

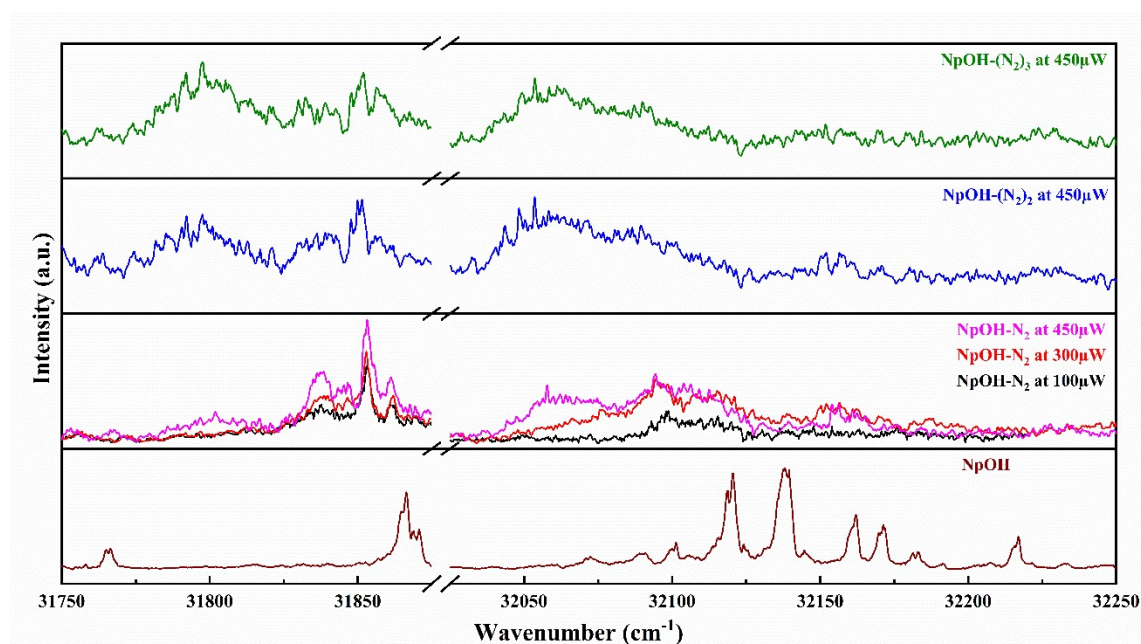
Supporting information for

Determination of intermolecular dissociation energies in the dispersion-bound N_2 and Xe complexes of 2-(2'-pyridyl) benzimidazole and 1-naphthol

