Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Azines: Synthesis, Structure, Electronic Structure and their Applications

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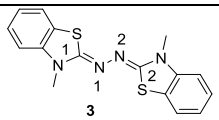
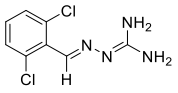
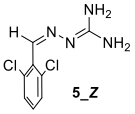
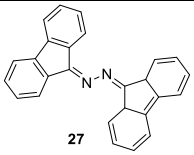
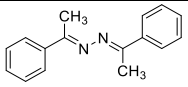
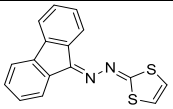
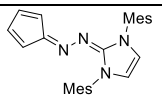
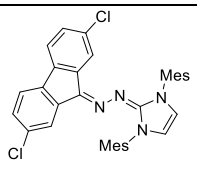
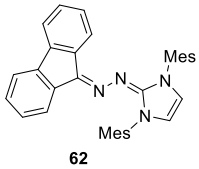
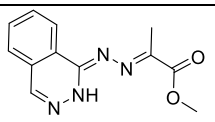
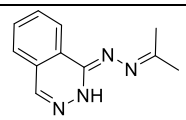
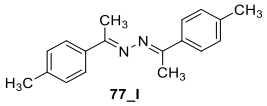
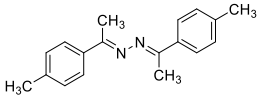
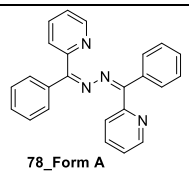
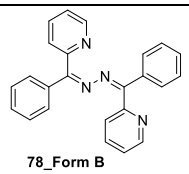
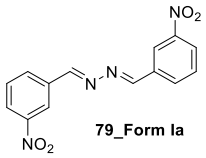
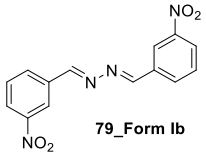
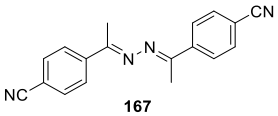
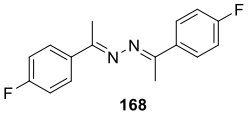
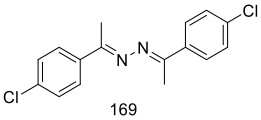
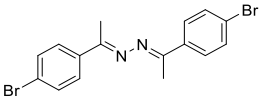
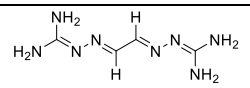
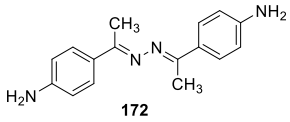
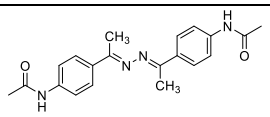
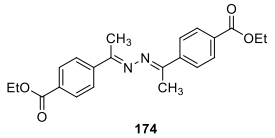
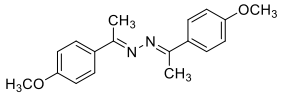
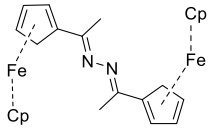
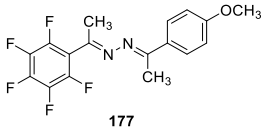
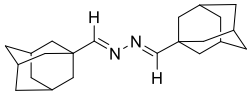
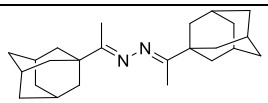
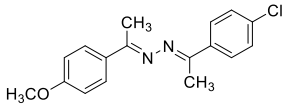
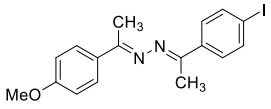
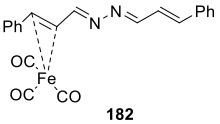
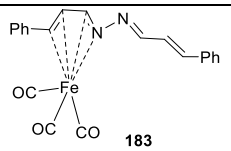
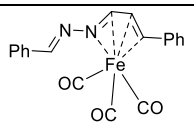
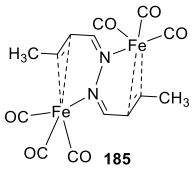
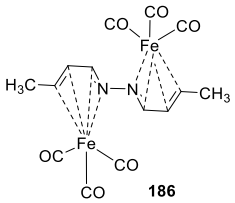
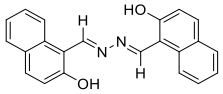
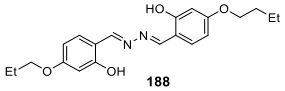
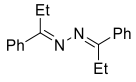
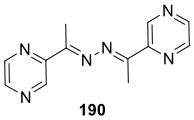
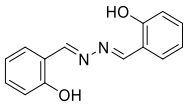
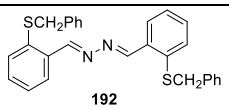
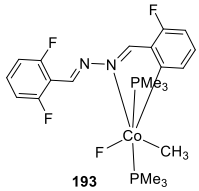
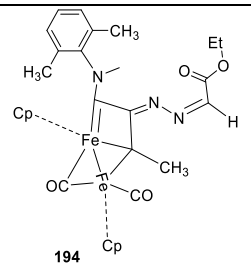
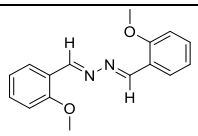
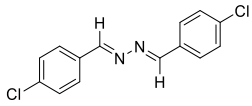
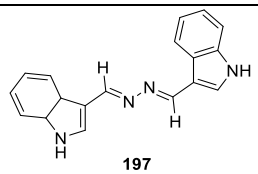
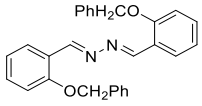
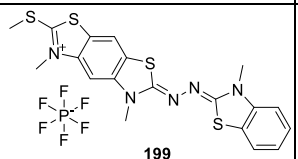
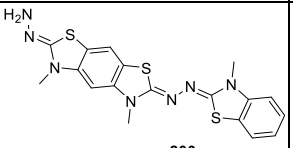
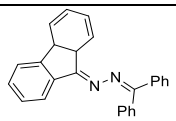
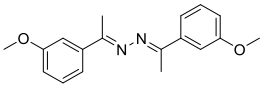
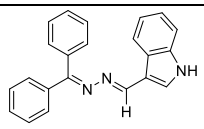
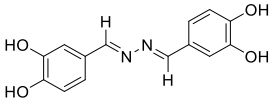
Table SI-1: The reported crystal structures of azine along with some important geometrical features.

