Electronic Supplementary Information

Syntheses, Structures, Photochromic and Magnetic Properties of Seven Lanthanide Complexes Based on 5-Azotetrazolyl Salicylic Acid Ligand

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Table S1 Cartesian coordinates of π⁻–π staking interaction in **1**.

	X	Y	Z
N(Fragment=1)	1.98040000	7.44020000	21.26570000
N(Fragment=1)	1.24120000	6.89410000	19.30610000
N(Fragment=1)	3.27330000	6.27980000	18.23920000
O(Fragment=1)	9.91950000	5.40770000	16.20080000
O(Fragment=1)	9.44400000	6.02510000	18.27470000
O(Fragment=1)	8.06590000	4.86620000	14.51550000
H(Fragment=1)	8.83920000	4.93700000	14.78020000
N(Fragment=1)	0.90940000	7.34950000	20.52150000
N(Fragment=1)	3.03910000	7.04400000	20.54950000
C(Fragment=1)	7.22650000	5.22640000	15.49170000
C(Fragment=1)	7.65340000	5.61180000	16.77220000
C(Fragment=1)	9.09660000	5.68890000	17.12700000
N(Fragment=1)	4.51230000	6.34310000	18.45710000
C(Fragment=1)	5.34400000	5.95380000	17.39830000
C(Fragment=1)	2.54770000	6.72100000	19.35940000
C(Fragment=1)	5.85610000	5.22940000	15.17910000
H(Fragment=1)	5.57400000	4.97720000	14.32850000
C(Fragment=1)	4.94130000	5.59940000	16.11140000
H(Fragment=1)	4.03760000	5.61570000	15.89000000
C(Fragment=1)	6.69280000	5.95480000	17.71010000
H(Fragment=1)	6.95920000	6.19110000	18.56830000
H(Fragment=1)	0.63333350	6.72332188	18.53064327
H(Fragment=1)	10.24285932	5.73301323	18.71979450
N(Fragment=2)	7.58820000	8.17640000	14.02180000
N(Fragment=2)	8.32740000	8.72250000	15.98140000
N(Fragment=2)	6.29530000	9.33680000	17.04830000
O(Fragment=2)	-0.35090000	10.20890000	19.08670000
O(Fragment=2)	0.12460000	9.59150000	17.01280000
O(Fragment=2)	1.50270000	10.75040000	20.77200000
H(Fragment=2)	0.72940000	10.67960000	20.50730000
N(Fragment=2)	8.65920000	8.26710000	14.76610000
N(Fragment=2)	6.52950000	8.57250000	14.73800000
C(Fragment=2)	2.34220000	10.39020000	19.79580000
C(Fragment=2)	1.91530000	10.00480000	18.51540000
C(Fragment=2)	0.47210000	9.92770000	18.16050000
N(Fragment=2)	5.05640000	9.27340000	16.83040000
C(Fragment=2)	4.22460000	9.66280000	17.88920000
C(Fragment=2)	7.02090000	8.89550000	15.92810000
C(Fragment=2)	3.71260000	10.38720000	20.10840000
H(Fragment=2)	3.99470000	10.63940000	20.95900000
C(Fragment=2)	4.62740000	10.01710000	19.17610000
H(Fragment=2)	5.53110000	10.00090000	19.39750000

C(Fragment=2)	2.87590000	9.66180000	17.57740000
H(Fragment=2)	2.60950000	9.42550000	16.71920000
H(Fragment=2)	-0.68748597	9.86192792	16.57807581

Table S2 Cartesian coordinates of π⁻–π staking interaction in **2**.

	X	Y	Z
O(Fragment=1)	4.73250187	-0.30559854	1.93769976
C(Fragment=1)	5.65630187	-1.14829854	1.90749976
C(Fragment=1)	6.22210187	-1.65929854	3.18849976
C(Fragment=1)	5.62250187	-1.26979854	4.36529976
H(Fragment=1)	4.87920187	-0.71269854	4.33609976
C(Fragment=1)	6.10930187	-1.69559854	5.59249976
C(Fragment=1)	7.35720187	-2.50519854	3.23999976
C(Fragment=1)	7.23380187	-2.52779854	5.62529976
H(Fragment=1)	7.56810187	-2.81339854	6.44379976
C(Fragment=1)	7.84460187	-2.92509854	4.47539976
H(Fragment=1)	8.59060187	-3.47859854	4.51519976
N(Fragment=1)	4.53120187	-0.60899854	6.79879976
N(Fragment=1)	5.56300187	-1.33849854	6.84109976
O(Fragment=1)	8.00590187	-2.91569854	2.15479976
H(Fragment=1)	7.65070187	-2.59839854	1.48709976
C(Fragment=1)	4.04180187	-0.28019854	8.06789976
N(Fragment=1)	4.50280187	-0.68729854	9.23929976
N(Fragment=1)	2.99510187	0.54590146	8.18499976
N(Fragment=1)	2.80120187	0.64400146	9.49529976
N(Fragment=1)	3.69790187	-0.08939854	10.12409976
O(Fragment=1)	6.14890187	-1.61279854	0.84059976
H(Fragment=1)	4.32846397	0.10169591	1.16798254
O(Fragment=2)	3.21149813	3.83869854	8.77950024
O(Fragment=2)	3.82849813	3.85519854	10.86770024
C(Fragment=2)	4.05229813	3.54499854	9.66280024
C(Fragment=2)	5.32439813	2.83529854	9.32900024
C(Fragment=2)	5.64319813	2.55039854	8.02460024
H(Fragment=2)	5.05369813	2.78789854	7.34540024
C(Fragment=2)	6.83839813	1.91059854	7.70370024
C(Fragment=2)	6.21639813	2.46629854	10.34070024
C(Fragment=2)	7.71159813	1.52319854	8.73180024
H(Fragment=2)	8.49959813	1.07479854	8.52690024
C(Fragment=2)	7.40639813	1.80259854	10.02460024
H(Fragment=2)	7.99199813	1.55169854	10.70260024
N(Fragment=2)	8.19179813	1.26279854	6.02380024
N(Fragment=2)	7.04529813	1.69309854	6.33540024
O(Fragment=2)	5.96269813	2.71119854	11.63560024

