

Supporting Material

Boron Beats Nitrogen:
Strained Boron-Boron Bonds as Molecular Proton Sponges

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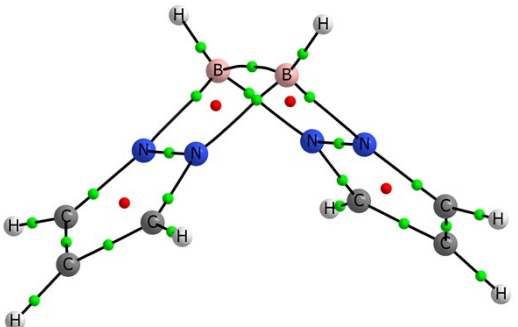
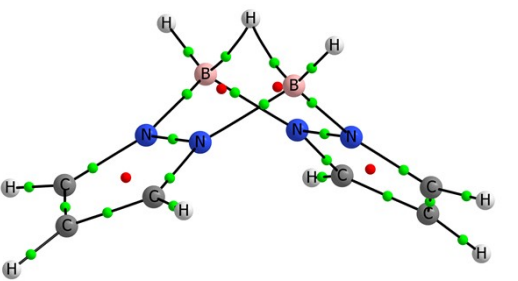
M. Merced Montero-Campillo, Otilia Mó, Manuel Yáñez