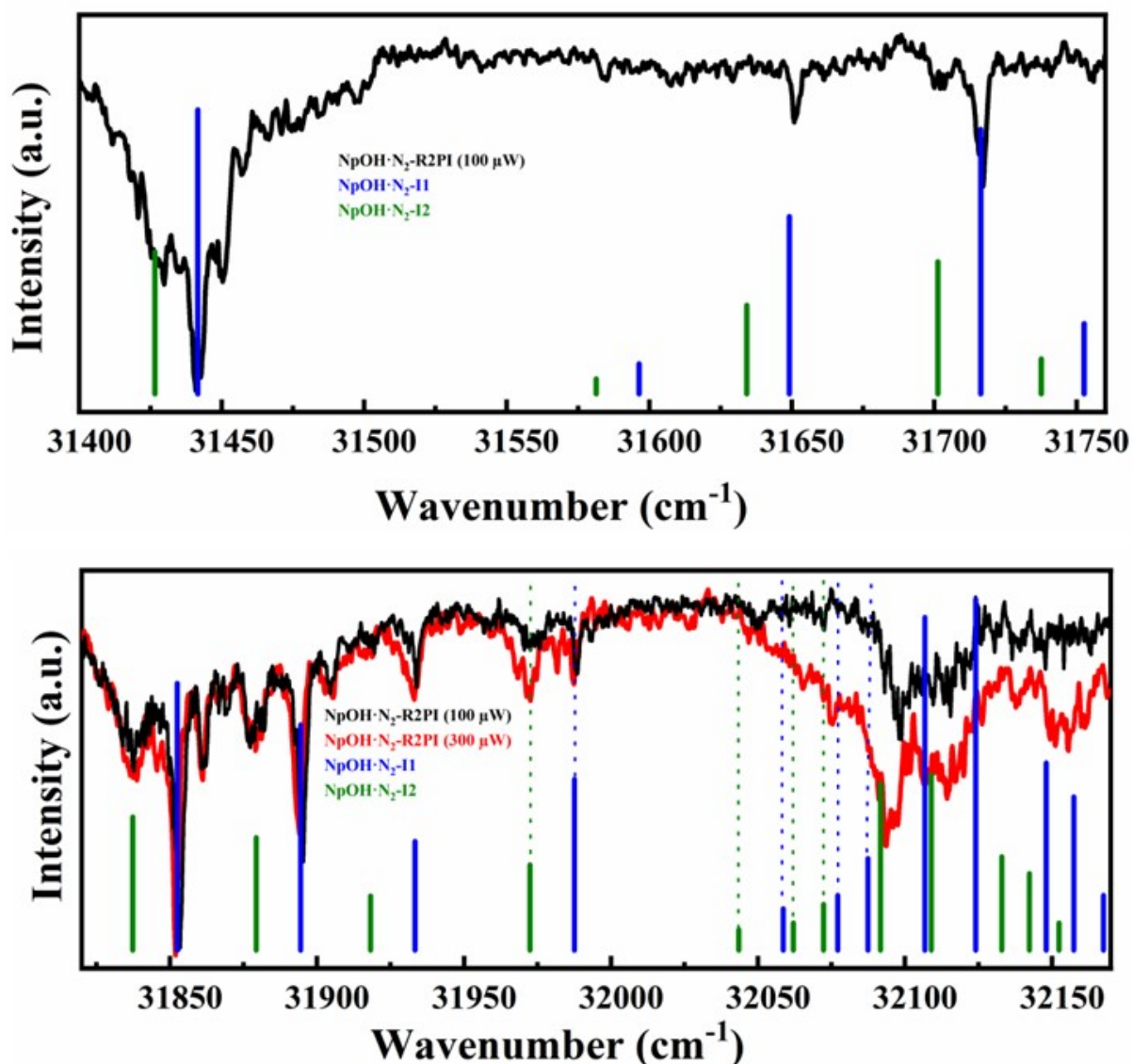
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SI Figure S1. The R2PI spectra of the $NpOH \cdot (N_2)_3$ (green) and $NpOH \cdot (N_2)_2$ (blue) complexes were recorded using 450 μW power of the excitation/ionization laser in the ‘cut-off region’. The R2PI spectra of the $NpOH \cdot N_2$ complex, recorded at three different laser powers 450 μW (pink), 300 μW (red), and 100 μW (black), are given along with the R2PI spectrum of $NpOH$ monomer in wavenumber (cm^{-1}). The broad band near 32050-32125 cm^{-1} region was obtained at each spectrum, including the 1:1 complex. However, in the lower energy region (below 32050 cm^{-1}), the contributions of higher order fragmentation from $NpOH \cdot (N_2)_3$ (green) and $NpOH \cdot (N_2)_2$ (blue) are insignificant in the Black-trace (recorded at 100 μW of laser power).



SI Figure S2. The R2PI spectra of the NpOH·N₂ complex recorded at two laser powers, 100 μW (black trace) and 300 μW (red trace), are presented as inverted peaks. The intramolecular vibrational modes of NpOH, referenced to the band origins of the NpOH·N₂-I1 (blue) and NpOH·N₂-I2 (green) isomers, are compared as stick spectra with the experimental R2PI spectrum of the NpOH·N₂ complex. The dissociation limit (D_0) of the complexes is inferred from the relative intensities of the intramolecular bands. We have compared all the intramolecular modes with the R2PI spectrum of the complex in the dissociation range, shown in vertical dashed lines.

Table S1. The ground state dissociation energy $D_0(S_0)$ of $PBI \cdot N_2$ complex, obtained by subtracting the origin band shift Δv of the complex from the origin PBI monomer. The calculated ZPE corrected $D_0(S_0)$ values are given at B3LYP-D2, B3LYP-D3 and B3LYP-D4 levels with def2-TZVPP basis set.

| System | Method | $D_0(S_0)$ (kJmol ⁻¹) (expt.) | $D_0(S_0)$ (kJmol ⁻¹) (calc.) | Minimum* and Mean** Error (%) |
|-----------------|----------|---|---|-------------------------------------|
| $PBI \cdot N_2$ | B3LYP-D2 | 6.15 ± 0.15 | 7.38 | 14.7; 16.7 |
| $PBI \cdot N_2$ | B3LYP-D3 | 6.15 ± 0.15 | 7.77 | 18.9; 20.9 |
| $PBI \cdot N_2$ | B3LYP-D4 | 6.15 ± 0.15 | 7.90 | 19.6; 22.2 |

*Minimum Error: calculated using the upper limit of the experimental dissociation energy;