H(Fragment=2)	5.20359813	3.00909854	11.71310024
C(Fragment=2)	8.34009813	1.07669854	4.64400024
N(Fragment=2)	7.44889813	1.32929854	3.69700024
N(Fragment=2)	9.48679813	0.62949854	4.14890024
H(Fragment=2)	10.19459813	0.40599854	4.58200024
N(Fragment=2)	8.07599813	1.02299854	2.56500024
N(Fragment=2)	9.29829813	0.60599854	2.83490024
H(Fragment=2)	2.33918404	4.20409896	8.94427480

Table S3 Cartesian coordinates of π⁻–π staking interaction in **3**.

	X	Y	Z
O(Fragment=1)	7.43150000	-2.78690000	5.14920000
O(Fragment=1)	7.02060000	-0.88390000	6.21270000
O(Fragment=1)	7.66460000	-2.78740000	2.55210000
H(Fragment=1)	7.82260000	-3.11920000	3.28620000
N(Fragment=1)	7.47720000	2.74520000	2.65220000
N(Fragment=1)	7.33960000	3.33360000	3.76650000
N(Fragment=1)	7.43460000	5.45930000	2.50710000
N(Fragment=1)	7.34050000	6.71860000	2.93800000
N(Fragment=1)	7.11170000	6.73530000	4.21920000
N(Fragment=1)	7.10580000	5.49710000	4.71970000
C(Fragment=1)	7.42670000	-0.80950000	3.89130000
C(Fragment=1)	7.62990000	-1.45440000	2.65800000
C(Fragment=1)	7.75730000	-0.69310000	1.50170000
H(Fragment=1)	7.88380000	-1.12180000	0.68630000
C(Fragment=1)	7.69910000	0.67320000	1.53650000
H(Fragment=1)	7.77670000	1.15850000	0.74720000
C(Fragment=1)	7.52470000	1.34330000	2.74510000
C(Fragment=1)	7.38850000	0.57430000	3.87670000
H(Fragment=1)	7.26250000	1.01330000	4.68630000
C(Fragment=1)	7.27050000	-1.52320000	5.18400000
C(Fragment=1)	7.31270000	4.72950000	3.62860000
H(Fragment=1)	6.95593656	-1.48721615	6.95662760
O(Fragment=2)	4.13680000	6.73110000	5.62510000
O(Fragment=2)	3.81380000	8.28210000	4.11470000
O(Fragment=2)	3.78700000	7.71370000	1.65400000
H(Fragment=2)	3.49990000	8.16410000	2.27640000
N(Fragment=2)	4.12310000	2.39650000	3.11650000
N(Fragment=2)	3.91300000	1.52330000	2.21980000
N(Fragment=2)	3.83380000	-0.84850000	1.95720000
H(Fragment=2)	3.67700000	-0.85340000	1.11140000
N(Fragment=2)	3.95520000	-1.87660000	2.74220000

N(Fragment=2)	4.21010000	-1.48340000	3.97540000
N(Fragment=2)	4.23850000	-0.14250000	3.98560000
C(Fragment=2)	3.97220000	6.02570000	3.34720000
C(Fragment=2)	3.85090000	6.40070000	2.02980000
C(Fragment=2)	3.84650000	5.44040000	1.00400000
H(Fragment=2)	3.79540000	5.70940000	0.11460000
C(Fragment=2)	3.91640000	4.12000000	1.31160000
H(Fragment=2)	3.89200000	3.48020000	0.63690000
C(Fragment=2)	4.02460000	3.72270000	2.66090000
C(Fragment=2)	4.05970000	4.68830000	3.64460000
H(Fragment=2)	4.14590000	4.42800000	4.53250000
C(Fragment=2)	3.98400000	7.03830000	4.41070000
C(Fragment=2)	4.01640000	0.20520000	2.72620000
H(Fragment=2)	4.17277952	7.35481181	6.35399578

Table S4 Cartesian coordinates of π⁻–π staking interaction in **4**.

