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A Computational Investigation of the Red and Blue Shifts in Hydrogen Bonded Systems[#]

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Footnote: Dedicated to the memory of the late Professor Charusita Chakravarty

Table S1: Calculated results on the bond distance, bond angle, total energy, frequency shift, atomic charges and bond order for $F_3CH\ldots NF_3$ system (a blue shifted system) as calculated by DFT using B3LYP exchange correlation function by regulating the H...Y distance.

Bond Length (Å)		X—H…Y Angle (°)	Total Energy (10^6 J/mol)	X—H bond stretching frequency (cm^{-1})	Mulliken Charge (e)		Lowdin Charge (e)		X—H Bond Order
H…Y	X—H				H	Y	H	Y	
1.0	1.44669	162.160	-1816.1845		0.36894	0.32226	0.18396	0.36776	0.462
1.2	1.21909	169.416	-1816.3222		0.35003	0.33724	0.16599	0.35314	0.703
1.4	1.13918	169.693	-1816.4143	2736.72	0.28379	0.40248	0.13698	0.35316	0.800
1.6	1.10778	166.509	-1816.4682	3039.57	0.23302	0.45757	0.11574	0.35590	0.832
1.8	1.09545	163.806	-1816.4969	3159.47	0.20206	0.49149	0.10424	0.35929	0.848
2.0	1.09124	179.128	-1816.5119	3195.86	0.18716	0.50571	0.09916	0.36232	0.860
2.2	1.08845	178.614	-1816.5191	3210.48	0.17946	0.51613	0.09809	0.35958	0.866
2.4	1.08739	178.284	-1816.5219	3211.03	0.17443	0.52260	0.09900	0.35772	0.872
2.6	1.08703	178.070	-1816.5228	3208.55	0.17153	0.52666	0.10038	0.35686	0.877
2.8	1.08694	177.846	-1816.5229	3206.57	0.17020	0.52922	0.10161	0.35686	0.88
3.0	1.08692	177.717	-1816.5227	3205.36	0.16986	0.53090	0.10253	0.35747	0.883
3.2	1.08693	177.585	-1816.5224	3204.52	0.17002	0.53215	0.10316	0.35847	0.885
3.4	1.08695	177.416	-1816.5220	3203.83	0.17034	0.53325	0.10357	0.35969	0.887
3.6	1.08699	168.351	-1816.5217	3203.86	0.17071	0.53434	0.10385	0.36097	0.887
3.8	1.08704	177.115	-1816.5215	3202.77	0.17092	0.53537	0.10401	0.36212	0.888
4.0	1.08709	177.042	-1816.5214	3202.38	0.17111	0.53635	0.10413	0.36316	0.888
4.2	1.08712	176.982	-1816.5213	3202.37	0.17118	0.53726	0.10418	0.36406	0.889
4.4	1.08715	174.143	-1816.5212	3202.13	0.17112	0.53826	0.10418	0.36497	0.889
4.6	1.08716	172.510	-1816.5213	3202.81	0.17123	0.53876	0.10423	0.36546	0.889
4.8	1.08717	176.048	-1816.5212	3202.02	0.17115	0.53963	0.10421	0.36621	0.889
5.0	1.08717	175.892	-1816.5213	3201.98	0.17120	0.54016	0.10424	0.36667	0.889
5.2	1.08715	176.560	-1816.5213	3202.23	0.17125	0.54061	0.10426	0.36705	0.889
5.4	1.08717	175.666	-1816.5213	3202.07	0.17133	0.54096	0.10431	0.36736	0.889
5.6	1.08717	174.219	-1816.5213	3201.95	0.17133	0.54160	0.10432	0.36787	0.889
5.8	1.08717	176.783	-1816.5214	3202.11	0.17142	0.54167	0.10436	0.36796	0.889
6.0	1.08716	173.327	-1816.5214	3202.20	0.17145	0.54212	0.10438	0.36831	0.889
∞	1.08713	180.000	-1816.5215	3202.64	0.17207	0.54463	0.10469	0.37052	0.89

Table S2: Calculated results on the bond distance, bond angle, total energy, frequency shift, atomic charges and bond order for $F_3CH\ldots NH_3$ system (a red shifted system) as calculated by DFT using B3LYP exchange correlation function by regulating the H...Y distance.

