Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Optimal arrangement of π-conjugated anionic groups in hydro-isocyanurates leads to large optical anisotropy and second-harmonic generation effect

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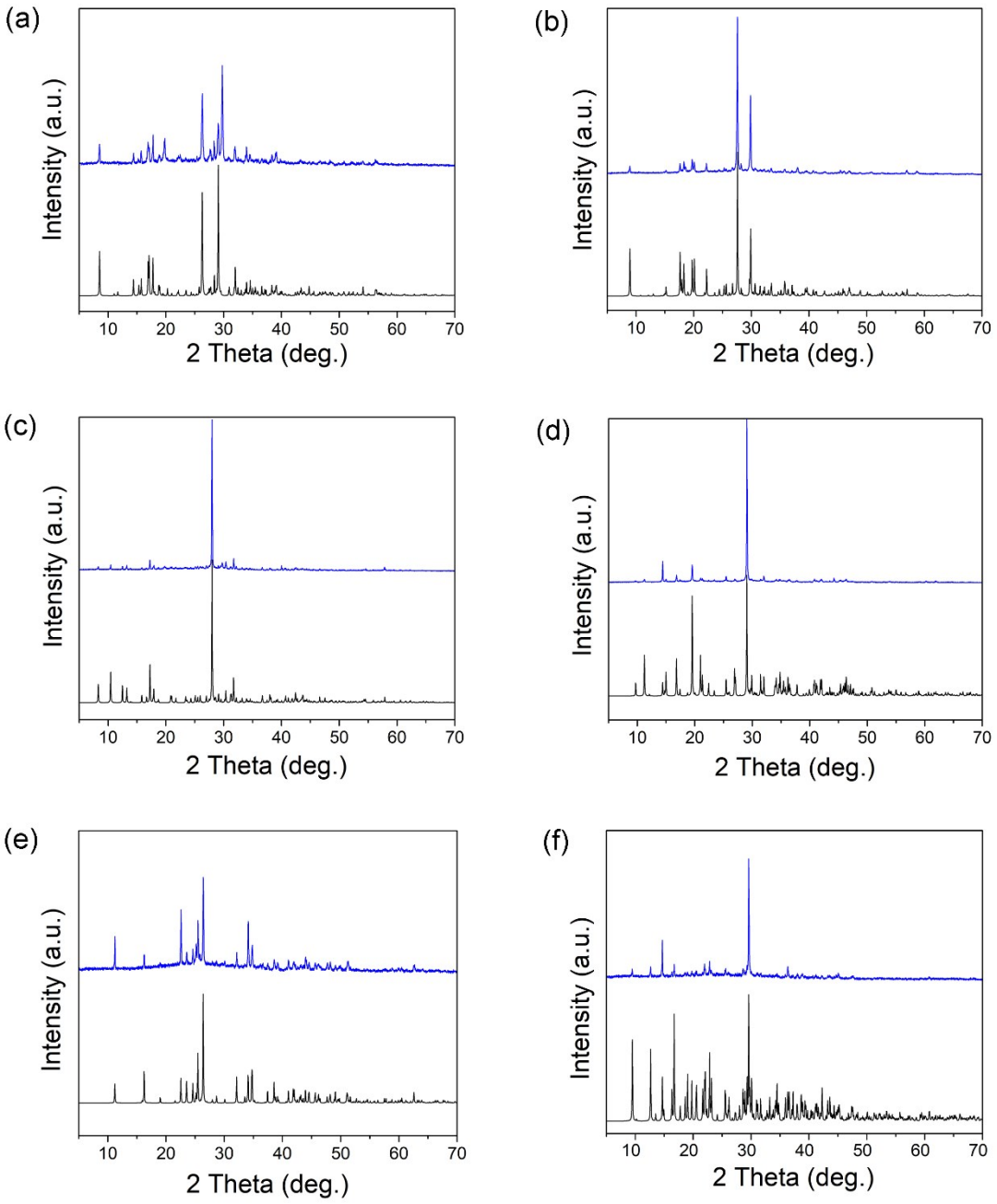

Figure S1. Powder XRD patterns of (a) **I**, (b) **II**, (c) **III**, (d) **IV**, (e) **VI** and (f) **VIII**.