	X	Y	Z
O(Fragment=1)	10.28780000	4.84980000	1.17500000
C(Fragment=1)	10.43400000	4.87690000	-0.06270000
C(Fragment=1)	10.37170000	3.57700000	-0.81420000
C(Fragment=1)	10.28260000	2.33860000	-0.21610000
C(Fragment=1)	10.24090000	1.16140000	-1.00620000
H(Fragment=1)	10.23960000	0.32530000	-0.59910000
C(Fragment=1)	10.19980000	1.26270000	-2.37410000
H(Fragment=1)	10.17880000	0.49510000	-2.89800000
C(Fragment=1)	10.19000000	2.50550000	-2.96650000
N(Fragment=1)	10.09290000	2.74090000	-4.40000000
N(Fragment=1)	9.75940000	1.70500000	-5.05310000
C(Fragment=1)	9.69170000	1.92910000	-6.43560000
N(Fragment=1)	9.77910000	2.73520000	-8.28780000
N(Fragment=1)	10.10240000	3.10620000	-7.08100000
H(Fragment=1)	10.45070000	3.83240000	-6.78000000
N(Fragment=1)	9.33500000	1.51670000	-8.39870000
N(Fragment=1)	9.25550000	0.97170000	-7.25940000
C(Fragment=1)	10.27970000	3.61700000	-2.23140000
H(Fragment=1)	10.28230000	4.44170000	-2.66070000
O(Fragment=1)	10.31680000	2.21300000	1.12970000
H(Fragment=1)	10.50400000	2.93780000	1.46730000
O(Fragment=1)	10.71850000	5.90700000	-0.73800000
H(Fragment=1)	10.79051674	6.66397970	-0.15200058

O(Fragment=2)	5.97420000	1.30840000	-8.33890000
C(Fragment=2)	6.38600000	2.29290000	-8.97080000
C(Fragment=2)	6.69080000	3.57130000	-8.31960000
C(Fragment=2)	6.99960000	4.89680000	-6.35360000
C(Fragment=2)	7.07470000	5.94840000	-8.48460000
H(Fragment=2)	7.18130000	6.71460000	-9.00070000
C(Fragment=2)	7.15530000	6.02690000	-7.14750000
H(Fragment=2)	7.31770000	6.85020000	-6.74520000
C(Fragment=2)	6.83670000	4.74700000	-9.09040000
N(Fragment=2)	7.15440000	5.16790000	-4.98080000
N(Fragment=2)	6.96670000	4.18060000	-4.31510000
C(Fragment=2)	7.16230000	4.55010000	-2.89700000
N(Fragment=2)	7.68250000	5.65160000	-2.33650000
N(Fragment=2)	6.87420000	3.69690000	-1.99020000
N(Fragment=2)	7.62880000	5.41910000	-0.92610000
N(Fragment=2)	7.12830000	4.21630000	-0.76210000
C(Fragment=2)	6.75180000	3.65270000	-6.96520000
H(Fragment=2)	6.63280000	2.89070000	-6.44520000
O(Fragment=2)	6.78230000	4.77560000	-10.39950000
H(Fragment=2)	6.74870000	4.00940000	-10.68900000
O(Fragment=2)	6.63440000	2.21730000	-10.23750000
H(Fragment=2)	5.86794689	0.56548396	-8.93755352

Table S5 Cartesian coordinates of π^{-}–π staking interaction in **5**.

	X	Y	Z
N(Fragment=1)	3.41260087	8.71140078	12.17629988
N(Fragment=1)	2.94130087	9.84390078	12.21209988
N(Fragment=1)	2.66400087	10.39800078	10.99289988
N(Fragment=1)	3.48860087	8.36610078	10.82379988
C(Fragment=1)	2.37760087	10.70060078	4.71149988
C(Fragment=1)	2.18540087	11.95950078	3.96859988
C(Fragment=1)	2.47040087	10.65380078	6.11429988
H(Fragment=1)	2.45220087	11.47220078	6.55669988
C(Fragment=1)	2.99680087	9.44600078	10.17949988
C(Fragment=1)	2.62180087	8.32070078	4.66609988
H(Fragment=1)	2.63190087	7.51650078	4.19949988
C(Fragment=1)	2.57770087	9.61650078	6.84559988
C(Fragment=1)	2.44310087	9.44170078	3.98019988
C(Fragment=1)	2.78290087	8.28520078	5.93939988
H(Fragment=1)	3.02170087	7.48520078	6.34899988
O(Fragment=1)	2.34450087	11.99650078	2.72819988