** Mean Error: calculated using the mean experimental dissociation energy values.

Table S2. The ground state vibrational frequencies (ν''_{calc}) of PBI, $PBI \cdot N_2$ and $PBI \cdot Xe$ complexes are calculated at B3LYP-D4/def2-TZVPP level of theory and the corresponding intramolecular and intermolecular vibrational modes are assigned.

| PBI | | $PBI \cdot N_2$ | | $PBI \cdot Xe$ | |
|-------------------|----------------|-------------------|----------------|-------------------|----------------|
| Vibrational Modes | ν''_{calc} | Vibrational Modes | ν''_{calc} | Vibrational Modes | ν''_{calc} |
| ν_1 | 3648.51 | ν_1 | 3646.2 | ν_1 | 3647.04 |
| ν_2 | 3218.36 | ν_2 | 3217.18 | ν_2 | 3219.55 |
| ν_3 | 3201.86 | ν_3 | 3201.65 | ν_3 | 3202.28 |
| ν_4 | 3201.8 | ν_4 | 3201.18 | ν_4 | 3201.9 |
| ν_5 | 3194.12 | ν_5 | 3193.87 | ν_5 | 3194.73 |
| ν_6 | 3183.39 | ν_6 | 3183.23 | ν_6 | 3184.04 |
| ν_7 | 3182.43 | ν_7 | 3181.84 | ν_7 | 3182.77 |

| | | | | | |
|-----------------|---------|-----------------|---------|-----------------|---------|
| v ₈ | 3173.19 | v ₈ | 3173.1 | v ₈ | 3173.66 |
| v ₉ | 3157.26 | v ₉ | 3156.9 | v ₉ | 3157.57 |
| v ₁₀ | 1666.52 | v ₁₀ | 1666.3 | v ₁₀ | 1667.52 |
| v ₁₁ | 1640.25 | v ₁₁ | 1639.92 | v ₁₁ | 1641.09 |
| v ₁₂ | 1626.92 | v ₁₂ | 1626.86 | v ₁₂ | 1627.87 |
| v ₁₃ | 1612.38 | v ₁₃ | 1611.93 | v ₁₃ | 1612.54 |
| v ₁₄ | 1584.09 | v ₁₄ | 1584.62 | v ₁₄ | 1585.77 |
| v ₁₅ | 1527.42 | v ₁₅ | 1527.05 | v ₁₅ | 1527.94 |
| v ₁₆ | 1498.24 | v ₁₆ | 1497.37 | v ₁₆ | 1498.38 |
| v ₁₇ | 1486.54 | v ₁₇ | 1485.42 | v ₁₇ | 1486.3 |
| v ₁₈ | 1471.52 | v ₁₈ | 1470.87 | v ₁₈ | 1471.85 |
| v ₁₉ | 1429.54 | v ₁₉ | 1427.72 | v ₁₉ | 1429.05 |
| v ₂₀ | 1405.78 | v ₂₀ | 1404.39 | v ₂₀ | 1406.3 |
| v ₂₁ | 1344.15 | v ₂₁ | 1343.03 | v ₂₁ | 1344.68 |
| v ₂₂ | 1316.89 | v ₂₂ | 1316.44 | v ₂₂ | 1316.99 |
| v ₂₃ | 1304.91 | v ₂₃ | 1301.82 | v ₂₃ | 1305.05 |
| v ₂₄ | 1302.01 | v ₂₄ | 1301.16 | v ₂₄ | 1302.03 |
| v ₂₅ | 1256.24 | v ₂₅ | 1255.99 | v ₂₅ | 1256.53 |
| v ₂₆ | 1248.38 | v ₂₆ | 1247.77 | v ₂₆ | 1249.17 |
| v ₂₇ | 1176.74 | v ₂₇ | 1175.68 | v ₂₇ | 1176.49 |
| v ₂₈ | 1172.71 | v ₂₈ | 1171.86 | v ₂₈ | 1172.76 |
| v ₂₉ | 1142.23 | v ₂₉ | 1141.85 | v ₂₉ | 1142.44 |
| v ₃₀ | 1121 | v ₃₀ | 1120.08 | v ₃₀ | 1121.56 |
| v ₃₁ | 1119.41 | v ₃₁ | 1118.71 | v ₃₁ | 1119.34 |
| v ₃₂ | 1066.18 | v ₃₂ | 1065.61 | v ₃₂ | 1066.18 |
| v ₃₃ | 1031.75 | v ₃₃ | 1030.86 | v ₃₃ | 1031.77 |
| v ₃₄ | 1016.68 | v ₃₄ | 1016.56 | v ₃₄ | 1016.81 |
| v ₃₅ | 980.95 | v ₃₅ | 981.12 | v ₃₅ | 981.81 |
| v ₃₆ | 915.28 | v ₃₆ | 914.94 | v ₃₆ | 915.71 |
| v ₃₇ | 835.52 | v ₃₇ | 835.93 | v ₃₇ | 836.45 |
| v ₃₈ | 729.19 | v ₃₈ | 729.31 | v ₃₈ | 729.82 |
| v ₃₉ | 644.45 | v ₃₉ | 644.25 | v ₃₉ | 644.81 |
| v ₄₀ | 633.77 | v ₄₀ | 633.48 | v ₄₀ | 634.1 |
| v ₄₁ | 581.56 | v ₄₁ | 581.55 | v ₄₁ | 581.98 |

