**Table S1** IR spectral data of free ligands (cm-1).

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Hsba** | **23dap** | **23da5Brp** | **23da5Clp** | **2a3bxp** | **2a3OHp** | **2a3mp** | **2a3m6Etp** | **2a3NO26mp** |
| ν(O-H) | 2900(br) | - | - | - | - | 3422(br) |  | - | - |
| ν(NH2) | 3364(m)3289(m) | 3311(m)3253(m)3143(m)3115(m) | 3374(m)3307(m)3281(m)3218(m) | 3377(m)3309(m)3287(m)3223(m) | 3309(m)3261(m) | 3346(m)3224(m) | 3325(m)3153(m) | 3344(m)3251(m) | 3329(m)3201(m) |
| ν(C-H)Ar | 3110(s) | 3053(w) | 3052(w) | 3058(w) | 3074(w) | 3062(w) | 3087(w) | 3057(w) | 3096(w) |
| ν(C-H)Al | 2994(w)2954(w)2850(w) | - | - | - | 3034(w)2967(w)2890(w) | - | 2989(w)2849(w)2727(w) | 2952(w)2895(w)2838(w) | 3012(w)2956(w)2904(w) |
| ν(C=O) | 1684(s)1480(s) | - | - | - | - | - | - | - | - |
| ν(C=N)ν(C=C) | 1578(s)1541(s)1492(s)1472(s)1435(s) | 1590(s)1552(s)1480(s)1445(s) | 1608(s)1588(s)1558(s)1476(s)1439(s) | 1619(s)1611(s)1588(s)1568(s)1476(s)1443(s) | 1609(s)1587(s)1497(s)1477(s)1437(s) | 1612(s)1634(s)1576(s)1482(s)1468(s) | 1614(s)1555(s)1476(s)1375(s) | 1614(s)1594(s)1581(s)1541(s)1471(s) | 1613(s)1587(s)1486(s)1472(s)1424(s) |
| ν(NO2) | - | - | - | - | - | - | - |  | 1531(s)1336(s) |
| ν(C-O) | 1357(s)1212(s)1052(s) | - | - | - | 1353(s)1276(s)1081(s) | 1354(s)1234(s)1082(s) | - | - | - |
| ν(S=O) | 1277(s)1189(s)1149(s) | - | - | - | - | - | - | - | - |
| ν(py) | - | 781(s) | 797(s) | 784(s) | 740(s) | 776(s) | 794(s) | 838(s) | 779(s) |

a abbreviations: w, weak; m, medium; s, strong; b, broad

**Table S2** IR spectral data of **1-9** (cm-1).

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
| ν(O-H) | 3488(br) | 3430(br) | 3446(br) | 3427(br) | - | 3568(br) | 3582(br) | 3526(br) | 3489(br) |
| ν(NH2) | 3370(m)3251(m) | 3396(m)3372(m)3336(m)3188(m) | 3384(m)3205(m) | 3302(m)3217(m) | 3319(m)3229(m)3280(m)3202(m) | 3372(m)3275(m) | 3476(m)3382(m)3321(m)3289(m) | 3435(m)3371(m)3266(m)3186(m) | 3428(m)3292(m)3231(m)3154(m) |
| ν(C-H)Ar | 3110(s) | 3105(s) | 3054(s) | 3074(s) | 3086(s) | 3103(s) | 3075(s) | 3027(s) | 3074(s) |
| ν(C-H)Alf. | 2994(w)2954(w)2850(w) | 2943(w)2900(w)2840(w) | 2948(w)2885(w)2828(w) | 2907(w)2840(w) | 2980(w)2885(w)2842(w) | 2948(w)2854(w) | 2942(w)2846(w)2746(w) | 2956(w)2849(w) | 2891(w)2801(w) |
| ν(C=O) | 1612(s)1467(s) | 1626(s)1475(s) | 1621(s)1475(s) | 1621(s)1469(s) | 1626(s)1472(s) | 1612(s)1463(s) | 1623(s)1481(s) | 1639(s)1484(s) | 1636(s)1486(s) |
| ν(C=N)ν(C=C) | 1581(s)1543(s)1468(s)1454(s)1437(s) | 1556(s)1518(s)1507(s)1497(s)1424(s) | 1604(s)1557(s)1506(s)1424(s) | 1555(s)1489(s) | 1583(s)1562(s)1492(s)1432(s) | 1581(s)1559(s)1531(s)1421(s) | 1583(s)1562(s)1459(s)1425(s) | 1604(s)1581(s)1548(s)1484(s)1413(s) | 1585(s)1558(s)1501(s)1417(s) |
| ν(NO2) | - | - | - | - | - | - | - |  | 1558(s)1335(s) |
| ν(C-O) | 1387(s)1257(s)1089(s) | 1355(s)1257(s)1030(s) | 1353(s)1254(s)1084(s) | 1371(s)1255(s)1088(s) | 1374(s)1283(s)1087(s) | 1375(s)1255(s)1087(s) | 1371(s)1258(s)1091(s) | 1382(s)1255(s)1089(s) | 1353(s)1249(s)1050(s) |
| ν(S=O) | 1277(s)1189(s)1149(s) | 1322(s)1157(s)1134(s) | 1331(s)1157(s)1131(s) | 1329(s)1167(s)1122(s) | 1335(s)1168(s)1123(s) | 1299(s)1166(s)1121(s) | 1295(s)1170(s)1124(s) | 1276(s)1171(s)1123(s) | 1304(s)1137(s) |
| ν(py) | - | 769(s) | 766(s) | 770(s) | 750(s) | 799(s) | 758(s) | 798(s) | 759(s) |
| ν(M-N) | - | 453(w) | 450(w) | 454(w) | 453(w) | 496(w) | 459(w) | 453(w) | 484(w) |
| ν(M-O) | 582(w) | 606(w) | 606(w) | 606(w) | 606(w) | 579(w) | 576(w) | 585(w) | 559(w) |