O(Fragment=1)	2.41490087	9.36220078	2.65669988
H(Fragment=1)	2.53460087	10.10670078	2.33599988
N(Fragment=1)	2.64060087	9.80690078	8.19709988
N(Fragment=1)	2.89150087	8.80240078	8.93419988
O(Fragment=1)	1.83700087	13.01950078	4.69119988
H(Fragment=1)	1.68043066	13.90036485	4.34311332
N(Fragment=2)	5.56279913	11.37269922	4.66800012
N(Fragment=2)	5.83809913	11.14679922	5.94130012
H(Fragment=2)	6.18079913	10.45059922	6.31130012
N(Fragment=2)	5.01489913	13.24119922	5.68720012
N(Fragment=2)	5.82529913	11.42959922	8.53810012
N(Fragment=2)	5.06999913	12.66709922	4.58110012
N(Fragment=2)	5.48349913	12.47109922	8.00000012
C(Fragment=2)	6.12549913	10.60399922	12.20150012
C(Fragment=2)	6.34939913	9.28829922	12.85930012
C(Fragment=2)	6.04239913	10.57559922	10.82290012
H(Fragment=2)	6.12639913	9.78279922	10.34270012
C(Fragment=2)	5.81659913	11.85719922	10.16020012
C(Fragment=2)	5.99539913	11.75489922	12.81880012
C(Fragment=2)	5.93949913	12.92719922	10.60550012
H(Fragment=2)	6.04249913	13.67599922	10.06260012
C(Fragment=2)	5.92079913	13.02949922	12.05750012
H(Fragment=2)	5.86699913	13.85219922	12.48740012
C(Fragment=2)	5.42219913	12.34319922	6.52480012
O(Fragment=2)	6.18419913	9.27549922	14.13940012
O(Fragment=2)	6.09139913	11.89419922	14.17420012
H(Fragment=2)	6.19349913	11.15669922	14.51810012
O(Fragment=2)	6.64669913	8.32489922	12.24490012
H(Fragment=2)	6.82407949	7.46022344	12.62235476

Table S6 Cartesian coordinates of π⁻–π staking interaction in **6**.

	X	Y	Z
O(Fragment=1)	3.12160000	0.20360000	16.91510000
O(Fragment=1)	2.40980000	1.62180000	18.44050000
O(Fragment=1)	-0.26610000	2.12770000	18.16960000
N(Fragment=1)	0.81440000	1.58940000	12.77560000
N(Fragment=1)	-0.09690000	1.77160000	11.91500000
N(Fragment=1)	-0.42900000	1.86470000	9.57160000
N(Fragment=1)	0.34760000	1.63420000	8.49800000
N(Fragment=1)	1.55020000	1.28160000	8.87770000
N(Fragment=1)	1.61540000	1.26980000	10.21700000

C(Fragment=1)	1.21670000	1.47140000	16.39930000
C(Fragment=1)	-0.01640000	1.98410000	16.89530000
C(Fragment=1)	-1.01220000	2.31750000	15.93470000
H(Fragment=1)	-1.83930000	2.62320000	16.22850000
C(Fragment=1)	-0.78630000	2.20080000	14.59740000
H(Fragment=1)	-1.45220000	2.44510000	13.99590000
C(Fragment=1)	0.43770000	1.71570000	14.12070000
C(Fragment=1)	1.41290000	1.35610000	15.03410000
H(Fragment=1)	2.22380000	1.02690000	14.72170000
C(Fragment=1)	2.29870000	1.06000000	17.30640000
C(Fragment=1)	0.38500000	1.63350000	10.60430000
H(Fragment=1)	3.74742309	-0.20924008	17.51469031
H(Fragment=1)	0.56115006	2.18224468	18.65362709
O(Fragment=2)	-2.66610000	6.69770000	8.19860000
O(Fragment=2)	-1.95420000	5.27950000	6.67320000
O(Fragment=2)	0.72170000	4.77360000	6.94420000
N(Fragment=2)	-0.35890000	5.31190000	12.33820000
N(Fragment=2)	0.55240000	5.12970000	13.19880000
N(Fragment=2)	0.88460000	5.03660000	15.54220000
N(Fragment=2)	0.10800000	5.26710000	16.61580000
N(Fragment=2)	-1.09460000	5.61970000	16.23610000
N(Fragment=2)	-1.15990000	5.63150000	14.89670000
C(Fragment=2)	-0.76120000	5.42990000	8.71450000
C(Fragment=2)	0.47200000	4.91720000	8.21850000
C(Fragment=2)	1.46780000	4.58380000	9.17910000
H(Fragment=2)	2.29490000	4.27810000	8.88530000
C(Fragment=2)	1.24190000	4.70050000	10.51640000
H(Fragment=2)	1.90780000	4.45620000	11.11790000
C(Fragment=2)	0.01780000	5.18560000	10.99310000
C(Fragment=2)	-0.95740000	5.54520000	10.07970000
H(Fragment=2)	-1.76830000	5.87440000	10.39210000
C(Fragment=2)	-1.84320000	5.84130000	7.80740000
C(Fragment=2)	0.07060000	5.26780000	14.50950000
H(Fragment=2)	1.84477374	4.75791494	15.52217426
H(Fragment=2)	-3.46687259	6.63569708	7.67274936
H(Fragment=2)	-0.00261607	4.70304637	6.31811022

Table S7. The results of π⁻-π staking interaction energies calculation of **1**–**6**