| | | | | | |
|-----------------|---------|----------------------------|---------|---------------------|---------|
| v ₄₂ | 547.27 | v ₄₂ | 546.54 | v ₄₂ | 547.38 |
| v ₄₃ | 342.38 | v ₄₃ | 341.48 | v ₄₃ | 342.51 |
| v ₄₄ | 301.59 | v ₄₄ | 301.96 | v ₄₄ | 302.37 |
| v ₄₅ | 108.04 | v ₄₅ | 106.02 | v ₄₅ | 107.81 |
| v ₄₆ | 1032.82 | v ₄₆ | 1029.26 | v ₄₆ | 1033.39 |
| v ₄₇ | 997.53 | v ₄₇ | 993.12 | v ₄₇ | 999.38 |
| v ₄₈ | 989.17 | v ₄₈ | 986.66 | v ₄₈ | 989.78 |
| v ₄₉ | 952.69 | v ₄₉ | 949.89 | v ₄₉ | 954.66 |
| v ₅₀ | 929.89 | v ₅₀ | 925.85 | v ₅₀ | 930.28 |
| v ₅₁ | 873.1 | v ₅₁ | 868.81 | v ₅₁ | 874.44 |
| v ₅₂ | 825.66 | v ₅₂ | 821.28 | v ₅₂ | 825.17 |
| v ₅₃ | 792.49 | v ₅₃ | 789.84 | v ₅₃ | 792.93 |
| v ₅₄ | 770.67 | v ₅₄ | 765.19 | v ₅₄ | 769.77 |
| v ₅₅ | 762.4 | v ₅₅ | 757.78 | v ₅₅ | 761.72 |
| v ₅₆ | 723.75 | v ₅₆ | 721.16 | v ₅₆ | 723.63 |
| v ₅₇ | 601.66 | v ₅₇ | 597.54 | v ₅₇ | 601.25 |
| v ₅₈ | 582.72 | v ₅₈ | 579.3 | v ₅₈ | 585.28 |
| v ₅₉ | 518.06 | v ₅₉ | 514.17 | v ₅₉ | 518.85 |
| v ₆₀ | 444.29 | v ₆₀ | 440.13 | v ₆₀ | 446.99 |
| v ₆₁ | 422.76 | v ₆₁ | 417.94 | v ₆₁ | 421.82 |
| v ₆₂ | 322.12 | v ₆₂ | 322.4 | v ₆₂ | 324.12 |
| v ₆₃ | 266.46 | v ₆₃ | 266.87 | v ₆₃ | 270.24 |
| v ₆₄ | 185.19 | v ₆₄ | 181.52 | v ₆₄ | 184.67 |
| v ₆₅ | 78.91 | v ₆₅ | 84.46 | v ₆₅ | 82.92 |
| v ₆₆ | 73.62 | v ₆₆ | 80.08 | v ₆₆ | 78.01 |
| | | Intermolecular mode | 69.43 | Intermolecular mode | 51.7 |
| | | Intermolecular mode | 55.68 | Intermolecular mode | 38.32 |
| | | Intermolecular mode | 33.36 | Intermolecular mode | 15.61 |
| | | Intermolecular mode | 29.12 | | |
| | | Intermolecular mode | 22.62 | | |
| | | N ₂ -stretching | 2447.61 | | |

Table S3. The ground state vibrational frequencies (ν''_{calc}) of NpOH, NpOH·N₂-I1, NpOH·N₂-I2 and NpOH·Xe complexes are calculated at B3LYP-D4/def2-TZVPP level of theory and the corresponding intramolecular and intermolecular vibrational modes are assigned.