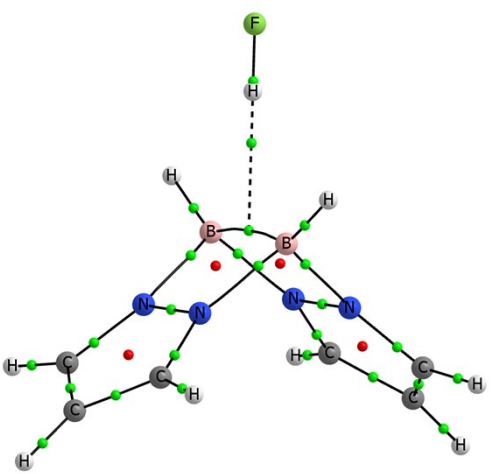
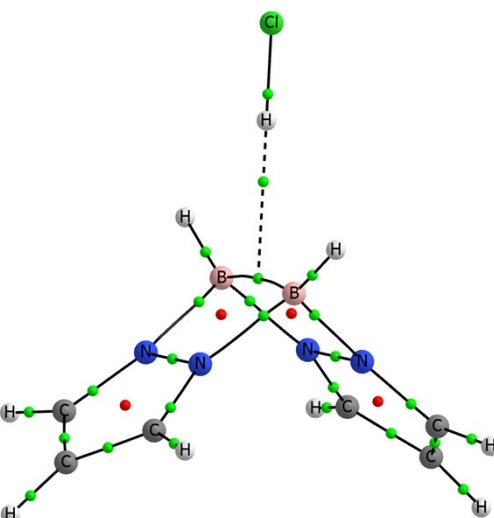
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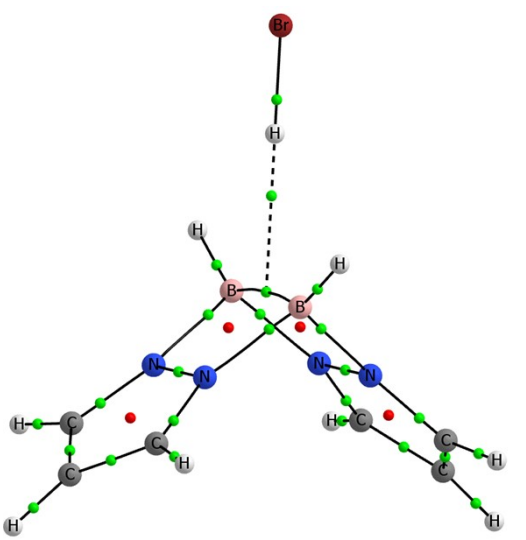
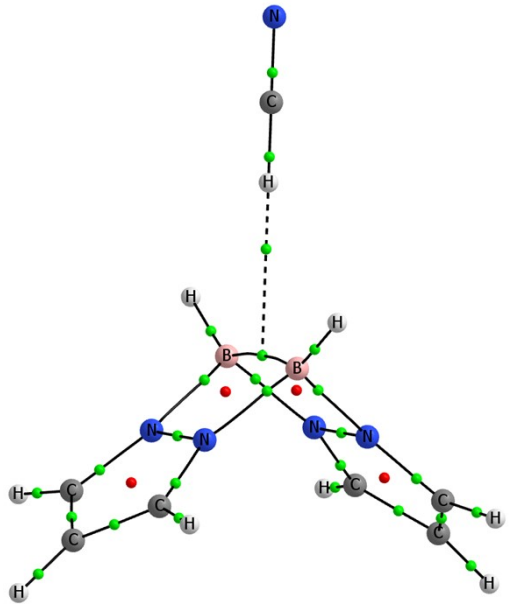
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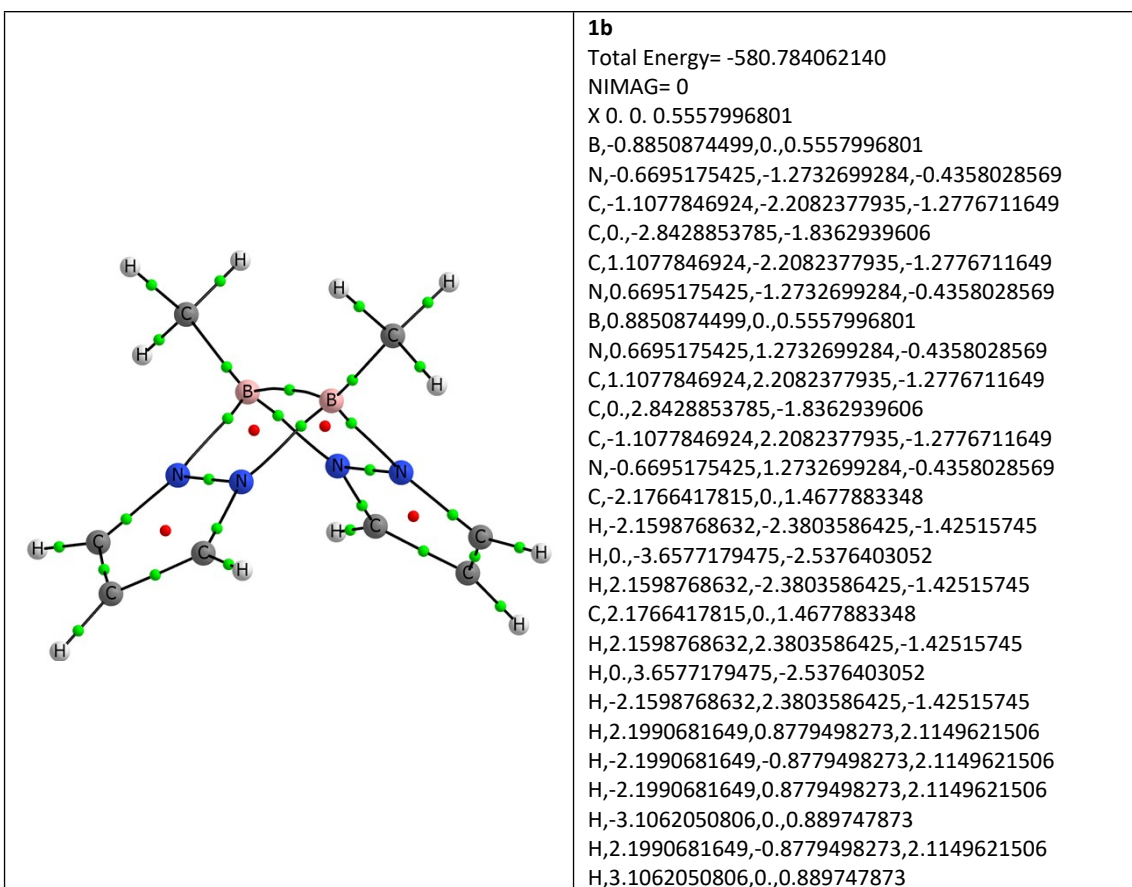
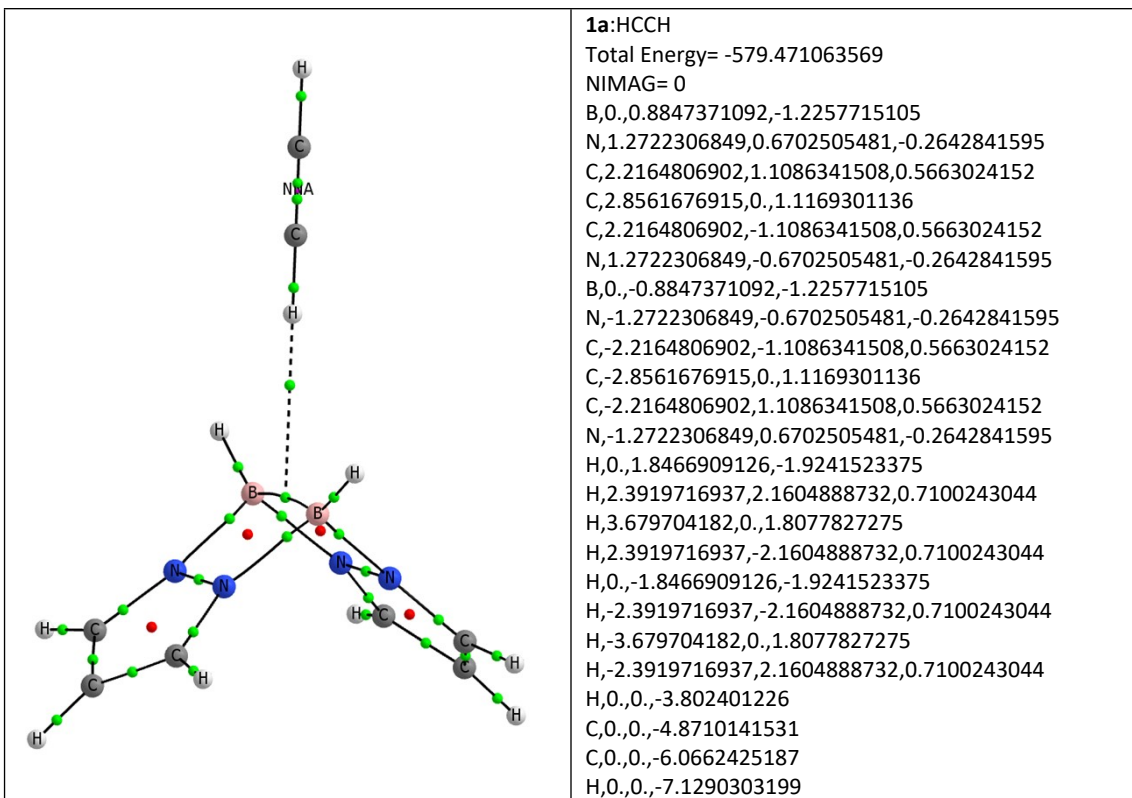
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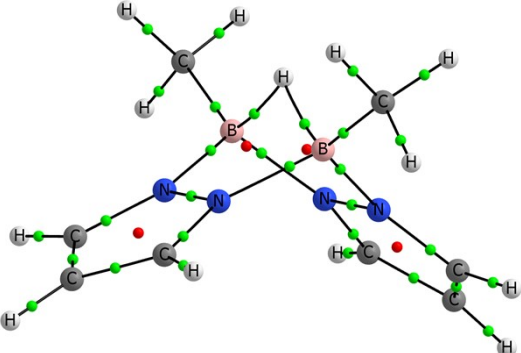
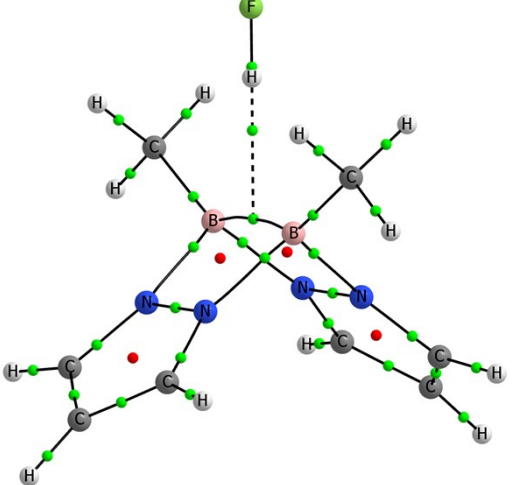
Table S1. Molecular graph, electronic energy (hartree) and optimized geometry (Å) of the systems at M06-2x/aug-cc-pVTZ computational level.