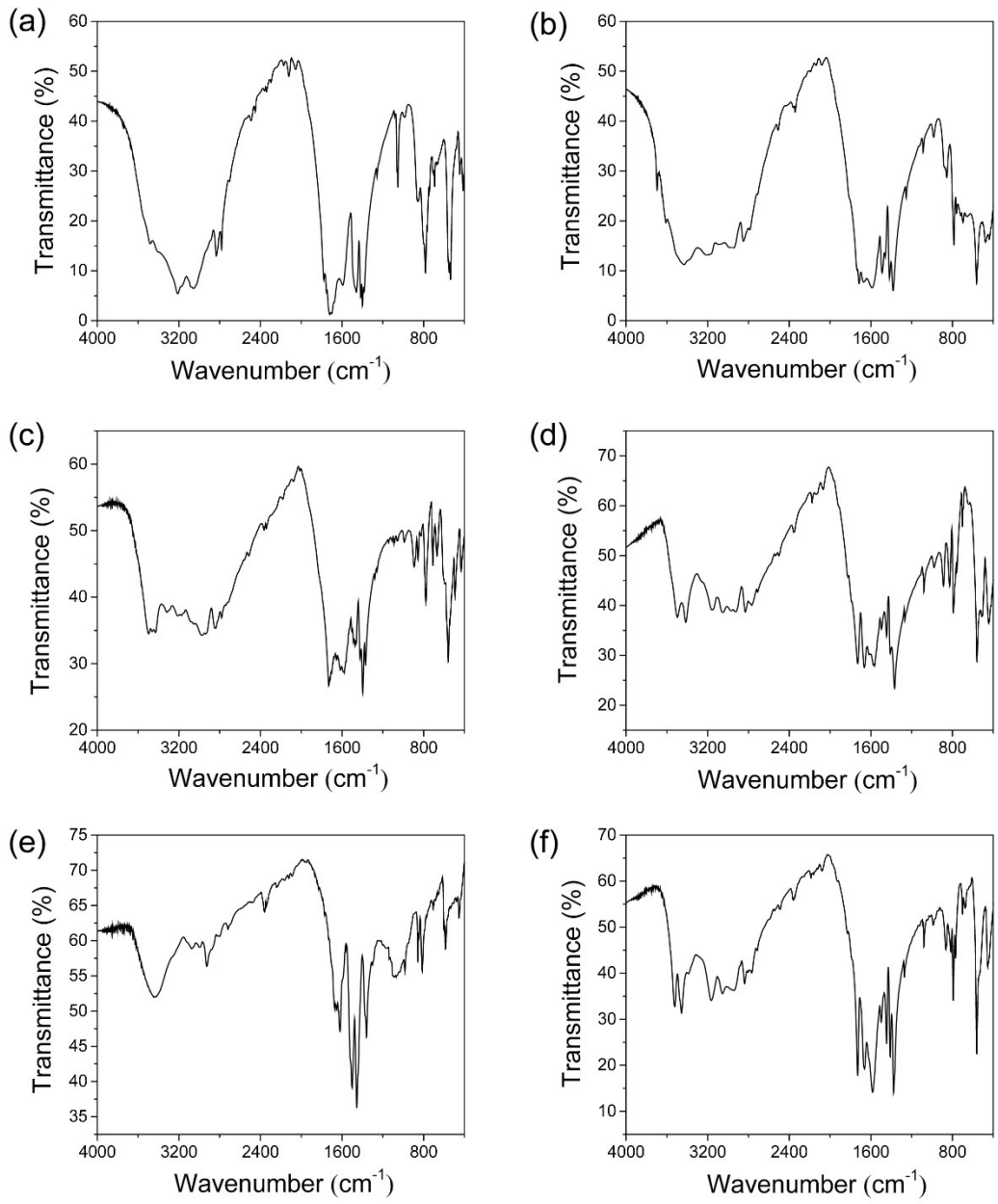

Figure S2. IR spectra of (a) **I**, (b) **II**, (c) **III**, (d) **IV**, (e) **VI** and (f) **VIII**.

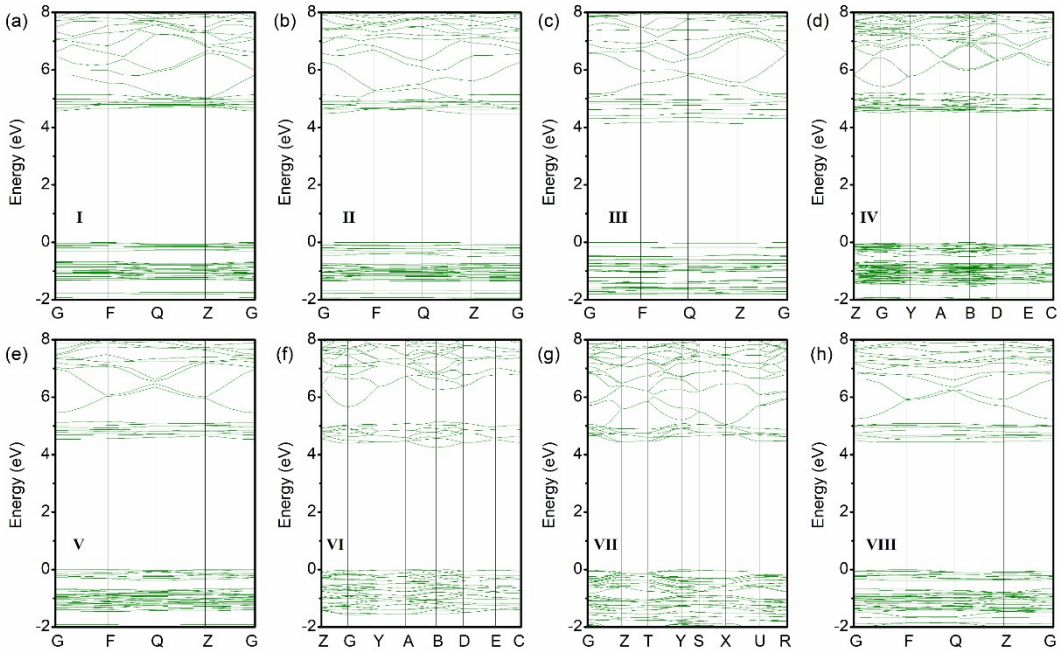

Figure S3. The simulated band structures of **I - VIII**.