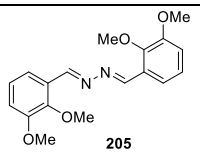
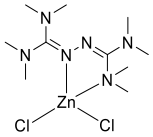
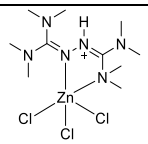
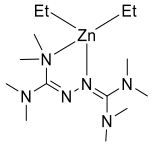
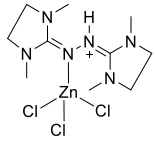
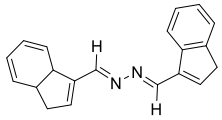
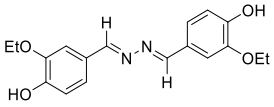
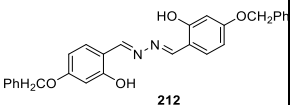
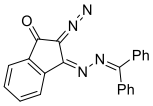
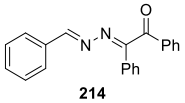
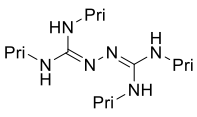
Entry	2-D structures	CCDC	Year	Purpose	Torsional angle (°) (C-N-N-C)	Bond length (Å)	
						C=N	N–N
1	 **3**	612474 [1]	2006	Crystal structure	178.92	1.286, 1.294	1.409
2	 ***5_E***	1866599[2]	2019	Polymorphism	179.76	1.268, 1.323	1.392
3	 ***5_Z***	1866600[2]	2019	Polymorphism	173.01	1.273, 1.332	1.389
4	 **27**	1448762[3]	2016	Conjugation	180.00	1.330	1.367
5	 **28b**	1207284[4]	1994	Stereochemistry and stereoelectronics	138.72	1.278	1.400
6	 **57**	236041[5]	2004	Push Pull donor acceptor azine for NLO material	169.75	1.299, 1.305	1.369
7	 **60**	236040[5]	2004	Push Pull donor acceptor azine	168.53	1.300, 1.310	1.353
8	 **61**	236035[5]	2004	Push Pull donor acceptor azine	173.77	1.316, 1.342	1.357
9	 **62**	236038[5]	2004	Push Pull donor acceptor azine	164.19	1.305, 1.325	1.368

