The Reactivity of 2,6-lutidine/BR_3 and Pyridine/BR_3 Lewis Pairs (R=F, Me, C_6F_5): A Density Functional Study

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Supporting Information: The geometry changes of Py/$B(C_6F_5)_3$ pair with the N-B bond length R ranged from 4.00 to 4.75 Å, atom-condensed Fukui functions calculated by Natural population analysis, and the optimized structures of the transition state and the two corresponding minima for dihydrogen activation by 2, 6-lutidine/$B(C_6F_5)_3$ and 2,6-lutidine/BMe_3 pairs.

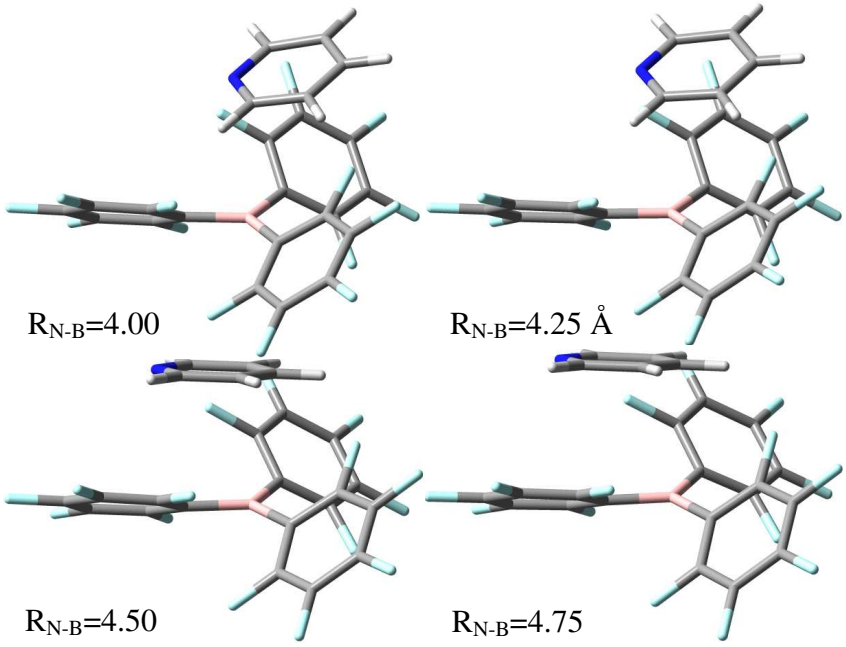

Figure S1. The geometry changes of Py/$B(C_6F_5)_3$ pair with the N-B bond length R ranged from 4.00 to 4.75 Å. Different color tubes correspond to atomic positions: gray, H; black, C; blue, N; pink, B; azure, F.