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **I**.

	x	*y*	*z*	*U*iso*/*U*eq
Mg1	0.0000	0.0000	1.0000	0.02032(14)
Mg2	0.5000	0.0000	0.5000	0.02025(14)
C1	0.76979(18)	0.60135(11)	0.69589(10)	0.0229(2)
C2	0.73785(17)	0.39841(11)	0.80084(10)	0.0214(2)
C3	0.74388(19)	0.40901(11)	0.60443(10)	0.0257(3)
C4	0.76431(18)	0.60182(11)	0.08850(10)	0.0233(2)
C5	0.75583(17)	0.60946(11)	0.28419(10)	0.0226(2)
C6	0.72814(17)	0.40819(11)	0.20648(10)	0.0219(2)
N1	0.75726(16)	0.52756(9)	0.79469(8)	0.0249(2)
N2	0.73705(15)	0.47967(9)	0.29563(8)	0.0242(2)
N3	0.76030(17)	0.53899(10)	0.60112(8)	0.0272(2)
N4	0.77118(16)	0.66829(9)	0.17935(8)	0.0244(2)
N5	0.73341(16)	0.34025(10)	0.70449(9)	0.0251(2)
N6	0.73971(16)	0.47343(10)	0.10298(8)	0.0250(2)
O1	0.72434(14)	0.34371(8)	0.89744(7)	0.0287(2)
O2	0.38003(16)	−0.15641(9)	0.57175(8)	0.0334(2)
O3	0.71061(14)	0.29343(8)	0.21764(8)	0.0301(2)
O4	0.78825(15)	0.71528(8)	0.69472(8)	0.0329(2)
O5	0.73900(18)	0.36147(9)	0.51249(8)	0.0416(3)
O6	0.75902(15)	0.66516(9)	0.37218(7)	0.0315(2)
O7	0.55583(15)	0.92698(10)	0.83560(9)	0.0354(2)
O8	0.46281(15)	0.08740(9)	0.64927(8)	0.0318(2)
O9	0.94115(14)	0.09038(10)	0.65427(8)	0.0312(2)
O10	0.78033(16)	0.64960(9)	−0.01053(8)	0.0343(2)
O11	0.28499(13)	−0.09205(9)	1.03376(8)	0.0287(2)
O12	0.21683(13)	0.08867(9)	0.46370(8)	0.0271(2)

O13	0.02993(14)	0.15244(8)	1.08916(8)	0.0291(2)
O14	0.11831(14)	0.08429(9)	0.85240(8)	0.0273(2)

Table S2. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **II**.

	x	*y*	*z*	*U*iso*/*U*eq
Mg1	0.0000	1.0000	0.0000	0.02778(16)
Mg2	0.5000	0.5000	0.0000	0.02731(16)
C1	0.33342(15)	0.43381(14)	0.47866(12)	0.0254(3)
C2	0.75833(15)	0.86838(14)	0.69237(12)	0.0265(3)
C3	0.13635(15)	0.63175(14)	0.47558(12)	0.0243(3)
C4	0.72630(16)	1.04044(14)	0.48709(12)	0.0270(3)
C5	0.56297(15)	1.06668(14)	0.70137(12)	0.0239(3)
C6	0.15771(16)	0.46591(14)	0.68711(13)	0.0262(3)
N1	0.80229(13)	0.91813(12)	0.55593(10)	0.0282(2)
H1	0.8813	0.8696	0.5124	0.034*
N2	0.60383(13)	1.11024(12)	0.56425(10)	0.0262(2)
H2	0.5488	1.1859	0.5252	0.031*
N3	0.63850(14)	0.94420(13)	0.76490(11)	0.0295(3)
N4	0.28111(13)	0.39088(12)	0.61517(11)	0.0286(3)
H4	0.3293	0.3125	0.6568	0.034*
N5	0.08878(13)	0.58756(12)	0.61259(11)	0.0277(2)
H5	0.0109	0.6402	0.6530	0.033*
N6	0.25884(13)	0.55344(12)	0.40902(10)	0.0263(2)
O1	0.06125(12)	0.74404(10)	0.41891(9)	0.0337(2)
O2	0.42972(15)	0.66077(14)	−0.15735(11)	0.0463(3)
O3	0.83296(13)	0.75352(11)	0.74410(10)	0.0381(3)
O4	0.45400(11)	1.14595(10)	0.76189(9)	0.0310(2)
O5	0.76265(14)	1.08505(12)	0.36595(10)	0.0440(3)
O6	0.11201(12)	0.42812(12)	0.80815(9)	0.0365(2)
O7	−0.01305(14)	0.94716(13)	0.20257(10)	0.0414(3)
O8	0.39024(16)	0.63639(12)	0.13891(11)	0.0452(3)

O9	0.24304(13)	1.03509(14)	−0.01206(10)	0.0423(3)
O10	0.44966(12)	0.35729(11)	0.42463(9)	0.0339(2)
O11	0.28943(15)	0.40339(15)	0.01698(11)	0.0498(3)
O12	0.07666(16)	0.77588(14)	−0.01603(15)	0.0557(3)

