468902
43	7	0	6.383687	0.787607	1.747177
44	7	0	8.998571	8.536218	9.591630
45	7	0	9.373747	5.479773	4.375552
46	7	0	5.320077	0.807761	0.840526
47	6	0	6.856629	7.979553	9.089883
48	6	0	7.231720	6.036478	3.873781
49	6	0	7.462061	1.364503	1.342317
50	6	0	5.700598	8.069764	8.176860
51	6	0	6.075791	5.946229	2.960748

52	6	0	8.618047	1.274233	2.255307
53	6	0	4.742144	7.065302	8.126912
54	6	0	5.117374	6.950718	2.910784
55	6	0	9.576491	2.278709	2.305224
56	6	0	3.674059	7.138075	7.230635
57	6	0	4.049258	6.877933	2.014545
58	6	0	10.644598	2.205955	3.201551
59	6	0	3.583140	8.227767	6.400134
60	6	0	3.958301	5.788233	1.184038
61	6	0	10.735571	1.116231	4.031924
62	6	0	4.503841	9.251904	6.438844
63	6	0	4.878943	4.764032	1.222885
64	6	0	9.814928	0.092004	3.993200
65	6	0	5.560262	9.167192	7.324226
66	6	0	5.935360	4.848767	2.108218
67	6	0	8.758492	0.176788	3.107842
68	6	0	6.727411	7.242529	10.379862
69	6	0	7.102769	6.773513	5.163598
70	6	0	7.591130	2.101508	0.052383
71	6	0	10.141951	8.226169	9.102058
72	6	0	10.517178	5.789820	3.885982
73	6	0	4.176716	1.117823	1.330113
74	6	0	11.288805	8.289952	10.027046
75	6	0	11.663963	5.726000	4.810976
76	6	0	3.029891	1.054048	0.405039
77	6	0	12.048714	9.203830	0.644365
78	6	0	11.673602	4.812141	5.860371
79	6	0	2.269861	0.140160	9.787860
80	6	0	13.113296	9.263679	1.524771
81	6	0	12.738211	4.752360	6.740733
82	6	0	1.205265	0.080355	8.907494
83	6	0	14.160845	8.380637	1.361177
84	6	0	13.785661	5.635365	6.577260
85	6	0	0.157814	0.963365	9.070964
86	6	0	14.173923	7.472389	0.347408
87	6	0	13.798744	6.543613	5.563479
88	6	0	0.144734	1.871608	10.084660
89	6	0	12.376391	7.435052	9.890046
90	6	0	12.751550	6.581000	4.674004
91	6	0	1.942271	1.908983	0.542150
92	6	0	10.358538	7.803177	7.678393
93	6	0	10.733681	6.212794	2.462510
94	6	0	3.959998	1.540800	2.753785
95	1	0	4.818834	6.210984	8.764887
96	1	0	5.191875	7.804729	3.551096
97	1	0	9.499887	3.132866	1.667022
98	1	0	2.936159	6.366861	7.191724
99	1	0	3.315011	7.653796	1.972307
100	1	0	11.382510	2.977159	3.240454
101	1	0	4.394856	0.337626	5.815617
102	1	0	4.770033	3.915233	0.581986
103	1	0	9.924058	9.006151	4.616310
104	1	0	6.288417	0.186688	7.394100
105	1	0	6.657134	4.063927	2.163890
106	1	0	8.030489	9.157128	3.037717
107	1	0	6.571841	7.547901	0.415645
108	1	0	6.167171	6.527341	5.642822
109	1	0	7.747940	1.798131	10.017832
110	1	0	8.325066	7.497465	0.563002
111	1	0	7.919942	6.519573	5.816963
112	1	0	5.994779	1.844448	9.868241
113	1	0	6.702959	6.170839	10.219020
114	1	0	7.122912	7.845964	4.997630

115	1	0	7.612629	3.173348	0.212886
116	1	0	11.216926	0.101194	0.793559