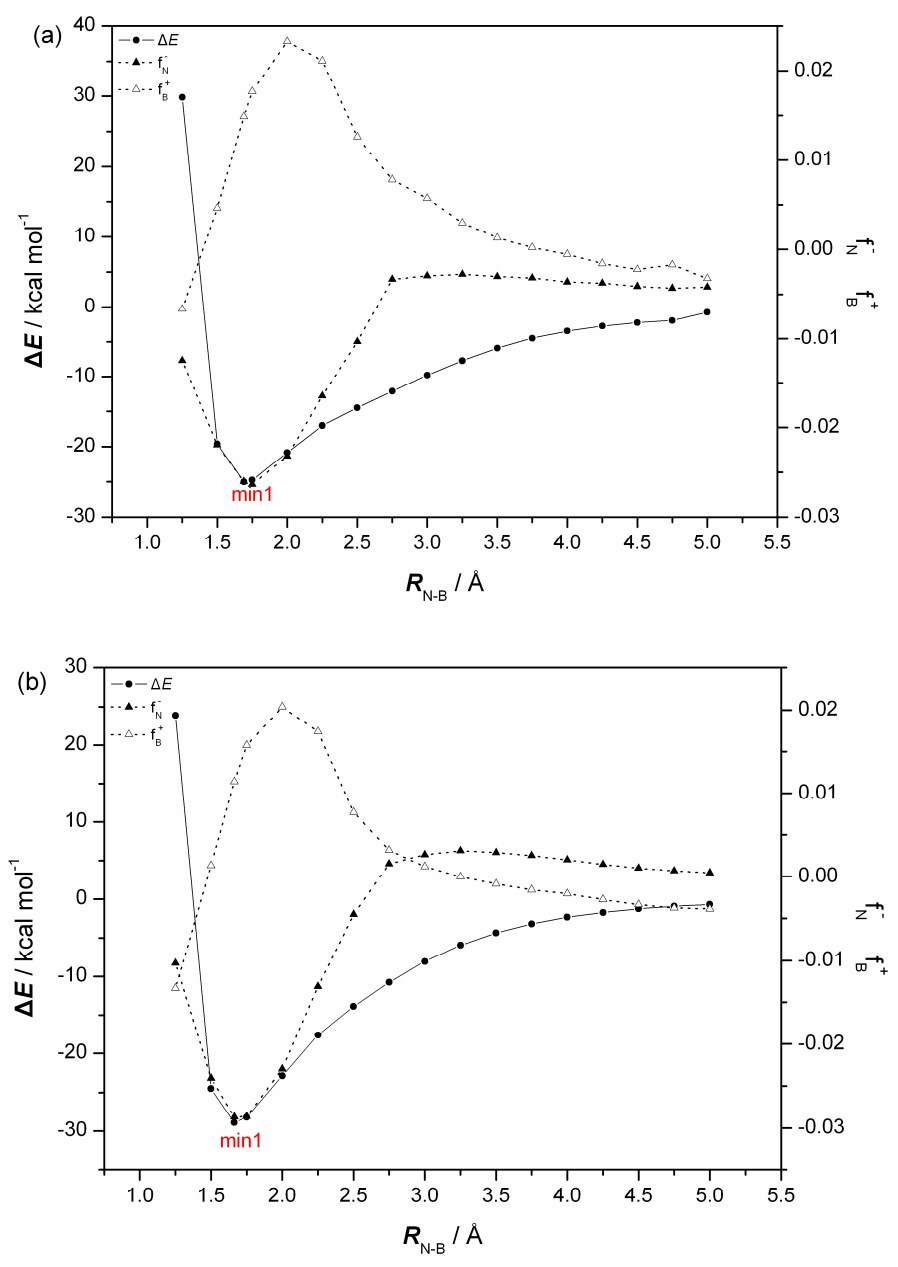

Figure S2. Potential energy curves for Lu/BF_3 (a) and Py/BF_3 (b) interactions. Values correspond to R_{N-B}=N-B bond length and ΔE=zero-point uncorrected electronic energy. Also shown is the profiles of local reactivity descriptors f_N^- and f_B^+, which obtained from natural population analysis. (Lu-2,6-lutidine, Py-pyridine)