Table S3. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **III.**

	x	y	z	Uiso*/Ueq
Ca1	0.04791(4)	−0.01366(3)	0.32517(3)	0.02231(11)
C1	0.0214(2)	0.64509(15)	0.29167(13)	0.0195(3)
C2	0.2334(2)	0.65422(15)	0.48824(13)	0.0211(3)
C3	0.5153(2)	0.39873(15)	0.75739(13)	0.0195(3)
C4	0.7126(2)	0.39302(15)	0.95615(13)	0.0206(3)
C5	0.6356(2)	0.64639(16)	0.89205(13)	0.0217(3)
C6	0.1154(2)	0.40102(15)	0.36031(13)	0.0204(3)
N1	0.01374(18)	0.48252(13)	0.27239(11)	0.0225(3)
N2	0.22519(18)	0.49062(13)	0.46640(11)	0.0228(3)
N3	0.60680(18)	0.31606(13)	0.84504(11)	0.0217(3)
N4	0.72539(19)	0.55659(13)	0.97728(11)	0.0240(3)
N5	0.52801(18)	0.56213(13)	0.78185(11)	0.0233(3)
N6	0.12771(18)	0.72874(13)	0.39901(11)	0.0216(3)
O1	−0.1728(2)	0.02256(14)	0.13476(12)	0.0509(4)
O2	0.33785(18)	−0.01752(13)	0.25172(12)	0.0338(3)
O3	0.10840(17)	0.25650(11)	0.34437(10)	0.0293(3)
O4	−0.07196(16)	0.71494(11)	0.20748(9)	0.0253(2)
O5	−0.22508(16)	−0.03533(12)	0.43552(10)	0.0262(2)
O6	0.41811(15)	0.33481(11)	0.65136(9)	0.0263(2)
O7	0.80103(17)	0.32482(12)	1.04252(10)	0.0299(3)
O8	0.65079(18)	0.79130(12)	0.91295(10)	0.0320(3)
O9	0.33625(17)	0.72500(12)	0.58918(10)	0.0309(3)

Table S4. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **IV.**

	x	*y*	*z*	*U*iso*/*U*eq
Sr1	0.09015(2)	0.518046(15)	0.203863(15)	0.01653(6)
C1	0.8068(3)	0.16837(17)	−0.07132(17)	0.0169(3)
C2	0.6255(3)	0.00913(17)	0.11481(17)	0.0164(3)
C3	0.5554(3)	0.27537(17)	0.11630(17)	0.0173(3)
C4	0.2173(3)	0.70124(17)	0.47662(18)	0.0180(3)
C5	0.0613(3)	0.80152(17)	0.69717(18)	0.0174(3)
C6	0.2413(3)	0.96050(17)	0.51012(17)	0.0177(3)
N1	0.6972(2)	0.28939(14)	−0.00817(15)	0.0184(3)
N2	0.7681(2)	0.03028(14)	−0.01092(15)	0.0172(3)
N3	0.5243(2)	0.13580(15)	0.17717(15)	0.0190(3)
N4	0.1068(2)	0.68522(15)	0.61202(15)	0.0200(3)
N5	0.1247(2)	0.93851(14)	0.64500(15)	0.0184(3)
N6	0.2902(2)	0.83793(15)	0.43015(15)	0.0210(3)
O1	0.9441(2)	0.17846(13)	−0.18464(13)	0.0245(3)
O2	0.45099(19)	0.38244(12)	0.18201(13)	0.0230(3)
O3	0.59045(19)	−0.11416(12)	0.16666(13)	0.0229(3)
O4	0.2607(2)	0.59982(12)	0.39081(13)	0.0235(3)
O5	0.2955(2)	1.08277(12)	0.46403(13)	0.0253(3)
O6	−0.0394(2)	0.78870(13)	0.82338(13)	0.0247(3)
O7	−0.2191(2)	0.58551(14)	0.08018(14)	0.0237(3)
O8	−0.2224(2)	0.63659(14)	0.39989(15)	0.0322(3)

Table S5. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **V**.

	x	*y*	*z*	*U*iso*/*U*eq
Sr1	0.09015(2)	0.518046(15)	0.203863(15)	0.01653(6)
C1	0.8068(3)	0.16837(17)	−0.07132(17)	0.0169(3)
C2	0.6255(3)	0.00913(17)	0.11481(17)	0.0164(3)
C3	0.5554(3)	0.27537(17)	0.11630(17)	0.0173(3)
C4	0.2173(3)	0.70124(17)	0.47662(18)	0.0180(3)
C5	0.0613(3)	0.80152(17)	0.69717(18)	0.0174(3)
C6	0.2413(3)	0.96050(17)	0.51012(17)	0.0177(3)
N1	0.6972(2)	0.28939(14)	−0.00817(15)	0.0184(3)
N2	0.7681(2)	0.03028(14)	−0.01092(15)	0.0172(3)
N3	0.5243(2)	0.13580(15)	0.17717(15)	0.0190(3)
N4	0.1068(2)	0.68522(15)	0.61202(15)	0.0200(3)
N5	0.1247(2)	0.93851(14)	0.64500(15)	0.0184(3)
N6	0.2902(2)	0.83793(15)	0.43015(15)	0.0210(3)
O1	0.9441(2)	0.17846(13)	−0.18464(13)	0.0245(3)
O2	0.45099(19)	0.38244(12)	0.18201(13)	0.0230(3)
O3	0.59045(19)	−0.11416(12)	0.16666(13)	0.0229(3)
O4	0.2607(2)	0.59982(12)	0.39081(13)	0.0235(3)
O5	0.2955(2)	1.08277(12)	0.46403(13)	0.0253(3)
O6	−0.0394(2)	0.78870(13)	0.82338(13)	0.0247(3)
O7	−0.2191(2)	0.58551(14)	0.08018(14)	0.0237(3)
O8	−0.2224(2)	0.63659(14)	0.39989(15)	0.0322(3)