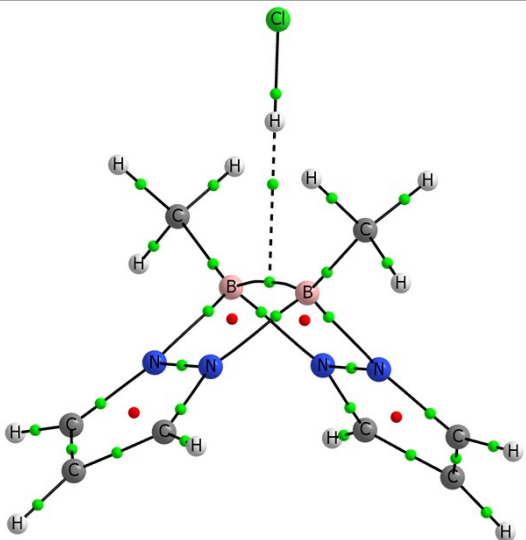
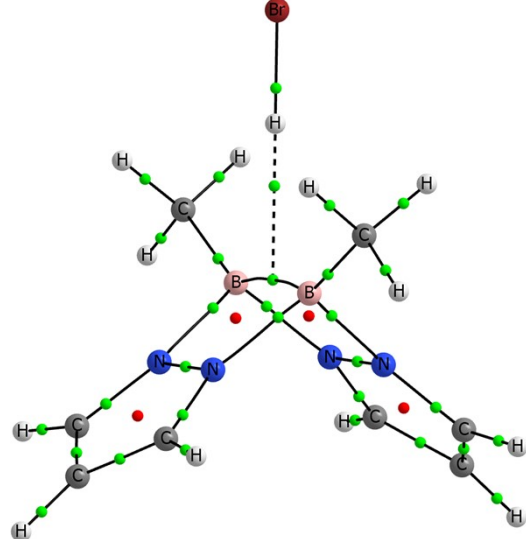
Molecular Graph	Electronic energy and optimized geometry
	1a Total Energy= -502.141187038 NIMAG= 0 B,0.,0.8808951592,-1.3626851601 N,1.2726348116,0.6701564421,-0.3926483625 C,2.212989624,1.1083891149,0.442470768 C,2.8505592811,0.,0.9963486993 C,2.212989624,-1.1083891149,0.442470768 N,1.2726348116,-0.6701564421,-0.3926483625 B,0.,-0.8808951592,-1.3626851601 N,-1.2726348116,-0.6701564421,-0.3926483625 C,-2.212989624,-1.1083891149,0.442470768 C,-2.8505592811,0.,0.9963486993 C,-2.212989624,1.1083891149,0.442470768 N,-1.2726348116,0.6701564421,-0.3926483625 H,0.,1.8465836554,-2.0554611583 H,2.3872671881,2.1602840591,0.5875273873 H,3.6706157082,0.,1.6914147857 H,2.3872671881,-2.1602840591,0.5875273873 H,0.,-1.8465836554,-2.0554611583 H,-2.3872671881,-2.1602840591,0.5875273873 H,-3.6706157082,0.,1.6914147857 H,-2.3872671881,2.1602840591,0.5875273873
	1a:H⁺ Total Energy= -502.557341211 NIMAG= 0 B,0.,1.099360993,-1.135486241 N,1.2572676728,0.6732066888,-0.3552130962 C,2.3088839595,1.1082868724,0.3415944503 C,3.0056337555,0.,0.8079659587 C,2.3088839595,-1.1082868724,0.3415944503 N,1.2572676728,-0.6732066888,-0.3552130962 B,0.,-1.099360993,-1.135486241 N,-1.2572676728,-0.6732066888,-0.3552130962 C,-2.3088839595,-1.1082868724,0.3415944503 C,-3.0056337555,0.,0.8079659587 C,-2.3088839595,1.1082868724,0.3415944503 N,-1.2572676728,0.6732066888,-0.3552130962 H,0.,2.0925369147,-1.767616878 H,2.509076124,2.160588077,0.4524623688 H,3.9094248236,0.,1.3893746621 H,2.509076124,-2.160588077,0.4524623688 H,0.,-2.0925369147,-1.767616878 H,-2.509076124,-2.160588077,0.4524623688 H,-3.9094248236,0.,1.3893746621 H,-2.509076124,2.160588077,0.4524623688 H,0.,0.,-1.98749883