| NpOH | | NpOH·N ₂ -I1 | | NpOH·N ₂ -I2 | | NpOH·Xe | |
|-------------------|-----------------------|-------------------------|-----------------------|-------------------------|-----------------------|-------------------|-----------------------|
| Vibrational Modes | ν''_{calc} | Vibrational Modes | ν''_{calc} | Vibrational Modes | ν''_{calc} | Vibrational Modes | ν''_{calc} |
| ν_1 | 3832.26 | ν_1 | 3827.71 | ν_1 | 3827.94 | ν_1 | 3827.89 |
| ν_2 | 3212.31 | ν_2 | 3211.52 | ν_2 | 3212.46 | ν_2 | 3211.79 |
| ν_3 | 3192.11 | ν_3 | 3192.94 | ν_3 | 3192.37 | ν_3 | 3192.49 |
| ν_4 | 3190.76 | ν_4 | 3190.57 | ν_4 | 3190.8 | ν_4 | 3190.43 |
| ν_5 | 3178.46 | ν_5 | 3178.32 | ν_5 | 3178.49 | ν_5 | 3178.02 |
| ν_6 | 3175.46 | ν_6 | 3175.76 | ν_6 | 3174.95 | ν_6 | 3175 |
| ν_7 | 3166.74 | ν_7 | 3166.58 | ν_7 | 3166.91 | ν_7 | 3166.06 |
| ν_8 | 3156.93 | ν_8 | 3156.92 | ν_8 | 3156.39 | ν_8 | 3156.73 |
| ν_9 | 1675.77 | ν_9 | 1674.44 | ν_9 | 1674.63 | ν_9 | 1675.09 |
| ν_{10} | 1644.65 | ν_{10} | 1643.36 | ν_{10} | 1643.39 | ν_{10} | 1643.92 |
| ν_{11} | 1621.44 | ν_{11} | 1620.63 | ν_{11} | 1620.88 | ν_{11} | 1621.08 |
| ν_{12} | 1558.21 | ν_{12} | 1557.78 | ν_{12} | 1557.74 | ν_{12} | 1557.88 |
| ν_{13} | 1503.65 | ν_{13} | 1503.59 | ν_{13} | 1503.63 | ν_{13} | 1503.77 |
| ν_{14} | 1495.09 | ν_{14} | 1494.36 | ν_{14} | 1494.33 | ν_{14} | 1494.45 |
| ν_{15} | 1440.7 | ν_{15} | 1440.46 | ν_{15} | 1440.38 | ν_{15} | 1440.48 |
| ν_{16} | 1415.78 | ν_{16} | 1414.61 | ν_{16} | 1413.95 | ν_{16} | 1414.68 |
| ν_{17} | 1394.9 | ν_{17} | 1392.76 | ν_{17} | 1393.41 | ν_{17} | 1393.09 |
| ν_{18} | 1308.74 | ν_{18} | 1308.89 | ν_{18} | 1308.54 | ν_{18} | 1308.48 |
| ν_{19} | 1276.14 | ν_{19} | 1275.06 | ν_{19} | 1275.04 | ν_{19} | 1275.05 |
| ν_{20} | 1260.85 | ν_{20} | 1259.66 | ν_{20} | 1259.63 | ν_{20} | 1259.66 |
| ν_{21} | 1224.72 | ν_{21} | 1223.61 | ν_{21} | 1223.46 | ν_{21} | 1223.64 |
| ν_{22} | 1192.32 | ν_{22} | 1190.9 | ν_{22} | 1190.82 | ν_{22} | 1190.88 |
| ν_{23} | 1176.86 | ν_{23} | 1174.98 | ν_{23} | 1174.97 | ν_{23} | 1174.93 |
| ν_{24} | 1171.2 | ν_{24} | 1169.88 | ν_{24} | 1169.93 | ν_{24} | 1170 |
| ν_{25} | 1107.22 | ν_{25} | 1106.91 | ν_{25} | 1106.43 | ν_{25} | 1106.61 |
| ν_{26} | 1067.09 | ν_{26} | 1066.55 | ν_{26} | 1066.29 | ν_{26} | 1066.29 |
| ν_{27} | 1044.55 | ν_{27} | 1043.86 | ν_{27} | 1044.27 | ν_{27} | 1043.94 |