117	1	0	10.847021	4.146661	5.983403
118	1	0	3.101656	9.242740	9.638659
119	1	0	13.121743	0.213302	2.342901
120	1	0	12.755071	4.032507	7.529428
121	1	0	1.196701	9.130671	8.089296
122	1	0	14.994470	6.796536	0.237522
123	1	0	14.626318	7.210006	5.447797
124	1	0	-0.675838	2.547450	10.194454
125	1	0	12.420238	6.738979	9.078777
126	1	0	12.785756	7.286813	3.870242
127	1	0	1.898557	2.605135	1.353324
128	1	0	11.316167	8.150182	7.314854
129	1	0	11.699812	5.889686	2.102837
130	1	0	3.002652	1.193191	3.117460
131	1	0	9.564738	8.196445	7.062567
132	1	0	9.950255	5.804665	1.843639
133	1	0	4.754229	1.148148	3.369476
134	1	0	10.338036	6.723908	7.589649
135	1	0	10.687706	7.293117	2.374054
136	1	0	3.979804	2.620102	2.842466
137	-2	0	15.139309	-0.004597	0.032468
138	-2	0	-0.000312	9.762028	-0.020607
139	-2	0	-0.764344	-0.025737	10.459367
Lengths of translation vectors:			15.139344	9.762050	10.487290
Angles of translation vectors:			90.261104	94.056667	90.019484

Polymorph **1M-II** partial optimization (Hs only) at RHF/3-21G

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.343625	5.345343	14.029112
2	7	0	-0.918642	4.334609	8.303043
3	6	0	0.266223	6.179401	12.511318
4	1	0	-0.019938	6.788179	13.342396
5	6	0	-0.476894	6.205032	11.334663
6	1	0	-1.334976	6.837974	11.292418
7	6	0	1.782520	4.597509	11.488035
8	1	0	2.657112	3.990447	11.556169
9	6	0	-0.124233	5.416145	10.234140
10	6	0	1.019636	4.615779	10.325476
11	1	0	1.309841	4.019704	9.486556
12	6	0	-0.962560	5.416007	9.004453
13	6	0	3.590140	6.636090	8.707696
14	1	0	3.166838	6.577268	7.724605
15	1	0	-1.172762	7.526797	8.787690
16	1	0	2.774845	6.711285	9.416116
17	6	0	1.387038	5.375838	12.569106
18	17	0	1.749019	0.992582	9.155928
19	17	0	0.384806	3.360157	1.427576
20	17	0	0.979412	7.712879	6.300766
21	7	0	-0.365189	8.687292	14.881921
22	7	0	3.647080	4.370854	7.153625
23	7	0	3.093781	0.018131	0.574682
24	6	0	-1.550151	1.826540	10.673837

25	6	0	2.462172	2.526014	2.945402
26	6	0	4.278654	6.878903	4.782929
27	1	0	-1.261115	2.438370	9.846129
28	1	0	2.749235	1.918345	2.113657
29	1	0	3.990117	6.267089	5.610964
30	6	0	-0.807114	1.852387	11.850328
31	6	0	3.205291	2.500409	4.121987
32	6	0	3.535518	6.853213	3.606379
33	1	0	0.050123	2.486691	11.890814
34	1	0	4.063374	1.867480	4.164077
35	1	0	2.678137	6.219100	3.565817
36	6	0	2.310128	0.244936	11.696867
37	6	0	0.945921	4.107951	3.968584
38	6	0	0.418265	8.460716	3.759964
39	1	0	1.439420	8.329906	11.636677
40	1	0	0.070792	4.714352	3.901012
41	1	0	1.288053	0.376968	3.820808
42	6	0	-1.159660	1.063361	12.950986
43	6	0	2.852687	3.289382	5.222664
44	6	0	3.888175	7.641994	2.505631