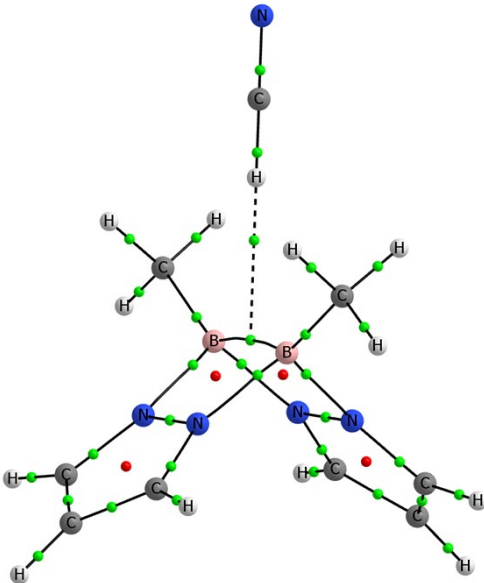
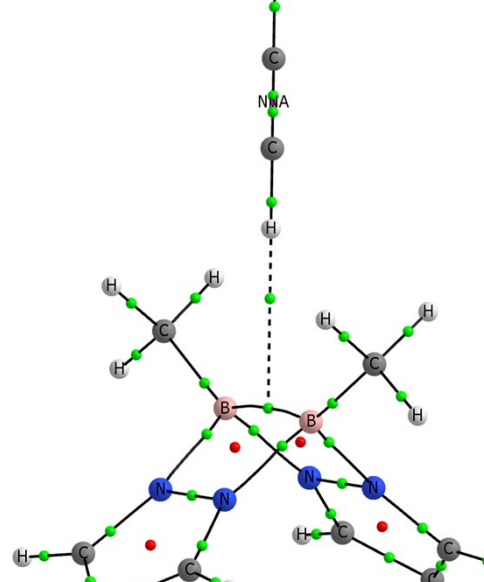
	1a:HF Total Energy= -602.608355888 NIMAG= 0 B,0.,0.8983741531,-1.2998167283 N,1.2698372563,0.6699987275,-0.3537106115 C,2.2231840243,1.1089759435,0.465922467 C,2.8680506014,0.,1.0091912963 C,2.2231840243,-1.1089759435,0.465922467 N,1.2698372563,-0.6699987275,-0.3537106115 B,0.,-0.8983741531,-1.2998167283 N,-1.2698372563,-0.6699987275,-0.3537106115 C,-2.2231840243,-1.1089759435,0.465922467 C,-2.8680506014,0.,1.0091912963 C,-2.2231840243,1.1089759435,0.465922467 N,-1.2698372563,0.6699987275,-0.3537106115 H,0.,1.862186945,-1.9933749572 H,2.4010155796,2.1608443933,0.6062634218 H,3.6992850265,0.,1.6905871389 H,2.4010155796,-2.1608443933,0.6062634218 H,0.,-1.862186945,-1.9933749572 H,-2.4010155796,-2.1608443933,0.6062634218 H,-3.6992850265,0.,1.6905871389 H,-2.4010155796,2.1608443933,0.6062634218 H,0.,0.,-3.330723261 F,0.,0.,-4.2677176697
	1a:HCl Total Energy= -962.958156915 NIMAG= 0 B,0.,0.8938119826,-1.2826408345 N,1.2709713284,0.6701286075,-0.3318592736 C,2.22225038,1.1088866414,0.4904193129 C,2.8659801057,0.,1.0354707668 C,2.22225038,-1.1088866414,0.4904193129 N,1.2709713284,-0.6701286075,-0.3318592736 B,0.,-0.8938119826,-1.2826408345 N,-1.2709713284,-0.6701286075,-0.3318592736 C,-2.22225038,-1.1088866414,0.4904193129 C,-2.8659801057,0.,1.0354707668 C,-2.22225038,1.1088866414,0.4904193129 N,-1.2709713284,0.6701286075,-0.3318592736 H,0.,1.858085059,-1.9762789948 H,2.3995596392,2.1607596699,0.6317153874 H,3.6954163172,0.,1.7191627338 H,2.3995596392,-2.1607596699,0.6317153874 H,0.,-1.858085059,-1.9762789948 H,-2.3995596392,-2.1607596699,0.6317153874 H,-3.6954163172,0.,1.7191627338 H,-2.3995596392,2.1607596699,0.6317153874 H,0.,0.,-3.4821959579 Cl,0.,0.,-4.7816995537

	1a:HBr Total Energy= -3076.98934534 NIMAG= 0 B,0.,0.8946357458,-1.2750663994 N,1.2710487379,0.6700841379,-0.3246498548 C,2.222738169,1.1088660601,0.4971520262 C,2.8666823705,0.,1.0419791313 C,2.222738169,-1.1088660601,0.4971520262 N,1.2710487379,-0.6700841379,-0.3246498548 B,0.,-0.8946357458,-1.2750663994 N,-1.2710487379,-0.6700841379,-0.3246498548 C,-2.222738169,-1.1088660601,0.4971520262 C,-2.8666823705,0.,1.0419791313 C,-2.222738169,1.1088660601,0.4971520262 N,-1.2710487379,0.6700841379,-0.3246498548 H,0.,1.8603492068,-1.966678995 H,2.4000944971,2.1607284351,0.6383181514 H,3.6964688675,0.,1.7252192342 H,2.4000944971,-2.1607284351,0.6383181514 H,0.,-1.8603492068,-1.966678995 H,-2.4000944971,-2.1607284351,0.6383181514 H,-3.6964688675,0.,1.7252192342 H,-2.4000944971,2.1607284351,0.6383181514 H,0.,0.,-3.4813910193 Br,0.,0.,-4.9241627439
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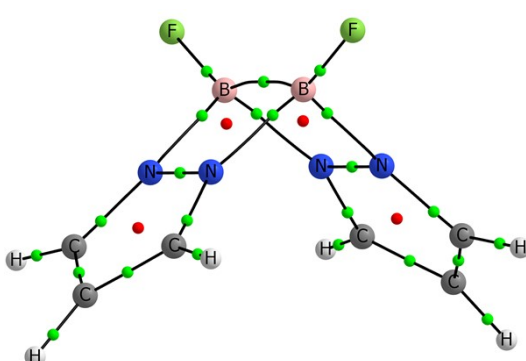
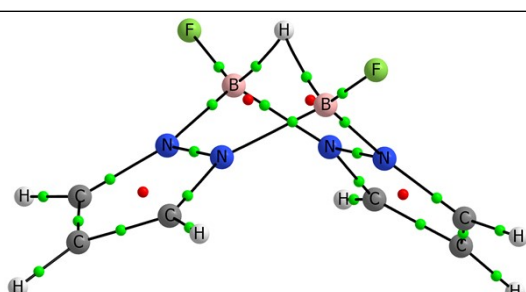


