

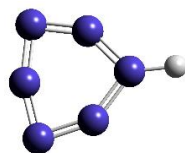
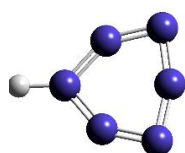
DFT calculation details.

The calculation was performed by using the m06/6-31G+(d,p) method in the gaussian 16 software package.¹ The M06 functional belongs to the density functional (DFT) calculation method.² The 6-31G+(d,p) basis set has sufficient accuracy for the calculation of C and H systems.^{3,4} The specific steps of calculation are as follows: firstly, a transition state (TS) in the system should be searched, and then Intrinsic Reaction Coordinate (IRC) should be conducted according to this transition state. so as to ensure that the reactants (RC), intermediates (IM) and products (PD) in the reaction path could be properly connected.

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, V.; Throssell, K.; A., M. J.; Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, 16 revision B.01. Gaussian Inc.: Wallingford, CT, USA 2016.
2. Y. Zhao and D. G. Truhlar, "The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals," *Theor. Chem. Acc.*, 120 (2008) 215-41.
3. G. A. Petersson, A. Bennett, T. G. Tensfeldt, M. A. Al-Laham, W. A. Shirley, and J. Mantzaris, "A complete basis set model chemistry. I. The total energies of closed-shell atoms and hydrides of the first-row atoms," *J. Chem. Phys.*, **89** (1988) 2193-218.
4. G. A. Petersson and M. A. Al-Laham, "A complete basis set model chemistry. II. Open-shell systems and the total energies of the first-row atoms," *J. Chem. Phys.*, **94** (1991) 6081-90.

Optimized structures and coordinated in figure 9 (a).

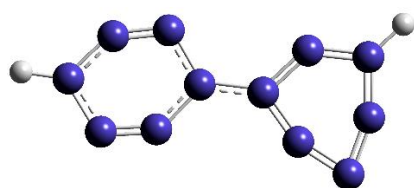
RC



C	5.45051099	-0.00682827	0.01463095
C	4.54190003	1.02851777	0.03366700
C	3.24099504	1.32023382	0.02511503
C	2.99738999	0.00436583	-0.01778902

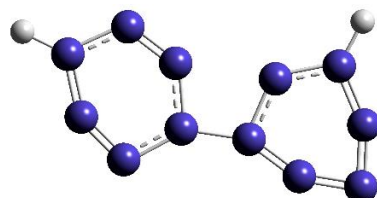
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C	4.53331195	-1.03384223	-0.02854708
H	6.52936399	-0.01175031	0.02886694
C	-5.44484102	-0.12435584	-0.01714993
C	-4.62828798	0.98503913	-0.03606889
C	-3.35719496	1.38720808	-0.02557389
C	-3.00177601	0.09712406	0.01973705
C	-3.12064706	-1.23595893	0.05783100
C	-4.44307005	-1.06890888	0.02923702
H	-6.51927102	-0.22175980	-0.03334992

IM1



C	2.93064100	1.22679400	-0.00000800
C	3.22024400	-0.10232100	0.00001100
C	2.99855700	-1.43335700	0.00002700
C	1.73731400	-0.95762400	0.00005000
C	0.75290200	-0.01415500	0.00004500
C	1.55504600	1.11790000	-0.00002300
H	3.56559400	2.09977200	-0.00002400
C	-3.66618000	0.03859400	0.00021900
C	-2.73814200	-0.99346400	-0.00004200
C	-1.49639400	-1.26472900	-0.00019600
C	-0.68972400	-0.10867900	0.00005300
C	-1.57996500	0.97860300	-0.00005300
C	-2.82722000	1.16604000	-0.00009300
H	-4.74805900	-0.02138100	0.00010000

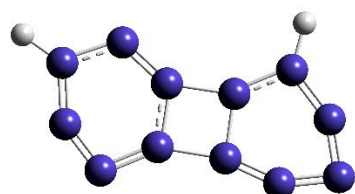
TS1



C	2.30123999	1.42052386	0.00000000
C	3.08630698	0.29986084	0.00000000
C	3.30870196	-1.00717316	0.00000000
C	1.97372996	-1.07501014	0.00000000
C	0.75519096	-0.52204112	0.00000000
C	1.03078999	0.86461188	0.00000000