45	6	0	3.072877	0.262864	12.859212
46	6	0	1.708670	4.089866	5.130858
47	6	0	-0.344449	8.442590	2.597429
48	1	0	2.784662	8.355583	13.702848
49	1	0	1.417795	4.685608	5.969683
50	1	0	-0.056608	0.351988	1.755415
51	6	0	-0.321397	1.063302	14.180611
52	6	0	3.690967	3.289554	6.452227
53	6	0	3.049856	7.642234	1.276088
54	6	0	0.502510	2.283439	14.477500
55	6	0	-0.861624	2.069350	6.749153
56	6	0	2.225751	6.422254	0.979204
57	1	0	0.939324	2.220968	15.455374
58	1	0	-0.439181	2.130435	7.732508
59	1	0	1.796460	6.479796	-0.002111
60	1	0	-0.109103	3.172620	14.401585
61	1	0	3.900203	1.178652	6.669589
62	1	0	2.833945	5.531885	1.065847
63	1	0	1.307773	2.361439	13.758467
64	1	0	-0.046555	1.994589	6.040527
65	1	0	1.413942	6.351572	1.691919
66	6	0	2.705612	1.023164	10.616066
67	6	0	1.341360	3.329614	2.887603
68	6	0	0.022847	7.682314	4.840705
69	-2	0	5.374687	-0.003139	0.009440
70	-2	0	0.004274	8.691901	0.006907
71	-2	0	-2.684306	-0.003602	15.516242

Lengths of translation vectors:	5.374697	8.691905	15.746723
Angles of translation vectors:	89.973047	99.714361	90.005208

Polymorph **2M-II** partial optimization (Hs only) at RHF/3-21G

```
Stoichiometry    C32H28Br4N4
Framework group  C1[X(C32H28Br4N4)]
Deg. of freedom   198
Full point group                 C1      NOp   1
                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	35	0	0.408991	7.730513	1.446575
2	6	0	3.097255	7.662155	5.276849
3	7	0	3.944845	0.011740	7.172538
4	6	0	1.500915	7.694802	2.999880
5	6	0	3.409939	6.872671	4.168757
6	1	0	4.272593	6.242534	4.180242
7	6	0	1.139558	8.467340	4.095803
8	1	0	0.244957	0.326851	4.079710
9	6	0	2.625315	6.896258	3.019838
10	1	0	2.884228	6.292253	2.177241
11	6	0	1.943285	8.454764	5.227341
12	1	0	1.664397	0.304620	6.098246
13	6	0	3.974685	7.675824	6.474389
14	6	0	-0.740913	6.471174	6.748372
15	1	0	4.234110	5.565206	6.666635
16	1	0	-0.307244	6.532187	7.726859
17	1	0	0.064567	6.424226	6.026596
18	35	0	1.177496	3.356867	6.285813
19	35	0	2.763997	1.016798	14.018192
20	35	0	1.995448	5.390488	9.178984
21	6	0	4.057412	3.288117	2.455238
22	6	0	0.076032	1.085365	10.187736
23	6	0	-0.884285	5.458941	13.009402
24	7	0	3.209497	4.385448	0.559829
25	7	0	-0.771832	8.735482	8.292253
26	7	0	-0.036234	4.361803	14.904859
27	6	0	0.085623	3.321163	4.732528
28	6	0	1.672050	1.052414	12.464958
29	6	0	3.087728	5.425529	10.731929
30	6	0	3.744088	2.499293	3.563878
31	6	0	-0.237119	1.874541	11.296045
32	6	0	-0.571299	6.248262	11.901085
33	1	0	2.881134	1.869816	3.555058
34	1	0	-1.099870	2.504622	11.284583
35	1	0	0.291174	6.878531	11.909680
36	6	0	0.446847	4.093800	3.636499