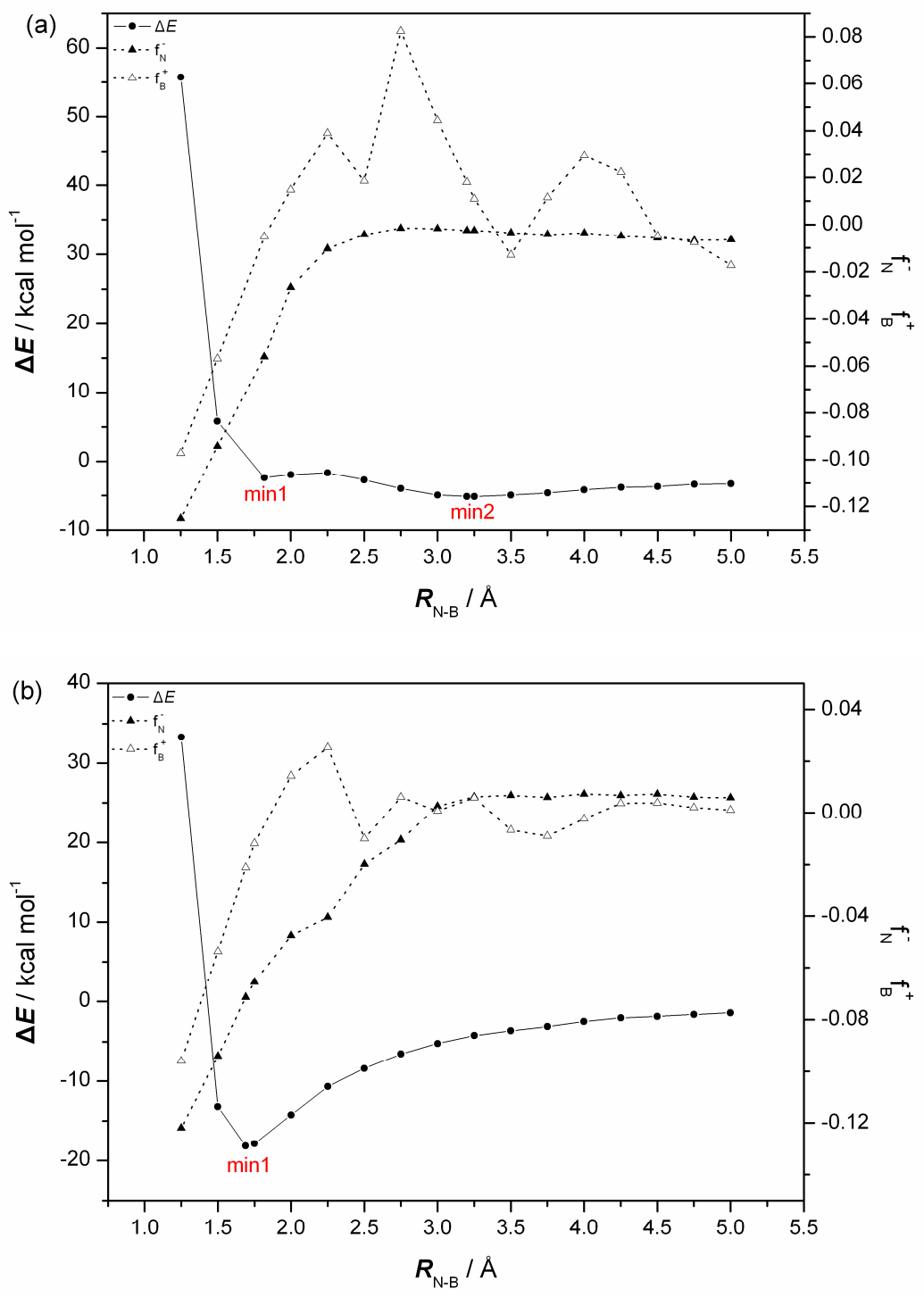

Figure S3. Potential energy curves for Lu/BMe_3 (a) and Py/BMe_3 (b) interactions. Also shown is the profiles of local reactivity descriptors f_N^- and f_B^+, which obtained from natural population analysis.