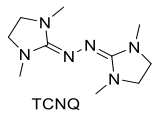
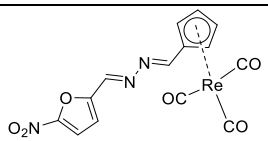
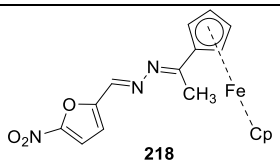
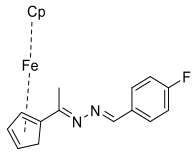
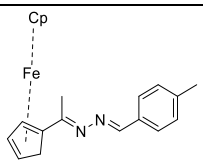
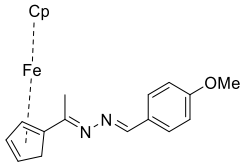
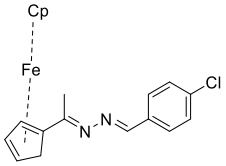
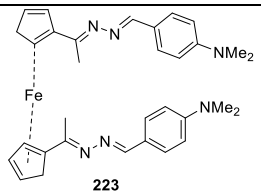
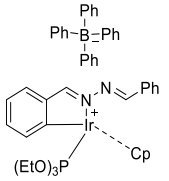
10	 75B	152755[5]	2000	isomerism/tautomerism	176.38	1.319, 1.291	1.397
11	 76	663787[6]	2007	Crystal Structure	178.93	1.294, 1.278	1.407
12	 77_I	1235039[7]	1994	Polymorphism and conformational isomerism	180.00	1.282	1.400
13	 77_II	1235041[7]	1994	Polymorphism and conformational isomerism	142.76	1.282, 1.277	1.400
14	 78_Form A	1239316[8]	1998	Polymorphism	180.00	1.289	1.415
15	 78_Form B	1239317[8]	1998	Polymorphism	123.34	1.289	1.384
16	 79_Form Ia	618474[9]	2006	Isomerism/Polymorphism	180.00	1.280	1.414
17	 79_Form Ib	618471[9]	2006	Isomerism/Polymorphism	180.00	1.273	1.418
18	 167	1207289[4]	1994	Stereochemistry and stereoelectronic study	180.00	1.277	1.397
19	 168	1207286[4]	1994	Stereochemistry and stereoelectronic study	137.99	1.280	1.396
20	 169	1207287[4]	1994	Stereochemistry and stereoelectronic study	134.70	1.280	1.398
21	 170	1207288[4]	1994	Stereochemistry and stereoelectronic study	124.56	1.269	1.380

