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Theoretical investigation of isomerization pathways of diazenes: Torsion *vs* inversion

SUPPORTING INFORMATION

Aarti Sindhu,[†] Renuka Pradhan,[‡] Upakarasamy Lourderaj,[‡] and Manikandan Paranjothy*,[†]

†*Department of Chemistry, Indian Institute of Technology Jodhpur, Jodhpur, Rajasthan, India*

‡*School of Chemical Sciences, National Institute of Science Education and Research (NISER), Bhubaneshwar, HBNI, P. O. Jatni, Khurda, India*

E-mail: pmanikandan@iitj.ac.in

Phone: +91 291 280 1306. Fax: +91 291 251 6823

Optimized Geometries

Optimized geometries of stationary points on the N_2H_2 and N_2F_2 potential energy surface computed using the CASSCF(2,2)/aug-cc-pVDZ level of electronic structure theory are given in Figure S1.

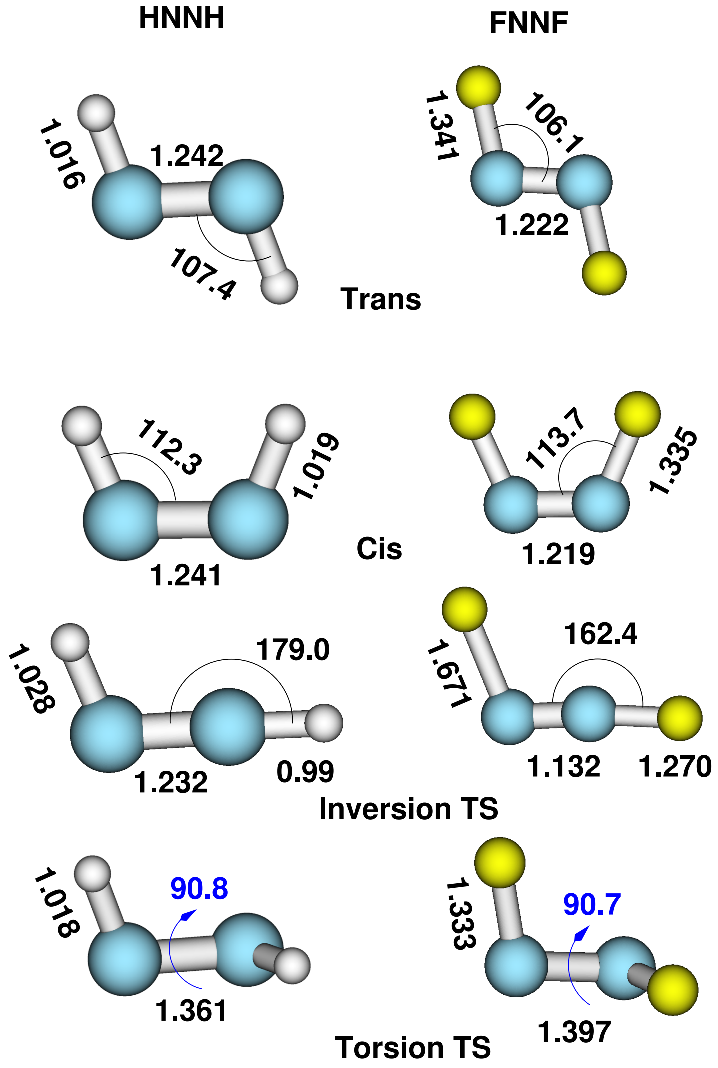

Figure S1: Optimized geometries of N_2H_2 and N_2F_2 using CASSCF(2,2)/aug-cc-pVDZ level of electronic structure theory. Distances are in units of Å and angles are in units of degrees.

Table S1: Normal mode frequencies (in cm^{-1}) associated with the stationary points on the N_2H_2 and N_2F_2 potential energy surface computed using CASSCF(2,2)/aug-cc-pVDZ theory.

Trans	Cis	Inversion TS	Torsion TS
N_2H_2			
1371	1289	-1706	-2954
1431	1463	497	1170
1681	1668	1623	1308
1715	1675	1706	1335
3564	3486	3360	3565
3603	3545	4085	3567
N_2F_2			
407	406	-739	-435
495	587	253	479
701	895	406	688
1215	1136	414	1105
1244	1174	1096	1144
1729	1730	2299	1193