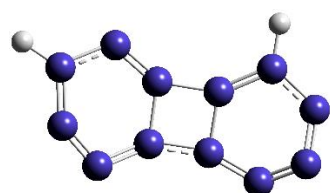
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C	-3.41482502	0.43268894	0.00000000
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C	-1.76495905	-1.52109508	0.00000000
C	-0.70639304	-0.61489310	0.00000000
C	-1.12376702	0.73583491	0.00000000
C	-2.28697501	1.28071893	0.00000000
H	-4.46646502	0.69777596	0.00000000

IM2



C	1.88239900	1.42631500	0.00006500
C	2.91267300	0.50260000	0.00043000
C	3.35937900	-0.71859900	0.00022000
C	2.07708300	-1.10260800	0.00023900
C	0.79701700	-0.78567700	-0.00091900
C	0.72228500	0.66265200	-0.00050600
H	1.96200200	2.50426100	-0.00009200
C	-3.17418700	0.61663800	0.00007500
C	-2.85355400	-0.71167600	0.00052000
C	-1.88479600	-1.57905100	-0.00005600
C	-0.73535800	-0.82709500	0.00001100
C	-0.79784000	0.60452800	-0.00011000
C	-1.93827900	1.31727000	0.00010700
H	-4.16294000	1.06395400	-0.00037100

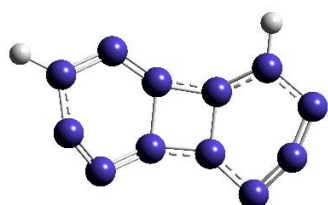
TS2



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C	3.03297400	0.60330200	0.05309900
C	3.01439600	-0.67128700	0.37600900
C	2.03337400	-1.31440000	-0.18911600
C	0.75083400	-0.82878800	-0.20083500
C	0.72814500	0.65051500	-0.11451100
H	1.86228100	2.48683500	0.05495400
C	-3.09504000	0.64134100	0.11198000

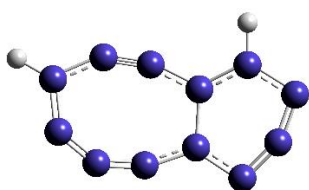
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C	-1.83769500	-1.52332200	0.11855300
C	-0.68362600	-0.84795700	-0.23477700
C	-0.74035900	0.64206500	-0.20664800
C	-1.87937500	1.35665600	-0.03698100
H	-4.08002200	1.08843100	0.00679300

IM3



C	-1.83000000	1.43080600	-0.09781200
C	-3.00904500	0.67247500	-0.35549400
C	-2.68961300	-0.59647100	-0.26984900
C	-1.90763700	-1.60756900	0.01016100
C	-0.77099500	-0.80986700	0.35110900
C	-0.73374300	0.67581600	0.31076800
H	-1.79071600	2.51631300	-0.16576100
C	2.98646000	0.65703600	-0.24251900
C	2.63659600	-0.67898700	-0.48302300
C	1.75953700	-1.51947300	-0.09290900
C	0.64363400	-0.87208300	0.40425800
C	0.69905100	0.71870300	0.39943300
C	1.84599900	1.34103900	0.11965800
H	4.00924400	1.01514100	-0.15693300

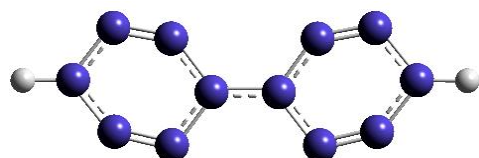
PD



C	-1.86796900	-1.35760200	0.00029300
C	-3.13290100	-0.68714500	0.11258800
C	-2.77951600	0.56241500	0.18218400
C	-1.93308200	1.54927200	0.05043100
C	-0.70585000	0.86878900	-0.19599800
C	-0.68768700	-0.63313600	-0.20125100
H	-1.79601400	-2.44566300	0.03246600
C	3.07087900	-0.66741000	0.02493100
C	2.84683700	0.64560700	0.30035800
C	1.81810200	1.41505900	-0.00814100

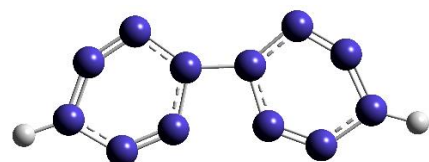
C	0.57803800	1.40913300	-0.20131100
C	0.60202900	-1.19533500	-0.09226000
C	1.82035700	-1.31722600	0.06650400
H	4.02059400	-1.10886800	-0.26243700

IM1'