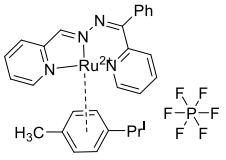
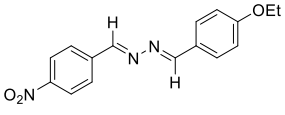
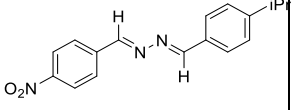
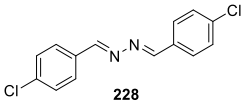
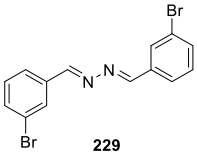
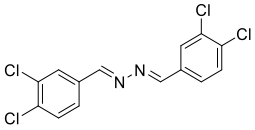
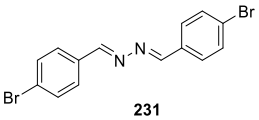
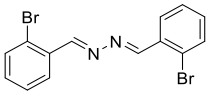
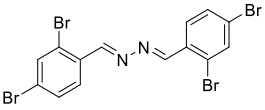
22	 **171**	1173133[10]	1993	Structural properties	167.03	1.332, 1.280	1.388
23	 **172**	1310586[11]	1995	Stereoelectronic, Crystal packing,	131.37°	1.287, 1.289	1.400
24	 **173**	1310587[11]	1995	Stereoelectronic, Crystal packing,	180.00	1.278	1.40 0
25	 **174**	1310589[11]	1995	Stereoelectronic, Crystal packing,	180.00	1.274	1.400
26	 **175**	1310584[11]	1995	Stereochemistry and stereoelectronics, Crystal packing	180.00	1.280	1.400
27	 **176**	1271227[12]	1996	Redox system	180.00	1.290	1.401
28	 **177**	131364[13]	1999	Stereochemistry and stereoelectronics, Crystal packing	174.77	1.282, 1.291	1.407
29	 **178**	101729[14]	1999	Structural studies	180.00	1.265	1.427
30	 **179**	101730[14]	1999	Structural studies	180.00	1.280	1.426
31	 **180**	143276[15]	2000	Solid state structure of mixed azine, application in NLO	137.05	1.288, 1.300	1.392
32	 **181**	165429[16]	2000	Stereoelectronic, stereochemistry, crystal packing for NLO property	144.34	1.300, 1.287	1.396
33	 **182**	200519[17]	2002	Metal coordination	176.00	1.287, 1.304	1.422

34	 **183**	200520[17]	2002	Metal coordination	140.01	1.331, 1.278	1.390
35	 **184**	200521[17]	2002	Metal coordination	140.01	1.286, 1.356	1.398
36	 **185**	200522[17]	2002	Metal coordination	169.89	1.299, 1.280	1.425
37	 **186**	200524[17]	2002	Metal coordination	180.00	1.356	1.448
38	 **187**	197370	2002	Single crystal XRD	180.00	1.286	1.387
39	 **188**	201672[18]	2003	Structural and thermal studies	180.00	1.294,	1.391
40	 **189**	231064[19]	2004	Crystal structure	180.00	1.293	1.400
41	 **190**	245919[20]	2004	Crystal structure	180.00	1.280	1.398
42	 **191**	224827[21]	2004	Crystals tructure and to study the possibility of intramolecular proton transfer	180.00	1.280, 1.280	1.400
43	 **192**	608352[22]	2006	Crystal structure, Can be used as a ligand	180.00	1.267	1.410
44	 **193**	600895[23]	2006	Complexation	169.05	1.260, 1.290	1.410