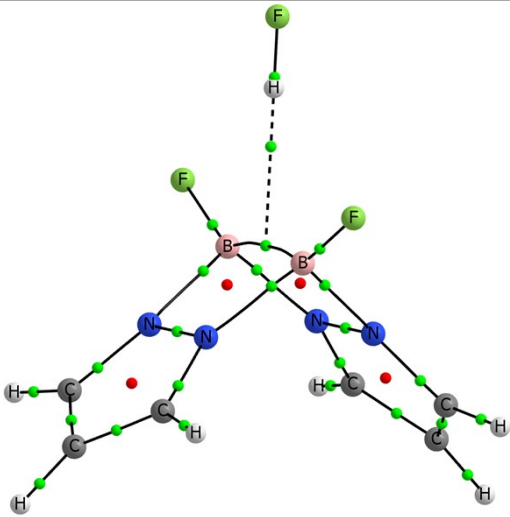
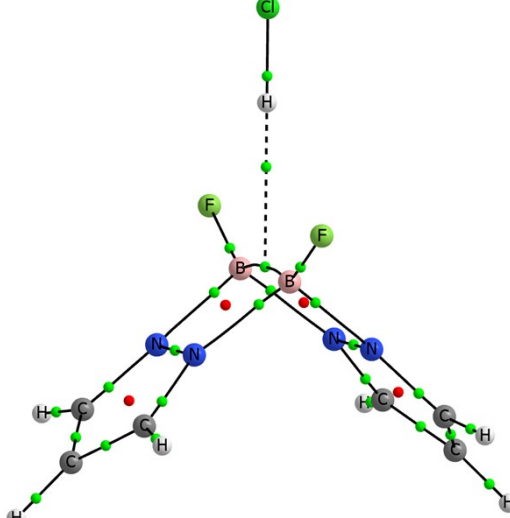
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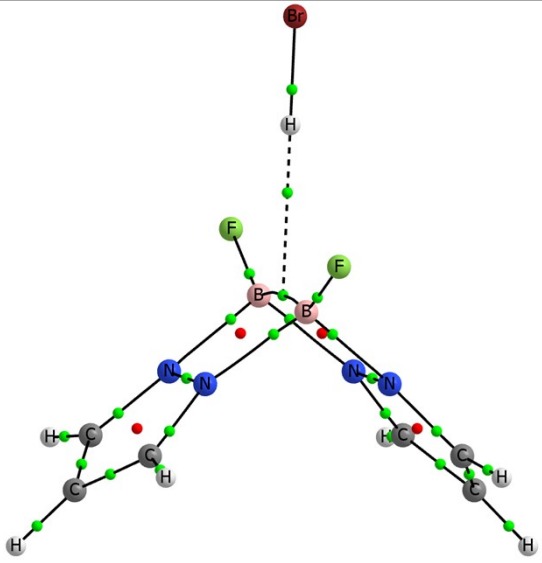
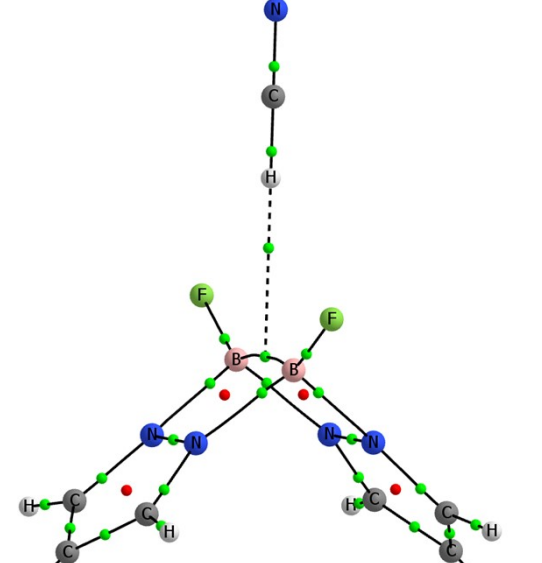
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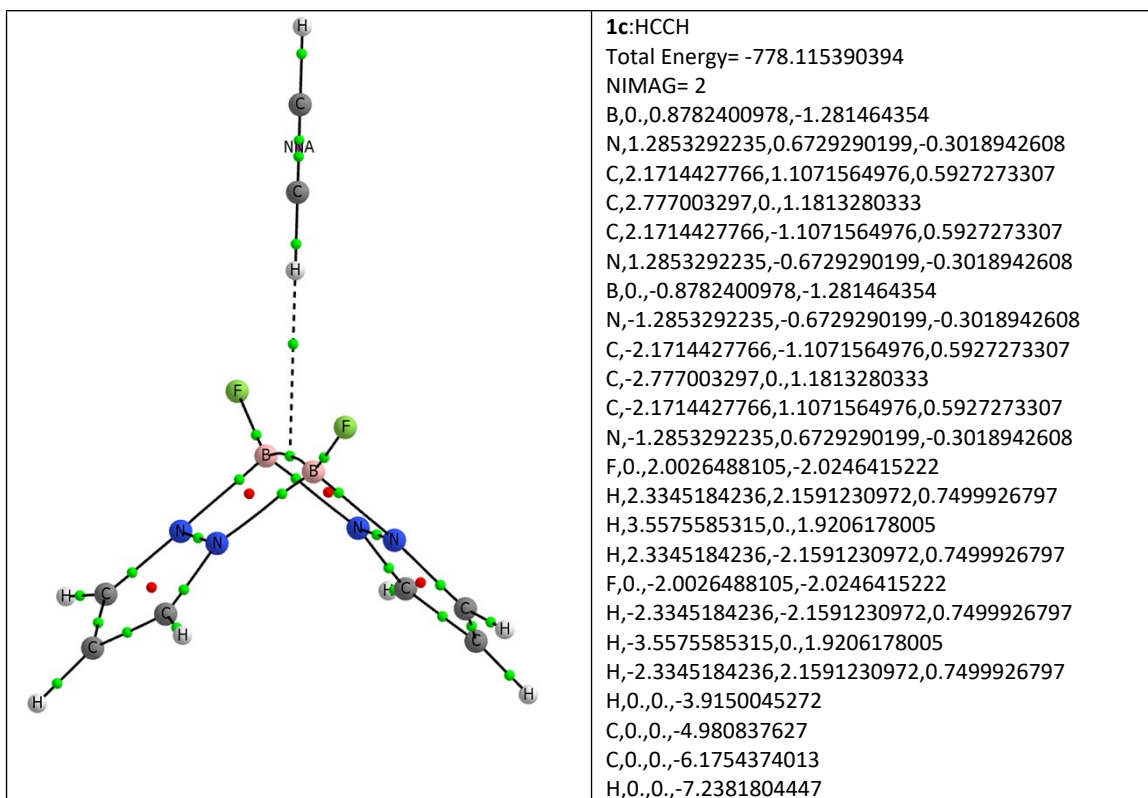
	H,3.1357885597,0.,-0.001168116 1b:HCN Total Energy= -674.218421534 NIMAG= 0 X 0. 0. 0.5695166 B,-0.8985454781,0.,0.5695166 N,-0.6694463968,-1.2704312803,-0.4041992349 C,-1.1082341841,-2.2098053201,-1.2409542863 C,0.,-2.8467140451,-1.7954447527 C,1.1082341841,-2.2098053201,-1.2409542863 N,0.6694463968,-1.2704312803,-0.4041992349 B,0.8985454781,0.,0.5695166 N,0.6694463968,1.2704312803,-0.4041992349 C,1.1082341841,2.2098053201,-1.2409542863 C,0.,2.8467140451,-1.7954447527 C,-1.1082341841,2.2098053201,-1.2409542863 N,-0.6694463968,1.2704312803,-0.4041992349 C,-2.20577945,0.,1.4621923614 H,-2.1602695658,-2.3835089378,-1.3868852432 H,0.,-3.6658666898,-2.4915627592 H,2.1602695658,-2.3835089378,-1.3868852432 C,2.20577945,0.,1.4621923614 H,2.1602695658,2.3835089378,-1.3868852432 H,0.,3.6658666898,-2.4915627592 H,-2.1602695658,2.3835089378,-1.3868852432 H,0.,0.,2.893429666 C,0.,0.,3.9706987067 N,0.,0.,5.1140707982 H,2.2528421639,0.878121504,2.1090853848 H,-2.2528421639,-0.878121504,2.1090853848 H,-2.2528421639,0.878121504,2.1090853848 H,-3.1183784375,0.,0.8583795286 H,2.2528421639,-0.878121504,2.1090853848 H,3.1183784375,0.,0.8583795286
	1b:HCCH Total Energy= -658.115291157 NIMAG= 0 X 0. 0. 0.5505404313 B,-0.8931071682,0.,0.5505404313 N,-0.6693424722,-1.2715178882,-0.4317155414 C,-1.1080336948,-2.211812471,-1.2672960609 C,0.,-2.8495806198,-1.8216279767 C,1.1080336948,-2.211812471,-1.2672960609 N,0.6693424722,-1.2715178882,-0.4317155414 B,0.8931071682,0.,0.5505404313 N,0.6693424722,1.2715178882,-0.4317155414 C,1.1080336948,2.211812471,-1.2672960609 C,0.,2.8495806198,-1.8216279767 C,-1.1080336948,2.211812471,-1.2672960609 N,-0.6693424722,1.2715178882,-0.4317155414 C,-2.1958991246,0.,1.4478868201 H,-2.1601387079,-2.3853411426,-1.4128810113 H,0.,-3.6692006135,-2.5172758435 H,2.1601387079,-2.3853411426,-1.4128810113 C,2.1958991246,0.,1.4478868201 H,2.1601387079,2.3853411426,-1.4128810113 H,0.,3.6692006135,-2.5172758435 H,-2.1601387079,2.3853411426,-1.4128810113 H,0.,0.,3.0318054092 C,0.,0.,4.1011224397 C,0.,0.,5.2964957669 H,0.,0.,6.3594144132 H,2.2330678613,0.8768956996,2.0965777724