Bond Length (Å)		X—H…Y Angle (°)	Total Energy (10^6 J/mol)	X—H bond stretching frequency (cm^{-1})	Mulliken Charge (e)		Lowdin Charge (e)		X—H Bond Order
H…Y	X—H				H	Y	H	Y	
1	1.6632	179.193	-1035.6255		0.18379	-0.75252	0.20213	-0.34809	0.64
1.2	1.37642	179.539	-1035.7060		0.26258	-0.83811	0.21849	-0.46485	0.710
1.4	1.21683	179.742	-1035.7635	1891.44	0.27195	-0.87454	0.19262	-0.53264	0.754
1.6	1.14843	179.749	-1035.8001	2487.53	0.26901	-0.87689	0.16327	-0.56192	0.781
1.8	1.11709	179.561	-1035.8177	2817.19	0.26034	-0.86887	0.14348	-0.57791	0.797
2.0	1.10161	179.362	-1035.8235	2994.02	0.24618	-0.86050	0.13195	-0.58980	0.810
2.2	1.09368	178.180	-1035.8232	3092.04	0.23012	-0.85505	0.12547	-0.59978	0.823
2.4	1.08956	177.081	-1035.8204	3148.28	0.21606	-0.85302	0.12170	-0.60813	0.835
2.6	1.08741	176.788	-1035.8169	3181.79	0.20574	-0.85366	0.11928	-0.61481	0.845
2.8	1.08622	176.765	-1035.8135	3202.48	0.19913	-0.85583	0.11759	-0.61990	0.854
3.0	1.08553	176.858	-1035.8101	3215.02	0.19537	-0.85839	0.11636	-0.62353	0.861
3.2	1.08516	176.840	-1035.8069	3221.49	0.19340	-0.86056	0.11547	-0.62595	0.868
3.4	1.08506	177.132	-1035.8038	3223.48	0.19230	-0.86192	0.11480	-0.62742	0.873
3.6	1.08519	176.587	-1035.8010	3222.45	0.19133	-0.86254	0.11420	-0.62824	0.877
3.8	1.08545	176.281	-1035.7987	3220.05	0.19016	-0.86260	0.11356	-0.62864	0.880
4.0	1.08576	174.447	-1035.7969	3217.40	0.18867	-0.86243	0.11282	-0.62884	0.882
4.2	1.08603	174.644	-1035.7955	3214.90	0.18705	-0.86217	0.11204	-0.62894	0.884
4.4	1.08625	174.090	-1035.7946	3212.98	0.18539	-0.86198	0.11124	-0.62903	0.885
4.6	1.08641	173.173	-1035.7938	3211.59	0.18373	-0.86184	0.11046	-0.62912	0.886
4.8	1.08653	173.140	-1035.7933	3210.29	0.18229	-0.86177	0.10977	-0.62921	0.886
5.0	1.08661	177.164	-1035.7929	3209.48	0.18106	-0.86175	0.10917	-0.62931	0.886
5.2	1.08668	174.289	-1035.7925	3208.48	0.17995	-0.86176	0.10864	-0.62941	0.887
5.4	1.08673	175.514	-1035.7922	3207.95	0.17903	-0.86180	0.10819	-0.62952	0.887
5.6	1.08678	173.674	-1035.7920	3207.23	0.17824	-0.86186	0.10781	-0.62963	0.887
5.8	1.08682	175.707	-1035.7918	3206.86	0.17757	-0.86191	0.10747	-0.62973	0.887
6.0	1.08685	173.459	-1035.7916	3206.30	0.17698	-0.86204	0.10719	-0.62988	0.887
∞	1.08713	180.000	-1035.7897	3202.75	0.17208	-0.86381	0.10469	-0.63166	0.889