Complex	$E_{(AB)}$/au	$E_{(A,bAB)}$ /au	$E_{(B,bAB)}$ /au	E(interaction energy) /au
1	-1717.0425180152	-858.77940345448	-858.25693688521	-0.00618767551
2	-1717.0363826789	-858.26447490954	-858.58697888269	-0.0152409855
3	-1717.0240094382	-858.26074907947	-858.75162610811	-0.01163425062
4	-1716.970376836	-858.72553264745	-858.22907352354	-0.01577151261
5	-1716.7332350464	-858.13083206516	-858.58697888269	-0.0152409855
6	-1717.1229962244	-858.29552568186	-858.81494581191	-0.01252473063

E(interaction energy) = $E_{(AB)} - (E_{(A,bAB)} + E_{(B,bAB)})$

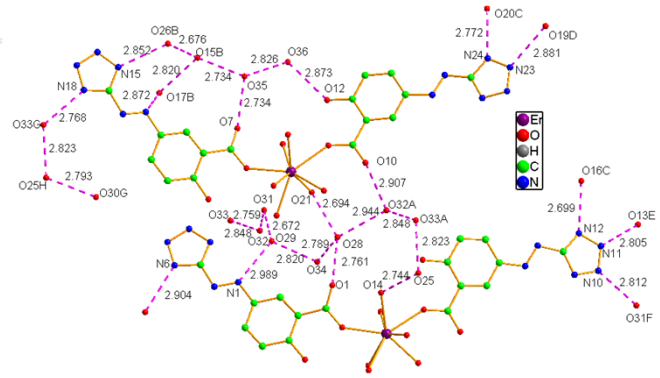


Figure S1 The diagram of hydrogen bonds in **1.** (Symmetry codes: A=1-x,1-y,1-z; B=x, y, -1+z; C=-1+x, y, z; D=-x,-y, 1-z; E=--x,1-y, 2-z; F=1-x, y,1+z; G=2-x,1-y, -z; H=1+x,1y, -1+z.)

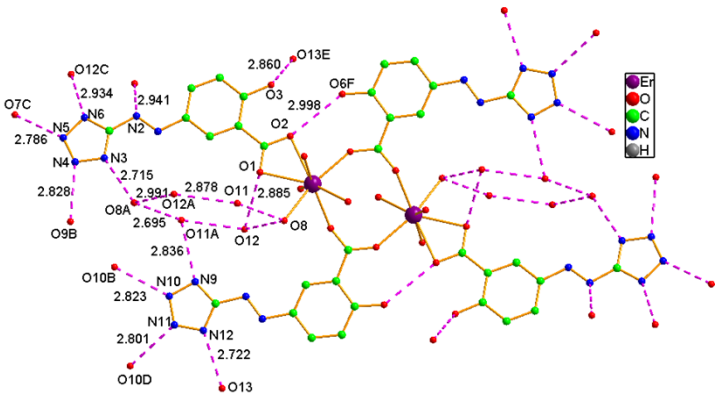


Figure S2 The diagram of hydrogen bonds in **2.** (Symmetry codes: A=1-x,1-y,2-z; B=1-x,1-y,1-z; C=-x,1-y,1-z; D=x,y, 1+z; E=-1+x,y,-1+z; F=1-x,-y,-z.)