Table S6. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **VI.**

	x	*y*	*z*	*U*iso*/*U*eq
Sr1	0.53346(2)	0.35554(2)	0.63197(2)	0.01400(12)
C1	0.0553(3)	0.1233(2)	0.4330(3)	0.0146(5)
C2	0.2137(3)	0.1211(2)	0.2475(3)	0.0151(5)
C3	0.3162(3)	0.1612(2)	0.4511(3)	0.0159(6)
C4	0.7440(3)	0.1605(2)	0.8059(3)	0.0147(5)
C5	1.0079(3)	0.1332(2)	0.8262(3)	0.0147(6)
C6	0.8484(3)	0.1299(2)	1.0101(3)	0.0151(6)
N1	0.0762(2)	0.1120(2)	0.3028(2)	0.0157(5)
N2	0.3316(3)	0.14610(19)	0.3220(2)	0.0177(5)
N3	0.1785(3)	0.14473(19)	0.5051(2)	0.0174(5)
N4	0.7296(3)	0.15125(19)	0.9353(2)	0.0168(5)
N5	0.8830(3)	0.14970(19)	0.7528(2)	0.0170(5)
N6	0.9857(3)	0.1233(2)	0.9561(2)	0.0156(5)
O1	0.6437(2)	0.4135(2)	0.8616(2)	0.0289(5)
O2	0.5780(2)	0.56955(18)	0.6137(2)	0.0211(4)
O3	−0.0679(2)	0.11705(18)	0.4812(2)	0.0203(4)
O4	0.2259(2)	0.1061(2)	0.12805(19)	0.0225(4)
O5	0.4186(2)	0.18789(18)	0.52517(19)	0.0207(4)
O6	0.6386(2)	0.17678(18)	0.72999(19)	0.0204(4)
O7	1.1308(2)	0.12851(18)	0.7780(2)	0.0217(5)
O8	0.8369(2)	0.11655(19)	1.12995(19)	0.0221(4)

Table S7. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **VII.**

	x	*y*	*z*	*U*iso*/*U*eq
Sr1	0.66629(2)	1.21699(3)	0.68446(2)	0.01068(10)
C1	0.6996(3)	0.5985(3)	0.9477(3)	0.0109(4)
C2	0.7403(3)	0.8988(3)	0.9807(2)	0.0105(4)
C3	0.9124(3)	0.6888(3)	1.1370(3)	0.0115(4)
N1	0.6549(3)	0.7673(2)	0.9036(2)	0.0133(4)
N2	0.8722(2)	0.8594(2)	1.0918(2)	0.0127(4)
H2	0.9322	0.9445	1.1349	0.015*
N3	0.8218(2)	0.5551(2)	1.0666(2)	0.0124(4)
O1	0.6153(2)	0.4730(2)	0.87623(19)	0.0159(3)
O2	0.7051(2)	1.0604(2)	0.95459(19)	0.0148(3)
O3	1.0315(2)	0.6657(2)	1.24402(19)	0.0165(3)

Table S8. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **VIII.**

	x	*y*	*z*	*U*iso*/*U*eq
Ba1	0.38630(3)	0.76755(3)	1.00001(3)	0.01815(10)
O1	−0.0157(4)	1.1853(4)	0.8767(3)	0.0256(7)
O2	0.6841(5)	0.5386(4)	0.8782(4)	0.0279(7)
O3	0.1448(5)	0.5993(4)	0.8818(4)	0.0311(8)
O4	0.7232(5)	0.9072(4)	0.9132(4)	0.0290(7)
O6	0.4367(5)	0.8028(4)	0.6844(3)	0.0272(7)
O7	0.1041(5)	1.1621(4)	0.3927(3)	0.0255(7)
O8	0.2048(4)	0.5321(4)	0.4069(3)	0.0240(7)
N1	0.2129(5)	0.9891(4)	0.7902(4)	0.0202(8)
N2	0.0415(5)	1.1737(4)	0.6370(4)	0.0209(8)
N3	0.2740(5)	0.9837(4)	0.5363(4)	0.0185(7)
N4	0.3548(5)	0.3871(4)	0.8001(4)	0.0218(8)
N5	0.3852(5)	0.3594(4)	0.5499(4)	0.0185(7)
N6	0.1700(5)	0.5611(4)	0.6468(4)	0.0222(8)
C1	0.1376(6)	1.1106(5)	0.5140(5)	0.0192(8)
C2	0.4386(6)	0.3089(5)	0.6853(5)	0.0173(8)
C3	0.2503(6)	0.4869(5)	0.5264(5)	0.0174(8)
C4	0.2221(6)	0.5170(5)	0.7829(5)	0.0202(9)
C5	0.0778(6)	1.1164(5)	0.7739(5)	0.0183(8)
C6	0.3106(6)	0.9210(5)	0.6735(5)	0.0186(8)
O5	0.5651(5)	0.1908(4)	0.6975(3)	0.0268(7)

Table S9. Select bond lengths (Å) and angles (°) for **I**.