C	-3.69781900	-0.11968292	0.00000000
C	-2.82415400	0.96330408	0.00000000
C	-1.59133500	1.24453808	0.00000000
C	-0.72366100	0.13199908	0.00000000
C	-1.57633400	-0.98912292	0.00000000
C	-2.81482100	-1.21288992	0.00000000
H	-4.78153300	-0.11033292	0.00000000
C	3.69781900	-0.11968292	0.00000000
C	2.81482100	-1.21288992	0.00000000
C	1.57633400	-0.98912292	0.00000000
C	0.72366100	0.13199908	0.00000000
C	1.59133500	1.24453808	0.00000000
C	2.82415400	0.96330408	0.00000000
H	4.78153300	-0.11033292	0.00000000

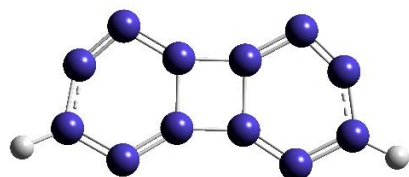
TS1'



C	3.44328605	-0.52676471	0.00000000
C	2.92754100	0.75803027	0.00000000
C	1.84350997	1.42200023	0.00000000
C	0.73326601	0.56898119	0.00000000
C	1.07611506	-0.81772880	0.00000000
C	2.26112908	-1.27148675	0.00000000
H	4.47691706	-0.85127067	0.00000000
C	-3.44097995	-0.52430597	0.00000000
C	-2.26500092	-1.28149592	0.00000000
C	-1.08639894	-0.80857188	0.00000000
C	-0.73347999	0.57393113	0.00000000
C	-1.83945603	1.43187309	0.00000000

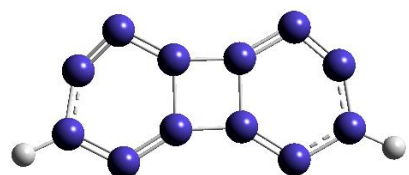
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H	-4.47721294	-0.84090901	0.00000000

IM2'



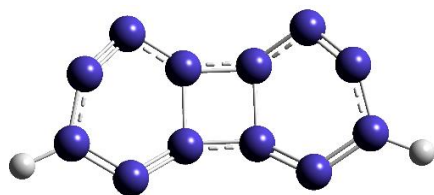
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C	1.87649300	-1.38502000	-0.11552000
C	0.72487600	-0.66962400	-0.06896700
C	0.72299200	0.83811200	-0.08138300
C	1.92881500	1.50367400	-0.00880500
C	2.86510900	0.64289400	0.17074600
H	4.07290700	-1.17278100	-0.17999300
C	-3.09454400	-0.73429900	0.00841800
C	-2.86678500	0.64331900	-0.16424700
C	-1.92870200	1.50320700	0.00947700
C	-0.72232800	0.83777900	0.07508300
C	-0.72471700	-0.66901100	0.06208300
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H	-4.07184500	-1.17360400	0.18929100

TS2'



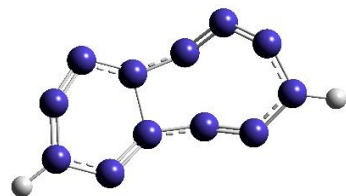
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C	-0.72057686	-0.65412306	-0.05479198
C	-0.70988796	0.84358094	-0.04196816
C	-1.92102201	1.49638587	0.01681876
C	-2.88399795	0.64814979	-0.04723014
H	-4.04386382	-1.19804625	0.31250009
C	3.07985215	-0.73883477	0.09044504
C	2.83091705	0.63469823	0.27986787
C	1.92813199	1.50676314	0.00973877
C	0.73161603	0.85309403	-0.18501316
C	0.72137114	-0.67917197	-0.18308097
C	1.87813919	-1.37606288	-0.13798288
H	4.07202718	-1.16638572	-0.02592391

IM3'



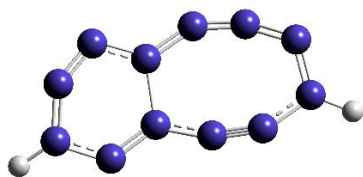
C	0.35351129	-0.70460242	2.97212897
C	-0.02381243	-1.37714970	1.82052199
C	-0.42424053	-0.71590157	0.71449100
C	-0.50783371	0.84813308	0.70236198
C	0.06969393	1.48552479	1.79218995
C	0.47229439	0.65143489	2.66765295
H	0.36232237	-1.12463442	3.97441198
C	0.35351129	-0.70460242	-2.97212897
C	0.47229439	0.65143489	-2.66765295
C	0.06969393	1.48552479	-1.79218995
C	-0.50783371	0.84813308	-0.70236198
C	-0.42424053	-0.71590157	-0.71449100
C	-0.02381243	-1.37714970	-1.82052199
H	0.36232237	-1.12463442	-3.97441198