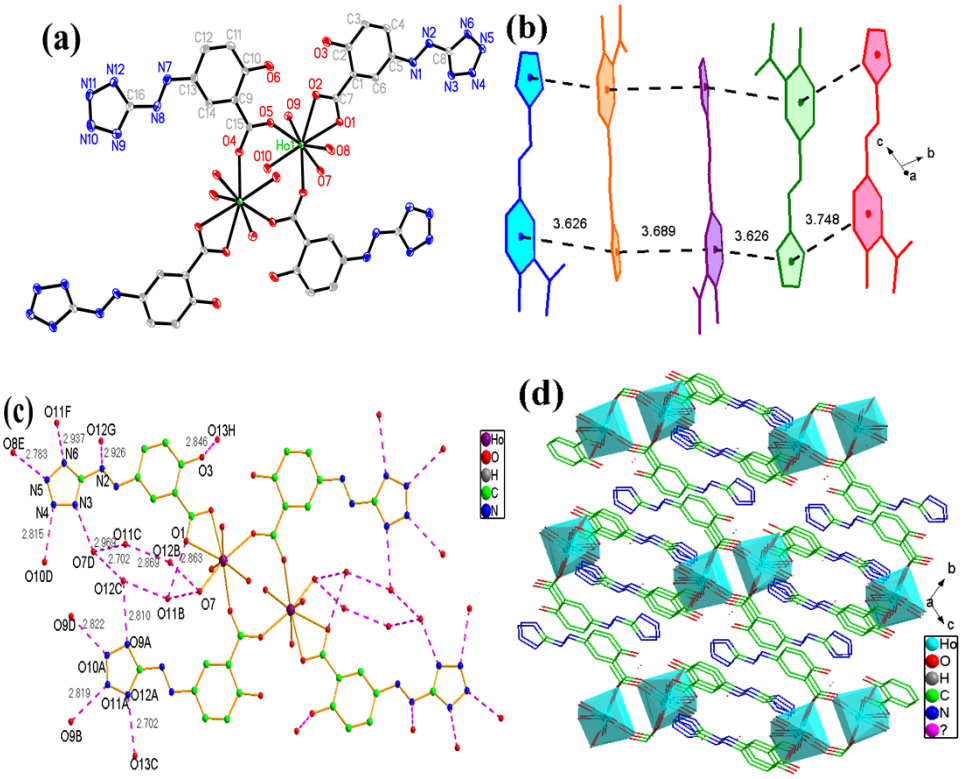


Figure S3 (a) ORTEP view (30% thermal ellipsoids) of **3**, all H atoms and lattice water molecules have been omitted for clarity, (b) the π⁻–π stacking interaction in **3**, (c) the diagram of hydrogen bonds in **3.** (Symmetry codes: A=1-x,1-y,2-z; B=x,y,1+z; C=1-x,1-y,2-z; D=1-x,1-y,3-z; E=-x,1-y,3-z; F=-x,1-y,2-z; G=-1+x,y,1+z; H=-x,1-y,1-z.) (d) the 3D supramolecular structure of **3**.

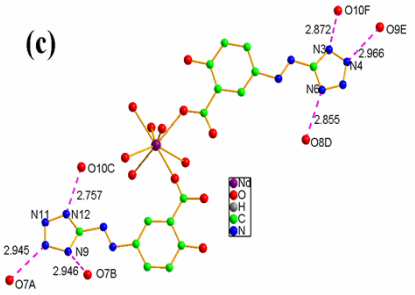


Figure S4 The diagram of hydrogen bonds in **4.** (Symmetry codes: A=0.5+x,-0.5+y,1+z; B=0.5+x,-0.5-y,0.5+z; C= x,-y,0.5+z; D= x,y,-1+z; E=-0.5+x,0.5-y,-1.5+z; F=-0.5+x,0.5+y,-1+z.)

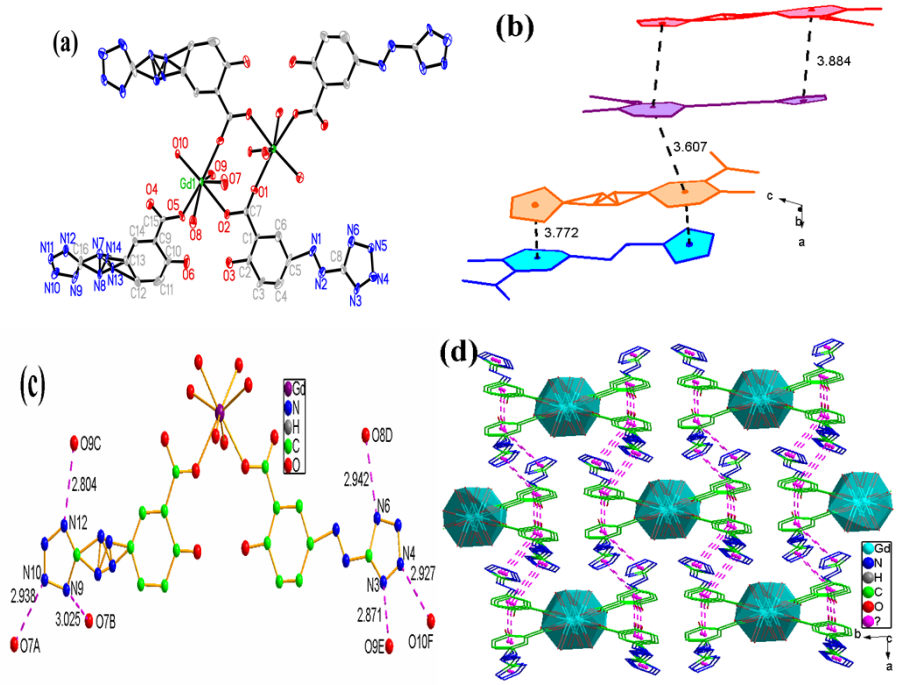


Figure S5 (a) ORTEP view (30% thermal ellipsoids) of **5**, all H atoms have been omitted for clarity, (b) the π-π stacking interaction in **5**, (c) the diagram of hydrogen bonds in **5** (Symmetry codes: A=0.5+x,0.5-y,1.5+z; B=0.5+x,0.5+y,1+z; C=x,y,1+z; D=x,y,-1+z; E=-0.5+x,0.5+y,-1+z; F=-0.5+x,0.5-y,-1.5+z), (d) the 3D supramolecular structure showing the π⁻–π stacking interaction.