a abbreviations: w, weak; m, medium; s, strong; b, broad

**Table S3** Optical properties all compounds in DMSO (nm(Lmol‑1cm-1)).

|  |  |  |  |
| --- | --- | --- | --- |
| **Compound** | **λ** | **Compound** | **λ** |
| **sba** | 301(32270) | **1** | 786(190)296(33260) |
| **2,3dap** | 321(28170)302(28680) | **2** | 794(290)300(31840)276(18500) |
| **2,3da5Brp** | 347(30460)295(34370) | **3** | 788(260)416(4980)296(13650) |
| **2,3da5Clp** | 329(38640)308(47900) | **4** | 773(250)561(12250)291(23880)269(11160) |
| **2a3bxp** | 321(39760)308(38660) | **5** | 770(140)395(14740)293(27270) |
| **2a3OHp** | 324(32740)309(32270) | **6** | 735(260)508(4660)295(19020) |
| **2a3mp** | 324(32740)300(31940) | **7** | 771(150)302(31740)296(31640) |
| **2a3m6Etp** | 321(32150)318(31840) | **8** | 798(160)290(26820) |
| **2a3NO26mp** | 396(26330)369(28040)286(22590) | **9** | 784(180)426(18850)366(22180)292(27620) |

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**Figure S1** FT-IR spectrum of compound **1**.

****

**Figure S2** FT-IR spectrum of compound **2**.

****

**Figure S3** FT-IR spectrum of compound **3**.

****

**Figure S4** FT-IR spectrum of compound **4**.

****

**Figure S5** FT-IR spectrum of compound **5**.

****

**Figure S6** FT-IR spectrum of compound **6**.

****

**Figure S7** FT-IR spectrum of compound **7**.

****

**Figure S8** FT-IR spectrum of compound **8**.

****

**Figure S9** FT-IR spectrum of compound **9**.



**Figure S10** UV–Vis spectrum of compound **1** and the free ligand, Hsba.



**Figure S11** UV–Vis spectrum of compound **2** and the free ligands, Hsba and 2,3dap.



**Figure S12** UV–Vis spectrum of compound **3** and the free ligands, Hsba and 2,3da5Brp.



**Figure S13** UV–Vis spectrum of compound **4** and the free ligands, Hsba and 2,3da5Clp.

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**Figure S14** UV–Vis spectrum of compound **5** and the free ligands, Hsba and 2a3bxp.

****

**Figure S15** UV–Vis spectrum of compound **6** and the free ligands, Hsba and 2a3OHp.



**Figure S16** UV–Vis spectrum of compound **7** and the free ligands, Hsba and 2a3mp.



**Figure S17** UV–Vis spectrum of compound **8** and the free ligands, Hsba and 2a3m6Etp.

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**Figure S18** UV–Vis spectrum of compound **9** and the free ligands, Hsba and 2a3NO26mp.