	H,-2.2330678613,-0.8768956996,2.0965777724 H,-2.2330678613,0.8768956996,2.0965777724 H,-3.1134698222,0.,0.8511095769 H,2.2330678613,-0.8768956996,2.0965777724 H,3.1134698222,0.,0.8511095769
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	1c Total Energy= -700.787046497 NIMAG= 0 B,0.,0.8745426483,-1.2920068985 N,1.2864066079,0.6727562779,-0.3043357039 C,2.169109312,1.1069510829,0.5936558205 C,2.7727731763,0.,1.1848324717 C,2.169109312,-1.1069510829,0.5936558205 N,1.2864066079,-0.6727562779,-0.3043357039 B,0.,-0.8745426483,-1.2920068985 N,-1.2864066079,-0.6727562779,-0.3043357039 C,-2.169109312,-1.1069510829,0.5936558205 C,-2.7727731763,0.,1.1848324717 C,-2.169109312,1.1069510829,0.5936558205 N,-1.2864066079,0.6727562779,-0.3043357039 F,0.,2.0050619182,-2.0255850849 H,2.3309401763,2.1589585436,0.7519812402 H,3.5500202005,0.,1.9276481363 H,2.3309401763,-2.1589585436,0.7519812402 F,0.,-2.0050619182,-2.0255850849 H,-2.3309401763,-2.1589585436,0.7519812402 H,-3.5500202005,0.,1.9276481363 H,-2.3309401763,2.1589585436,0.7519812402
	1c:H⁺ Total Energy= -701.192599246 NIMAG= 0 X 0. 0. -1.1346060449 B,0.,1.1315743922,-1.1346060449 N,1.2673217295,0.6742524456,-0.3844322856 C,2.2961251848,1.1073844012,0.3488846488 C,2.982725197,0.,0.8304376255 C,2.2961251848,-1.1073844012,0.3488846488 N,1.2673217295,-0.6742524456,-0.3844322856 B,0.,-1.1315743922,-1.1346060449 N,-1.2673217295,-0.6742524456,-0.3844322856 C,-2.2961251848,-1.1073844012,0.3488846488 C,-2.982725197,0.,0.8304376255 C,-2.2961251848,1.1073844012,0.3488846488 N,-1.2673217295,0.6742524456,-0.3844322856 F,0.,2.3019290204,-1.729636092 H,2.4872139517,2.1607102259,0.4690730102 H,3.8735249575,0.,1.4318392268 H,2.4872139517,-2.1607102259,0.4690730102 F,0.,-2.3019290204,-1.729636092 H,-2.4872139517,-2.1607102259,0.4690730102 H,-3.8735249575,0.,1.4318392268 H,-2.4872139517,2.1607102259,0.4690730102 H,0.,0.,-1.9916031251

	1c:HF Total Energy= -801.247966591 NIMAG= 0 X 0. 0. -1.3532005097 B,0.,0.89299414,-1.3532005097 N,1.2817602126,0.6725506923,-0.3884533722 C,2.1703004711,1.1074923424,0.5034341814 C,2.7773610295,0.,1.0894793778 C,2.1703004711,-1.1074923424,0.5034341814 N,1.2817602126,-0.6725506923,-0.3884533722 B,0.,-0.89299414,-1.3532005097 N,-1.2817602126,-0.6725506923,-0.3884533722 C,-2.1703004711,-1.1074923424,0.5034341814 C,-2.7773610295,0.,1.0894793778 C,-2.1703004711,1.1074923424,0.5034341814 N,-1.2817602126,0.6725506923,-0.3884533722 F,0.,2.0276539925,-2.0795147531 H,2.3342406377,2.1595284722,0.6590859775 H,3.5612283931,0.,1.8251114493 H,2.3342406377,-2.1595284722,0.6590859775 F,0.,-2.0276539925,-2.0795147531 H,-2.3342406377,-2.1595284722,0.6590859775 H,-3.5612283931,0.,1.8251114493 H,-2.3342406377,2.1595284722,0.6590859775 H,0.,0.,-3.5214505035 F,0.,0.,-4.4499342806
	1c:HCl Total Energy= -1161.60033866 NIMAG= 1 B,0.,0.8858327693,-1.3252341441 N,1.2836356441,0.6727932671,-0.3545180272 C,2.1728493569,1.1073691491,0.5368831804 C,2.7802866466,0.,1.1229207826 C,2.1728493569,-1.1073691491,0.5368831804 N,1.2836356441,-0.6727932671,-0.3545180272 B,0.,-0.8858327693,-1.3252341441 N,-1.2836356441,-0.6727932671,-0.3545180272 C,-2.1728493569,-1.1073691491,0.5368831804 C,-2.7802866466,0.,1.1229207826 C,-2.1728493569,1.1073691491,0.5368831804 N,-1.2836356441,0.6727932671,-0.3545180272 F,0.,2.0148634123,-2.0612675269 H,2.3367530838,2.1593585474,0.6930198137 H,3.5639936074,0.,1.8587945887 H,2.3367530838,-2.1593585474,0.6930198137 F,0.,-2.0148634123,-2.0612675269 H,-2.3367530838,-2.1593585474,0.6930198137 H,-3.5639936074,0.,1.8587945887 H,-2.3367530838,2.1593585474,0.6930198137 H,0.,0.,-3.6575255714 Cl,0.,0.,-4.9458080585