| | | | | | | | |
|-----------------|--------|----------------------------|---------|----------------------------|---------|---------------------|---------|
| v ₂₈ | 895.35 | v ₂₈ | 895.11 | v ₂₈ | 895.07 | v ₂₈ | 895.04 |
| v ₂₉ | 806.07 | v ₂₉ | 805.34 | v ₂₉ | 805.3 | v ₂₉ | 805.21 |
| v ₃₀ | 728.02 | v ₃₀ | 727.95 | v ₃₀ | 727.89 | v ₃₀ | 728.09 |
| v ₃₁ | 586.22 | v ₃₁ | 585.87 | v ₃₁ | 585.8 | v ₃₁ | 585.73 |
| v ₃₂ | 535.42 | v ₃₂ | 534.51 | v ₃₂ | 534.47 | v ₃₂ | 534.58 |
| v ₃₃ | 488.47 | v ₃₃ | 488.46 | v ₃₃ | 488.5 | v ₃₃ | 488.54 |
| v ₃₄ | 473.08 | v ₃₄ | 471.64 | v ₃₄ | 471.46 | v ₃₄ | 471.54 |
| v ₃₅ | 288.67 | v ₃₅ | 287.11 | v ₃₅ | 287.04 | v ₃₅ | 287.18 |
| v ₃₆ | 1013.1 | v ₃₆ | 1006.31 | v ₃₆ | 1007.46 | v ₃₆ | 1006.23 |
| v ₃₇ | 992.74 | v ₃₇ | 984.47 | v ₃₇ | 985.7 | v ₃₇ | 984.36 |
| v ₃₈ | 975.13 | v ₃₈ | 970.16 | v ₃₈ | 968.14 | v ₃₈ | 969.3 |
| v ₃₉ | 905.4 | v ₃₉ | 896.3 | v ₃₉ | 897.17 | v ₃₉ | 896.16 |
| v ₄₀ | 874.39 | v ₄₀ | 865.9 | v ₄₀ | 864.67 | v ₄₀ | 864.68 |
| v ₄₁ | 813.76 | v ₄₁ | 807.88 | v ₄₁ | 807.99 | v ₄₁ | 807.52 |
| v ₄₂ | 800.91 | v ₄₂ | 789.16 | v ₄₂ | 789.79 | v ₄₂ | 789.09 |
| v ₄₃ | 760.05 | v ₄₃ | 744.86 | v ₄₃ | 744.69 | v ₄₃ | 744.64 |
| v ₄₄ | 652.2 | v ₄₄ | 648.71 | v ₄₄ | 648.64 | v ₄₄ | 648.21 |
| v ₄₅ | 592.18 | v ₄₅ | 586.27 | v ₄₅ | 586.34 | v ₄₅ | 586.36 |
| v ₄₆ | 485.49 | v ₄₆ | 478.17 | v ₄₆ | 478.28 | v ₄₆ | 477.67 |
| v ₄₇ | 440.24 | v ₄₇ | 430.85 | v ₄₇ | 430.35 | v ₄₇ | 430.69 |
| v ₄₈ | 370.68 | v ₄₈ | 358.53 | v ₄₈ | 359.49 | v ₄₈ | 360.18 |
| v ₄₉ | 270.27 | v ₄₉ | 264.47 | v ₄₉ | 262.13 | v ₄₉ | 263.51 |
| v ₅₀ | 186.58 | v ₅₀ | 177.2 | v ₅₀ | 177.91 | v ₅₀ | 177.46 |
| v ₅₁ | 153.62 | v ₅₁ | 141.2 | v ₅₁ | 143.73 | v ₅₁ | 140.95 |
| | | Intermolecular mode | 85.25 | Intermolecular mode | 81.3 | Intermolecular mode | 43.91 |
| | | Intermolecular mode | 71.27 | Intermolecular mode | 67.73 | Intermolecular mode | 25 |
| | | Intermolecular mode | 36.96 | Intermolecular mode | 33.7 | Intermolecular mode | 13.12 |
| | | Intermolecular mode | 29.06 | Intermolecular mode | 19.31 | | |
| | | Intermolecular mode | 24.85 | Intermolecular mode | 17.99 | | |
| | | N ₂ -stretching | 2448.4 | N ₂ -stretching | 2449.55 | | |

Table S4. Coordinates of the optimized structures of PBI, PBI·N₂ and PBI·Xe complexes in ground state S₀ calculated at B3LYP-D4/def2-TZVPP level of theory are provided.