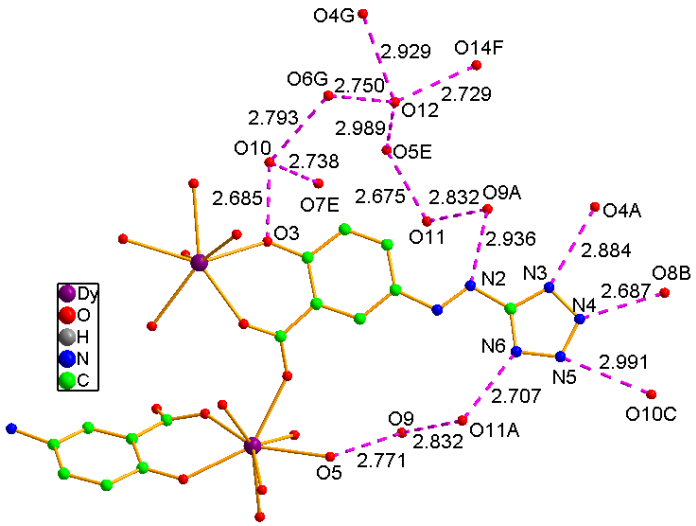


Figure S6 The diagram of hydrogen bonds in **6** (Symmetry codes: A=1-x,1-y,2-z; B=1+x,1.5-y,0.5+z; C=x,1.5-y,0.5+z; D=1+x,y,z; E=1+x,y,1+z; F=1+x,1+y,z)

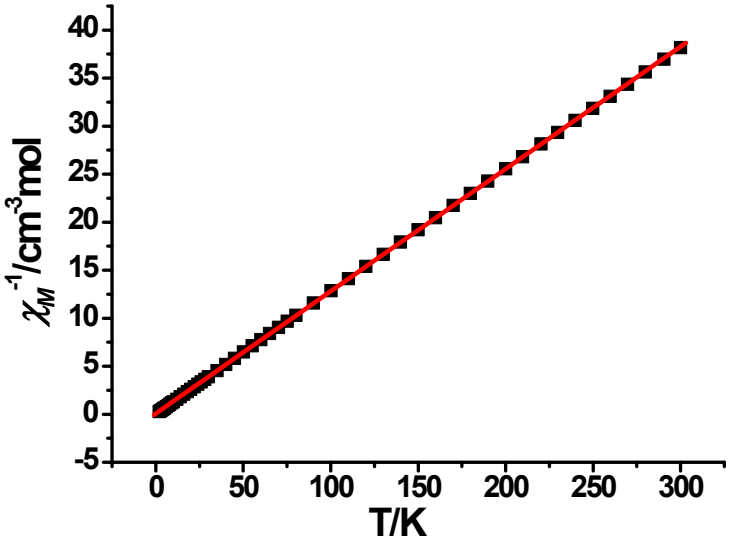
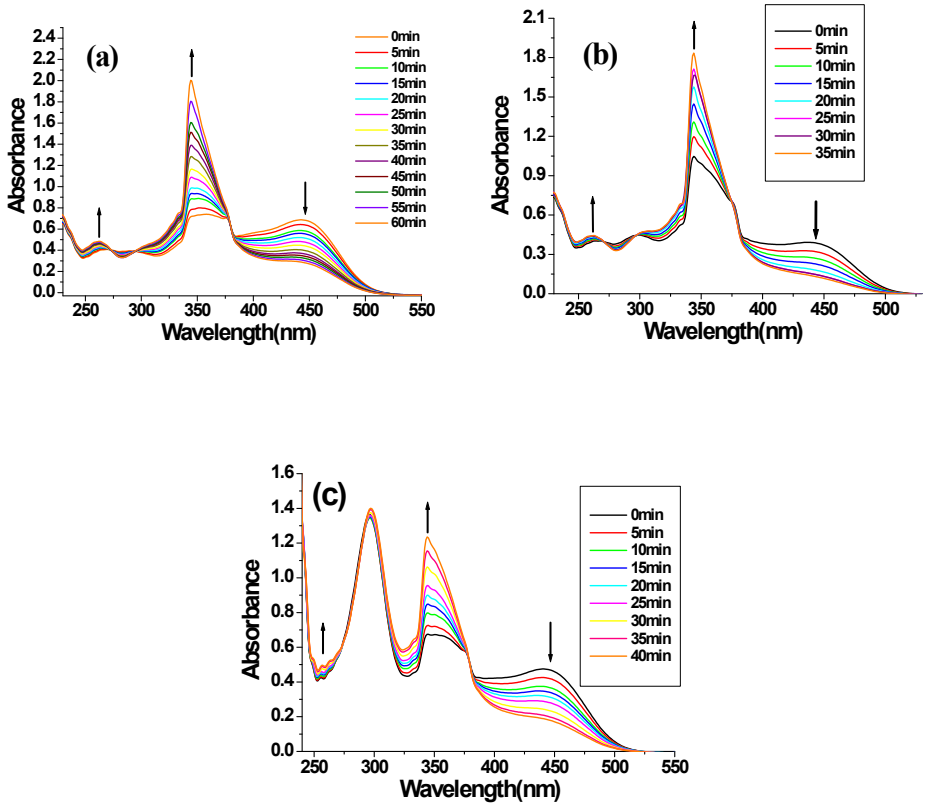


Figure S7. Plots of χ_M^{-1} vs. T for **6**. The red lines represent the fitting results.