	1c:HBr Total Energy= -3275.63202835 NIMAG= 0 X 0. 0. -1.3175209516 B,0.,0.8854251743,-1.3175209516 N,1.2839267237,0.6727771184,-0.3463498671 C,2.1735016357,1.1073503713,0.5447067884 C,2.7811849351,0.,1.1305611572 C,2.1735016357,-1.1073503713,0.5447067884 N,1.2839267237,-0.6727771184,-0.3463498671 B,0.,-0.8854251743,-1.3175209516 N,-1.2839267237,-0.6727771184,-0.3463498671 C,-2.1735016357,-1.1073503713,0.5447067884 C,-2.7811849351,0.,1.1305611572 C,-2.1735016357,1.1073503713,0.5447067884 N,-1.2839267237,0.6727771184,-0.3463498671 F,0.,2.015002969,-2.0528032411 H,2.3374357012,2.159343551,0.7007948716 H,3.5651178534,0.,1.8662106676 H,2.3374357012,-2.159343551,0.7007948716 F,0.,-2.015002969,-2.0528032411 H,-2.3374357012,-2.159343551,0.7007948716 H,-3.5651178534,0.,1.8662106676 H,-2.3374357012,2.159343551,0.7007948716 H,0.,0.,-3.6657718422 Br,0.,0.,-5.0950970228
	1c:HCN Total Energy= -794.218176968 NIMAG= 0 X 0. 0. -1.3071540631 B,0.,0.8799684687,-1.3071540631 N,1.28454435,0.6734383056,-0.3361778048 C,2.1706230788,1.1074000405,0.5587927313 C,2.775959262,0.,1.1467137218 C,2.1706230788,-1.1074000405,0.5587927313 N,1.28454435,-0.6734383056,-0.3361778048 B,0.,-0.8799684687,-1.3071540631 N,-1.28454435,-0.6734383056,-0.3361778048 C,-2.1706230788,-1.1074000405,0.5587927313 C,-2.775959262,0.,1.1467137218 C,-2.1706230788,1.1074000405,0.5587927313 N,-1.28454435,0.6734383056,-0.3361778048 F,0.,1.9965783902,-2.0652826046 H,2.3341530506,2.159265358,0.7163673398 H,3.5568449492,0.,1.8855731271 H,2.3341530506,-2.159265358,0.7163673398 F,0.,-1.9965783902,-2.0652826046 H,-2.3341530506,-2.159265358,0.7163673398 H,-3.5568449492,0.,1.8855731271 H,-2.3341530506,2.159265358,0.7163673398 H,0.,0.,-3.7633591795 C,0.,0.,-4.8346226656 N,0.,0.,-5.9773331211



