The crucial role of the inter-ring hydrogen bond to explain morin properties

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Electronic Supplementary Information

Contents:

Cartesian coordinates for the optimized geometry of morin

C	-4.316466	-2.103019	1.507256
C	-2.978670	-2.085447	0.982755
C	-2.481411	-0.811046	0.573410
C	-3.295610	0.322021	0.709187
C	-5.052035	-0.967596	1.654158
C	-1.190858	-0.657452	0.009339
C	-2.877945	1.580112	0.312902
C	-1.603795	1.697366	-0.236106
C	-0.756934	0.592574	-0.390103
H	-3.518450	2.444947	0.427203
H	0.232011	0.704743	-0.821224
O	-4.530660	0.221489	1.251828
O	-4.807068	-3.328321	1.829344
H	-4.074167	-3.952356	1.676894
O	-0.396344	-1.722048	-0.138258
H	-0.895233	-2.505126	0.194831
O	-1.221071	2.931553	-0.614688
H	-0.332570	2.908059	-0.984686
C	-6.408910	-0.828215	2.172359
C	-7.216385	0.191214	1.638752
C	-6.946774	-1.608516	3.222994
C	-8.492725	0.441311	2.095804
H	-6.817027	0.799371	0.835699
C	-8.232782	-1.352442	3.689435
C	-9.002796	-0.339351	3.138010
H	-9.090755	1.231148	1.652845
H	-8.625534	-1.956150	4.499278
O	-6.265783	-2.569316	3.878269
H	-5.619713	-2.997062	3.285524
O	-10.240709	-0.155071	3.646116
H	-10.682701	0.565854	3.186744
O	-2.342858	-3.161956	0.888918

Cartesian coordinates for the optimized geometry of H_{34}

C	3.723076	-2.809487	-0.017309
C	3.316921	-1.491468	-0.050969
C	1.930377	-1.178264	-0.053568
C	1.007576	-2.236206	-0.016220
C	1.401068	-3.562966	0.019566
C	2.764817	-3.832970	0.019209
H	4.783058	-3.040032	-0.016264
C	1.432302	0.146749	-0.071813
H	0.671716	-4.361968	0.046471
C	-0.827235	-0.723855	-0.032435
C	0.019090	0.365774	-0.041789
C	-2.282784	-0.732433	0.005444
C	-2.927078	-1.857985	0.553300
C	-3.101755	0.294359	-0.533428
C	-4.298366	-1.987571	0.584737
H	-2.317603	-2.651471	0.968549
C	-4.488971	0.158260	-0.503968
C	-5.086642	-0.966071	0.043071
H	-4.758704	-2.867250	1.022908
H	-5.099457	0.947927	-0.926524
O	-0.313151	-1.980634	-0.023840
O	2.215041	1.164943	-0.084066
O	-0.394375	1.626376	0.001839
O	4.235130	-0.519050	-0.079402
H	3.761022	0.339019	-0.090788
O	3.127316	-5.128227	0.055685
H	4.086740	-5.208841	0.055598
O	-2.622849	1.388439	-1.137692
H	-1.718057	1.605871	-0.765014
O	-6.436735	-1.022868	0.030656
H	-6.735169	-1.841883	0.438481
Zn	1.153075	2.876658	-0.020238
O	1.684888	4.607634	-0.947333
H	1.897595	4.599606	-1.886830
H	1.087590	5.348777	-0.796049
O	0.618681	4.121696	1.570755
H	-0.092026	3.793264	2.132339
H	1.308068	4.444821	2.161125

Cartesian coordinates for the optimized geometry of H_{45}

C	-4.645695	-2.516867	0.447739
C	-3.204628	-2.514664	0.429610
C	-2.538550	-1.285025	0.163489
C	-3.347149	-0.140469	-0.041010
C	-5.350633	-1.379246	0.211326
C	-1.100501	-1.111172	0.097687
C	-2.837441	1.120493	-0.289070
C	-1.452578	1.257868	-0.344977
C	-0.606161	0.171147	-0.158934
H	-3.509889	1.956788	-0.439328
H	0.467212	0.311387	-0.209957
O	-4.695088	-0.219263	-0.016536
O	-5.244588	-3.679849	0.762624
H	-4.515011	-4.307221	0.901379
O	-0.258996	-2.085056	0.253428
O	-0.869750	2.450732	-0.584080
H	-1.540781	3.131579	-0.696776
C	-6.800412	-1.206782	0.241088
C	-7.347921	-0.158572	0.989044
C	-7.675958	-2.023783	-0.494725
C	-8.710762	0.063030	1.052893
H	-6.678282	0.488592	1.545166
C	-9.049344	-1.813370	-0.434335
C	-9.565387	-0.778243	0.337154
H	-9.110909	0.873756	1.652766
H	-9.726654	-2.439368	-1.006511
O	-7.143295	-2.975033	-1.288400
H	-7.843504	-3.446071	-1.750980
O	-10.908577	-0.629702	0.346818
H	-11.152771	0.120935	0.897444
O	-2.672757	-3.647003	0.685500
Zn	-0.699362	-3.875946	0.835802
O	0.563629	-5.493125	1.223210
H	0.401465	-6.056081	1.986975
O	-0.743417	-3.489930	2.948892
H	0.075885	-3.404486	3.446649
O	-0.445350	-4.666562	-1.205830
H	-1.239629	-5.010281	-1.628235
H	-0.126120	-3.961377	-1.779445
H	0.661559	-6.068946	0.456491
H	-1.356857	-3.974230	3.510563

Cartesian coordinates for the optimized geometry of H_{32},

C	-4.470042	-1.672337	0.315754
C	-3.223534	-1.437158	1.011105
C	-2.792519	-0.079183	1.152431
C	-3.624894	0.964753	0.725298
C	-5.294507	-0.587710	0.091892
C	-1.527949	0.254606	1.706980
C	-3.241677	2.297666	0.800833
C	-1.990414	2.584454	1.329781
C	-1.130521	1.576184	1.786619
H	-3.903860	3.087603	0.470176
H	-0.159384	1.819829	2.204876
O	-4.856925	0.696916	0.260660
O	-4.791083	-2.901041	-0.020672
O	-0.717081	-0.716658	2.140659
H	-1.213431	-1.567448	2.004190
O	-1.637975	3.887034	1.394919
H	-0.761237	3.972915	1.782132
C	-6.673980	-0.653769	-0.368943
C	-7.105781	0.251958	-1.348018
C	-7.618440	-1.568527	0.193956
C	-8.400461	0.265225	-1.832042
H	-6.386530	0.958218	-1.750808
C	-8.929096	-1.549635	-0.324780
C	-9.313672	-0.658018	-1.310790
H	-8.699762	0.967865	-2.603644
H	-9.657097	-2.240932	0.087102
O	-7.348988	-2.365004	1.200303
O	-10.604057	-0.713109	-1.739630
H	-10.744637	-0.048509	-2.420542
O	-2.534770	-2.401792	1.469353
Zn	-5.983913	-3.788565	1.248662
O	-7.444065	-4.686250	2.548533
H	-8.078008	-3.954848	2.530778
O	-6.004927	-5.634554	0.196061
H	-6.253588	-6.416737	0.698443
O	-4.290114	-4.202614	2.437079
H	-3.572806	-3.620391	2.071737
H	-4.302344	-4.071667	3.389605
H	-7.265593	-4.880259	3.473833
H	-5.192948	-5.852472	-0.272341