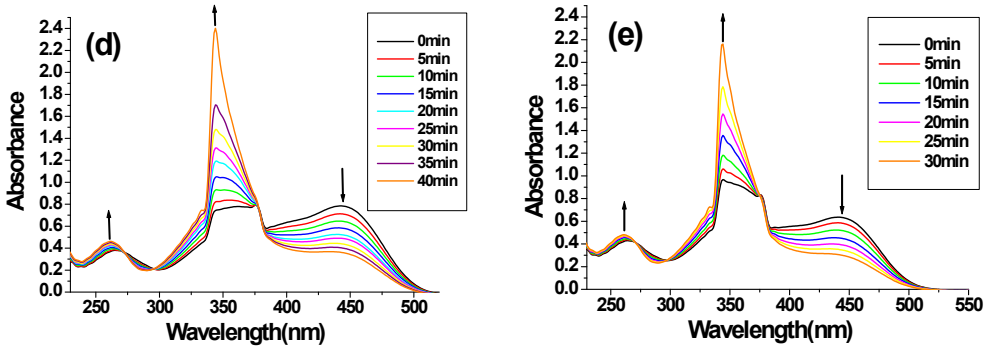
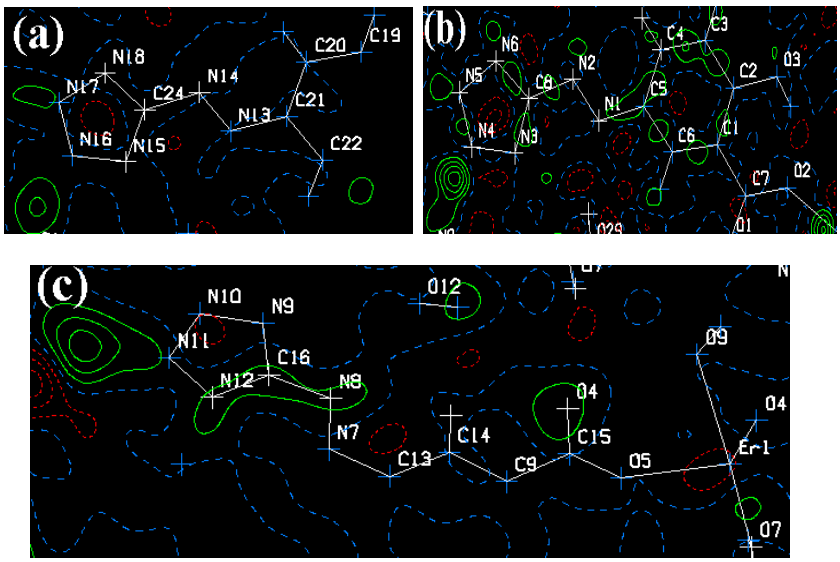


Figure S8 (a)–(e) UV-vis spectral change of **2–6** in alkaline aqueous solution with the concentration of 2.0×10^{-5} mol·L^{-1} upon repeated irradiation at 365 nm at 5 min interval at room temperature.



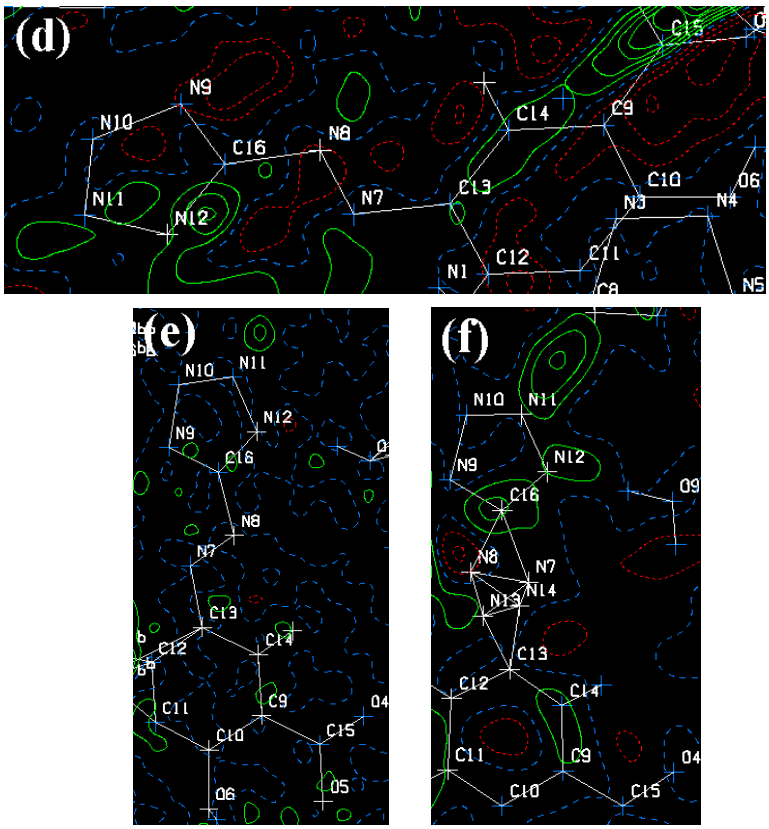


Figure S9. (a) and (b) Difference-map plots of the azotetrazolyl rings for complex **1**.(c)-(f) Difference-map plots of the azotetrazolyl rings for complexes **2**-**5**, respectively.