45	 **194**	659988[24]	2007	Metal coordination	176.02	1.363, 1.302	1.360
46	 **195**	651498[25]	2007	Crystal structure	180.00	1.268	1.268
47	 **196**	641726	2007	Crystal structure	180.00	1.280, 1.280	1.400
48	 **197**	680631[26]	2008	Crystal structure	180.00	1.280	1.400
49	 **198**	758263[27]	2009	Crystal structure	180.00	1.267	1.412
50	 **199**	766128[28]	2010	Building block for conducting molecular materials	179.34	1.303, 1.303	1.410
51	 **200**	766128[28]	2010	Building block for conducting molecular materials	177.00	1.290, 1.300	1.421
52	 **201**	765127[29]	2010	Crystal structure, (previously identified as NLO)	148.47	1.290	1.387
53	 **202**		2010	Antibacterial azines	150.43	1.285	1.400
54	 **203**	786543[30]	2010	Crystal structure	164.25	1.290, 1.275	1.410
55	 **204**	741032[31]	2010	Structure and theoretical studies	180.00	1.280	1.410

56	 **205**	811460[32]	2011	Crystal structure	180.00	1.280	1.410
57	 **206**	770438[33]	2011	To study the coordination mode of azines (Chances for catalysis)	158.00	1.320, 1.284	1.416
58	 **207**	784039[33]	2011	To study the coordination mode of azines (Chances for catalysis)	111.00	1.340, 1.350	1.436
59	 **208**	770440[34]	2011	Tuning the properties	158.81	1.287, 1.300	1.413
60	 **209**	770441[34]	2011	Tuning the properties	114.26	1.330, 1.340	1.420
61	 **210**	899718[35]	2012	Structural prosperty (NLO)	180.00	1.280	1.410
62	 **211**	907483[36]	2012	Crystal structure	180.00	1.280	1.410
63	 **212**	969910[37]	2013	analogous to salicylaldehyde azine (analogous to salicylaldehyde azine)	180.00	1.280	1.391
64	 **213**	885009[38]	2013	To Study bent C-N-N angle	167.69	1.288, 1.297	1.396
65	 **214**	1036846[39]	2015	To study Schiff base azine	179.87	1.270	1.280
66	 **215**	1043736[40]	2015	Electronic structure, redox property and coordination chemistry	180.00	1.295	1.427

67	 TCNQ **216**	1043732[40]	2015	Electronic structure, redox property and coordination chemistry	170.91	1.345 1.346	1.335
68	 **217**	1415028[41]	2015	Structural chemistry and electrochemistry	170.79	1.280, 1.278	1.420
69	 **218**	1415029[41]	2015	Structural chemistry and electrochemistry	170.65	1.257, 1.280	1.421
70	 **219**	1548571[36]	2017	To study extent of conjugation	177.04	1.280 , 1.265	1.409
71	 **220**	1548572[42]	2017	To study extent of conjugation	177.72	1.283, 1.267	1.413
72	 **221**	1548573[36]	2017	To study extent of conjugation	174.23	1.273, 1.268	1.402
73	 **222**	1548574[36]	2017	To study extent of conjugation	162.16°	1.284 Å, 1.268 Å	1.400 Å
74	 **223**	1548575[36]	2017	To study extent of conjugation	163.58	1.280, 1.278	1.412
75	 **224**	1553138[43]	2017	Coordination chemistry	154.07	1.296, 1.278	1.400

76	 **225**	1554273[44]	2017	Coordination chemistry	113.00	1.280, 1.290	1.392
77	 **226**	1533855[39]	2017	Solid state structure and polarization effect	165.21	1.282, 1.278	1.400
78	 **227**	1489316	2017	Quantum chemical and structural investigation (directional dihedral interactions)	173.67	1.277, 1.280	1.400
79	 **228**	1551264[45]	2018	Crystal structure determination	180.00	1.282	1.412
80	 **229**	1551265[45]	2018	Crystal structure determination	180.00	1.284	1.407
81	 **230**	1551266[45]	2018	Crystal structure determination	180.00	1.277	1.402
82	 **231**	1551267[45]	2018	Crystal structure determination	180.00	1.282	1.410
83	 **232**	1551268[45]	2018	Crystal structure determination	180.00	1.279	1.412
84	 **233**	1551268[45]	2018	Crystal structure determination	180.00	1.266	1.409

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