

Supplementary Information

Seeking the Most Stable Isomer of Azahomocubanes

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Table 1SI. T1-diagnostic values obtained from CCSD(T1diag) computations for **1-4** and their corresponding protonation species.

	T1-diagnostic value
1	0.0102
2	0.0098
3	0.0103
4	0.0100
1-H⁺	0.0093
2-H⁺	0.0098
3-H⁺	0.0096
4-H⁺	0.0098

Table 2SI. Relative energies in kcal/mol computed in the gas phase at the CCSD(T)/cc-pVTZ//M06-2X-D3/def2-TZVP and at M06-2X-D3/def2-TZVP levels. Solvent effects were taken into account at the M06-2X-D3/def2-TZVP level by employing the polarizable continuum model (PCM).

	gas phase	gas phase DFT	H ₂ O	CH ₃ OH	C ₆ H ₆	CH ₃ COOH	CH ₂ Cl ₂	CHCl ₃
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	1.9	3.3	2.6	2.6	2.9	2.7	2.7	2.7
3	3.2	3.8	3.9	3.9	3.8	3.8	3.9	3.9
4	3.4	4.6	4.3	4.3	4.5	4.4	4.3	4.3