TS3'



C	3.03352104	-0.67358609	-0.28274081
C	1.85932702	-1.36899611	0.00825105
C	0.72575001	-0.69950213	0.35977008
C	0.68204503	0.82891986	0.43866527
C	1.78443607	1.49073691	-0.10799961
C	2.71426607	0.66763093	-0.39971266
H	4.03392004	-1.09546611	-0.23912682
C	-3.01498196	-0.69041101	-0.27093108
C	-2.75031593	0.65627201	-0.47536291
C	-1.83477694	1.43565495	-0.02160577
C	-0.69799597	0.98151687	0.50249922
C	-0.67802299	-0.89756111	0.33471500
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H	-4.01271297	-1.10142801	-0.13944718

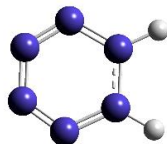
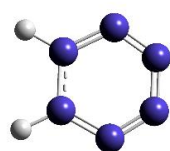
PD'



C	-3.11838992	-0.68184003	-0.01096288
C	-1.89199889	-1.31930399	-0.15461485
C	-0.68687092	-0.70610094	-0.20203593
C	-0.62494799	0.89797307	-0.18406206
C	-1.83363900	1.43591105	0.26187392
C	-2.80822597	0.61757701	0.31778201
H	-4.08589091	-1.07825109	-0.30445082
C	3.08901509	-0.71751875	0.09114400
C	2.98983303	0.65486225	0.13948288
C	1.86492900	1.27923618	-0.14372115
C	0.62382799	1.47623711	-0.26678314
C	0.59407211	-1.23521386	0.02357009
C	1.81446111	-1.31033680	0.18738807
H	4.01349711	-1.27064272	-0.04991498

Optimized structures and coordinated in figure 9 (b).

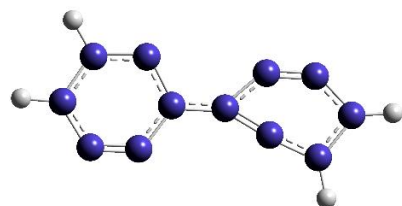
RC



C	-4.17531293	-1.36898892	0.02191898
C	-3.05625594	-0.76114792	0.07420000
C	-2.94524795	0.54995209	0.06973805
C	-3.94620896	1.33691808	0.01271208
C	-5.22491196	0.80687107	-0.04829493
C	-5.34673194	-0.63192393	-0.04339899
H	-6.14421796	1.38420506	-0.09954691
H	-6.35004694	-1.04681094	-0.09127500
C	3.95372707	-1.33838584	-0.02492503
C	2.94705306	-0.55675185	-0.03700800
C	3.05051504	0.75490915	-0.02417095
C	4.16725804	1.36868016	0.00156807
C	5.34428805	0.63785217	0.01722104
C	5.23074906	-0.80155983	0.00313399

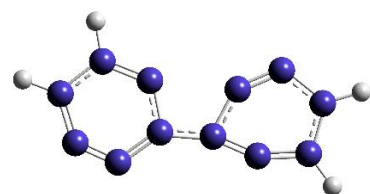
H	6.34629004	1.05805818	0.03922905
H	6.15445107	-1.37399882	0.01542696

IM1



C	3.69476600	0.17879500	-0.00009800
C	2.98432500	-1.05929900	-0.00008200
C	1.60123100	-1.16806700	0.00000000
C	0.84819100	0.03682800	0.00009000
C	1.61206000	1.23074700	0.00011000
C	2.87399300	1.29685100	0.00003300
H	4.78469100	0.18209100	-0.00016400
H	3.60225300	-1.95860400	-0.00018800
C	-3.85860700	-0.10534500	-0.00006500
C	-3.07747600	1.05726900	-0.00010200
C	-1.76579200	0.58216300	-0.00001600
C	-0.54970400	-0.01291800	0.00011100
C	-1.55153600	-1.00982700	0.00010000
C	-2.82484500	-1.03844200	0.00002800
H	-4.92790200	-0.25393200	-0.00010900
H	-3.37869100	2.09790200	-0.00019900