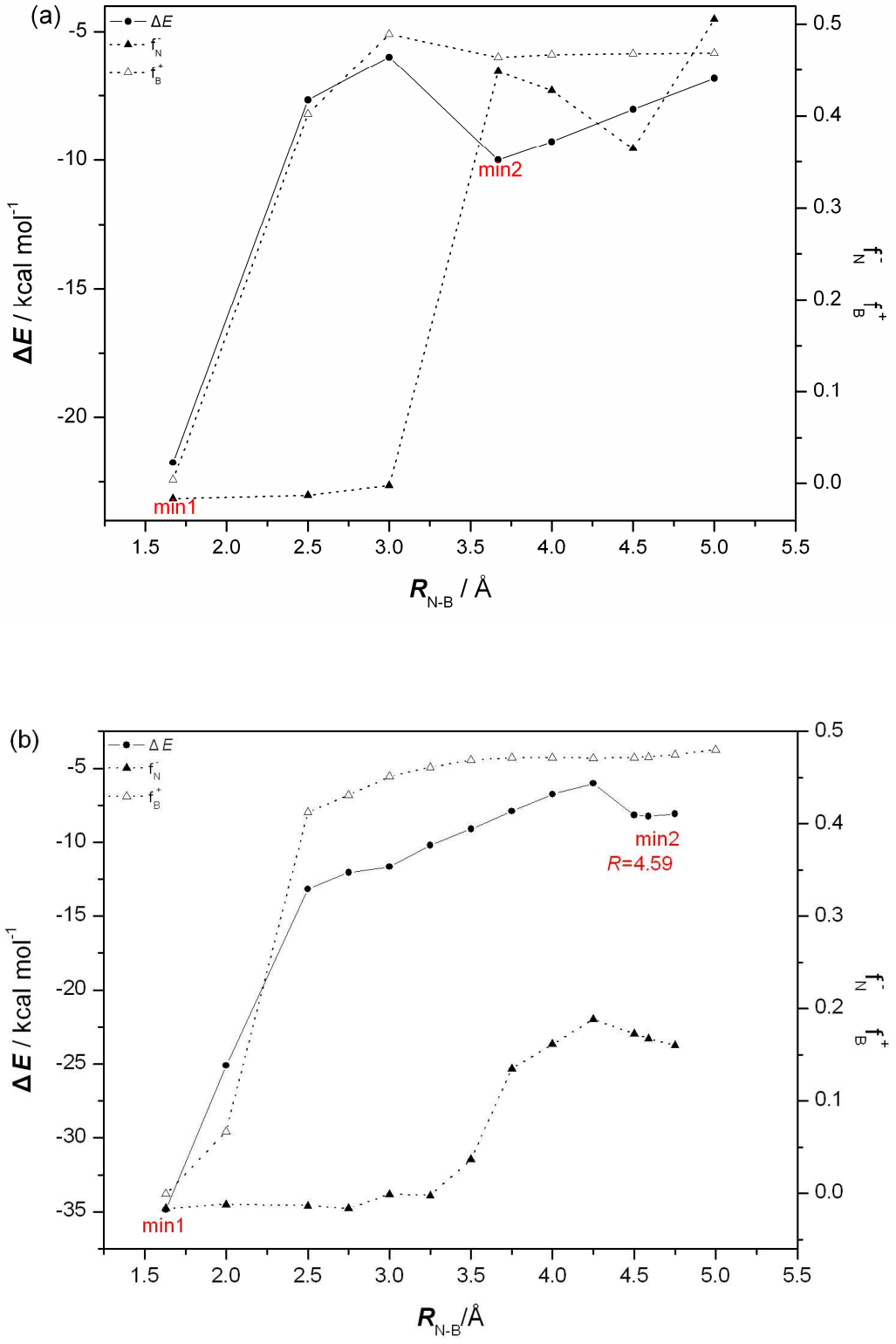

Figure S4. Potential energy curve for Lu/B(C_6F_5)$_3$ (a) and Py/B(C_6F_5)$_3$ (b) with respect to N-B distance. Also shown is the profiles of local reactivity descriptors f_N^- and f_B^+, which obtained from natural population analysis.