Mg1-O13^{i}	2.0398(9)	C2-O1	1.2425(15)
Mg1-O13	2.0398(9)	C2-N5	1.3402(16)
Mg1-O14^{i}	2.0506(9)	C2-N1	1.3874(15)
Mg1-O14	2.0506(9)	C3-O5	1.2378(16)
Mg1-O11^{i}	2.1059(9)	C3-N5	1.3427(16)
Mg1-O11	2.1059(9)	C3-N3	1.3922(16)
Mg2-O8^{ii}	2.0226(9)	C4-O10	1.2412(15)
Mg2-O8	2.0226(9)	C4-N4	1.3363(16)
Mg2-O2	2.0589(9)	C4-N6	1.3894(15)
Mg2-O2^{ii}	2.0589(9)	C5-O6	1.2373(15)
Mg2-O12^{ii}	2.0932(9)	C5-N4	1.3464(16)
Mg2-O12	2.0932(9)	C5-N2	1.3924(15)
C1-O4	1.2290(15)	C6-O3	1.2329(15)
C1-N3	1.3554(16)	C6-N2	1.3547(16)
C1-N1	1.3579(15)	C6-N6	1.3602(15)
O4-C1-N3	123.85(11)	O6-C5-N4	123.04(11)
O4-C1-N1	121.59(11)	O6-C5-N2	117.69(11)
N3-C1-N1	114.55(10)	N4-C5-N2	119.27(10)
O1-C2-N5	123.90(11)	O3-C6-N2	123.06(11)
O1-C2-N1	116.85(10)	O3-C6-N6	122.43(11)
N5-C2-N1	119.25(10)	N2-C6-N6	114.51(10)
O5-C3-N5	122.48(11)	C1-N1-C2	123.98(10)
O5-C3-N3	117.31(11)	C6-N2-C5	123.61(10)
N5-C3-N3	120.21(11)	C1-N3-C3	122.76(10)
O10-C4-N4	122.75(11)	C4-N4-C5	119.45(10)
O10-C4-N6	117.36(11)	C2-N5-C3	119.22(10)
N4-C4-N6	119.89(10)	C6-N6-C4	123.23(10)

Symmetry codes: (i) $-x$, $-y$, $-z+2$; (ii) $-x+1$, $-y$, $-z+1$.

Table S10. Select bond lengths (Å) and angles (°) for **II**.

Mg1-O7^{i}	2.0142(9)	C2-O3	1.2393(16)
Mg1-O7	2.0142(9)	C2-N3	1.3481(17)
Mg1-O9	2.0642(11)	C2-N1	1.3807(16)
Mg1-O9^{i}	2.0642(11)	C3-O1	1.2433(16)
Mg1-O12^{i}	2.1109(12)	C3-N6	1.3437(17)
Mg1-O12	2.1109(12)	C3-N5	1.3822(16)
Mg2-O11	2.0178(11)	C4-O5	1.2237(16)
Mg2-O11^{ii}	2.0178(11)	C4-N2	1.3580(16)
Mg2-O2	2.0824(10)	C4-N1	1.3616(17)
Mg2-O2^{ii}	2.0824(10)	C5-O4	1.2516(15)
Mg2-O8^{ii}	2.0870(10)	C5-N3	1.3380(17)
Mg2-O8	2.0870(10)	C5-N2	1.3747(16)
C1-O10	1.2448(16)	C6-O6	1.2246(16)
C1-N6	1.3432(16)	C6-N5	1.3580(17)
C1-N4	1.3827(17)	C6-N4	1.3593(17)
O10-C1-N6	122.37(11)	O4-C5-N3	122.60(11)
O10-C1-N4	117.50(11)	O4-C5-N2	117.19(11)
N6-C1-N4	120.14(11)	N3-C5-N2	120.21(11)
O3-C2-N3	122.15(11)	O6-C6-N5	122.62(12)
O3-C2-N1	117.66(11)	O6-C6-N4	123.48(12)
N3-C2-N1	120.19(11)	N5-C6-N4	113.91(11)
O1-C3-N6	122.73(11)	C4-N1-C2	123.05(11)
O1-C3-N5	117.40(11)	C4-N2-C5	123.64(11)
N6-C3-N5	119.87(11)	C5-N3-C2	118.53(11)
O5-C4-N2	121.89(12)	C6-N4-C1	123.56(11)
O5-C4-N1	123.84(12)	C6-N5-C3	123.89(11)
N2-C4-N1	114.27(11)	C1-N6-C3	118.61(11)

Symmetry codes: (i) $-x$, $-y+2$, $-z$; (ii) $-x+1$, $-y+1$, $-z$.

Table S11. Select bond lengths (Å) and angles (°) for **III**.

Ca1-O3	2.2913(10)	C3-O6	1.2477(17)
Ca1-O2	2.3201(12)	C3-N3	1.3379(18)
Ca1-O1	2.3689(12)	C3-N5	1.3885(17)
Ca1-O5	2.4601(11)	C4-O7	1.2428(17)
Ca1-N6^{i}	2.5003(11)	C4-N3	1.3425(18)
Ca1-O4^{i}	2.5078(10)	C4-N4	1.3877(18)
Ca1-O5^{ii}	2.6147(11)	C5-O8	1.2290(17)
C1-O4	1.2478(17)	C5-N4	1.3568(18)
C1-N6	1.3345(18)	C5-N5	1.3617(19)
C1-N1	1.3813(17)	C6-O3	1.2274(16)
C2-O9	1.2363(17)	C6-N2	1.3531(18)
C2-N6	1.3444(18)	C6-N1	1.3604(17)
C2-N2	1.3911(17)	O8-C5-N4	122.65(13)
O4-C1-N1	119.60(12)	O8-C5-N5	123.14(13)
N6-C1-N1	120.96(12)	N4-C5-N5	114.21(12)
O9-C2-N6	122.69(12)	O3-C6-N2	122.40(13)
O9-C2-N2	118.75(12)	O3-C6-N1	122.35(13)
N6-C2-N2	118.56(12)	N2-C6-N1	115.25(11)
O6-C3-N3	122.46(12)	C6-N1-C1	121.90(12)
O6-C3-N5	117.29(12)	C6-N2-C2	123.78(12)
N3-C3-N5	120.25(12)	C3-N3-C4	119.25(12)
O7-C4-N3	123.15(12)	C5-N4-C4	124.04(12)
O7-C4-N4	117.59(12)	C5-N5-C3	122.97(12)
N3-C4-N4	119.26(12)	C1-N6-C2	119.53(11)
O4-C1-N6	119.45(12)		