37	6	0	2.033362	0.279934	11.368917
38	6	0	2.725810	4.654039	11.828487
39	1	0	1.326920	4.695472	3.671265
40	1	0	2.927954	8.419842	11.384888
41	1	0	1.844908	4.053473	11.794484
42	6	0	4.529128	2.522609	4.712565
43	6	0	0.547740	1.850890	12.444944
44	6	0	-1.356141	6.224698	10.752238
45	1	0	4.264241	1.915984	5.551432
46	1	0	0.287489	2.454415	13.287464
47	1	0	-1.092163	6.831631	9.913558
48	6	0	-0.356755	4.080975	2.505006
49	6	0	1.229756	0.292684	10.237370
50	6	0	3.529771	4.666253	12.959748
51	1	0	-0.088497	4.674879	1.657543
52	1	0	1.508597	8.442461	9.366551
53	1	0	3.261567	4.072362	13.807207
54	6	0	3.179226	3.302205	1.258224
55	6	0	-0.802058	1.071379	8.990609
56	6	0	-0.006261	5.445076	14.206492
57	6	0	2.327431	2.097647	0.984034
58	6	0	3.914016	2.276260	8.716376
59	6	0	0.845261	6.649796	14.480861
60	1	0	2.922975	1.197157	1.050933
61	1	0	-1.060581	3.181854	8.797887

62	1	0	0.246257	7.549007	14.427888
63	1	0	1.873341	2.168732	0.014309
64	1	0	3.480552	2.215042	7.737853
65	1	0	1.310168	6.571872	15.444937
66	1	0	1.537126	2.038800	1.721599
67	1	0	3.108342	2.323766	9.438217
68	1	0	1.627133	6.717484	13.735248
69	-2	0	5.567083	-0.005981	0.009592
70	-2	0	0.014133	8.741053	-0.020819
71	-2	0	-2.422040	-0.006783	15.531251
Lengths of translation vectors:			5.567094	8.741089	15.718972
Angles of translation vectors:			90.173834	98.764917	89.969151

Polymorph **8M-I** partial optimization (Hs only) at RHF/3-21G

Stoichiometry C72H80N8
Framework group C1[X(C72H80N8)]
Deg. of freedom 474
Full point group C1 NOp 1

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	10.081629	5.953163	1.109874
2	7	0	9.036460	6.043730	17.459436
3	6	0	9.225553	5.347091	1.837897
4	6	0	9.539246	5.273087	3.295639
5	6	0	8.683107	4.644980	4.187676
6	6	0	8.999494	4.578700	5.545357
7	6	0	10.175321	5.121041	6.032316
8	6	0	11.017756	5.744415	5.135354
9	6	0	10.710783	5.834459	3.799413
10	6	0	7.977962	4.718067	1.309330
11	6	0	10.534537	5.001235	7.494636
12	6	0	10.034092	5.923650	16.662782
13	6	0	9.751216	6.084895	15.218172
14	6	0	10.624607	5.595278	14.254398
15	6	0	10.342338	5.733057	12.902751
16	6	0	9.208812	6.391795	12.470918
17	6	0	8.350373	6.888279	13.428293
18	6	0	8.613287	6.734398	14.777127
19	6	0	-0.012903	5.627966	17.122168
20	6	0	8.901849	6.570725	10.993454
21	1	0	7.773444	4.190417	3.857468
22	1	0	8.323146	4.078466	6.206932
23	1	0	0.467937	6.183200	5.520074
24	1	0	-0.092775	6.344671	3.170415
25	1	0	7.883562	4.914219	0.256247
26	1	0	7.111772	5.112340	1.826001
27	1	0	7.997504	3.648193	1.480794
28	1	0	9.762993	4.475617	8.043015
29	1	0	10.664862	5.980289	7.943356