| PBI | | | | PBI·N ₂ | | | | PBI·Xe | | | |
|-----|---------|---------|---------|--------------------|---------|---------|---------|--------|---------|---------|---------|
| C | -2.7993 | -1.5421 | 0.0119 | C | -2.7849 | -1.5356 | 0.0677 | C | -2.5374 | -1.5119 | 0.0758 |
| C | -1.6715 | -0.728 | 0.0044 | C | -1.6599 | -0.7191 | 0.0229 | C | -1.3916 | -0.7303 | -0.0251 |
| C | -1.7547 | 0.6822 | 0.1084 | C | -1.7454 | 0.693 | 0.0959 | C | -1.4419 | 0.6841 | -0.0812 |
| C | -3.0023 | 1.2973 | 0.2248 | C | -2.9927 | 1.3077 | 0.2163 | C | -2.6744 | 1.3373 | -0.037 |
| C | -4.1267 | 0.4897 | 0.2332 | C | -4.1143 | 0.4978 | 0.2605 | C | -3.8171 | 0.5621 | 0.0628 |
| C | -4.0267 | -0.9084 | 0.128 | C | -4.0119 | -0.9021 | 0.1874 | C | -3.7495 | -0.8408 | 0.1186 |
| N | -0.4895 | 1.2329 | 0.0734 | N | -0.4817 | 1.2448 | 0.0434 | N | -0.1632 | 1.198 | -0.1592 |
| C | 0.329 | 0.2125 | -0.0454 | C | 0.3388 | 0.2237 | -0.0556 | C | 0.6319 | 0.1523 | -0.1501 |
| N | -0.3254 | -0.9912 | -0.0918 | N | -0.3142 | -0.9816 | -0.0755 | N | -0.0517 | -1.0334 | -0.0754 |
| C | 1.7847 | 0.2757 | -0.1249 | C | 1.7944 | 0.2858 | -0.1312 | C | 2.0898 | 0.1724 | -0.1944 |
| C | 2.451 | 1.5014 | -0.0902 | C | 2.4616 | 1.5107 | -0.0954 | C | 2.7879 | 1.3789 | -0.2583 |
| C | 3.8326 | 1.5 | -0.1693 | C | 3.8437 | 1.5073 | -0.1652 | C | 4.1707 | 1.3359 | -0.2925 |
| C | 4.5012 | 0.2857 | -0.2788 | C | 4.5113 | 0.292 | -0.2679 | C | 4.8086 | 0.1008 | -0.262 |
| C | 3.7493 | -0.8824 | -0.3053 | C | 3.7581 | -0.8754 | -0.2968 | C | 4.0261 | -1.0456 | -0.1978 |
| N | 2.4214 | -0.8987 | -0.2313 | N | 2.4298 | -0.8896 | -0.2306 | N | 2.6967 | -1.0219 | -0.1641 |
| H | -2.728 | -2.6183 | -0.0687 | H | -2.7117 | -2.6133 | 0.0143 | H | -2.4907 | -2.5914 | 0.1226 |
| H | -3.0752 | 2.373 | 0.3051 | H | -3.0671 | 2.3846 | 0.2752 | H | -2.7221 | 2.4166 | -0.0767 |
| H | -5.1062 | 0.9396 | 0.3223 | H | -5.0935 | 0.947 | 0.3553 | H | -4.7857 | 1.0417 | 0.1005 |
| H | -4.9298 | -1.5035 | 0.138 | H | -4.913 | -1.499 | 0.2273 | H | -4.666 | -1.4096 | 0.1982 |
| H | 0.1478 | -1.8745 | -0.179 | H | 0.1613 | -1.8656 | -0.1434 | H | 0.4012 | -1.9311 | -0.0471 |
| H | 1.8765 | 2.4115 | -0.0034 | H | 1.8877 | 2.4216 | -0.0137 | H | 2.2362 | 2.3069 | -0.2783 |
| H | 4.3827 | 2.4312 | -0.1462 | H | 4.395 | 2.4377 | -0.1394 | H | 4.7454 | 2.2511 | -0.3418 |
| H | 5.5793 | 0.2408 | -0.3425 | H | 5.5896 | 0.2455 | -0.3243 | H | 5.8864 | 0.0235 | -0.2866 |
| H | 4.236 | -1.8473 | -0.3899 | H | 4.2441 | -1.841 | -0.3764 | H | 4.4883 | -2.0258 | -0.172 |
| | | | | N | -0.0661 | -0.1194 | 3.1639 | Xe | -0.3285 | 0.1049 | 3.5435 |
| | | | | N | -1.1521 | -0.1195 | 3.2706 | | | | |

Table S5. Coordinates of the optimized structures of NpOH, NpOH·N₂-I1, NpOH·N₂-I2 and NpOH·Xe complexes in ground state S₀ calculated at B3LYP-D4/def2-TZVPP level of theory are provided.