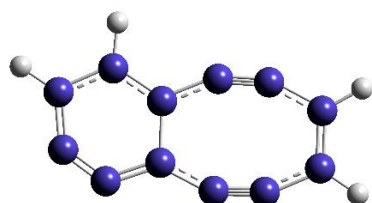
TS1



C	3.55764990	0.30339509	0.00000000
C	2.48768788	1.24823806	0.00000000
C	1.17305089	0.82250103	0.00000000
C	0.81213892	-0.54353598	0.00000000
C	1.88503594	-1.41964295	0.00000000
C	3.06598293	-0.97972493	0.00000000
H	4.59825289	0.61529911	0.00000000
H	2.74031885	2.30692607	0.00000000
C	-3.51748310	0.52599991	0.00000000
C	-3.22954007	-0.84296708	0.00000000
C	-1.86202707	-0.99628005	0.00000000
C	-0.62210308	-0.55488502	0.00000000

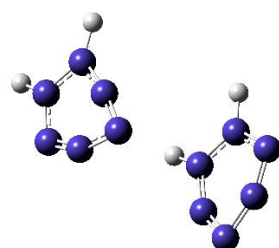
C	-1.20673011	0.74592197	0.00000000
C	-2.35558012	1.33240394	0.00000000
H	-4.53853911	0.90225489	0.00000000
H	-3.92853005	-1.67302410	0.00000000

PD



C	-3.22101800	0.52576300	0.00000400
C	-1.98941300	1.23051600	0.00002700
C	-0.75023200	0.59102400	0.00003300
C	-0.63201200	-0.86432400	0.00000900
C	-1.87705000	-1.44266000	-0.00004100
C	-2.96426900	-0.81750100	-0.00003300
H	-4.18312600	1.02665500	-0.00002300
H	-2.00573400	2.31875500	0.00003300
C	3.07022500	0.79182600	-0.00003500
C	3.16451900	-0.56539400	0.00002800
C	1.91673200	-1.26731000	0.00002900
C	0.70460700	-1.38253100	-0.00000200
C	0.52320500	1.26364300	0.00007000
C	1.73942700	1.32086600	-0.00009400
H	3.95493600	1.42185000	-0.00006000
H	4.12560100	-1.07076300	0.00007600

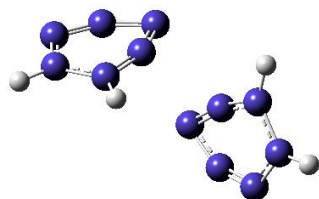
IM1'



C	4.75834500	0.01412900	-0.01219600
C	3.95194600	-0.57529400	0.95904900
C	2.64203300	-0.29949700	0.54588400
C	1.52001700	0.09356100	-0.06283900
C	2.62464800	0.53015600	-0.79377700
C	3.88564700	0.60871100	-0.95065400
H	5.84174800	0.02039400	-0.04905400
H	4.22507900	-1.13029200	1.84787000
C	-2.79114400	-1.13871100	-0.40613500

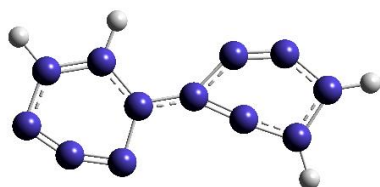
C	-2.01065800	-0.01075300	-0.04395200
C	-2.89496800	0.96446400	0.33196700
C	-4.12279800	1.32054900	0.50514100
C	-4.49431000	0.09593200	0.09293000
C	-4.21569200	-1.08747100	-0.33107600
H	-2.25982300	-2.03164000	-0.73959600
H	-0.92540000	0.04688100	-0.06527500

TS1'



C	4.61810404	0.24542296	-0.02633288
C	3.74491501	0.61946296	0.99302110
C	2.49529003	0.13812393	0.58368009
C	1.45240205	-0.41461510	-0.03913492
C	2.59835806	-0.59787910	-0.80973689
C	3.84853006	-0.44026908	-0.99365188
H	5.68375003	0.43895698	-0.07604387
H	3.93792099	1.15958699	1.91150409
C	-3.27068094	-1.25912719	0.37918303
C	-2.06925995	-0.59569717	0.07922503
C	-2.42653497	0.69210482	-0.26556200
C	-3.26270799	1.66883679	-0.47718004
C	-4.14966497	0.70480079	-0.11745103
C	-4.46155296	-0.48096221	0.25638100
H	-3.27146993	-2.30427018	0.68502006
H	-1.05338594	-0.97548815	0.10487606