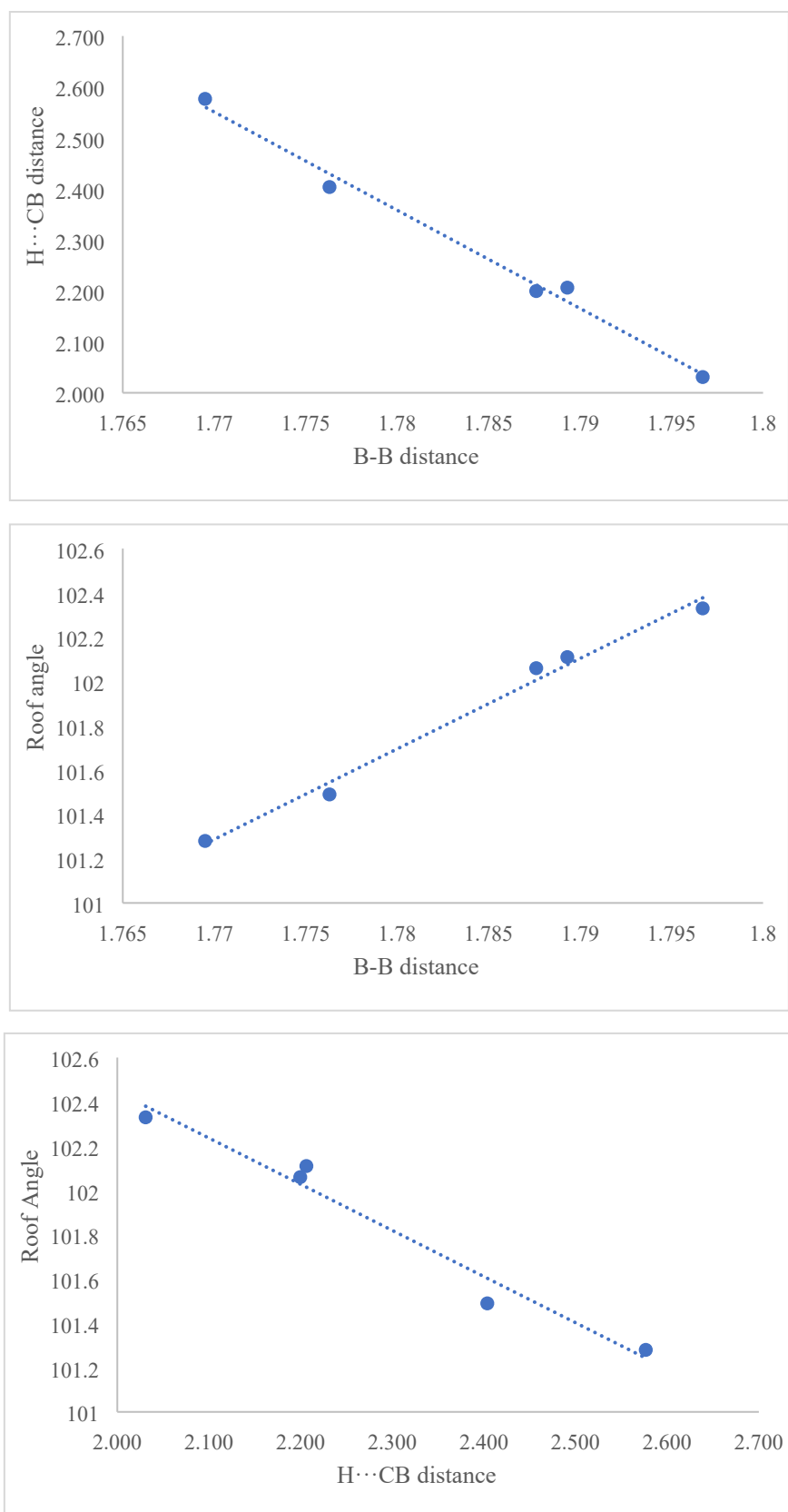


Figure S1. Linear correlations between the geometrical parameters (Å and °) in the complexes of **1a**. CB indicate a dummy in the center of the B-B bond.

Table S2. Geometrical parameters (Å and °) of the complexes of **1a**.

System	B-B distance	H...CB* distance	Roof angle
1a:	1.7618		
1a: HF	1.7967	2.031	102.33
1a: HCl	1.7876	2.200	102.06
1a: HBr	1.7893	2.206	102.11
1a: HCN	1.7763	2.404	101.49
1a: HCCH	1.7695	2.577	101.28

*CB indicate a dummy in the center of the B-B bond

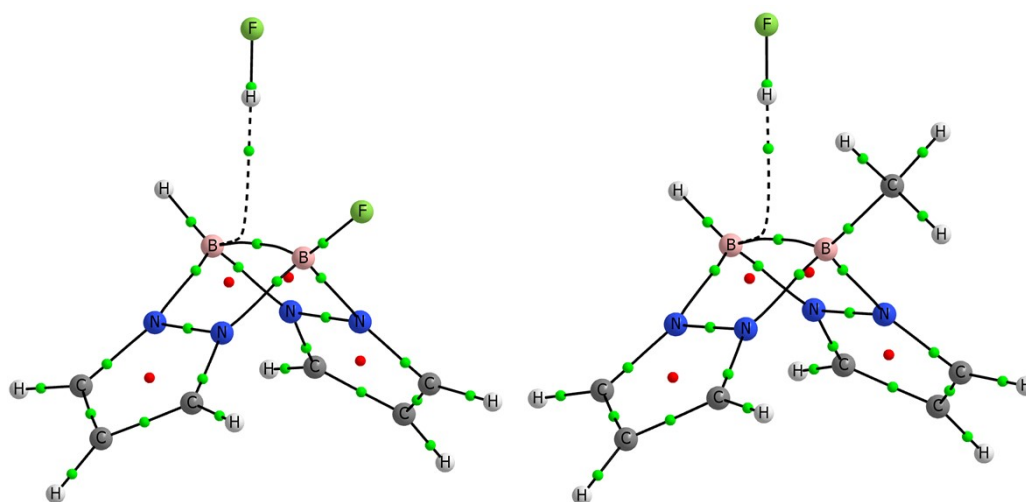


Figure S2. Molecular graph with two systems were one of the H...B bond paths is absent.

Table S2. Free-Wilson Matrix.

Complex	D_e	1a	1b	1c	HF	HCl	HBr	HCN	HCCH
1a :HF	37.17	1	0	0	1	0	0	0	0
1a :HCl	24.84	1	0	0	0	1	0	0	0
1a :HBr	22.67	1	0	0	0	0	1	0	0
1a :HCN	24.58	1	0	0	0	0	0	1	0
1a :HCCH	11.99	1	0	0	0	0	0	0	1
1b :HF	39.76	0	1	0	1	0	0	0	0
1b :HCl	28.42	0	1	0	0	1	0	0	0
1b :HBr	27.03	0	1	0	0	0	1	0	0
1b :HCN	27.19	0	1	0	0	0	0	1	0
1b :HCCH	15.54	0	1	0	0	0	0	0	1
1c :HF	20.76	0	0	1	1	0	0	0	0
1c :HCl	15.19	0	0	1	0	1	0	0	0
1c :HBr	14.34	0	0	1	0	0	1	0	0
1c :HCN	18.71	0	0	1	0	0	0	1	0
1c :HCCH	7.97	0	0	1	0	0	0	0	1

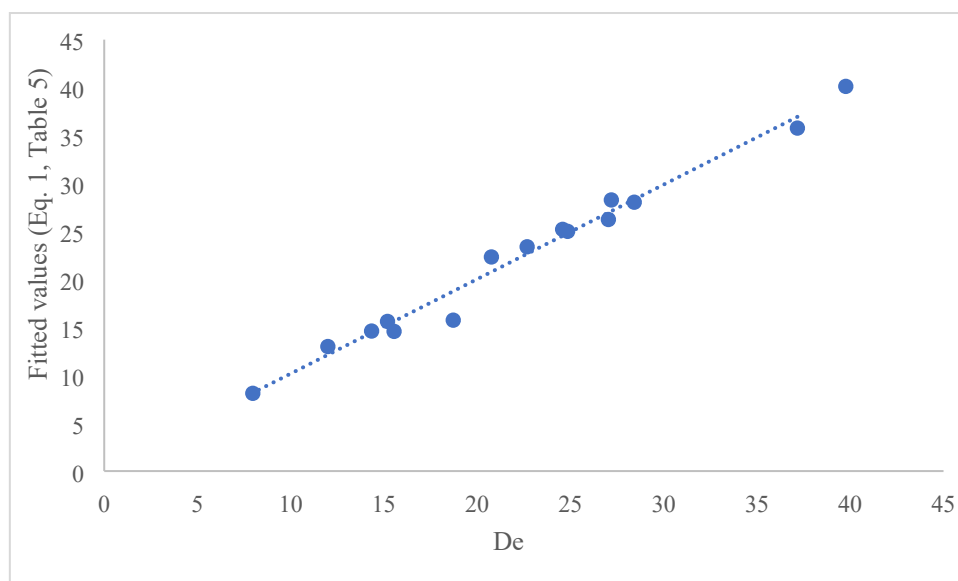


Figure S3. Fitted values vs. the calculated D_e energies (kJ mol⁻¹) following Equation [1]. Note: Removing only one value from the 15 used, (**1c**:HCN), results in R^2 above 0.98.