30	1	0	-0.003798	4.473878	7.654298
31	1	0	0.047636	5.093721	14.575399
32	1	0	-0.441558	5.330167	12.235014
33	1	0	7.466845	7.415257	13.129353
34	1	0	7.929754	7.125801	15.501562
35	1	0	0.214182	4.589257	16.911098
36	1	0	0.832274	5.815464	0.431312
37	1	0	0.674165	6.258217	16.576364

38	1	0	9.797307	6.460229	10.394755
39	1	0	8.350694	-0.370284	10.934125
40	1	0	8.182477	5.827849	10.667534
41	7	0	6.723175	2.145819	7.746541
42	7	0	0.649568	1.661529	16.602968
43	7	0	4.008005	5.468874	9.966316
44	7	0	7.060364	2.236411	9.109901
45	7	0	1.694767	1.570913	0.253471
46	7	0	3.670826	5.378258	8.602957
47	6	0	7.579218	1.539690	7.018533
48	6	0	1.505607	2.267652	15.874979
49	6	0	3.151956	6.074973	10.694302
50	6	0	7.265597	1.465831	5.560774
51	6	0	1.191984	2.341530	14.417204
52	6	0	3.465599	6.148894	12.152075
53	6	0	8.121677	0.837617	4.668755
54	6	0	2.048069	2.969722	13.525180
55	6	0	2.609511	6.777061	13.044104
56	6	0	7.805310	0.771367	3.311069
57	6	0	1.731690	3.036007	12.167497
58	6	0	2.925873	6.843350	14.401785
59	6	0	6.629370	1.313516	2.824143
60	6	0	0.555834	2.493733	11.680543
61	6	0	4.101828	6.301204	14.888709
62	6	0	5.787066	1.937209	3.721109
63	6	0	-0.286551	1.870177	12.577546
64	6	0	4.944106	5.677476	13.991748
65	6	0	6.093996	2.027025	5.057020
66	6	0	0.020389	1.780317	13.913448
67	6	0	4.637187	5.587673	12.655836
68	6	0	8.826809	0.910722	7.547115
69	6	0	2.753201	2.896629	16.403500
70	6	0	1.904369	6.704027	10.165777
71	6	0	6.270303	1.193987	1.361764
72	6	0	0.196594	2.613478	10.218201
73	6	0	4.460877	6.420703	16.351093
74	6	0	6.062587	2.116120	9.906483
75	6	0	0.697001	1.691225	1.050018
76	6	0	4.668582	5.498601	7.806410
77	6	0	6.345599	2.277609	11.351105
78	6	0	0.980026	1.529792	2.494686
79	6	0	4.385590	5.337114	6.361727
80	6	0	5.472157	1.787919	12.314862
81	6	0	0.106559	2.019419	3.458435
82	6	0	5.259025	5.826752	5.397994
83	6	0	5.754417	1.925778	13.666540
84	6	0	0.388847	1.881600	4.810103
85	6	0	4.976786	5.688943	4.046281
86	6	0	6.887968	2.584403	14.098371
87	6	0	1.522378	1.222910	5.241921
88	6	0	3.843215	5.030262	3.614510
89	6	0	7.746416	3.080909	13.140990
90	6	0	2.380784	0.726448	4.284635
91	6	0	2.984805	4.533764	4.571859
92	6	0	7.483469	2.927082	11.792157
93	6	0	2.117896	0.880250	2.935728
94	6	0	3.247556	4.687688	5.920838
95	6	0	4.670548	1.820662	9.447070
96	6	0	10.744103	1.986676	0.590730
97	6	0	6.060687	5.794016	8.265710
98	6	0	7.194966	2.763392	15.575798
99	6	0	1.829445	1.043963	6.719235
100	6	0	3.536267	4.851319	2.137064

101	1	0	9.031014	0.382287	4.999731
102	1	0	2.957711	3.424350	13.855378
103	1	0	1.700159	7.232362	12.713106