| NpOH | | | | NpOH·N ₂ -I1 | | | |
|------|---------|---------|---------|-------------------------|---------|---------|---------|
| C | 1.2804 | -1.0915 | -0.0105 | C | 1.3095 | -1.0469 | -0.0879 |
| C | 2.3686 | -0.2543 | -0.0211 | C | 2.3963 | -0.2089 | -0.1391 |
| C | 2.1879 | 1.1427 | -0.0585 | C | 2.2132 | 1.1835 | -0.2469 |
| C | 0.9319 | 1.6859 | -0.0843 | C | 0.9562 | 1.7221 | -0.3038 |
| C | -0.2081 | 0.8462 | -0.0742 | C | -0.1821 | 0.8818 | -0.2534 |
| C | -0.0412 | -0.5692 | -0.0371 | C | -0.0127 | -0.529 | -0.1428 |
| C | -1.1808 | -1.4052 | -0.0279 | C | -1.1501 | -1.3668 | -0.106 |
| C | -2.4403 | -0.8636 | -0.0538 | C | -2.4102 | -0.8307 | -0.1758 |
| C | -2.6131 | 0.5352 | -0.09 | C | -2.5855 | 0.5639 | -0.2851 |

| | | | | | | | |
|------------------------------|---------|---------|-----------|----------------|---------|---------|---------|
| C | -1.5237 | 1.3666 | -0.1 | C | -1.4978 | 1.3969 | -0.3224 |
| O | 1.3962 | -2.4516 | 0.0258 | O | 1.4273 | -2.4025 | 0.0126 |
| H | 3.3695 | -0.6696 | -2.00E-04 | H | 3.3978 | -0.6212 | -0.099 |
| H | 3.059 | 1.784 | -0.0664 | H | 3.083 | 1.8252 | -0.288 |
| H | 0.7943 | 2.7585 | -0.1126 | H | 0.8166 | 2.7911 | -0.3919 |
| H | -1.0418 | -2.4758 | 1.00E-04 | H | -1.0088 | -2.4343 | -0.0245 |
| H | -3.3074 | -1.5104 | -0.0465 | H | -3.2758 | -1.4789 | -0.1482 |
| H | -3.6118 | 0.9509 | -0.1099 | H | -3.5846 | 0.9752 | -0.3408 |
| H | -1.6548 | 2.4409 | -0.128 | H | -1.6305 | 2.4677 | -0.4092 |
| H | 2.3266 | -2.6937 | 0.0402 | H | 2.3579 | -2.6441 | 0.0238 |
| NpOH·N₂-I2 | | | | NpOH·Xe | | | |
| C | 1.2586 | -1.0575 | -0.1311 | C | 1.2448 | -1.0818 | -0.0693 |
| C | 2.3484 | -0.2264 | -0.2158 | C | 2.3322 | -0.2454 | -0.123 |
| C | 2.1705 | 1.1675 | -0.3205 | C | 2.1527 | 1.152 | -0.1131 |
| C | 0.9156 | 1.7139 | -0.3401 | C | 0.8987 | 1.6964 | -0.0495 |
| C | -0.2254 | 0.8802 | -0.2568 | C | -0.2398 | 0.8576 | 0.0119 |
| C | -0.0613 | -0.5314 | -0.1501 | C | -0.0741 | -0.558 | 0.0013 |
| C | -1.2022 | -1.3626 | -0.0841 | C | -1.2105 | -1.3934 | 0.0848 |
| C | -2.4607 | -0.8198 | -0.1236 | C | -2.4661 | -0.8507 | 0.1791 |
| C | -2.6308 | 0.5754 | -0.2295 | C | -2.6379 | 0.5486 | 0.1898 |
| C | -1.5397 | 1.4023 | -0.2932 | C | -1.5512 | 1.3794 | 0.1058 |
| O | 1.3708 | -2.4139 | -0.0303 | O | 1.3595 | -2.442 | -0.0679 |
| H | 3.3483 | -0.6442 | -0.2026 | H | 3.3317 | -0.6616 | -0.1694 |
| H | 3.0428 | 1.8038 | -0.3864 | H | 3.0234 | 1.7926 | -0.1542 |
| H | 0.78 | 2.784 | -0.4226 | H | 0.7622 | 2.7694 | -0.0377 |
| H | -1.0648 | -2.4309 | -0.0079 | H | -1.072 | -2.4642 | 0.0793 |
| H | -3.3288 | -1.4635 | -0.076 | H | -3.3309 | -1.497 | 0.2468 |
| H | -3.6286 | 0.9923 | -0.2628 | H | -3.6335 | 0.9652 | 0.2656 |
| H | -1.6689 | 2.4736 | -0.3789 | H | -1.6812 | 2.4541 | 0.1166 |
| H | 2.3001 | -2.6606 | -0.0369 | H | 2.2883 | -2.6857 | -0.117 |
| N | -0.6763 | -0.6747 | -3.427 | Xe | 0.5399 | 0.1012 | 3.6627 |
| N | -1.0622 | 0.334 | -3.5815 | | | | |