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, -y, -z+1$; (iii) $x, y+1, z$.

Table S12. Select bond lengths (Å) and angles (°) for **IV**.

Sr1-O5	2.546(2)	C2-N1	1.388(3)
Sr1-O6	2.589(2)	C3-O5	1.234(3)
Sr1-O1	2.637(2)	C3-N2	1.346(4)
Sr1-O2	2.666(2)	C3-N3	1.394(4)
Sr1-N2^{i}	2.704(2)	C4-O6	1.238(3)
Sr1-N4^{ii}	2.720(2)	C4-N4	1.341(4)
Sr1-O8^{ii}	2.781(2)	C4-N5	1.393(4)
Sr1-O4^{i}	2.836(2)	C5-O7	1.233(4)
Sr1-O2^{iii}	2.848(2)	C5-N6	1.357(4)
C1-O3	1.236(3)	C5-N5	1.364(4)
C1-N3	1.356(4)	C6-O8	1.246(3)
C1-N1	1.358(4)	C6-N4	1.338(4)
C2-O4	1.246(3)	C6-N6	1.379(4)
C2-N2	1.339(4)	O7-C5-N6	122.9(2)
O3-C1-N3	122.7(3)	O7-C5-N5	122.5(3)
O3-C1-N1	122.2(3)	N6-C5-N5	114.5(2)
N3-C1-N1	115.1(2)	O8-C6-N4	120.5(3)
O4-C2-N2	120.5(3)	O8-C6-N6	118.9(3)
O4-C2-N1	119.2(2)	N4-C6-N6	120.6(3)
N2-C2-N1	120.2(2)	C1-N1-C2	122.5(2)
O5-C3-N2	123.3(3)	C2-N2-C3	119.6(2)
O5-C3-N3	117.8(3)	C1-N3-C3	123.4(2)
N2-C3-N3	118.9(2)	C6-N4-C4	119.3(2)
O6-C4-N4	123.0(3)	C5-N5-C4	123.5(2)
O6-C4-N5	117.9(2)	C5-N6-C6	122.9(2)
N4-C4-N5	119.1(2)		

Symmetry codes: (i) x, $-y+1/2$, $z+1/2$; (ii) x, $-y+1/2$, $z-1/2$; (iii) $-x+1$, $-y+1$, $-z+1$.

Table S13. Select bond lengths (Å) and angles (°) for **V**.

Sr1-O2	2.5640(12)	C2-N3	1.363(2)
Sr1-O4	2.5689(12)	C3-O2	1.2411(19)
Sr1-O8	2.6109(13)	C3-N1	1.337(2)
Sr1-O7	2.6761(13)	C3-N3	1.390(2)
Sr1-N4^{i}	2.7006(14)	C4-O4	1.238(2)
Sr1-N1^{ii}	2.7331(14)	C4-N4	1.343(2)
Sr1-O1^{ii}	2.7566(11)	C4-N6	1.392(2)
Sr1-O7^{iii}	2.8584(13)	C5-O6	1.245(2)
Sr1-O6^{i}	2.8771(12)	C5-N4	1.339(2)
C1-O1	1.241(2)	C5-N5	1.387(2)
C1-N1	1.342(2)	C6-O5	1.232(2)
C1-N2	1.383(2)	C6-N6	1.356(2)
C2-N2	1.358(2)	C6-N5	1.358(2)
C2-O3	1.229(2)	O6-C5-N4	120.71(15)
O1-C1-N1	120.64(14)	O6-C5-N5	119.17(14)
O1-C1-N2	118.96(14)	N4-C5-N5	120.11(15)
N1-C1-N2	120.40(14)	O5-C6-N6	122.88(15)
O3-C2-N2	122.46(14)	O5-C6-N5	122.41(15)
O3-C2-N3	123.27(15)	N6-C6-N5	114.70(14)
N2-C2-N3	114.26(14)	C3-N1-C1	119.22(14)
O2-C3-N1	122.80(15)	C2-N2-C1	122.99(13)
O2-C3-N3	117.92(15)	C2-N3-C3	123.77(14)
N1-C3-N3	119.27(14)	C5-N4-C4	119.71(14)
O4-C4-N4	123.36(15)	C6-N5-C5	122.73(14)
O4-C4-N6	117.94(15)	C6-N6-C4	123.79(14)
N4-C4-N6	118.70(14)		

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*, −*y*+1, −*z*.

Table S14. Select bond lengths (Å) and angles (°) for **VI**.