104	1	0	8.480110	0.265830	2.649532
105	1	0	2.407997	3.536286	11.505927
106	1	0	2.251108	7.348867	15.063361
107	1	0	4.868024	2.366546	3.378396
108	1	0	10.263384	1.431195	12.193033
109	1	0	5.863233	5.248292	14.334415
110	1	0	5.426489	2.527900	5.724022
111	1	0	10.823977	1.270078	14.542498
112	1	0	5.304750	5.086899	11.988820
113	1	0	8.926378	1.105457	8.599750
114	1	0	2.847542	2.700708	17.456661
115	1	0	1.805590	6.510640	9.112825
116	1	0	9.692602	1.300989	7.026094
117	1	0	3.619339	2.502085	15.886958
118	1	0	1.038441	6.312436	10.685650
119	1	0	8.930729	7.759648	7.247967
120	1	0	2.733736	3.966445	16.231764
121	1	0	1.799699	-0.145167	10.466434
122	1	0	7.083528	0.758499	0.794430
123	1	0	0.963944	3.146858	9.671469
124	1	0	3.650542	6.863325	16.917048
125	1	0	6.035415	2.163544	0.937113
126	1	0	0.075352	1.634128	9.767540
127	1	0	4.687986	5.450141	16.777709
128	1	0	5.395219	0.564863	1.236935
129	1	0	10.730247	3.132548	10.058885
130	1	0	5.340683	7.043278	16.475456
131	1	0	4.576293	1.275646	12.031336
132	1	0	10.683504	2.520890	3.137449
133	1	0	6.154904	6.338998	5.681550
134	1	0	5.067213	1.510305	14.376656
135	1	0	11.172965	2.284936	5.477792
136	1	0	5.663846	6.104738	3.336199
137	1	0	8.630258	3.606203	13.438852
138	1	0	3.264426	0.199645	4.583608
139	1	0	2.101002	4.008403	4.273988
140	1	0	8.168630	3.315588	11.068205
141	1	0	2.801470	0.488947	2.211270
142	1	0	2.562271	4.299223	6.644659
143	1	0	4.444946	0.767902	9.595167
144	1	0	10.517163	3.025640	0.800842
145	1	0	6.286814	6.846462	8.116256
146	1	0	4.574492	2.046810	8.400206
147	1	0	9.898743	1.798422	17.281706
148	1	0	6.156390	5.569145	9.312882
149	1	0	3.958565	2.406547	10.009882
150	1	0	10.056990	1.357019	1.137062
151	1	0	6.772423	5.207026	7.703712
152	1	0	6.284049	2.778827	16.161921
153	1	0	0.937310	1.171743	7.319406
154	1	0	4.447819	4.826169	1.552226
155	1	0	7.735064	3.685231	15.749648
156	1	0	2.364154	7.978373	6.780683
157	1	0	2.987858	3.934254	1.964151
158	1	0	7.809746	1.942499	15.930681
159	1	0	2.562314	1.775131	7.041422
160	1	0	2.929964	5.677472	1.779790
161	-2	0	11.471534	-0.012098	-0.040941
162	-2	0	0.127148	7.920197	-0.129092
163	-2	0	-0.734314	-0.016813	17.748328

```
 ---------------------------------------------------------------------
 Lengths of translation vectors:     11.471613    7.922269   17.763520
 Angles of translation vectors:     91.025108   92.573610   89.137482
 ---------------------------------------------------------------------

%mem=800GB
%NProcShared=256
Job cpu time:     887 days 20 hours 28 minutes 56.0 seconds.
Elapsed time:       5 days  0 hours  6 minutes 53.5 seconds.