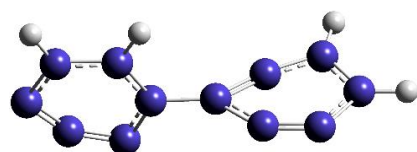
IM2'



C	-3.79386500	-0.07833400	-0.00022900
C	-2.96201800	1.05262300	-0.00068900
C	-1.67115900	0.53067200	-0.00015800
C	-0.46660900	-0.09748100	0.00056100
C	-1.51052900	-1.06529400	-0.00057100
C	-2.78231300	-1.03121500	0.00131700
H	-4.86672900	-0.19296500	-0.00026700

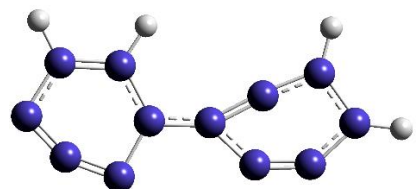
H	-3.21790400	2.10511000	-0.00081700
C	3.15575100	-0.93958200	-0.00004600
C	1.77973700	-1.09134000	-0.00020200
C	0.92175200	0.05819900	-0.00022800
C	1.40571500	1.42792400	0.00061200
C	2.69298100	1.17713200	0.00047000
C	3.72279900	0.38923200	-0.00046600
H	3.79730400	-1.82104100	-0.00044900
H	1.33387500	-2.08632200	-0.00069600

TS2'



C	-3.77324386	0.04349800	-0.02491187
C	-2.95635184	0.07218805	1.10594114
C	-1.65188884	0.02446245	0.61375108
C	-0.51893686	-0.04197497	-0.09044600
C	-1.58066087	-0.04410720	-0.99749798
C	-2.86570087	-0.01679911	-1.09106094
H	-4.85433186	0.06065306	-0.07917884
H	-3.23039982	0.11547518	2.15275618
C	3.09630015	1.03468591	0.01358684
C	1.69444015	1.07568296	-0.03394210
C	0.95061514	-0.12586704	-0.02558110
C	1.55262713	-1.39342310	0.04533883
C	2.82998114	-1.10986913	0.06138205
C	3.76527714	-0.21654316	0.09256378
H	3.64795716	1.97599192	-0.00336438
H	1.18202816	2.03627801	-0.08495529

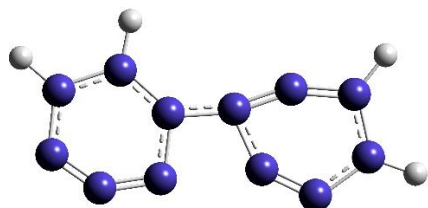
IM3'



C	-3.79376000	0.00997600	-0.00009700
C	-2.93062500	1.11566000	0.00006900
C	-1.65627100	0.54657100	0.00004600
C	-0.46799200	-0.12024300	0.00002900
C	-1.54151500	-1.04372700	0.00001000
C	-2.81200400	-0.97516600	-0.00003000

H	-4.86956100	-0.07331100	-0.00019400
H	-3.15944900	2.17445500	0.00012600
C	3.03665600	1.10946600	-0.00003900
C	1.65219700	1.10003500	-0.00000400
C	0.92963400	-0.14049600	0.00003200
C	1.57092100	-1.44409700	0.00005900
C	2.82085300	-1.04633700	0.00000300
C	3.75205900	-0.14484600	-0.00005100
H	3.57113100	2.05953500	-0.00008400
H	1.09696200	2.03855400	-0.00000800

TS3'



C	-3.49558709	-0.38984398	0.00000000
C	-3.12432406	0.95494801	0.00000000
C	-1.74681906	0.99625998	0.00000000
C	-0.53153707	0.50715996	0.00000000
C	-1.19620109	-0.77118303	0.00000000
C	-2.38780710	-1.27417100	0.00000000
H	-4.53809309	-0.70207996	0.00000000
H	-3.75877104	1.83548302	0.00000000
C	3.30055594	0.71776888	0.00000000
C	1.98763095	1.22356891	0.00000000
C	0.89801093	0.34444893	0.00000000
C	0.99560990	-1.08380907	0.00000000
C	2.30506289	-1.34896310	0.00000000
C	3.38101991	-0.67892412	0.00000000
H	4.15963695	1.38386186	0.00000000
H	1.82353697	2.29917291	0.00000000