Sr1-O2	2.5224(15)	C1-N1	1.365(3)
Sr1-O1^{i}	2.5525(16)	C1-N3	1.362(3)
Sr1-O3^{ii}	2.5728(17)	C2-O2	1.267(3)
Sr1-O2^{iii}	2.5727(16)	C2-N1	1.335(3)
Sr1-N1^{iv}	2.613(2)	C2-N2	1.366(3)
Sr1-N3^{v}	2.6225(18)	C3-O3	1.252(3)
Sr1-O1^{iv}	2.9032(17)	C3-N3	1.343(3)
Sr1-O1^{v}	2.9227(17)	C3-N2	1.372(3)
C1-O1	1.277(3)	O3-C3-N3	123.1(2)
O1-C1-N1	117.1(2)	O3-C3-N2	117.9(2)
O1-C1-N3	117.97(19)	N3-C3-N2	119.0(2)
N1-C1-N3	124.8(2)	C2-N1-C1	117.2(2)
O2-C2-N1	122.7(2)	C2-N2-C3	122.39(19)
O2-C2-N2	118.1(2)	C3-N3-C1	117.02(18)
N1-C2-N2	119.22(19)		

Symmetry codes: (i) *x*, *y*+1, *z*;(ii) −*x*+2, −*y*+2, −*z*+2;(iii) *x*, −*y*+5/2, *z*−1/2;(iv) −*x*+1, *y*+1/2, −*z*+3/2;(v) *x*, −*y*+3/2, *z*−1/2;(vi) *x*, −*y*+5/2, *z*+1/2;(vii) *x*, −*y*+3/2, *z*+1/2;(viii) −*x*+1, *y*−1/2, −*z*+3/2;(ix) *x*, *y*−1, *z*.

Table S15. Select bond lengths (Å) and angles (°) for **VII**.

Sr1-O1	2.5789(18)	C1-O2	1.262(3)
Sr1-N1^{i}	2.617(2)	C1-N2	1.340(4)
Sr1-O3^{i}	2.6230(17)	C1-N3	1.367(4)
Sr1-O4	2.628(3)	C2-O1	1.262(4)
Sr1-O6	2.6377(19)	C2-N1	1.324(5)
Sr1-O4^{ii}	2.671(3)	C2-N3	1.377(4)
Sr1-O6^{iii}	2.706(2)	C3-O3	1.254(4)
Sr1-O1^{iv}	2.8091(17)	C3-N2	1.360(3)
Sr1-O5	2.9179(18)	C3-N1	1.365(4)
O2-C1-N2	120.8(3)	O3-C3-N2	119.5(2)
O2-C1-N3	119.1(3)	O3-C3-N1	116.4(2)
N2-C1-N3	120.1(3)	N2-C3-N1	124.1(2)
O1-C2-N1	122.3(3)	C2-N1-C3	118.6(2)
O1-C2-N3	119.0(4)	C1-N2-C3	116.8(2)
N1-C2-N3	118.7(3)	C1-N3-C2	121.5(3)

Symmetry codes: (i) x, y, z+1; (ii) x, −y+3/2, z−1/2; (iii) −x+2, −y+1, z; (iv) x, −y+3/2, z+1/2; (v) x, y, z−1.

Table S16. Select bond lengths (Å) and angles (°) for **VIII**.

Ba1-O1^{i}	2.724(3)	O8-C3	1.224(5)
Ba1-O2	2.830(3)	N1-C6	1.343(6)
Ba1-O3	2.878(4)	N1-C5	1.344(5)
Ba1-N1	2.880(4)	N2-C1	1.368(6)
Ba1-N4^{ii}	2.884(4)	N2-C5	1.381(6)
Ba1-O4	2.925(4)	N3-C1	1.356(5)
Ba1-O6	2.941(3)	N3-C6	1.396(6)
Ba1-O2^{ii}	2.965(4)	N4-C2	1.341(6)
Ba1-O5^{ii}	2.974(3)	N4-C4	1.351(5)
Ba1-O4^{iii}	2.984(4)	N5-C3	1.355(5)
O1-C5	1.235(5)	N5-C2	1.390(5)
O3-C4	1.234(5)	N6-C3	1.360(6)
O6-C6	1.245(5)	N6-C4	1.383(6)
O7-C1	1.228(5)	C2-O5	1.248(5)
C6-N1-C5	119.5(4)	O8-C3-N5	122.9(4)
C1-N2-C5	124.1(4)	O8-C3-N6	122.7(4)
C1-N3-C6	122.7(4)	N5-C3-N6	114.4(4)
C2-N4-C4	119.7(4)	O3-C4-N4	123.8(4)
C3-N5-C2	123.0(4)	O3-C4-N6	117.9(4)
C3-N6-C4	124.5(4)	N4-C4-N6	118.4(4)
O7-C1-N3	121.9(4)	O1-C5-N1	122.6(4)
O7-C1-N2	123.7(4)	O1-C5-N2	118.2(4)
N3-C1-N2	114.4(4)	N1-C5-N2	119.1(4)
O5-C2-N4	121.1(4)	O6-C6-N1	121.3(4)
O5-C2-N5	118.9(4)	O6-C6-N3	118.6(4)
N4-C2-N5	120.0(4)	N1-C6-N3	120.1(4)

Symmetry codes: (i) −*x*, −*y*+2, −*z*+2; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) −*x*+1, −*y*+2, −*z*+2.