```

Polymorph **8M-II** partial optimization (Hs only) at RHF/3-21G

```
 Stoichiometry    C36H40N4
 Framework group  C1[X(C36H40N4)]
 Deg. of freedom   234
 Full point group                 C1      NOp   1
                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        0.738516    1.009475   -6.487986
      2          6           0       -0.084502    1.024905   -5.256613
      3          6           0        0.277398    1.788938   -4.159988
      4          6           0       -0.472369    1.764833   -2.990722
      5          6           0       -1.605964    0.985078   -2.886970
      6          6           0       -1.979577    0.243575   -3.992291
      7          6           0       -1.243047    0.249649   -5.151339
      8          6           0        1.615827    2.178176   -6.780221
      9          6           0       -2.435699    0.989904   -1.633539
     10          1           0        1.142841    2.417480   -4.196619
     11          1           0       -0.166766    2.387502   -2.173500
     12          1           0        3.308703   -0.380505   -4.098029
     13          1           0       -1.553339   -0.334111   -5.992456
     14          1           0        1.948783    2.157835   -7.802238
     15          1           0        2.492731    2.137041   -6.140518
     16          1           0        1.099302    3.105961   -6.571783
     17          1           0        3.760744   -0.009621   -1.303690
     18          1           0        2.710153    1.196923   -2.011025
     19          1           0       -2.068065    1.722190   -0.925788
     20          7           0        0.634832   -0.035523   -7.218928
     21          6           0       -0.738002   -1.008058    6.487369
     22          6           0        0.083923   -1.022651    5.253751
     23          6           0       -0.273939   -1.789067    4.162425
     24          6           0        0.474081   -1.762023    2.994268
     25          6           0        1.607708   -0.982283    2.889304
     26          6           0        1.987193   -0.237711    4.001461
     27          6           0        1.236290   -0.250392    5.147277
     28          6           0       -1.621240   -2.179240    6.790244
     29          6           0        2.432245   -0.995265    1.620010
     30          1           0       -1.137641   -2.420333    4.199353
     31          1           0        0.169887   -2.385096    2.176910
     32          1           0       -3.300983    0.385485    4.112508
     33          1           0        1.540112    0.333429    5.991512
     34          1           0       -1.940512   -2.156362    7.816259
     35          1           0       -2.504733   -2.132484    6.160228
     36          1           0       -1.109720   -3.108099    6.574822
     37          1           0       -3.802056   -0.010051    1.265160
     38          1           0       -2.705104   -1.162688    1.994995
     39          1           0        2.079181   -1.758801    0.938730
     40          7           0       -0.632683    0.037031    7.221430
     41          6           0        0.280627   -3.364965   -1.306663
```

42	6	0	-0.280868	3.365096	1.308214
43	6	0	1.103031	-3.362177	-2.542426
44	6	0	-1.104434	3.360717	2.540935
45	6	0	0.752696	-2.596281	-3.635932
46	6	0	-0.749709	2.597249	3.638194
47	6	0	1.501119	-2.628044	-4.801559
48	6	0	-1.497185	2.633186	4.806326
49	6	0	2.625425	-3.421328	-4.907987
50	6	0	-2.626242	3.421667	4.907308
51	6	0	2.991168	-4.167065	-3.801850
52	6	0	-2.994544	4.163064	3.799736
53	6	0	2.251828	-4.144680	-2.644577
54	6	0	-2.252388	4.144128	2.641341
55	6	0	-0.585746	-2.185827	-1.008742
56	6	0	0.586225	2.187178	1.017404
57	6	0	3.463040	-3.423996	-6.174949
58	6	0	-3.455030	3.427332	6.160380
59	1	0	-0.106398	-1.958715	-3.600371
60	1	0	0.110861	1.961873	3.603343
61	1	0	1.202514	-2.002741	-5.619740
62	1	0	-1.196603	2.012873	5.627555
63	1	0	-2.255788	4.023890	-3.693751
64	1	0	2.250745	-4.030292	3.690929
65	1	0	2.603795	4.040304	-1.802336
66	1	0	-2.604375	-4.041348	1.798963
67	1	0	-0.874073	-2.171846	0.025781
68	1	0	0.877149	2.168494	-0.016557
69	1	0	-1.490438	-2.249472	-1.607275
70	1	0	1.489878	2.254532	1.617133
71	1	0	-0.081468	-1.265442	-1.270816
72	1	0	0.082910	1.267127	1.282119
73	1	0	-2.763939	-4.361465	-6.515107
74	1	0	2.758924	4.369053	6.493919
75	1	0	-1.677746	-3.193004	-5.792052
76	1	0	1.686573	3.183893	5.783186
77	1	0	3.112206	-2.671482	-6.869776
78	1	0	-3.100001	2.686211	6.865613
79	7	0	0.415885	4.362162	-0.585837
80	7	0	-0.413440	-4.360807	0.590825
81	-2	0	6.180037	-0.027835	-0.149934
82	-2	0	0.048140	8.769386	-0.001250
83	-2	0	-2.041695	0.060607	15.650323
Lengths of translation vectors:			6.181918	8.769518	15.783054
Angles of translation vectors:			89.828767	98.823287	89.943355