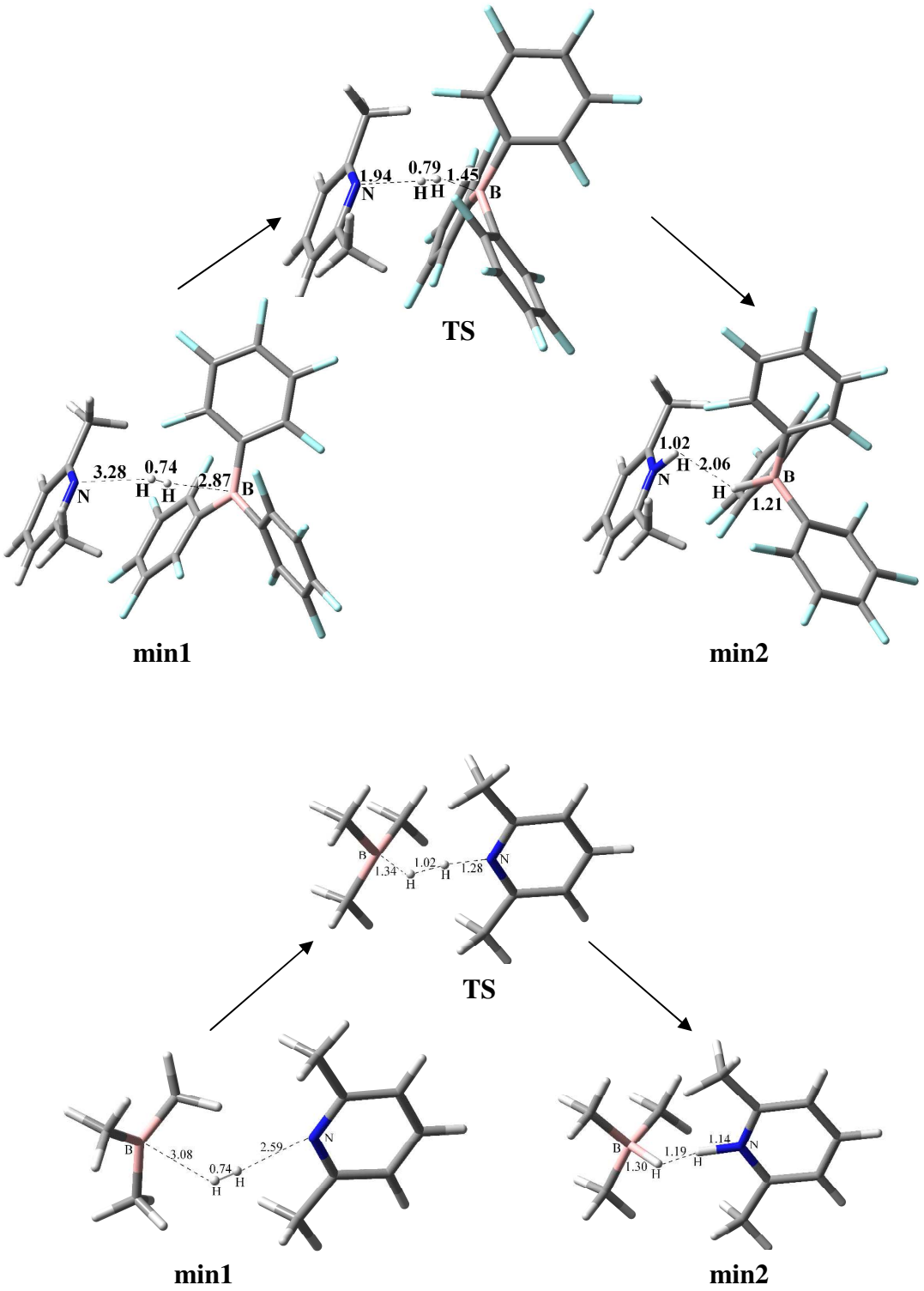

Figure S5. Optimized structures of the TS and the two corresponding minima for the dihydrogen activation by 2,6-lutidine/$B(C_6F_5)_3$ (up) and 2,6-lutidine/BMe_3 (down) pairs, respectively.